

Copyright
by
Michael Allen Basden
2014

**The Dissertation Committee for Michael Allen Basden Certifies that this is the
approved version of the following dissertation:**

**Characterization of Structured Packing via Computational Fluid
Dynamics**

Committee:

Roger T. Bonnecaze, Supervisor

R. Bruce Eldridge, Co-Supervisor

Venkat Ganesan

Gary T. Rochelle

Frank Seibert

Gerald McGlamery

**Characterization of Structured Packing via Computational Fluid
Dynamics**

by

Michael Allen Basden, B.S.C.E.; M.S.

Dissertation

Presented to the Faculty of the Graduate School of
The University of Texas at Austin
in Partial Fulfillment
of the Requirements
for the Degree of

Doctor of Philosophy

**The University of Texas at Austin
December 2014**

Dedication

This work is dedicated to my father and grandmother. I am immeasurably grateful for your unwavering support and belief in me.

Acknowledgements

This project would not have been possible without the great deal of help I received from so many people. The first person I wish to thank is my adviser, Dr. Bruce Eldridge. Without his words of encouragement and advice, I would have been completely lost. He also proved to be an invaluable resource, capable of either answering questions immediately or connecting me with contacts in a wide variety of industries whenever a vexing question would arise.

Next, I wish to thank the talented researchers who I had the pleasure to work with on a variety of research projects. In particular, Jose Delgado and Shawn Grush were fantastic undergraduate assistants who helped in the collection and analysis of experimental data. Christian Waas, a research intern from Technische Universität München, proved to be extremely competent in both experimental work and model development. His ability to clearly visualize and organize data made analysis significantly easier.

SRP personnel proved to be fantastic resources for all manner of problems. Frank Seibert, Robert Montgomery, Steve Briggs, and Micah Perry guided me in the development and design of equipment and experiments. Micah Perry, SRP's Renaissance man, could always be counted on for help on any issue, no matter how big or small. Susan Tedter proved to be a source of great help regarding any and all questions about how best to navigate the university's extensive organization.

The other graduate students within my group were a godsend. Scott Owens proved to be a fount of knowledge and advice long after he had graduated. Without his initial guidance, I would have spent significantly more time becoming operational. Bailee

Roache brought new life to the group, and it was a pleasure to share the experience of graduate school with her.

This research would not have been completed without the support from a myriad of organizations. Sulzer Chemtech provided equipment for experiments. In particular, I owe a debt of gratitude to Mark Pilling for being so generous with packing donations. TACC provided computational resources on their super computers. CD-adapco provided software licenses. The PSTC provided funding for the project, and the Cockrell School of Engineering provided additional support in the form of fellowships. UTCT aided in computational geometry generation by scanning the packing.

I owe a debt of gratitude to old friends who kept me grounded along the way. Benjamin Anderson, Jonathan Zumwalt, Sophie Schwarz, and Estevan Vidales were always there for support and encouragement. Thank you all.

Finally, I wish to thank all of my family. This wouldn't have been possible without you.

Characterization of Structured Packing via Computational Fluid Dynamics

Michael Allen Basden, PhD

The University of Texas at Austin, 2014

Supervisors: Roger T. Bonnecaze, R. Bruce Eldridge

CFD simulations were used to study single phase and multiphase flows through structured packing. Simulations utilizing a high fidelity, digital copy of a packing element were validated against experimental results for both single phase and multiphase flows. Single phase simulations were carried out on a variety of periodic packing elements to examine the impact of packing channel geometry on pressure drop. Multiphase simulations on periodic elements were used to examine the effect of hydrodynamic properties and boundary conditions.

Single-phase simulations of nitrogen flow through the high fidelity geometry produced via X-ray CT scans showed average deviations less than 15% when compared to experimental measurements. This error was reduced to 7% when a mesh utilizing prism layers to accurately resolve the boundary layer was used. With a validated model for single phase flow, the application of CFD to packing design was investigated on periodic geometries with varied packing parameters (e.g. channel corrugation angle and channel side length). It was found that current industrial packings have channel geometries maximizing pressure drop, indicating some degree of optimization around channel geometry is possible depending on separation needs.

Multiphase simulations using the Volume of Fluid model examined the effects of liquid density, viscosity, surface tension, and contact angle on small-scale packing geometries. Contact angle had the most pronounced influence on predicted wetting, and simulations demonstrated that using experimentally determined static contact angles was not an appropriate choice for the simulation contact angle. The predicted influence of surface tension qualitatively matched experimental data for wetted area. Liquid viscosity and density also demonstrated qualitative agreement with semi-empirical models derived from experimental data.

Experimental data collected via absorption of CO₂ into 0.1 mol/L NaOH were compared to simulation predictions using a geometry generated via X-ray CT scans. Wetted area predictions matched experimental data best when a fully wetting static contact angle (0°) was used, yielding simulated results 3.4% lower than experimental data on average. Irrigated pressure drop and holdup predictions were significantly higher than experimental data.

Table of Contents

List of Tables	xiii
List of Figures	xv
Chapter 1: Introduction	1
Summary of Work.....	1
Motivation.....	2
Gas-Liquid Separations.....	4
Structured Packing	5
Computational Fluid Dynamics (CFD).....	6
Mesh Generation.....	7
Turbulence Modeling.....	10
Direct Numerical Simulation	10
Large Eddy Simulation	11
Reynolds Averaged Navier-Stokes Equations	12
Two-Equation RANS Models: k- ϵ model.....	13
Two-Equation RANS Models: k- ω	16
Other RANS Models.....	17
Multiphase Modeling.....	17
Volume of Fluid Model Equations	19
Numerical Solutions.....	22
Chapter 2: Literature Review	27
Semi-Empirical Model Development	27
CFD Simulations of Structured Packing.....	31
Summary	50
Chapter 3: Simulation Details.....	51
Single Phase Flow Geometry Generation – CT Geometry	51
Single Phase Flow Meshing and Simulations– CT Geometry.....	56
Simulation Settings	56
Mesh Settings.....	58

Impact of Prism Layers	60
Single Phase Flow Geometry Generation– Periodic Geometry Generation	61
Single Phase Flow Meshing and Simulations– Periodic Geometry.....	65
Simulation Settings and Method	65
Mesh Settings	66
Multiphase Flow Geometry Generation–Small-Scale Geometries.....	66
Periodic Geometry	67
Small Inlet Geometry	67
Large Inlet Geometry	67
Multiphase Meshing and Simulations– Small-Scale Geometries	70
Simulation Settings and Method	70
Multiphase Geometry Generation– CT Geometry	74
Multiphase Meshing and Simulations– CT Geometry.....	77
Chapter 4: Experimental Methods	79
Single Phase Pressure Drop Equipment and Instrumentation.....	79
Single Phase Pressure Drop Method.....	83
Irrigated Pressure Drop and Wetted Area Equipment and Instrumentation .	83
Irrigated Pressure Drop Method.....	87
Wetted area Method	89
Liquid Holdup Equipment and Instrumentation	90
Liquid Holdup Method	92
Chapter 5: Single Phase Results	95
Mesh Independent Solution	95
Joint Rotation Comparisons.....	99
Turbulence Model Comparisons.....	107
Impact of A Boundary Layer Mesh	109
Wiper Bands and Pressure Drop	113
Development of Pressure Drop Model	114
Pressure Drop due to Friction between the Gas and Packing Surface	117
Final Model Proposal	120

Packing Analysis.....	123
Functional Comparison to Semi-Empirical Models	128
Turbulence Model Comparisons.....	133
Effect of Geometry and Flow Field	137
Chapter 6: Evaluation of CFD to Simulate Multiphase Flow	145
Small-Scale Simulations	145
Grid Sensitivity – Periodic Simulations.....	146
Impact of Contact Angle – Periodic Simulations	149
Impact of Surface Tension – Periodic Simulations.....	152
Impact of Density – Periodic Simulations	156
Impact of Viscosity – Periodic Simulations.....	161
Impact of Boundary Conditions.....	166
Effect of Turbulence Model – Periodic Geometry	173
Comparison to a Semi-Empirical Models.....	176
Pilot-Scale Simulations and Experimental Results.....	182
Experimental Data Analysis	182
Simulation Results	185
Comparison Between Simulated Data and Experimental Data	194
Chapter 7: Conclusions and Recommendations	200
Summary of Work and Conclusions	200
Single Phase Conclusions	200
Multiphase Conclusions.....	203
Future Work	208
Geometry Generation.....	208
Pressure Drop Mechanism Refinement	213
Packing Design and Experimental Validation	213
Model Enhancement and Evaluation	215
Gas and Liquid Phase Mass Transfer.....	215

Appendix A: Simulation and Mesh Settings.....	217
Appendix B: SOP for Air-Water Column Operation.....	230
B-1. Process Description.....	230
B-2. List of Equipment, Chemicals, and Instrumentation Used	232
B-3. Air-Water System Flowsheet & Pictures	234
B-4. Start-up Procedure	248
B-5. Steady-State Operation	252
B-6. Shutdown Procedure	253
B-7. Method of Data Acquisition.....	255
B-8. Data Analysis Example.....	255
B-9. Safety and Risks.....	255
Appendix C: Wetted Area Calculations and Experimental Conditions.....	257
Wetted Area Calculations	257
Chemical Reactions and Kinetics	258
Mass Transfer Enhanced by Chemical Reaction	258
Model Equations	260
Appendix D: Liquid Holdup at the Contact Points.....	262
Method.....	262
Glossary	267
Greek Letters.....	269
References.....	272
Vita	277

List of Tables

Table 3-1:	Packed bed orientations examined for single phase nitrogen flow...	55
Table 3-2:	Flow rates examined using the CT geometry.	57
Table 3-3:	Mesh settings examined for the mesh independence study.	60
Table 3-4:	Description of packing variables examined.	62
Table 3-5:	Periodic geometries examined for pressure drop studies. Geometries highlighted in blue were examined using the realizable k- ϵ , SST k- ω and LES turbulence models. Geometries highlighted in green were examined using the realizable k- ϵ and SST k- ω turbulence models. The remaining geometries were only examined with the realizable k- ϵ turbulence model.....	64
Table 3-6:	Packing geometry parameters for multiphase simulations.	67
Table 3-7:	Summary of hypothetical fluids examined for all small-scale geometries utilized in multiphase fluid flow simulations.....	71
Table 4-1:	Summary of experimental conditions examined for irrigated pressure drop and wetted area experiments.	89
Table 4-2:	Summary of experimental conditions examined for irrigated pressure drop and wetted area experiments.	93
Table 5-1:	Pressure drop results for the three meshes examined.	97
Table 5-2:	Impact of prism layer on pressure drop predictions on a small-scale CT geometry at an F-factor of 3.05 Pa ^{0.5} using the two-layer realizable k- ϵ turbulence model. Shaded prism layers were used in the full-scale CT geometry of three half elements.....	112

Table 5-3:	Pressure drop as a function of prism layers in a packed bed of three half-elements at an F-factor of $3.05 \text{ Pa}^{0.5}$. The experimental extrapolation was produced using the power law regression of experimental data shown in Figure 5-9.....	113
Table 5-4	Vertical rhombus channel dimensions examined to determine pressure drop due to friction between the gas and packing surface.	119
Table 5-5:	Summary of functional forms of friction factors between CFD- derived pressure drop model and two semi-empirical models.....	131
Table 5-6:	Packing examined with different turbulence models. Blue shaded packings were used in LES simulations in addition to the SST k- ω and realizable k- ϵ turbulence models.....	134
Table 6-1:	Physical properties used for grid convergence study.....	146
Table 6-2:	Results summary for the grid sensitivity study for multiphase simulations.	149
Table 6-3:	Summary of the impact of contact angle and surface tension.	156
Table 6-4:	Liquid and gas physical properties used for multiphase CT geometry simulations.	185
Table 6-5:	Summary of irrigated pressure drop predictions.....	198
Table B-1:	Valves associated with air-water tower (shown in above figures). ...	233
Table C-1:	Wetted area experimental conditions.....	257
Table D-1:	Location of the four contact point sphere centers for contact point studies.	262

List of Figures

Figure 1-1: Process diagrams from distillation (left) and gas absorption (right)...	5
Figure 1-2: Structured packing element shown from the side (left), top (middle), and a single sheet pulled from the element (right).	6
Figure 1-3: Example of a structured (left) and unstructured (right) mesh for CFD simulations.	8
Figure 1-4: Example of a polyhedral mesh with prism layers (left) and a mesh constructed of only polyhedral cells (right).	9
Figure 1-5: Figure showing the smearing of the interfacial region due to the VOF model. Figure taken from Brackbill <i>et al.</i> ¹⁹	20
Figure 1-6: Example uniform, one-dimensional grid showing the spatial discretization.	23
Figure 1-7: Example of successively finer grids from left to right.....	24
Figure 1-8: Discretization of a volume into several control volumes.....	26
Figure 2-1: Illustration of the criss-crossing channels of structured packing. The liquid flows with uniform thickness down the channel walls, and the gas flows in the opposite direction at the center of the channels. Figure from Olujic <i>et al.</i> ²⁴	29
Figure 2-2: Impact of surface tension and liquid load on fractional wetted area of Mellapak 250.Y. High surface tension experiments (72 mN/m) are shown on the left. Low surface tension experiments (35 mN/m) are shown on the right. Figure taken from Tsai <i>et al.</i> ²⁸	31

Figure 2-3: Computational geometry used by van Gulijk for dispersion simulations. ³⁰ In particular, the geometry illustrated by (b), (c), and (d) was simulated.....	32
Figure 2-4: Sandwich of packing used by Van Baten and Krishna to examine liquid phase mass transfer coefficients in KATAPAK-S packing. ³¹⁻³³	34
Figure 2-5: REUs employed by Petre <i>et al.</i> ³⁴	36
Figure 2-6: REUs employed by Larachi <i>et al.</i> ³⁵	37
Figure 2-7: Geometries employed by Raynal <i>et al</i> to predict pressure drop and liquid holdup. ³⁷ A) is the elementary geometry used to predict pressure drop. B) indicates the complex geometry to predict pressure drop. C) shows the two-dimensional geometry used for multiphase simulations to predict liquid holdup.	39
Figure 2-8: Computational domain employed by Ataki <i>et al.</i> to estimate wetted area of Rombopak. ³⁸	40
Figure 2-9: Different scales used by Raynal and Royon-Lebeaud to simulate overall column performance. ⁴¹	42
Figure 2-10: Examples of increasing liquid load causing the liquid profile to transition from a liquid film following the packing crimp to a liquid pool filling the packing cavity. Figure taken from Haroun <i>et al.</i> ⁵³	47
Figure 2-11: Periodic geometries examined by Armstrong <i>et al.</i> ⁵⁵	48
Figure 3-1: Example of the partial volume effect impacting the wiper band geometry.	53
Figure 3-2: Geometry used to correct wiper band defects and generate a packing element with a uniform diameter.	53
Figure 3-3: Wiper band section that has been corrected via Boolean subtraction.	54

Figure 3-4: Final packed bed for simulations (left), and a simulation schematic (right) showing boundary conditions and packed bed placement.....	56
Figure 3-5: Cross-section of geometry to used examine the impact of prism layers on pressure drop and skin friction coefficient.....	61
Figure 3-6: Schematic for prism layer studies geometry.....	62
Figure 3-7: Example periodic geometry viewed from different angles with boundary conditions indicated. View showing 3D geometry (left), view of the packing element front (middle) and view from the top (right).	63
Figure 3-8: Packing sheet showing the main packing variables. Top left shows the triangular channel formed when looking down the corrugation angle. The right figure shows the definition of the corrugation angle. Bottom left shows a three-dimensional representation of the packing dimensions.	63
Figure 3-9: Small Inlet Geometry. Top shows the side view of the liquid inlet geometry. Middle shows the top view of the inlet geometry. The bottom shows a 3D representation of how the geometry is arranged.	68
Figure 3-10: Large Inlet Geometry shown from an offset view.	69
Figure 3-11: Initial conditions to generate a uniform film thickness using a user-defined field function called initial_vol_frac.....	72
Figure 3-12: Initial conditions to generate a uniform film thickness by using an extracted table called vol_frac_init.....	73
Figure 3-13: Multiphase CT Geometry used in present studies.	76
Figure 3-14: Top view of liquid velocity inlet geometry used in multiphase simulations.	77

Figure 4-1: Sample half element of Mellapak N250.Y used in experimental work.	79
Figure 4-2: Schematic (left) and picture (right) of experimental test system used for dry pressure drop validation experiments.	81
Figure 4-3: Top view of the vapor distributor used in dry pressure drop studies.	82
Figure 4-4: Packing support used in single phase dry pressure drop studies. Figure taken from Owens. ⁶²	82
Figure 4-5 Process flow diagram for single phase nitrogen validation experiments.	84
Figure 4-6: Picture (left) and experimental schematic (right) of column used in wetted area and irrigated pressure drop experiments. Figure from Waas. ⁶³	85
Figure 4-7: Process flow diagram for irrigated pressure drop and wetted area measurements.	88
Figure 4-8: Experimental schematic (left) and apparatus (right) for liquid holdup experiments.	91
Figure 4-9: Process flow diagram for liquid holdup experiments.	93
Figure 5-1: Meshes generated for the grid convergence studies. The Coarse mesh is shown at the top, Medium mesh at center, and Fine mesh at bottom.	98
Figure 5-2: Meshes generated for the grid convergence studies. The Coarse mesh is shown at left, the Medium mesh at center, and the Fine mesh at right.	99
Figure 5-3: Joint rotation angles examined to determine the impact on pressure drop. The central element is the first element viewed from the top. An element shown after an arrow is the view from the top of the second (rotated) element.	100

Figure 5-4: Simulated pressure drop through a bed of three Mellapak N250.Y half elements with varying joint rotation angles.	101
Figure 5-5: Area-weighted pressures for the 0° rotation and 90° rotation cases. F-factor was $3.05 \text{ Pa}^{0.5}$, and simulations were carried out using an SST k- ω . Joints are at 163 and 326 mm. There were two wiper bands per half element located at roughly.	103
Figure 5-6: Cross-section of middle packing element showing the variation in pressure. Indicated regions are the wiper bands.	104
Figure 5-7: Negative z-direction velocities for the 90° (left) and 0° (right) joint rotation cases. Flow rate is an F-factor of $3.05 \text{ Pa}^{0.5}$. Vertical positions are indicated relative to the joint on the right side.	106
Figure 5-8: Simulated pressure drop vs. experimental pressure drop for the 90° and 0° joint rotation geometries. Error bars indicate 95% confidence interval. Turbulence model used was the SST k- ω model.	107
Figure 5-9: Experimental and predicted pressure drops through a bed of packing with a joint rotation angle of 90°.	109
Figure 5-10: Example volume mesh with a prism layer near the wall.	111
Figure 5-11: Packing used by Owens <i>et al.</i> shown at left. Packing used in present studies shown at right. Current studies have two wiper bands per half element. Owens <i>et al.</i> used one wiper band per half element.	114
Figure 5-12: Comparisons between two beds of equivalent height of Mellapak N250.Y. One wiper band pressure drop data (1 WB) taken from Owens <i>et al.</i> ¹⁰	114
Figure 5-13: Two-dimensional mixing layer.	115

Figure 5-14: Initial non-dimensionalization of the pressure drop using only the horizontal gas velocities. Corrugation angles for each packing examined are given in the legend. All packings examined had packing parameters of $b=26.05$ mm, $h=10.53$ mm, and $s=16.75$ mm.	117
Figure 5-15: Cross-section of vertical channels used to determine pressure drop due to friction of the gas and packing surface.	118
Figure 5-16: Results of non-dimensionalization of pressure drop in vertical channels.	119
Figure 5-17: Results of the non-dimensionalization of shear pressure drop. Corrugation angles for each packing examined are given in the legend. All packings examined had packing parameters of $b=26.05$ mm, $h=10.53$ mm, and $s=16.75$ mm.....	120
Figure 5-18: Non-dimensionalization of the shear pressure drop for all periodic geometries examined.	121
Figure 5-19: Comparison of simulated pressure drop vs. predicted pressure drop from the proposed non-dimensionalization.	122
Figure 5-20: Comparisons between water and nitrogen using the proposed non-dimensionalization.	123
Figure 5-21: Pressure drop in a hypothetical packing as a function of the channel height, h , with constant corrugation angle and packing specific area. Superficial gas velocity was 1 m/s.	124
Figure 5-22: Pressure drop in a hypothetical packing as a function of the channel opening angle, θ with constant channel corrugation angle and packing specific area. Superficial gas velocity was 1 m/s.	125

Figure 5-23: Pressure drop in a hypothetical packing as a function of the packing corrugation angle, α , with constant channel opening angle and specific surface area. Superficial gas velocity was 1 m/s.....	126
Figure 5-24: Pressure drop in a hypothetical packing as a function of the packing specific area, a_p , with constant corrugation angle and channel opening angle. Superficial gas velocity was 1 m/s.	127
Figure 5-25: Parity plot showing calculated CFD pressure drops vs. model predictions of asymptotic model (i.e. a constant value of fH) generated with $Re_{GH} > 500$	132
Figure 5-26: Impact of changing the channel height-to-base on structured packing performance in the Delft model. Figure taken from Olujic <i>et al.</i> ²⁶	133
Figure 5-27: Effect of turbulence model choice on calculated flow rates for packings designated by 650-45-150 and 650-70-150.	135
Figure 5-28: Effect of turbulence model choice on calculated flow rates for packings designated by 650-45-30 and 650-70-30.	135
Figure 5-29: Effect of turbulence model choice on calculated flow rates for packings designated by 500-45-90.....	136
Figure 5-30: Velocity field at the top of the packing element. Top left is geometry 650-45-30. Top right is 500-45-90. Bottom is 650-45-150 at 0.04147s and 0.066552s.	138
Figure 5-31: Perpendicular view to the preferred flow direction of one set of triangular channels.	139

Figure 5-32: Velocity field perpendicular to preferred flow direction for the three different packings. Top left is geometry 650-45-30. Top right is 500-45-90. Bottom left is 650-45-150 at 0.040940s. Bottom right is 650-45-150 at 0.061352s.	141
Figure 5-33: Central vertical plane cut from the packing to examine the x-velocity magnitude.....	142
Figure 5-34: X-velocities in the vertical plane at the center of the packing. Top figures are for packing 500-45-90 at $t=0.424173$ s (left) and $t=0.428373$ s (right). Bottom figures are for packing 650-45-150 at $t=0.041147$ s (left), $t=0.0504657$ s (middle), and $t=0.059352$ s (right).	144
Figure 6-1: Impact of number of prism layers on predicted liquid load.	147
Figure 6-2: Effect of number of prism layers on fractional wetted area predictions.	148
Figure 6-3: Definition of the contact angle. Figure taken from Starov <i>et al.</i> ⁶⁹	150
Figure 6-4: Impact of changing the contact angle on periodic simulations.	151
Figure 6-5: Impact of varying simulation contact angle and liquid holdup on fractional wetted area (top) and liquid load (bottom). Surface tension was constant at 0.074 N/m.	153
Figure 6-6: Influence of surface tension on wetted area predictions with a static contact angle of 0°	154
Figure 6-7: Influence of surface tension on wetted area predictions with a static contact angle of 30°	155
Figure 6-8: Impact of varying density at constant surface tension (0.074 N/m) and contact angle (30°). Liquid holdup was 7.6-7.9%.	157

Figure 6-9: Impact of density and surface tension on periodic simulations using a contact angle of 30° (top) and 0° (bottom). Black markers are simulations with liquid a liquid density of 1500 kg/m³. Colored markers have a density of 500 kg/m³. Triangle markers have a surface tension of 0.018 N/m. Diamond markers have a surface tension of 0.074 N/m.158

Figure 6-10: Impact of predicted liquid load on fractional wetted area for simulations of different densities. Contact angle of 30° shown at top. Contact angle of 0° shown at bottom. Black markers are simulations with liquid a liquid density of 1500 kg/m³. Colored markers have a density of 500 kg/m³. Triangle markers have a surface tension of 0.018 N/m. Diamond markers have a surface tension of 0.074 N/m. 160

Figure 6-11: Impact of increasing liquid viscosity for periodic simulations. Contact angle was set at 0°, surface tension was 0.074 N/m, and liquid density was 997.561 kg/m³ 161

Figure 6-12: Summary of the increased viscosity results for a contact angle of 0°. Black markers are 20x base viscosity, solid colored markers are 10x base viscosity, and hollow markers are base viscosity. Diamonds are the high surface tension case. Triangles are the low surface tension case. Top shows the impact of liquid load on fractional wetted area. Bottom shows the impact of holdup on predicted liquid load. 163

Figure 6-13: Liquid film showing the impact of increased viscosity on predicted wetted area for a contact angle of 30° and a surface tension of 0.018 N/m. High viscosity shown at left. Base viscosity shown at right. .164

Figure 6-14: Summary of the increased viscosity results for a contact angle of 30°.	
Black markers are 20x base viscosity, solid colored markers are 10x base viscosity, and hollow markers are base viscosity. Diamonds are the high surface tension case. Triangles are the low surface tension case. Top shows the impact of liquid load on fractional wetted area. Bottom shows the impact of holdup on predicted liquid load.	165
Figure 6-15: Periodic geometry vs. the Small Inlet geometry. Top shows the predicted wetted areas for three contact angles. Bottom shows the liquid holdup vs. liquid load for three different contact angles. Hollow markers are the periodic geometry.	167
Figure 6-16: Effect of contact angle on Large Inlet geometry flow field.	168
Figure 6-17: Impact of geometry and inlet conditions on fractional wetted area (top) and liquid holdup (bottom) with a contact angle of 0° and a surface tension of 0.074 N/m.	170
Figure 6-18: Impact of geometry and inlet conditions on fractional wetted area (top) and liquid holdup (bottom) with a contact angle of 30° and a surface tension of 0.074 N/m.	171
Figure 6-19: Impact of geometry and inlet conditions on fractional wetted area (top) and liquid holdup (bottom) with a contact angle of 75° and a surface tension of 0.074 N/m.	172

Figure 6-20: Fractional wetted area as a function of liquid holdup and flow regime choice. Laminar simulations are solid markers. Turbulent simulations are hollow markers. High surface tension simulations are diamonds. Low surface tension simulations are triangles. Results for a contact angle of 0° are shown at top. At bottom are results for a contact angle of 30°.	174
Figure 6-21: Predicted liquid loads as a function of liquid holdup and flow regime. Laminar simulations are solid markers. Turbulent simulations are hollow markers. High surface tension simulations are diamonds. Low surface tension simulations are triangles. Results for a contact angle of 0° are shown at top. At bottom are results for a contact angle of 30°.	175
Figure 6-22: Scaled holdup as a function of the liquid Reynolds number.	177
Figure 6-23: Comparison between CFD holdup predictions (at contact angles of 0° and 30°), the Tsai model, and the Delft model for different liquid physical properties. CFD model equations are shown in Figure 6-22. Top: $\rho_L=997.561 \text{ kg/m}^3$, $\mu_L=0.00088714 \text{ Pa-s}$. Middle: $\rho_L=1500 \text{ kg/m}^3$, $\mu_L=0.00088714 \text{ Pa-s}$. Bottom: $\rho_L=997.561 \text{ kg/m}^3$, $\mu_L=0.0088714 \text{ Pa-s}$.	179
Figure 6-24: Periodic simulations compared to the Tsai correlation. Surface tension was set at 0.074 N/m.	180
Figure 6-25: Periodic simulations compared to the Tsai correlation. Surface tension was set at 0.037 N/m.	181
Figure 6-26: Periodic simulations compared to Tsai correlation. Surface tension was set at 0.018 N/m.	182
Figure 6-27: Summary of fractional wetted area experimental results.	184

Figure 6-28: Experimental liquid holdup as a function of liquid load.....	185
Figure 6-29: Liquid surface generated at a liquid load of $48.9 \text{ m}^3/\text{m}^2\text{-hr}$ (20 GPM/ft ²) for a fluid with a contact angle of 0° . Red arrows indicate remnants of the adjacent packing sheet that were not clipped. The green arrow indicates the packing texture. The purple arrow indicates a perforation that has been completely covered by liquid.	187
Figure 6-30: Liquid layer isosurface (blue) overlaid on a dry packing image (gray) as viewed from different angles. Images were generated via X-ray CT scans. Liquid load was $36.7 \text{ m}^3/\text{m}^2\text{-hr}$ (15 GPM/ft ²). F-factor of the gas was $1.6 \text{ Pa}^{0.5}$. Figure taken from Green. ⁷³	188
Figure 6-31: Liquid surface generated at a liquid load of $48.9 \text{ m}^3/\text{m}^2\text{-hr}$ (20 GPM/ft ²) for a fluid with a contact angle of 30° . The red arrow indicates where perforations enhance wetting by splitting rivulets. The green arrow indicates where the surface texture influences the film. The purple arrow indicates a contact point between adjacent packing sheets. The black arrow indicates a preferred flow direction of the liquid.	190
Figure 6-32: Liquid surface generated by stitching periodic packing geometries together. Contact angle was 30° , surface tension was 0.074 N/m , and predicted liquid load was $54 \text{ m}^3/\text{m}^2\text{-hr}$ (22 GPM/ft ²).	191
Figure 6-33: Velocity field in a vertical plane where two packing sheets meet. .	192
Figure 6-34: Velocity field at a plane halfway within a triangular channel.	193
Figure 6-35: Illustration of where the two planes are located for the velocity fields shown in Figures 6-33 and 6-34.....	194
Figure 6-36: Comparison between experimental predictions and CFD simulations for fractional wetted area.	195

Figure 6-37: Comparison between experimental predictions and CFD simulations for liquid holdup. All liquid volume fraction was used to calculate the holdup in the CFD simulations.	197
Figure 6-38: Comparison between experimental predictions and CFD simulations for liquid holdup. Only liquid volume fractions greater than 0.5 were used to calculate the CFD values.	197
Figure 6-39: Comparison between experimental data and CFD simulations for irrigated pressure drop. Top is a liquid load of 10 GPM/ft ² , middle is 15 GPM/ft ² , and bottom is 20 GPM/ft ² (24.5, 36.7, and 48.9 m ³ /m ² -hr respectively).....	199
Figure 7-1: Example of prism layer mesh applied to the multiphase CT-generated geometry. Pure liquid is indicated by red shading. Pure gas is blue.	204
Figure 7-2: Schematic showing one possible method to generate novel packing geometries for CFD simulations.	210
Figure 7-3: Schematic showing how to generate a packing geometry capable of simulating pressure drop in large columns	211
Figure 7-4: Possible geometric arrangement for arbitrary shaped packing element domain. Periodic interfaces are coupled with matching periodic boundaries. Interfaces 3 and 4 are coupled via a field function to mimic a joint.	212
Figure 7-5: Hypothetical detector setup for stereoscopic particle image velocimetry.	214
Figure A-1: Physics continuum values for single-phase k- ω simulations on CT geometry.	217
Figure A-2: Solver settings for single-phase k- ω simulations on CT geometry.	218

Figure A-3: Physics continuum values for single-phase k- ϵ simulations on CT geometry	219
Figure A-4: Solver settings for single-phase k- ϵ simulations on CT geometry.....	220
Figure A-5: Mesh settings for “Coarse” CT geometry mesh	221
Figure A-6: Mesh settings for “Medium” CT geometry mesh	222
Figure A-7: Mesh settings for “Fine” CT geometry mesh	223
Figure A-8: Physics continuum values for periodic LES simulations.....	224
Figure A-9: Solver settings for periodic LES simulations.....	225
Figure A-10: Mesh settings for single-phase periodic RANS simulations.....	226
Figure A-11: Physics continuum settings for multiphase turbulent simulations.....	227
Figure A-12: Solver settings for multiphase turbulent simulations.....	228
Figure A-13: Mesh continuum settings for multiphase CT geometry simulations.....	229
Figure B-1: Air-water system flow diagram	231
Figure B-2: Process water source	235
Figure B-3: Liquid line valves (north)	236
Figure B-4: Liquid line valves (south).....	237
Figure B-5: Pump and associated valves.	238
Figure B-6: Column sump.	239
Figure B-7: MicroMotion outlet pipes and associated valves.	240
Figure B-8: Associated valves and drains.....	241
Figure B-9: MicroMotion outlet flow associated valve.....	242
Figure B-10: Air sampling system.....	243
Figure B-11: Power for air sampling system.....	244
Figure B-12: Storage tank and gas cylinders.....	244
Figure B-13: Column mid-section.....	245

Figure B-14: Column top	245
Figure B-15: Plant Nitrogen Supply Valve	246
Figure B-16: Nitrogen Control Valve.....	247
Figure D-1: Threshold geometries used to determine the contact point liquid holdup.	263
Figure D-2: Summary of local liquid holdup for simulations with a contact angle of 0°. Diamonds are high surface tension. Squares are middle surface tension. Triangles are low surface tension. Solid black markers are a base case with a liquid density of 997.561 kg/m ³ and viscosity of 0.0008871 Pa-s. Hollow black markers have a density of 1500 kg/m ³ . Grey markers have a density of 500 kg/m ³ . Blue markers have a viscosity of 0.008871 Pa-s. Green markers have a viscosity of 0.01774 Pa-s.....	265
Figure D-3: Summary of local liquid holdup for simulations with a contact angle of 0° with a surface tension correction. Diamonds are high surface tension. Squares are middle surface tension. Triangles are low surface tension. Solid black markers are a base case with a liquid density of 997.561 kg/m ³ and viscosity of 0.0008871 Pa-s. Hollow black markers have a density of 1500 kg/m ³ . Grey markers have a density of 500 kg/m ³ . Blue markers have a viscosity of 0.008871 Pa-s. Green markers have a viscosity of 0.01774 Pa-s. A Power law model generated is shown as the red line (Equation 5-2).....	266

Chapter 1: Introduction

SUMMARY OF WORK

This research explored the use of computational fluid dynamics (CFD) to characterize the hydraulic performance of structured packing using both single phase and multiphase simulations. Single phase simulations were carried out to determine which features of packing contribute to pressure drop, and computational efforts were made to determine more optimal packing geometries. Multiphase simulations were performed in an effort to understand the impact various hydrodynamic properties had on wetted area and liquid holdup.

The first set of single phase simulations was performed to validate the use of CFD as a tool for packing performance prediction. Pressure drop due to the packing joint was examined as part of this study. For the validation work, a high fidelity model of a Mellapak N250.Y packing was generated via X-ray computed tomography (CT). The CT geometry was imported into a commercial CFD program. The geometry was then meshed to perform the simulations. Flow was imposed axially through a bed of packing at flow rates analogous to those found in industrially operating columns. Pressure drop across the bed of packing was monitored for convergence. This data was compared to experiments utilizing a bed height and packing geometry that matched the CFD simulations.

Single phase simulations were then carried out on idealized representative elementary units (REUs) of structured packing where channel geometry and packing corrugation angle could be varied to examine the impact of a wide range of packing geometries. Periodic boundary conditions were imposed on all sides of the REU with a pressure drop between the top and bottom interface used to drive the flow. Mass flow rate through the packing was monitored for convergence. The pressure drop and mass flow

data were used to non-dimensionalize the pressure drop through structured packing to generate correlations for packing design.

Multiphase simulations were performed on an REU with channel dimensions matching those of Mellapak N.250Y. Periodic boundary conditions were imposed on all sides once again with a pressure drop between the top and bottom boundaries. Initially, a uniform liquid film was introduced near the packing surface, and stagnant gas filled the rest of the domain. Transient simulations were allowed to run until a pseudo-steady state was achieved for interfacial area and liquid mass flow rate. The impact of liquid holdup, viscosity, density, surface tension, and static contact angle were examined in this REU geometry.

Experimental data was also collected in an effort to determine if CFD is an appropriate tool capable of predicting wetted area and liquid holdup. Experiments using CO₂ absorption into a caustic solution were carried out with a bed of Mellapak N250.Y packing. From this data, packing wetted area was determined for comparison with simulation results. The CT generated geometry was utilized for large-scale multiphase simulations. Due to the simulation size, only the impact of varying liquid load and simulation contact angle were examined. Liquid viscosity and surface tension were chosen to match that of the experiments.

MOTIVATION

Distillation continues to be a primary method of separation in the petrochemical and chemicals industries.¹ There are over 40,000 operating distillation columns in the United States, and they account for 40% of the processing energy in refineries and chemical plants². This amounts to roughly 5% of the total energy used in the United

States. As such, a small increase in efficiency will result in a significant amount of energy savings.

As anthropogenic climate change continues to be a primary concern, curbing CO₂ emissions continues to be an area of great research interest.³ Because distillation columns are ultimately heated by burning fossil fuels, any energy savings will result in a reduction in CO₂ emissions. Furthermore, it may be necessary for coal-fired power plants to capture and store their CO₂ emissions in the future. One promising technique to remove CO₂ from flue gas is gas absorption using amine systems. These systems rely heavily on efficient packing internals, and specially designed packings can significantly reduce both capital and operating expenses for the CO₂ capture system.³ Like the aerospace and automotive industries, CFD can be applied to evaluate and develop novel designs.

Distillation and absorption columns rely on semi-empirical equations to estimate pressure drop, capacity, mass transfer coefficients, and interfacial area.⁴ The correlations rely on a limited set of data from a limited amount of test systems to predict column performance, with the accuracy of such models relying heavily on the accuracy of the experimental databases.⁵ Furthermore, data regression will often obfuscate the impact of individual system properties. Essentially, models are developed based on overall mass transfer in a column (e.g. HETP) with assumed forms for mass transfer coefficients and interfacial area. This leads to an irreversible coupling between the mass transfer coefficients and interfacial area with the equations designed to fit the HETP data.⁶ The impact of individual variables (e.g. liquid viscosity or flow rate) is masked by generating correlations this way.

Unfortunately, direct observation of the flow field within packed columns is a difficult problem to overcome.⁷⁻⁹ Various imaging techniques have been used, but there are often problems with acquisition time, sample size, spatial resolution, and temporal

resolution. Experimental limitations have thus far precluded the development of more accurate design equations based on localized flow data.

With the advent of high-performance computing clusters, it is increasingly possible to simulate complex fluid flow in and around complex geometries. CFD programs have been used in the design of aerospace, marine, and automotive products. They are also increasingly finding application within the chemical processing and oil and gas industries. Mixing, reactor engineering, combustion, and oil/gas separators are all processes to which CFD has been applied successfully.

Validated CFD simulations offer access to a wealth of data not available with traditional experimental techniques. Both macroscopic and localized data are available as part of the simulation process, allowing researchers and engineers to rigorously analyze the impact of system properties and geometry on quantities of interest. These parameters can be examined individually and independently within the CFD program, an advantage traditional experimental systems cannot match easily. A parametric study using CFD to simulate flow through structured packing will allow a fundamental understanding of the flow field for a wide variety of geometries and system properties. From these digital experiments, new packings and design equations can be generated.

GAS-LIQUID SEPARATIONS

Distillation, gas absorption, and stripping all rely on efficient contact between gas and liquid phases to produce the desired separation. Distillation relies on the difference in relative volatilities between components to perform the separation. Gas absorption and stripping rely on the preference of a solute to distribute between the gas and liquid phases to achieve a given separation. These operations are usually performed in vertical towers

filled with packing or trays. Figure 1-1 shows an example of distillation (left) and gas absorption (right).

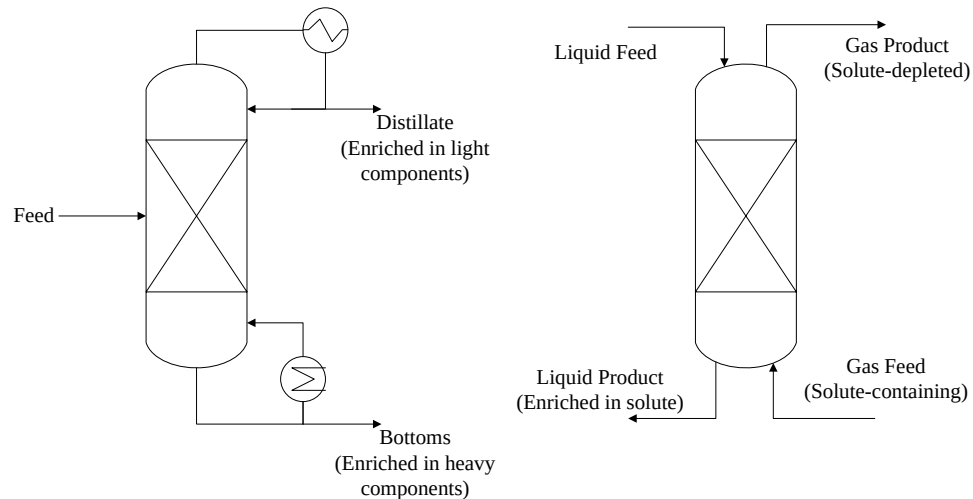


Figure 1-1: Process diagrams from distillation (left) and gas absorption (right).

STRUCTURED PACKING

Structured packings are made of crimped layers of corrugated sheets bundled together. Figure 1-2 shows an example of structured packing and the corrugated sheets it is built from. Adjacent sheets are rotated 180° with respect to each other and bundled together to form an element of structured packing. Typical specific areas for structured packing range from $100\text{--}500\text{ m}^2/\text{m}^3$.¹ Packed element heights range from $0.203\text{--}0.305\text{ m}$. Adjacent elements of structured packing are typically rotated 90° with respect to each other. This rotation allows for liquid and vapor redistribution at the interface between elements. This region between two layers (i.e. the joint) is associated with increased pressure drop and increased liquid holdup.^{7,10} Structured packings are made from wire mesh, stainless steel sheets, ceramic, and polypropylene. Wiper bands, indicated in Figure 1-2, are present in structured packing to redirect any liquid and vapor flowing along the wall back into the packing to ensure efficient contact between the two phases.

In small columns, the wiper bands act to increase pressure drop when compared to large-diameter columns.¹¹

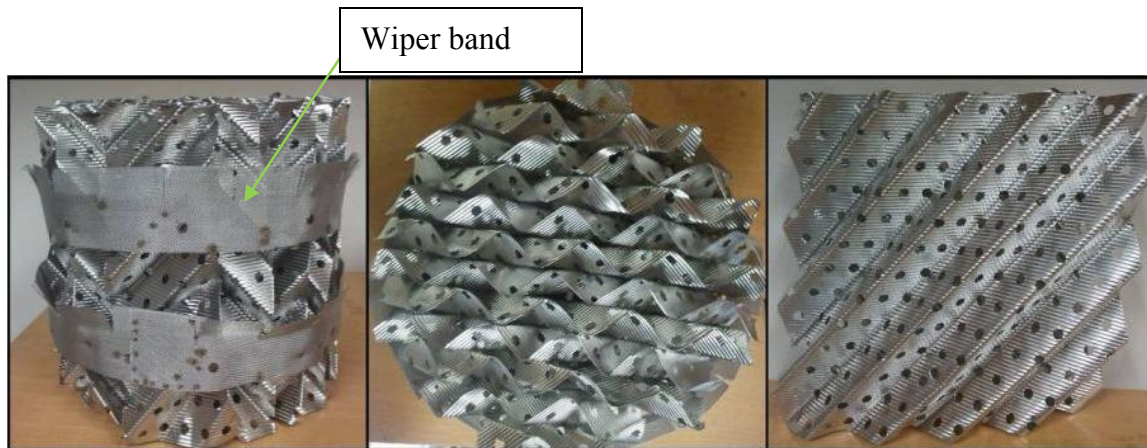


Figure 1-2: Structured packing element shown from the side (left), top (middle), and a single sheet pulled from the element (right).

The high specific surface areas, high porosities (typically greater than 0.9 for stainless steel corrugated packings), and regular geometries provide for lower pressure drop than trays or random packings. Structured packings typically cost significantly more on a per-volume basis than random packings. Due to differences in capacities and efficiencies, however, cost comparisons should only be made between complete designs. Structured packings will typically result in smaller columns, lower operational cost, and lower reflux than random packings.⁵

COMPUTATIONAL FLUID DYNAMICS (CFD)

CFD is the use of computers to solve fluid flow problems numerically. The following steps are necessary to perform a CFD analysis:

1. Model the geometry. This is traditionally done via CAD or importing a surface file from scanned data.

2. Generate the mesh/grid. The generated mesh will directly impact the quality of results, and it is necessary to ensure the presence of a high quality mesh before beginning simulations.
3. Determine appropriate physical models and equations to describe the flow. This ranges from choosing an equation of state for the fluid to an appropriate turbulence model.
4. Run the simulations. Simulation residuals and engineering quantities of interest should be monitored for convergence. As part of the simulations, a mesh sensitivity study should be performed to ensure the solution is mesh-independent.
5. Post-process the data to gain maximum understanding of the fluid flow.

An introduction to mesh generation, turbulence modeling, choice of multiphase models, and numerical solutions is presented in the following sections.

Mesh Generation

Mesh generation can be largely divided into two classes, as shown in Figure 1-3.¹² A structured mesh is shown on the left. At right, an unstructured mesh is presented. Structured meshes are built from quadrilaterals in 2D and hexahedra in 3D. A structured grid is laid out in a regular and repeating fashion, but it is not necessarily a Cartesian grid. In a 2D structured grid, point (i,j) will always have neighbors $(i-1,j)$, $(i+1,j)$, $(i,j-1)$, and $(i,j+1)$. This same idea also applies to 3D grids with each point having six neighbors. This regular structure of cells allows simulations to be executed in a lower amount of time with significantly less memory required than unstructured grids. Unstructured grids can be made up of arbitrarily shaped cells to fill a domain. In general, the mesh is made up of triangles or polygons in 2D, and tetrahedrons, prisms, or polyhedrons in 3D. There is no logical structure between the location of grid points in the domain and in system

memory, and each grid point can have an arbitrary number of neighbors. This acts to increase memory requirements due to the fact the connectivity and location of all points needs to be stored. The creation of unstructured meshes is significantly more robust when compared to structured meshes, though, and they are more easily adapted to arbitrary geometries.

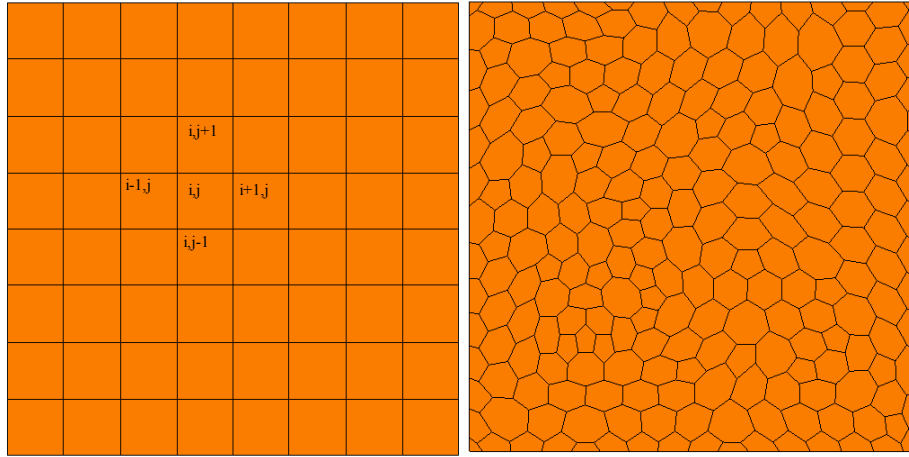


Figure 1-3: Example of a structured (left) and unstructured (right) mesh for CFD simulations.

One final concern with mesh generation, especially in the case of turbulence modeling, is the resolution of the near-wall region. Generally, this is measured with a dimensionless wall distance:

$$y^+ = \frac{u_* y}{\nu} \quad \text{Equation 1-1}$$

with u_* defined as the friction velocity:

$$u_* = \sqrt{\frac{\tau_w}{\rho}} \quad \text{Equation 1-2}$$

where τ_w is the wall shear stress, and ρ is the fluid density. For accurate skin friction and pressure drop results, the wall y^+ of the first cell should be of order unity, and an appropriate turbulence model formulation should be chosen.^{13,14} Refinement of a

tetrahedral or polyhedral mesh to ensure a y^+ near unity everywhere is often not possible due to the refinement in both the wall normal and wall tangent directions occurring simultaneously. This leads to a significant increase in computational cells, and thus, computational time and memory required. To resolve the near-wall region in an efficient manner, the use of prism layers is recommended. This also allows for more accurate predictions of skin friction.¹⁴ An example of a mesh with and without prism layers is shown in Figure 1-4. Through the use of prism layers, the large gradients in the near-wall region are captured efficiently. Also, the y^+ values can be readily controlled through prism layer parameters (e.g. number of prism layers, prism layer thickness, and stretching factor between prism layers). The wall tangent direction, where gradients are often significantly smaller than the wall normal direction, is not excessively resolved in this case.

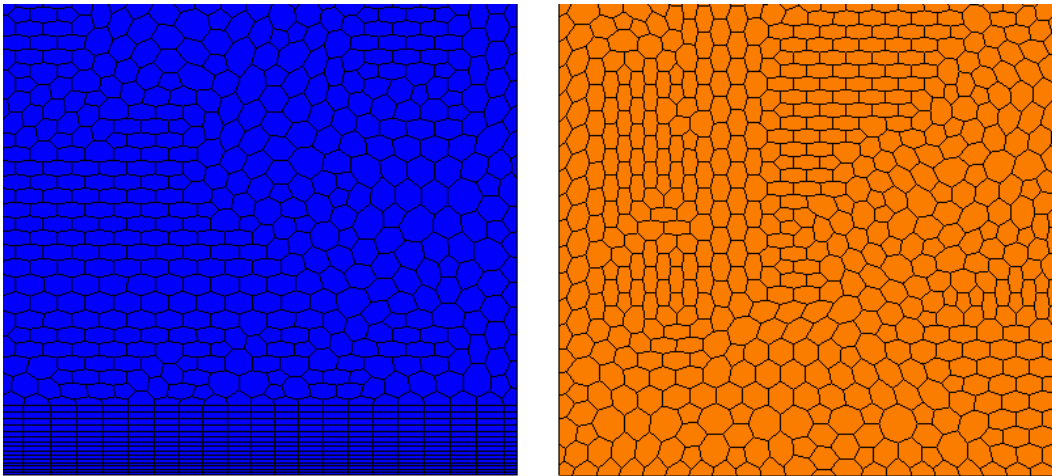


Figure 1-4: Example of a polyhedral mesh with prism layers (left) and a mesh constructed of only polyhedral cells (right).

Turbulence Modeling

Simulation of turbulent flow can be broken down based on whether the turbulence is simulated or modeled. In the case of turbulent flow simulation, methods available include direct numerical simulation (DNS) and large-eddy simulation (LES). Turbulence modeling generally involves assuming a relationship between the mean velocity field and turbulent velocity fluctuations. It generally involves solving the Reynolds-averaged Navier-Stokes (RANS) equations. These methods can be broken down further into Reynolds-stress models (RSM) and eddy viscosity models. When using an RSM approach, the Reynolds stresses each have individual transport equations which are solved. In eddy viscosity models, the Reynolds stresses are related to the mean-strain rate tensor. Basic details for LES and RANS models are presented below. For a more detailed discussion of turbulence and modeling turbulent flows, interested readers are referred to the textbook *Turbulent Flows* by Stephen Pope.¹⁵

Direct Numerical Simulation

In DNS, the time-dependent Navier-Stokes equations are solved exactly to determine the velocity field, including all turbulent fluctuations. The continuity equation (Equation 1-3) and the conservative form of the Navier-Stokes equation (Equation 1-4) are presented below for an incompressible fluid:

$$\frac{\partial U_i}{\partial x_i} = 0 \quad \text{Equation 1-3}$$

$$\frac{\partial U_i}{\partial t} + \frac{\partial}{\partial x_j} U_i U_j = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} + f_i \quad \text{Equation 1-4}$$

where U_i is the velocity vector, ρ is the density, p is the pressure, ν is the kinematic velocity, and f_i represents body forces that may be present (e.g. gravity). Commonly, a modified pressure is used:

$$p = p_{ref} + \rho g_i x_i + P \quad \text{Equation 1-5}$$

where p_{ref} is a constant reference pressure, g_i is the gravitational vector, and P is the modified pressure. If gravity is the only body force present (i.e. $f_i = g_i$), Equation 1-4 becomes:

$$\frac{\partial U_i}{\partial t} + \frac{\partial}{\partial x_j} U_i U_j = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} \quad \text{Equation 1-6}$$

The exact solution to the above equations requires all length and time scales to be resolved, making DNS computationally expensive. Because of this, DNS is strictly reserved for low-to-moderate Reynolds number flows. Although of limited engineering interest, DNS results have been used to extract results of turbulent quantities that are difficult or impossible to measure experimentally.¹⁵ These results can then be applied to develop or enhance turbulence models.

Large Eddy Simulation

Large eddy simulations filter the Navier-Stokes equations. In this manner, the larger unsteady turbulent motions are directly simulated. The turbulent structures smaller than the filter used are modeled. This approach places LES somewhere between DNS and RANS models in terms of computational cost.

The first step in LES is filtering the velocity field by the convolution of the velocity field with a filtering kernel:

$$\bar{U}(\vec{x}, t) = \int G(\vec{x} - \vec{\xi}) U(\vec{\xi}) d\vec{\xi} \quad \text{Equation 1-7}$$

where $\bar{U}$ is the filtered velocity and G is the convolution kernel. Applying the filter to Equation 1-3 and Equation 1-6 yields:

$$\frac{\partial \bar{U}_i}{\partial x_i} = 0 \quad \text{Equation 1-8}$$

$$\frac{\partial \bar{U}_i}{\partial t} + \frac{\partial}{\partial x_j} \overline{U_i U_j} = -\frac{1}{\rho} \frac{\partial \bar{P}}{\partial x_i} + \nu \frac{\partial^2 \bar{U}_i}{\partial x_j \partial x_j} \quad \text{Equation 1-9}$$

At this point, it is useful to define the residual-stress tensor:

$$\tau_{ij}^R \stackrel{\text{def}}{=} \overline{U_i U_j} - \bar{U}_i \bar{U}_j \quad \text{Equation 1-10}$$

It should be noted that the residual-stress tensor is formally defined as $-\rho\tau_{ij}^R$, but Equation 1-10 is more convenient to work with here. Substituting τ_{ij}^R into Equation 1-8 yields:

$$\frac{\partial \bar{U}_i}{\partial t} + \frac{\partial}{\partial x_j} \bar{U}_i \bar{U}_j = -\frac{1}{\rho} \frac{\partial \bar{P}}{\partial x_i} + \nu \frac{\partial^2 \bar{U}_i}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j} \tau_{ij}^R \quad \text{Equation 1-11}$$

With these equations, only τ_{ij}^R needs to be modeled to achieve closure. A common approach to achieve closure is through the use of an eddy viscosity model. For an incompressible fluid, the linear eddy-viscosity model is given by:

$$\tau_{ij}^R = -2\nu_r \bar{S}_{ij} + \frac{2}{3} k_{SGS} \delta_{ij} \quad \text{Equation 1-12}$$

where ν_r is the eddy viscosity of the residual motions, $\bar{S}_{ij}$ is the filtered strain-rate tensor, δ_{ij} is the Kronecker delta, and k_{SGS} is the subgrid turbulent kinetic energy defined by:

$$k_{SGS} = \frac{1}{2} \tau_{ii}^R \quad \text{Equation 1-13}$$

Both k_{SGS} and ν_r are determined by the specific subgrid stress model chosen. The full formulations used in present research can be found in the STAR-CCM+ user manual.¹⁴ By solving for the large-scale velocity fluctuations due to turbulence, more of the flow information is retained for the simulation, providing a more accurate picture of the flow. Furthermore, the small scales of turbulence are more universal in nature, making the development of a universal subgrid stress model more feasible.¹⁵

Reynolds Averaged Navier-Stokes Equations

The RANS equations can be derived by time-averaging the Navier-Stokes equations. Time-averaging Equations 1-3 and 1-6 yields:

$$\frac{\partial \langle U_i \rangle}{\partial x_i} = 0 \quad \text{Equation 1-14}$$

$$\frac{\partial \langle U_i \rangle}{\partial t} + \frac{\partial}{\partial x_j} \langle U_i U_j \rangle = -\frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial x_i} + \nu \frac{\partial^2 \langle U_i \rangle}{\partial x_j \partial x_j} \quad \text{Equation 1-15}$$

where bracketed terms indicate the time-average. The velocity field is broken into an average and a fluctuating part:

$$U_i = \langle U_i \rangle + u'_i \quad \text{Equation 1-16}$$

where u'_i is the fluctuating part of the velocity. Noting that $\langle u'_i \rangle = 0$, Equation 1-15 can be transformed into:

$$\frac{\partial \langle U_i \rangle}{\partial t} + \frac{\partial}{\partial x_j} \langle U_i \rangle \langle U_j \rangle = -\frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial x_i} + \nu \frac{\partial^2 \langle U_i \rangle}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j} \langle u'_i u'_j \rangle \quad \text{Equation 1-17}$$

The Reynolds stresses can now be identified as:

$$\tau_{ij} = -\rho \langle u'_i u'_j \rangle \quad \text{Equation 1-18}$$

$\langle u'_i u'_j \rangle$ is a positive semi-definite, symmetric 2nd-order tensor.¹⁵ As such, it contains six unknown flow variables, preventing the Equations 1-17 and 1-14 from forming a closed system of equations. To achieve closure, $\langle u'_i u'_j \rangle$ must be determined in some way.

One of the most common methods of achieving closure for the Reynolds stresses is through the use of an eddy-viscosity model. This is analogous to what was shown for LES:

$$\langle u'_i u'_j \rangle = -2\nu_t \langle S_{ij} \rangle + \frac{2}{3} k \delta_{ij} \quad \text{Equation 1-19}$$

where ν_t is the eddy viscosity, $\langle S_{ij} \rangle$ is the mean strain-rate tensor, and k is the turbulent kinetic energy defined as half the trace of the Reynolds stress tensor:

$$k \stackrel{\text{def}}{=} \frac{1}{2} \langle u'_i u'_i \rangle \quad \text{Equation 1-20}$$

To calculate the eddy viscosity, a turbulent length scale and turbulent time scale must be calculated or assumed.

Two-Equation RANS Models: k-ε model

In the k-ε model, model equations for the turbulent kinetic energy (k) and the dissipation of turbulent kinetic energy (ϵ) are solved. From these two quantities, a turbulent length scale ($L_T = k^{\frac{3}{2}}/\epsilon$) and a turbulent time scale ($\tau_T = k/\epsilon$) can be used to define the eddy viscosity as:

$$\nu_t = C_\mu \frac{L_T^2}{\tau_T} = C_\mu \frac{k^2}{\epsilon} \quad \text{Equation 1-21}$$

where C_μ is a constant. In the original formulation, C_μ is set at 0.09. This can lead to negative and, thus, non-physical values for diagonal elements of the Reynolds stress tensor (i.e. $\langle u'_1 u'_1 \rangle$, $\langle u'_2 u'_2 \rangle$ and $\langle u'_3 u'_3 \rangle$). To ensure the values remained positive (i.e. realizable), the realizable k- ϵ model was developed where C_μ is determined dynamically to ensure the diagonal elements of $\langle u'_i u'_j \rangle$ remain greater than or equal to 0.

The model equation for the turbulent kinetic energy is given by:

$$\frac{\partial k}{\partial t} + \langle U_j \rangle \frac{\partial k}{\partial x_j} = -\langle u'_i u'_j \rangle \frac{\partial \langle U_i \rangle}{\partial x_j} - \epsilon + \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] \quad \text{Equation 1-22}$$

where σ_k is a constant equal to 1.0. The first term on the right-hand side of Equation 1-22 is generally positive, and is thus considered a source of turbulent kinetic energy. It is more normally known as the production of turbulent kinetic energy. The second term is the dissipation of kinetic energy. The final term is the diffusion of turbulent energy.

The model equation for dissipation is given by:

$$\frac{\partial \epsilon}{\partial t} + \langle U_j \rangle \frac{\partial \epsilon}{\partial x_j} = -C_{\epsilon 1} \langle u'_i u'_j \rangle \frac{\partial \langle U_i \rangle}{\partial x_j} \frac{\epsilon}{k} - C_{\epsilon 2} \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] \quad \text{Equation 1-23}$$

where $C_{\epsilon 1} = 1.44$, $C_{\epsilon 2} = 1.92$, and $\sigma_\epsilon = 1.3$ are constants in the standard formulation.¹⁶

The terms on the right hand side are, in order from left to right, production of dissipation, dissipation of dissipation, and diffusion of dissipation. Unlike the turbulent kinetic energy equation, the equation for dissipation cannot be systematically derived. Instead, the dissipation equation is chosen to be a dimensionally consistent analog to Equation 1-22.¹⁶

The realizable k- ϵ has a slightly different form in which some of the constants are replaced by expressions involving the mean flow. The exact formulation used can be found in the STAR-CCM+ user manual.¹⁴

As mentioned in the mesh generation section, the near-wall resolution and the wall formulation chosen are key for accurate results.^{14,17} There are three classes of wall formulations broadly used: 1) wall functions, 2) low-Reynolds-number turbulence modeling, and 3) two-layer zonal modeling. Wall functions are the cheapest computationally. Rather than resolving the flow through the viscous sublayer in the near-wall region, the first mesh point is placed at a dimensionless wall distance in the range of $30 < y^+ < 100$. Boundary conditions for the velocity, turbulent kinetic energy, and dissipation are assumed forms derived from boundary layer theory.¹⁷

Low-Reynolds-number turbulence modeling allows for the integration of turbulent and flow quantities all the way to the wall. The name of this method only refers to the ability to integrate to the wall, where viscous effects dominate (i.e. where the local Reynolds number is low). By needing to resolve the boundary layer, computational costs are necessarily increased. The computational cell closest to the wall should have a y^+ near 1. However, due to the poor behavior of the k - ϵ model in the near wall region, arbitrary damping functions and modifications to the ϵ model equation are necessary. Because of this, low-Reynolds-number formulations for the k - ϵ model are of limited benefit in practical cases.¹⁶

Two-layer zonal modeling serves as a compromise between the assumption of a universal wall layer used in wall functions and simulating the near-wall region in its entirety. Two-layer models break the simulation regime into two regions. In the outer region, the full equations for k - ϵ are solved. In the inner region (i.e. near the wall), the equation for k is still solved, but an algebraic model for the turbulent length scale is used instead of the ϵ equation. This avoids the numeric stiffness associated with the ϵ equation in the near wall region. The solutions of the inner layer and outer layer are patched together or blended in the transition region between the layers.^{16,17} The two-layer model

yields better predictions than wall functions, but it does require more computational points in the near wall region.¹⁶ For the studies employing a realizable k- ϵ turbulence model, the two-layer wall modeling approach was used.

Two-Equation RANS Models: k- ω

Rather than solve for k and ϵ , the k- ω model solves two equations for turbulent kinetic energy (k) and the specific dissipation rate, ω , defined as:

$$\omega \stackrel{\text{def}}{=} \frac{\epsilon}{k} \quad \text{Equation 1-24}$$

k- ω models have the primary advantage of being well-behaved through the boundary layer. This allows the equations to be integrated all the way to the wall without the need for damping functions or two-layer formulations. It is still an eddy viscosity model with the eddy viscosity given as:

$$\nu_t = C_\mu \frac{k}{\omega} \quad \text{Equation 1-24}$$

where C_μ is a constant of value 0.09. The model equations for k and ω are:

$$\frac{\partial k}{\partial t} + \langle U_j \rangle \frac{\partial k}{\partial x_j} = -\langle u'_i u'_j \rangle \frac{\partial \langle U_i \rangle}{\partial x_j} - k\omega + \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] \quad \text{Equation 1-26}$$

$$\frac{\partial \omega}{\partial t} + \langle U_j \rangle \frac{\partial \omega}{\partial x_j} = -C_{\omega 1} \langle u'_i u'_j \rangle \frac{\partial \langle U_i \rangle}{\partial x_j} \frac{\omega}{k} - C_{\omega 2} \omega^2 + \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_\omega} \right) \frac{\partial \omega}{\partial x_j} \right]$$

$$\text{Equation 1-27}$$

where $\sigma_k = 2$, $C_{\omega 1} = 5/9$, $C_{\omega 2} = 5/6$, and $\sigma_\omega = 2$.¹⁶ On the right hand side of the equations, the terms are production, dissipation, and turbulent transport of the respective variables.

The wall formulations typically seen for k- ω are wall functions and direct integration to the wall. No modifications to the ω equation are necessary to find a solution near the wall, but the first cell should have a y^+ near 1. Wall function considerations are similar to what was mentioned for the k- ϵ turbulence models.

The standard formulation $k-\omega$ model is sensitive to inlet turbulent boundary conditions.¹⁴ The $k-\epsilon$ model does not demonstrate this weakness. This led to the development of the shear stress transport (SST) formulation of the $k-\omega$ model. The SST $k-\omega$ includes an additional term. This additional term causes the turbulence model to behave similar to the $k-\epsilon$ model in the free-stream, while maintaining the superior performance of the $k-\omega$ model in the near-wall region. For the studies employing the $k-\omega$ model, the SST $k-\omega$ was used.

Other RANS Models

There are several other models developed for specific applications.¹⁵ The models range in complexity from using a single algebraic equation to the Reynolds-stress models, where seven additional transport equations are solved. For a discussion of other turbulence models and their applications, the reader is referred to “Turbulent Flows” by Pope.¹⁵

In RSM, seven model transport equations are solved for the turbulent quantities (i.e. the six independent terms of $\langle u'_i u'_j \rangle$ and a dissipation equation). The additional transport equations in RSM require more computational time. When compared to a $k-\epsilon$ simulation, the CPU time required for an RSM simulation can be more than a factor of two.¹⁵ This increase in CPU time, though, is offset by increased accuracy. This is especially important when turbulent viscosity models fail (e.g. flows with significant streamline curvature and flows with strong swirl).

Multiphase Modeling

Multiphase simulations involve solving equations of motions for two or more phases. Phase is taken to mean liquid, solid, and vapor state. In the context of multiphase modeling, two immiscible liquids would be considered distinct phases for simulation.

The choice of multiphase model depends on many variables, but the two primary concerns are whether the two phases are separated or dispersed and how much of each phase is present.¹⁷ STAR-CCM+ offers many different models, depending on the specific application.¹⁴ The five primary choices of multiphase models in STAR-CCM+ are:

1. Lagrangian Multiphase model. This method is also known as the Euler-Lagrange model.¹⁷ In the Lagrangian Multiphase model, the fluid is treated in a continuous framework and relatively few particles (e.g. droplets or catalyst particles) are simulated individually. Closure for mass and momentum balance between phases is achieved with semi-empirical expressions. These simulations may or may not account for particle-particle interaction, and are generally reserved for low volume fractions of the dispersed phase (less than 0.001).¹⁷
2. Multiphase Segregated Flow model. This method is more commonly known as the Euler-Euler or Eulerian Multiphase model in the literature.¹⁴ The two (or more fluids) are treated as fully interpenetrating fluids. Each fluid is simulated by solving separate continuity and momentum equations for each phase. Phase interaction models are required to predict mass, momentum, and energy transfer between phases. It is generally used to simulate dispersed flows.
3. Volume of Fluid (VOF) model. These models track the local value of the volume fraction to describe the position of the interface. Two or more immiscible phases are simulated using a shared-field approach (i.e. only one set of conservation equations must be solved). The volume fraction is tracked via an additional advection equation. This method is most appropriate for free-surface or stratified flow simulations where each fluid constitutes a large structure of the flow.
4. Discrete Element Method. This method is an extension of the Lagrangian Multiphase model in which each particle is individually simulated. Inter-particle

contact forces are rigorously calculated. It is most suited for granular flow applications.

5. Fluid Film model. This model is a more recent addition to STAR-CCM+. The simulation is split into two regions. In the first, the gas phase is rigorously calculated using the Navier-Stokes equations. In the second region, a liquid film is modeled using laminar film equations, and a parabolic profile is used for the liquid velocity.

Liquid flow on structured packing has been observed as a film on the packing surface via X-ray CT scans.⁷ Because the gas and liquid flows are largely separate and immiscible, the flow regime would be considered stratified. This flow regime precludes the use of the Lagrangian and Discrete Element models. As the Euler-Euler model is generally for dispersed flow, it can also be eliminated as a viable option. This leaves the Fluid Film model and VOF model to simulate the free surface. The Fluid Film model was not available when this research started and does not allow the wettability of the surface to be defined via a contact angle.¹⁴ The VOF method was developed as an interface tracking method where accurate simulation of the free surface was desired. It also allows for wall adhesion to be accounted for with a contact angle, making it the most appropriate choice for multiphase flow through structured packing.

Volume of Fluid Model Equations

The VOF model assumes a shared-field between the two phases. This approximation is also known as the one-fluid model.¹⁸ To track the interface, a scalar known as the volume fraction is advected with a conservation law of the form:

$$\frac{\partial \alpha_L}{\partial t} + U_i \frac{\partial \alpha_L}{\partial x_i} = 0 \quad \text{Equation 1-28}$$

where α_L is the volume fraction of the liquid. This approach necessarily smears the interfacial region across one or more computational cells as shown in Figure 1-5.

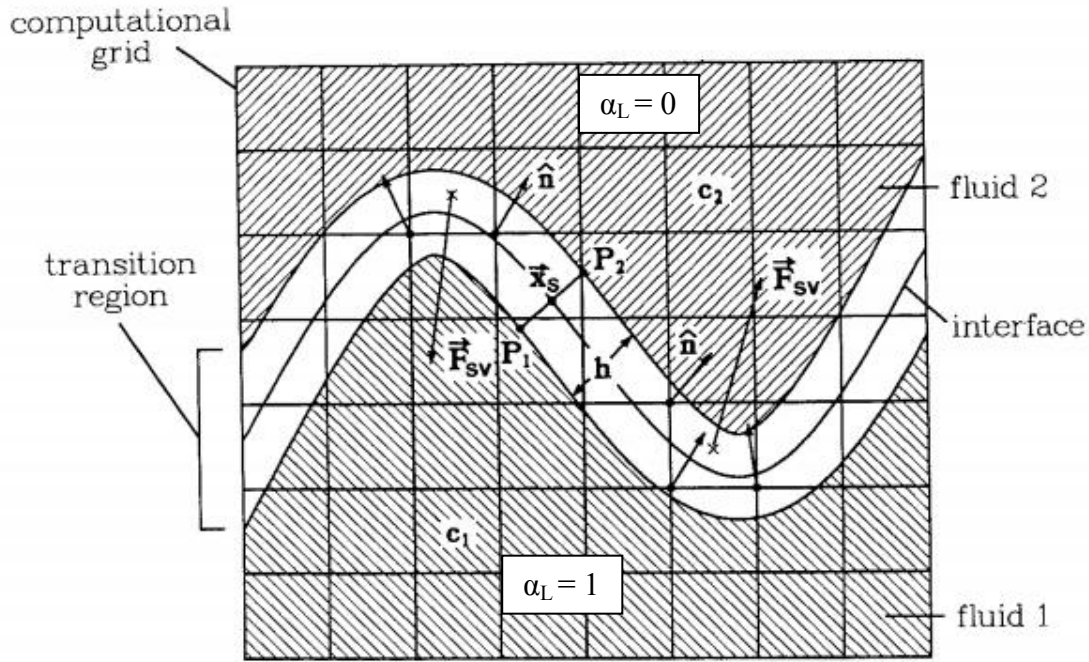


Figure 1-5: Figure showing the smearing of the interfacial region due to the VOF model. Figure taken from Brackbill *et al.*¹⁹

The volume fraction of liquid is defined as the ratio of the volume occupied by the liquid to the total volume of the cell. It can only take values ranging from 0 to 1, with 0 indicating the cell is pure vapor and 1 indicating the cell is occupied by liquid. With the volume fraction defined, the density and viscosity in each cell are taken to be averages defined as:

$$\rho = \alpha_L \rho_L + (1 - \alpha_L) \rho_G \quad \text{Equation 1-29}$$

$$\mu = \alpha_L \mu_L + (1 - \alpha_L) \mu_G \quad \text{Equation 1-30}$$

where ρ_L and ρ_G are the densities of the liquid and gas respectively, and μ_L and μ_G are the dynamic viscosities of the liquid and gas. To write these averages, the fact the volume fractions of gas and liquid must add up to one in each cell (i.e. $\alpha_L + \alpha_G = 1$).

Surface tension is modeled using the continuum surface force (CSF) approach of Brackbill *et al.*¹⁹ The Navier-Stokes equations are presented again with the surface tension force explicitly shown:

$$\rho \frac{\partial U_i}{\partial t} + \rho \frac{\partial}{\partial x_j} U_i U_j = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_k} \left[\mu \left(\frac{\partial u_k}{\partial x_j} + \frac{\partial u_j}{\partial x_k} \right) \right] + \rho g_i + F_i^\gamma$$

Equation 1-31

where F_i^γ is the surface tension force. ρ and μ are now given by Equations 1-29 and 1-30. Strictly speaking, the surface tension force acts only at the interface between fluids. Following Brackbill *et al.*, the surface tension force per unit area is given by:

$$\mathbf{F}_{sa} = \gamma \kappa \hat{\mathbf{n}}$$

Equation 1-32

where γ is the surface tension of the fluid, κ is the curvature of the surface taken to be positive if the center of curvature is in the heavy phase, and $\hat{\mathbf{n}}$ is the unit normal vector pointing into the heavy phase.¹⁹ $\hat{\mathbf{n}}$ is calculated at the free surface located at position $\mathbf{x}_s$.

This surface force can be rewritten as a volume force using the Dirac delta function:

$$\int_A \gamma \kappa \hat{\mathbf{n}} dA = \int_V \gamma \kappa \hat{\mathbf{n}} \delta(\hat{\mathbf{n}} \cdot (\mathbf{x} - \mathbf{x}_s)) dV$$

Equation 1-33

Brackbill *et al.* showed that:

$$\hat{\mathbf{n}} \delta(\hat{\mathbf{n}} \cdot (\mathbf{x} - \mathbf{x}_s)) = \nabla \alpha_L$$

Equation 1-34

in the limit the interface was infinitely thin. If the interface is not infinitely thin, the Equation 1-34 is an approximation, and the following can be written:

$$\int_A \gamma \kappa \hat{\mathbf{n}} dA \cong \int_V \gamma \kappa \nabla \alpha_L dV$$

Equation 1-34

From this, the volume body force for surface tension in equation 1-31 can be identified as:

$$F_i^\gamma = \gamma \kappa \frac{\partial \alpha_L}{\partial x_i} \quad \text{Equation 1-35}$$

In this manner, the surface tension body force only has non-zero values in the interfacial region. This is the only location where the gradient of the volume fraction is non-zero.

The unit normal and curvature can also be computed as a function of α_L :

$$\hat{n}_i = \frac{\frac{\partial \alpha_L}{\partial x_i}}{\left(\frac{\partial \alpha_L}{\partial x_j} \frac{\partial \alpha_L}{\partial x_j} \right)^{\frac{1}{2}}} \quad \text{Equation 1-36}$$

$$\kappa = - \frac{\partial}{\partial x_i} \frac{\hat{n}_i}{(\hat{n}_j \hat{n}_j)^{\frac{1}{2}}} \quad \text{Equation 1-37}$$

Wall adhesion is handled by modifying the unit normal when the interfacial region of the fluid (i.e. $0 < \alpha_L < 1$) contacts the wall. Instead of using Equation 1-36 to calculate the normal, the following is used:²⁰

$$\hat{n}_i = \hat{n}_i^{wall} \cos(\theta_c) + \hat{t}_i^{wall} \sin(\theta_c) \quad \text{Equation 1-38}$$

where $\hat{n}_i^{wall}$ is the unit normal of the wall directed into the surface, $\hat{t}_i^{wall}$ is the unit tangent of the wall directed into the liquid phase, and θ_c is the contact angle.

Numerical Solutions

As the numeric values at each mesh point are the only thing available to the computer, it is necessary to discretize the equations themselves. This process transforms the continuous equations describing fluid flow into algebraic equations described by the discrete numeric values at each mesh point. Finite difference methods (FDM), finite volume methods (FVM), and finite element methods (FEM) have all been successfully applied for fluid flow simulation.¹² A brief description of FDM and FVM are presented below. Interested readers are referred to the text *Numerical Computation of Internal and*

External Flows: The Fundamentals of Computational Fluid Dynamics by Charles Hirsch for a more detailed discussion of numerical methods.¹²

Finite difference methods are based on the Taylor series expansion of functions, making their application straightforward and relatively simple to apply.¹² Their simplicity, however, requires meshes to be structured in some way. As a simple example, consider some function $f(x)$ and the uniform grid (i.e. $x_j - x_{j-1} = \Delta x = \text{constant}$) shown in Figure 1-6.

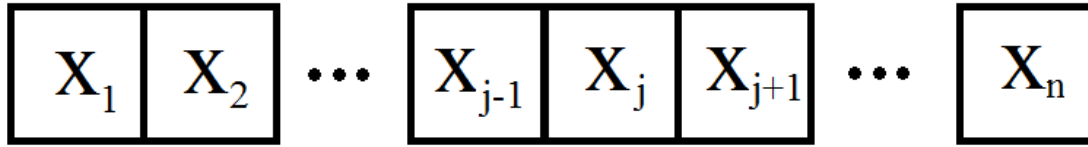


Figure 1-6: Example uniform, one-dimensional grid showing the spatial discretization.

As part of the discretization process, $f(x)$ will be represented by discrete values at the grid points (i.e. $f(x) \cong f(x_j)$ for $j = 1, 2, \dots, n$). A Taylor series expansion about x_j is given by:

$$f(x_{j+1}) = f(x_j) + f'(x_j)\Delta x + f''(x_j)\frac{\Delta x^2}{2} + \dots \quad \text{Equation 1-39}$$

Solving for $f'(x_j)$ yields:

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_j)}{\Delta x} - \left[f''(x_j)\frac{\Delta x}{2} + \dots \right] \quad \text{Equation 1-40}$$

The bracketed term is truncated, introducing an error in the approximation of $O(\Delta x)$. Because the scheme presented in Equation 1-40 uses information at points x_j and x_{j+1} , this scheme presented is called a forward difference method. With a truncation error of $O(\Delta x)$, this scheme could be further characterized as a first order forward difference method. If instead information at points x_{j-1} and x_j were used, the first order backward difference scheme could be generated:

$$f'(x_j) = \frac{f(x_j) - f(x_{j-1}))}{\Delta x} + \left[f''(x_j) \frac{\Delta x}{2} + \dots \right] \quad \text{Equation 1-41}$$

Noticing that the leading order of the truncation errors in the forward difference and backward difference schemes are equal but opposite, it is possible to write the central difference scheme summing Equations 1-40 and 1-41:

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_{j-1}))}{2\Delta x} + O(\Delta x^2) \quad \text{Equation 1-42}$$

The leading truncation errors canceled out, leaving a scheme that is $O(\Delta x^2)$ in accuracy. It is possible to write higher order schemes by using Taylor series expansions involving more mesh points. Higher order derivatives can also be approximated using finite differences.¹² As the mesh becomes finer, the discretization errors shrink, and the discrete solution will typically result in a closer approximation to the continuous solution. An example of a successively finer mesh is shown in Figure 1-7. However, finer meshes require more memory and more computational time to reach a solution.

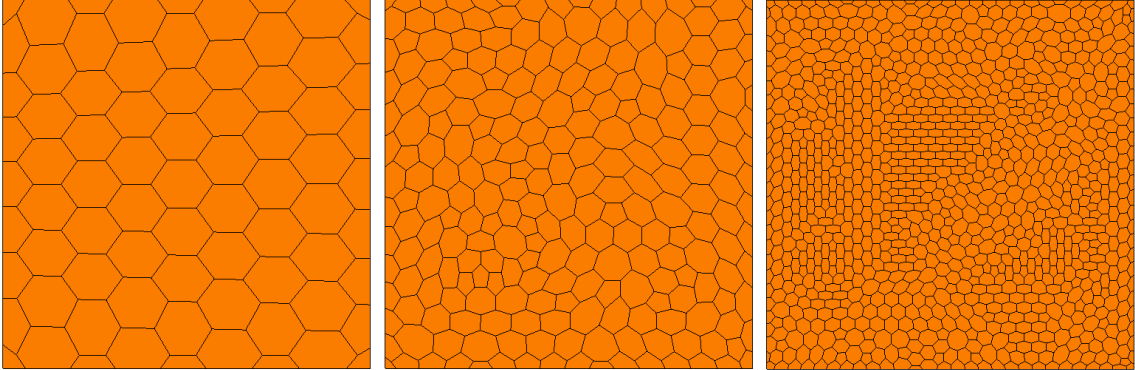


Figure 1-7: Example of successively finer grids from left to right.

While finite differences provide a simple base case for understanding, the difficulty in creating structured grids on arbitrary geometries makes the use of FDM difficult, if not impossible, to use in many cases.¹² On the other hand, finite volume

methods are generally applicable to arbitrary grids, making FVM the most widely applied method in CFD solvers today, including in STAR-CCM+. ^{12,14} The starting point for a FVM is the integral formulation of a scalar or vector conservation law. As an example, consider a conservation equation for an arbitrary scalar written as:

$$\frac{\partial}{\partial t} \int_V M dV + \oint_S F_j dS_j = \int_V Q dV \quad \text{Equation 1-43}$$

where V is an arbitrary control volume, S is the bounding surface, F_j is the flux vector for M , and Q is a volumetric source term. S_j is $\hat{n}_j S$ where $\hat{n}_j$ is the outward pointing normal of the surface. Note that one benefit of using the integral equations is the order of equations is reduced by one. Instead of using the gradient of flux as would be necessary in FDM, the flux term itself is used in the FVM. The conservation equation can be written in discrete form as for the discrete volume V_j as:

$$\frac{\partial}{\partial t} (M_j V_j) + \sum_{faces} F_j \Delta S_j = Q_j V_j \quad \text{Equation 1-44}$$

As an example, consider the 2D volume V_A shown in Figure 1-8. Equation 1-44 for a steady state problem can be written as:

$$F_j^{(AB)} \hat{n}_j^{(AB)} S_{AB} + F_j^{(AC)} \hat{n}_j^{(AC)} S_{AC} + F_j^{(AL)} \hat{n}_j^{(AL)} S_{AL} + F_j^{(AT)} \hat{n}_j^{(AT)} S_{AT} = Q_A V_A \quad \text{Equation 1-45}$$

where $F_j^{(ik)}$ is the flux computed at face ik , S_{ik} is the length of the face ik , and $\hat{n}_j^{(ik)}$ is the outward pointing vector of face ik .

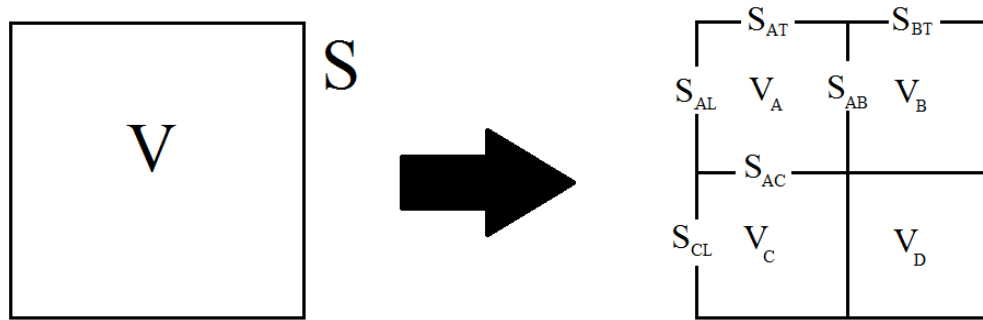


Figure 1-8: Discretization of a volume into several control volumes.

No matter the discretization scheme chosen, an algebraic system of equations can be formed by writing the discrete equations for all computational cells within the domain. Initial conditions/guesses are provided for all grid points. For steady state, an iterative solution method is used until convergence is achieved.¹² This is typically monitored by monitoring engineering quantities of interest (e.g. pressure drop) and how much the solutions to the conservation equations change between iterations.¹⁴ For time-dependent simulations, the solution is numerically integrated in time to calculate a new solution at each time step.

Chapter 2: Literature Review

This work serves to characterize the hydraulic performance of structured packing using CFD simulations. Traditionally, column performance has been characterized by macro-scale data (e.g. HETP, total column pressure drop), which necessarily limits the understanding of the underlying physics. In the first section of this chapter, several semi-empirical models and the assumptions implicit in their development are detailed demonstrating disagreement regarding the relevant parameters for predicting hydraulic performance. The second section of this chapter details the use of CFD to simulate flow through structured packing. The geometries examined tended to be simplified through the use of small periodic geometries or a porous media approximation. These simplifications necessarily complicate comparisons between CFD predictions and experimental data, leading to disagreement in simulation parameters used (e.g. choice turbulence model).

SEMI-EMPIRICAL MODEL DEVELOPMENT

Distillation column design relies on various empirical and semi-empirical models to accurately design and predict column performance. Two models commonly employed are the Rocha-Bravo-Fair model and the Delft model. Summaries of other column performance models for both random and structured packing can be found in a review by Wang *et al.*⁶

The SRP model represents the bed of structured packing as a series of parallel inclined wetted wall columns.^{21–23} The flow channels are assumed to be diamond shaped with a hydraulic diameter equal to the packing corrugation side length. Additional packing-specific parameters are required to be regressed from experimental data to predict dry pressure drop and to account for variations in distillation performance due to packing material and surface texture. Dry pressure drop is modeled by treating the bed as

a porous media. A form of the Forchheimer equation is used to break the pressure drop into the laminar and turbulent components. An expression for wetted area was based on expressions derived for liquid flow over an inclined plate, including the impact of contact angle.²¹

The Delft model was developed in an effort to predict column performance as a function of packing geometry.^{11,24-26} The packing is considered to be a series of criss-crossing triangular channels as shown in Figure 2-1. Packing corrugation angle, specific surface area, and channel dimensions are the only packing specific details needed to predict packing performance. Pressure drop performance is broken into three mechanisms:

1. Friction between the gas and the liquid. In the case of dry pressure drop, this term becomes the friction between the gas and packing surface. To properly predict dry pressure drop, experimental data must be regressed to calculate a friction factor.
2. The gas-gas interaction which accounts for friction between criss-crossing gas channels.
3. The pressure drop due to direction changes. This term accounts for the pressure drop due to channels terminating at the column wall and the pressure drop due to the packing joints.

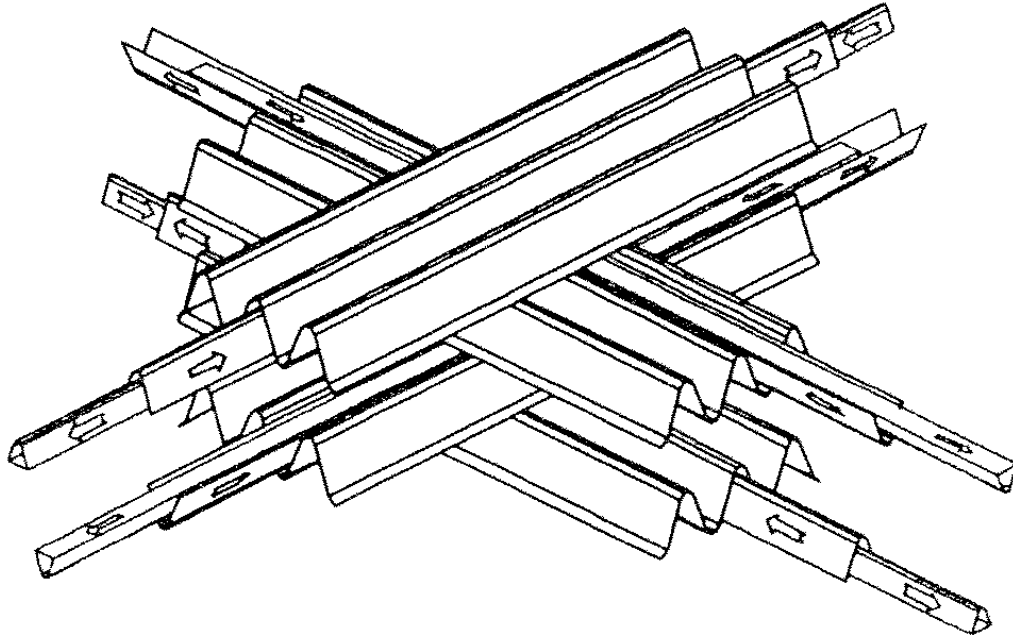


Figure 2-1: Illustration of the criss-crossing channels of structured packing. The liquid flows with uniform thickness down the channel walls, and the gas flows in the opposite direction at the center of the channels. Figure from Olujić *et al.*²⁴

Originally, the wetting was assumed to only be a function of liquid load in the Delft model.²⁴ This was later modified using the Onda equation to better account for the lower degree of wetting at low liquid loads.^{23,27} The Onda equation does explicitly depend on the contact angle.

Tsai *et al.* examined the impact of surface tension on effective wetted area of Mellapak 250.Y and Mellapak 500.Y.²⁸ Effective areas (a_e) were measured through absorption of CO₂ into a dilute caustic solution. Areas were measured under a range of liquid and gas loads, with all data captured in the pre-loading regime. Surface tension of the aqueous system was varied through the addition of a surfactant, allowing the authors to examine surface tensions from 35-72 mN/m. Their results for fractional wetted area

($a_f = a_w/a_p$) of Mellapak 250.Y ($a_p = 250 \text{ m}^2 \text{ m}^{-3}$) are presented in Figure 2-2. The results are compared to various literature models for wetted area prediction. None of the models proved adequate for predicting all experimental data trends and numerical values, underscoring the need for new wetted area models.

Tsai *et al.* developed a dimensionless model for predicting fractional wetted area.²⁹ Wetted area was strongly dependent on packing surface area and liquid load. Surface tension played a weaker, but still important role in wetted area. Packing corrugation angle and liquid viscosity, however, were found to have no noticeable effect on effective area. The impact of surface texture on wetted area was less clear. Embossed Mellapak 250.Y showed roughly 10% increase in effective area when compared to smooth packing. It was unclear if this increase was due to increased turbulence caused by the texture or if the embossed packing itself had a higher specific surface area. Contact angle was found to directly scale with surface tension in this work, and the two parameters were presumed to have the same meaning.

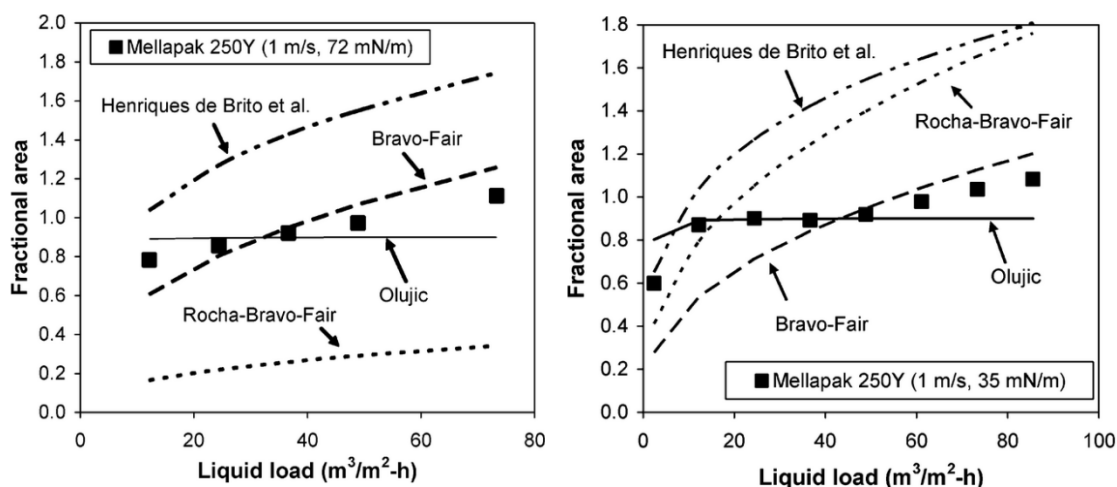


Figure 2-2: Impact of surface tension and liquid load on fractional wetted area of Mellapak 250.Y. High surface tension experiments (72 mN/m) are shown on the left. Low surface tension experiments (35 mN/m) are shown on the right. Figure taken from Tsai *et al.*²⁸

CFD SIMULATIONS OF STRUCTURED PACKING

Early CFD simulations in structured packing focused on simplifying the geometry in an effort to limit the computational resources needed. These simplifications include treating the packing as a porous media, treating the packed bed as small representative units, and performing two-dimensional simulations.

An early model proposed by van Gulijk used simplified geometry to simulate single phase flow in a hypothetical structured packing.³⁰ The computational domain is shown in Figure 2-3. The structured packing geometry was simplified as intersecting triangular channels. The author performed transient simulations of a single-phase liquid flow to calculate liquid transversal dispersion coefficients in a bed of packing with catalyst particles sandwiched between two sheets of packing, concluding that structured packing offered superior liquid dispersion when compared to a conventional catalyst bed.

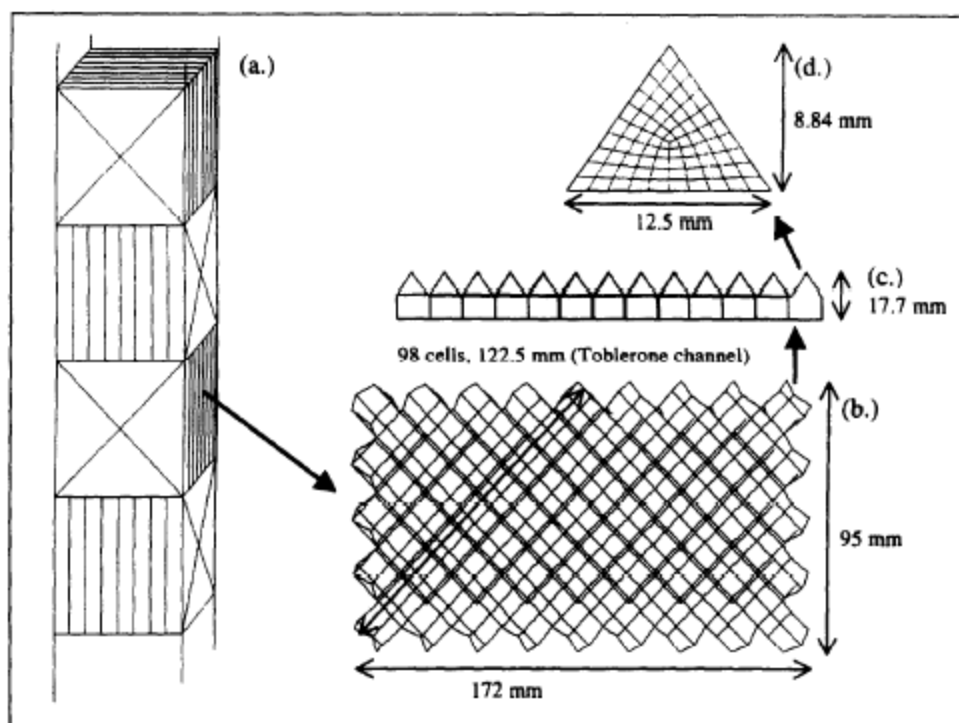


Figure 2-3: Computational geometry used by van Gulijk for dispersion simulations.³⁰ In particular, the geometry illustrated by (b), (c), and (d) was simulated.

Van Baten and Krishna used a similar sandwich structure model to simulate single phase flow between two sheets of KATAPAK-S catalytic structured packing.^{31–33} The authors used the geometry similar to that shown in Figure 2-4.³¹ Simulation results for axial dispersion compared poorly to experiments due to an oversimplification of the physics involved. Namely, their model did not account for the possibility of liquid flow outside of the wire-gauze envelopes of catalyst. Radial dispersion simulation results compared favorably to experimental results because liquid flow outside of the envelopes did not significantly distort the values for radial dispersion coefficients. It was again concluded that structured packing offered superior liquid dispersion when compared to a traditional (random) catalyst bed.

Expanding on their dispersion simulations, Van Baten and Krishna sought to simulate liquid-phase mass transfer within KATAPAK-S utilizing CFD simulations.³² A mass transfer coefficient was calculated by simulating the amount of tracer absorbed into the bulk liquid from all external surfaces (e.g. channel wall/packing surface), which had a mass fraction of 1 for the tracer. Five geometries were considered for comparison: a single empty round tube, a round tube packed with particles, a single packed triangular channel, a single crossover consisting of two packed triangular channels, and an entire sandwich of packing consisting of 16 packed triangular channels with 32 total crossovers. This sandwich geometry can be seen in Figure 2-4. Simulations showed that the triangular channels were superior to the round tube for liquid phase mass transfer. Furthermore, the single crossover and entire sandwich geometries demonstrated very similar mass transfer coefficients, leading the authors to conclude the triangular shape and junction between two channels were the most important geometric parameters for mass transfer in the packing.

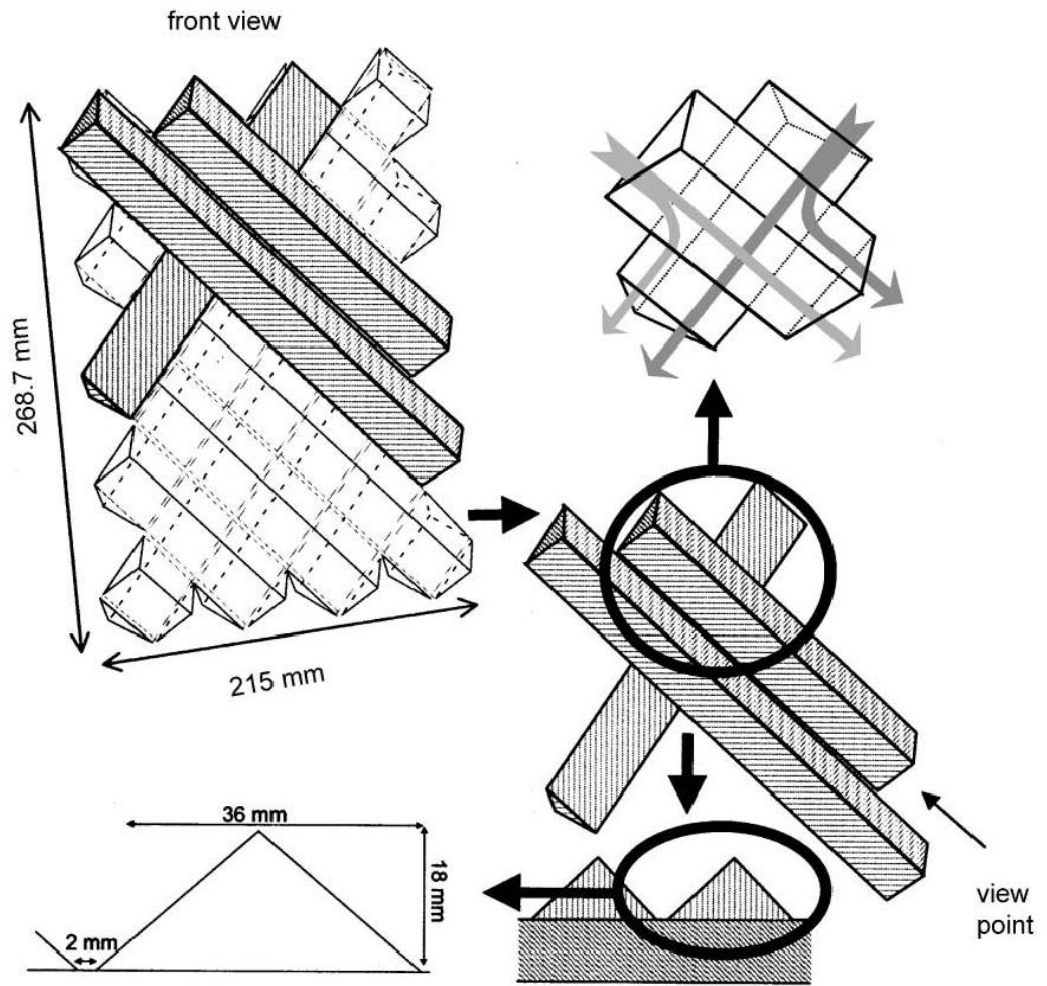


Figure 2-4: Sandwich of packing used by Van Baten and Krishna to examine liquid phase mass transfer coefficients in KATAPAK-S packing.^{31–33}

Van Baten and Krishna performed simulations for gas and liquid flow separately in various geometries to predict mass transfer coefficients.³³ Simulation results for flow through an empty circular tube compared well to the classical Graetz solution. Mass transfer coefficients in the KATAPAK-S packing were compared to correlations generated for catalytic bales. Gas phase mass transfer coefficients were similar between the two structures, leading the authors to conclude the criss-crossing geometry does little

to enhance the turbulence in the gas phase when compared to catalytic bales. Liquid phase mass transfer coefficients for KATAPAK-S were an order of magnitude below the predictions for catalyst bales. The authors concluded this was due to their model not accounting for liquid flow bypassing the catalyst sandwiches and contacting countercurrent gas directly, which would have caused significant turbulence in the liquid phase and enhanced mass transfer.

Petre *et al.* modeled single phase vapor flow through simplified geometrical elements termed Representative Elementary Units (REUs).³⁴ Four REUs were modeled to determine the impact of each geometric feature on the total pressure drop of a packed bed. The REUs employed can be seen in Figure 2-5. CFD simulations varied in Reynolds number from creeping flow to fully turbulent flow in which pressure drop was measured directly from the simulations. Empirically determining the number of each REU present in the packing, the authors were able to determine the total pressure drop in the bed. The macro-scale pressure drop was then used to fit an empirical correlation. The predictions from this correlation were shown to be more accurate than other semi-empirical models for predicting pressure drop.

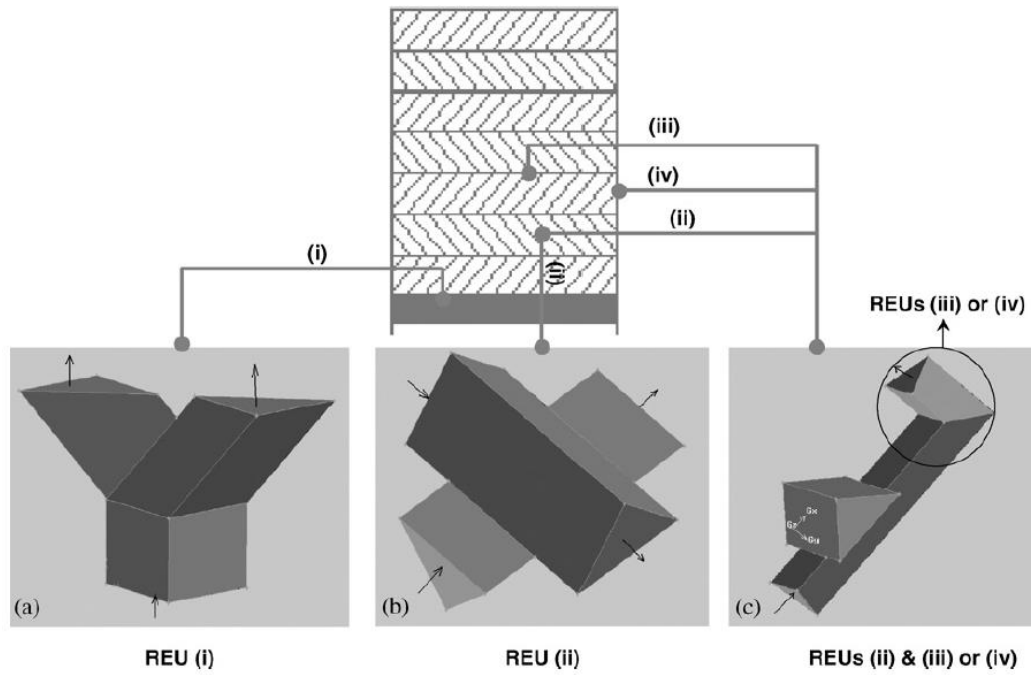


Figure 2-5: REUs employed by Petre *et al.*³⁴

Larachi *et al.* expanded on the use of REUs to evaluate the benefits of high capacity packings.³⁵ Two packings were compared, Montz B1-250.45 and the high capacity version, Montz B1-250.45+B1V. The REUs simulated are shown in Figure 2-6. To facilitate the transition between two layers of packing, the top and bottom ends of the corrugated sheet are bent in a vertical direction in high capacity packings. The pressure drop in the vertical channel REU was shown to be significantly lower than the traditional joint transition between 45° channels. Overall, it was shown that the pressure drop at the joint is a minor contribution to the macro-scale pressure loss of the packed bed. The pressure drop due to the criss-crossing packing channels accounted for 60-70% of the overall pressure drop in the CFD simulations.

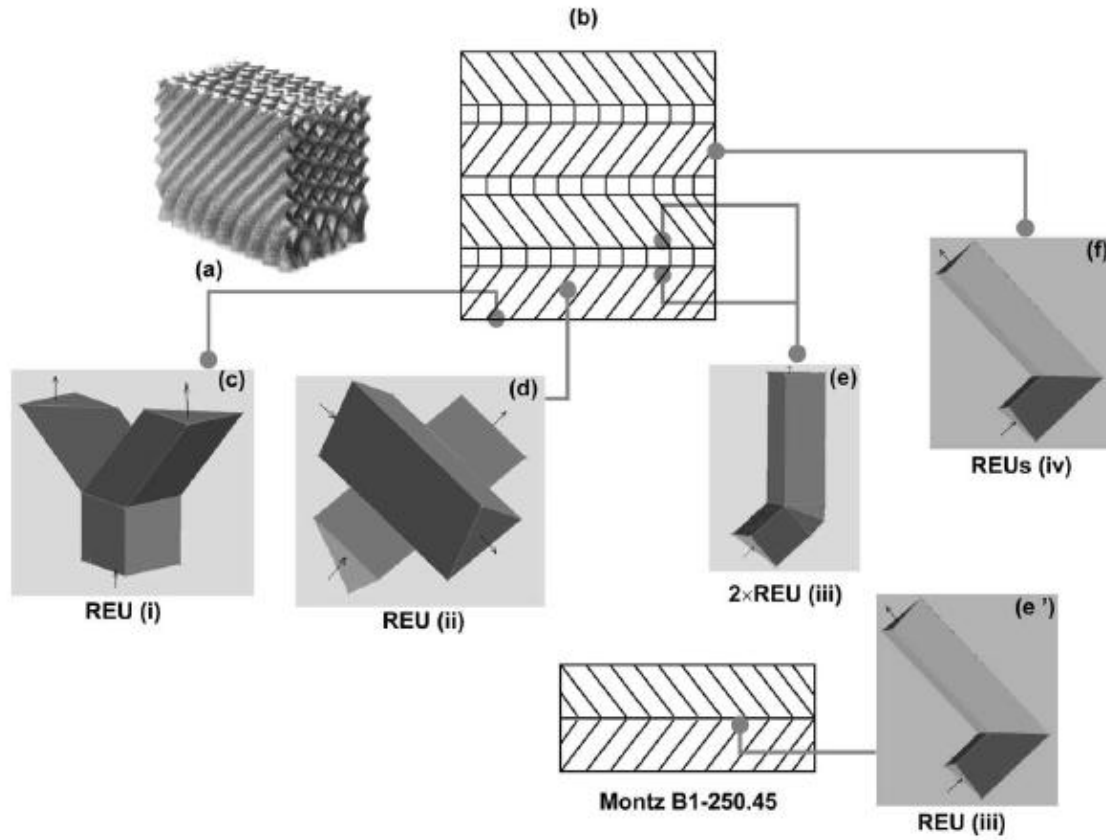


Figure 2-6: REUs employed by Larachi *et al.*³⁵

Szulczewska *et al.* employed a two-dimensional CFD model to study the formation of interfacial area in structured packing and on a vertical plate.³⁶ Countercurrent simulations were performed on two geometries: a vertical, flat plate and a vertical, corrugated plate (corresponding to the dimensions of Mellapak 250Y). Liquid was introduced via a velocity inlet at the top of the geometry. Gas was introduced at the bottom via a pressure boundary condition; this boundary also served as the liquid outlet. Another pressure boundary condition at the top served as the gas outlet. Water flowrates varying from 50-100 $\text{m}^3/\text{m}^2\text{h}$ and toluene flowrates from 10-50 $\text{m}^3/\text{m}^2\text{h}$ were simulated. High water flows simulated with a contact angle of 45° achieved total wetting of the plate and corrugated geometries. When the contact angle was increased to 65° , complete

coverage was not achieved. Experiments performed on steel corrugated sheets also demonstrated water preferred to form rivulets on both geometries, thus preventing total coverage. In contrast, toluene simulations and experiments were able to achieve complete wetting at flowrates above $15 \text{ m}^3/\text{m}^2\text{-hr}$. Further increases in the flowrate increased the interfacial area slightly due to wave formation.

Raynal *et al.* employed CFD on several different geometries to determine pressure drop and liquid holdup.³⁷ In an attempt to simulate pressure, the researchers used a simplified model consisting of two intersecting, triangular channels shown in Figure 2-7A. However, due to the choice of boundary conditions, the pressure drop was over-estimated, and the researchers concluded that this representation was too simplistic for any quantitative measurements. The second geometry simulated was the space between two sheets of structured packing (200mm wide and 100 mm tall) shown in Figure 2-7B. To eliminate end effects, pressure was measured at 23 mm and 78.55mm. This geometry was able to predict pressure drop within 20% of experimental values 90% of the time. A two-dimensional cross section of the second geometry was used to simulate two-phase co-current flow using a Volume of Fluid (VOF) package. This geometry can be observed in Figure 2-7C. The film thickness calculated via CFD was extrapolated to calculate volumetric holdup in the packed bed. Comparisons to gamma ray tomography showed the simulation results under predicted holdup by roughly 20%.

Ataki *et al.* performed VOF calculations using a representative geometry for Rombopak 4M.³⁸ Rombopak is composed of strips of metal arranged to form a repeating pattern of X-shaped structures. The authors simulated a single X-shape structure at different flowrates and physiochemical properties (contact angle, surface tension, and viscosity) to determine the effect these parameters would have on interfacial area. The computational geometry is shown in Figure 2-8. Liquid was introduced at the top of the

two upper legs with a pressure outlet boundary on the bottom. Stagnant gas filled any volume without liquid. CFD predictions for holdup and wetted area were more accurate over a wider range of fluid properties and liquid flowrates when compared to the Rocha-Bravo-Fair, Delft, Shi-Mersmann, Billet-Schultes, and Onda models.

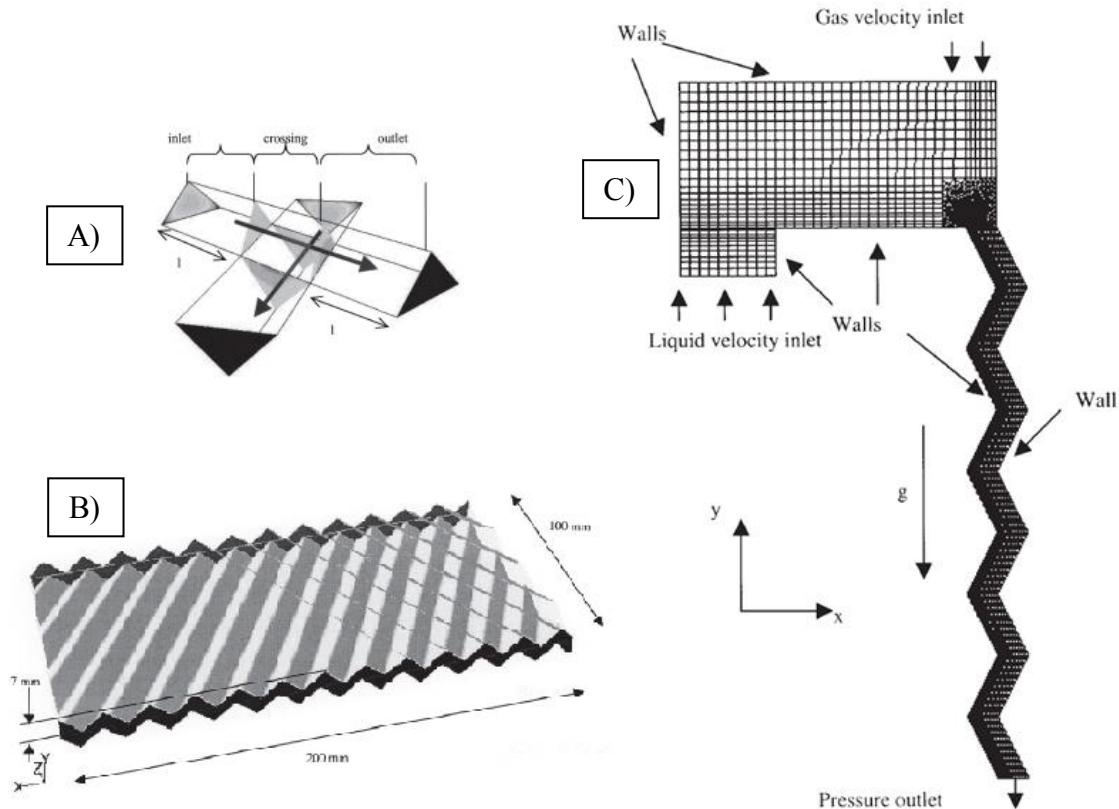


Figure 2-7: Geometries employed by Raynal *et al* to predict pressure drop and liquid holdup.³⁷ A) is the elementary geometry used to predict pressure drop. B) indicates the complex geometry to predict pressure drop. C) shows the two-dimensional geometry used for multiphase simulations to predict liquid holdup.

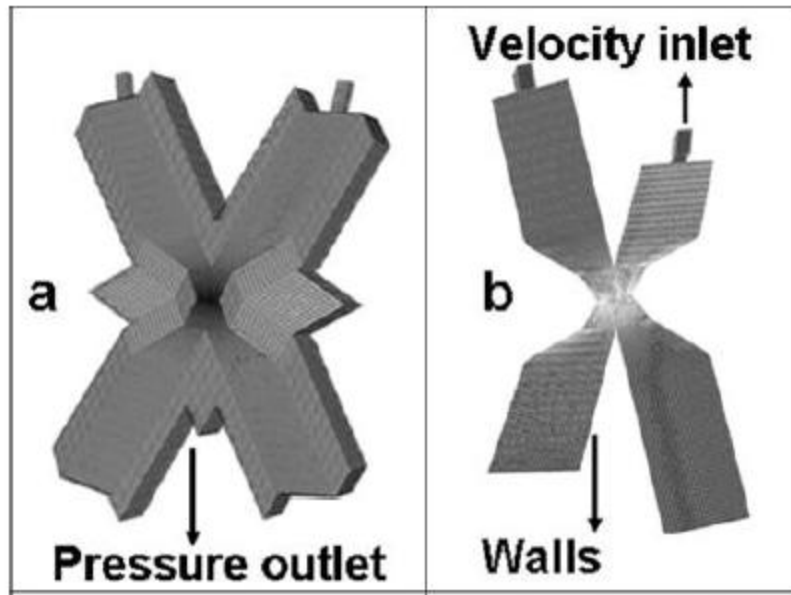


Figure 2-8: Computational domain employed by Ataki *et al.* to estimate wetted area of Rombopak.³⁸

Fard *et al.* used an Eulerian-Eulerian approach to predict pressure drop and mass transfer performance in a ceramic packing element of MELLADUR 450Y.³⁹ The predicted dry and irrigated pressure drops were 20.3% and 23%, lower than experimental data. The authors utilized the Rocha-Bravo-Fair semi-empirical correlations implemented to account for interphase mass transfer in each computational cell. Mean relative error between experimental data and CFD predictions for HETP was 9.15%.

Wen *et al.* simulated single phase flow through a variety of packing types.⁴⁰ The authors demonstrated the ability of CFD to predict the impact of varying geometry on dry pressure drop performance. The authors simulated two different Sulzer BX packings ($a_p=500\text{m}^2\text{m}^{-3}$ and $\alpha=45^\circ$ and 60°) and a Flexipac 3Y. Simulated pressure drop compared favorably to experimental data. The authors also performed multi-component, single phase simulations in which a small amount of CO_2 was injected into a stream of air. The authors concluded the qualitative behavior of the tracer was correct, demonstrating the

viability of CFD to predict packing performance with no closure models necessary for the fluid-solid interaction. Only a three-dimensional representation of the packing was needed to account for the anisotropic flow through structured packing.

Raynal and Royon-Lebeaud simulated the performance of an industrial-scale column filled with structured packing by utilizing multiple scales as shown in Figure 2-9.⁴¹ First, liquid holdup and interfacial velocity was calculated using a VOF simulation on a 2D geometry meant to capture all surface effects. Using the holdup and interfacial velocity, irrigated pressure drop could be calculated in a mesoscale geometry consisting of two criss-crossing channels. Vapor velocity was corrected by accounting for liquid holdup. The interfacial velocity was implemented as a boundary condition on the walls of the packing. The irrigated pressure drop data was then used to fine-tune a porous media approximation for the macro scale simulations. By changing the magnitudes of the permeabilities between layers of packing, the researchers were able to account for the different orientations of successive layers to examine column-scale gas distribution.

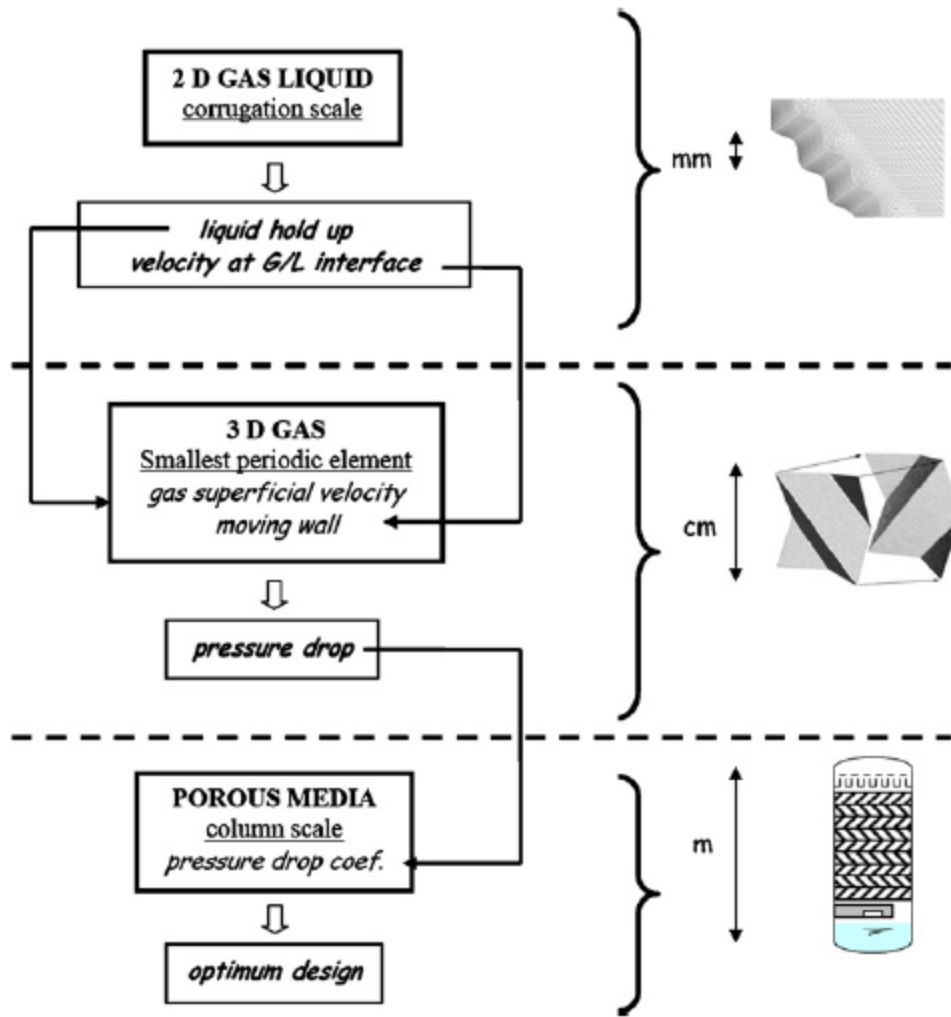


Figure 2-9: Different scales used by Raynal and Royon-Lebeaud to simulate overall column performance.⁴¹

Mahr and Mewes approximated structured packing (Mellapak N250.Y) as a porous media.^{42,43} While the flow field varies significantly within a periodic structure of packing (i.e. an elementary cell), the authors noted the velocities at the boundaries of these elementary cells were quite similar. By using the elementary cell model, the authors were able to model a macroscopic column operating under countercurrent flow. In a

novel approach, the authors treated the liquid as two distinct phases to account for the anisotropy of the packing. Permeability for the first liquid phase was set to give it a preferential flow direction $+19^\circ$ from the vertical. For the second liquid phase, a preferential flow direction of -19° was used. This flow direction was an analytical derivation based on the forces on the liquid phase. Gas phase permeabilities were derived from experiments and small-scale simulations of an elementary cell. The liquid spreading observed from the simulations matched experiments performed using x-ray radiography, and an increase in liquid holdup was observed at the joint between elements of packing. The authors demonstrated that the CFD predictions could be used to predict the onset of flooding.

In 2008, Fernandes *et al.* compared the performance of CFD simulations to experimental studies involving air and CO₂.⁴⁴ Both laminar and turbulent flows were examined in two geometries. The first geometry consisted of two contacting corrugated sheets of SULZER EX Gauze packing. Velocity inlet (bottom) and pressure outlet (top) conditions were specified. Average deviation of pressure for the supercritical CO₂ flows was 15%. The second geometry examined was a cylinder of 13 corrugated sheets bundled together into a single piece of packing with a diameter of 24mm. In this case, a CFD model was able to predict the pressure drop with an average deviation of 6%.

Expanding on their previous work, Fernandes *et al.* simulated two-phase pressure drop in SULZER EX Gauze packing.⁴⁵ Utilizing a 2D geometry, a VOF model was used to calculate liquid holdup, film thickness, and interfacial velocity. With this data, a pseudo-single phase simulation was carried out in a small piece of packing consisting of 13 corrugated sheets. By accounting for liquid holdup via a uniform film thickness and interfacial velocities, the simulations were able to accurately predict irrigated pressure drop. To show that the assumption of complete wetting was valid, a VOF simulation on a

small piece of packing (13 sheets, 24 mm diameter, and 18 mm height) was performed showing a thin liquid film ($\gamma = 0.046$ N/m, $\theta_c = 27.3^\circ$) did wet the bulk of the packing.

Raynal *et al.* expanded on previous work on multi-scale modeling of column performance by examining the impact of small-scale wetting performance using a VOF model.⁴⁶ The authors examined the impact of varying contact angle, flow rate, surface tension, and liquid injector width on predicted rivulet thickness and width on an inclined plate. CFD simulations and experimental data demonstrated similar functional behavior on the Reynolds, Weber, and Froude numbers. The authors concluded CFD simulations would allow for researchers to investigate the impact of solvent properties on hydrodynamic and mass transfer performance without the need for costly experiments.

Haroun *et al.* performed simulations of reactive absorption of laminar gas-liquid flow on a two-dimensional geometry representative of structured packing.⁴⁷ Co-current flow of gas and liquid were simulated with a second-order chemical reaction taking place in the liquid phase. The authors represented the vapor-liquid equilibrium as an additional flux present at the gas-liquid interface. Simulation results compared favorably with Higbie penetration theory. Mass transfer on the corrugated sheet was superior to mass transfer on a plane liquid film.

Rafati *et al.* performed single phase and multiphase simulations on a packing geometry similar to MellapakPlus 752.Y.⁴⁸ Single phase simulations were carried out to determine the impact of turbulence model choice on pressure drop. The authors examined the choice of standard k- ϵ , standard k- ω , renormalized group (RNG) k- ϵ , and baseline (BSL) k- ω . The authors concluded the BSL k- ω matched experimental data best. It should be noted, however, that the simulation packing geometry was only two solid packing sheets sandwiched together. That is, the authors neglected any impact on pressure drop that the column wall, joints between packing layers, packing surface

texture, and packing perforations may have had. Simulated dry pressure drop results were an average of 19% lower than experimental data. Irrigated pressure drop results were predicted using an Eulerian-Eulerian simulation approach. Predicted irrigated pressure drop was 22.5% lower than reported experimental results. Simulation results comparing MellapakPlus 752.Y to Mellapak 500.Y demonstrated a reduced pressure drop in the MellapakPlus geometry. The predicted pressure drop in the enhanced geometry (MellapakPlus) was roughly 10% lower than traditional packing (Mellapak). The researchers also simulated a sandwich structure with a solid sheet placed between the two corrugated sheets. This change was meant to decrease the gas-gas interaction, which is known to be a major cause of pressure loss in structured packing. This modification reduced dry pressure drop by 16% and wet pressure drop by 9% at moderate F-factors.

Said *et al.* developed a CFD model to predict the contribution to dry pressure drop from wall friction and gas-gas interaction in the packing channels.⁴⁹ Two different periodic elements were simulated. In each case, periodic boundary conditions were enforced on opposite faces, and a pressure gradient was imposed in the z-direction. No appreciable differences in results were observed between the two different periodic elements chosen. Pressure drop results for Montz-Pak B1-250.45 compared favorably to experimental data. The study also examined the effect of corrugation channel height and the channel opening angle. Larger channel opening angles and larger channel heights led to decreased pressure drop.

Shojaee *et al.* used CFD simulations of a two corrugated sheets to predict the effective interfacial area under countercurrent flow.^{50,51} A velocity boundary condition was imposed at the bottom of the geometry to simulate air entering the geometry and water leaving. A pressure boundary condition was used at the top of packing, and no slip walls were prescribed elsewhere. Utilizing the baseline k- ω turbulence model, researchers

were able to show good agreement between experimental and simulated pressure drop. Rather than calculate interfacial area directly from the VOF simulations through the use of an isosurface, the authors utilized predicted film thicknesses from the simulations to estimate fractional wetted area. Wetted area predictions compared favorably to the semi-empirical model of Brunazzi *et al.*⁵²

Haroun *et al.* utilized a VOF model on a two-dimensional corrugated sheet to examine the impact of liquid flow rate on liquid holdup and mass transfer under co-current gas-liquid flow.⁵³ The authors assumed complete wetting of the packing with surface tension having a negligible impact on holdup and mass transfer. As the liquid Reynolds number was increased, a transition from a smooth film closely following the packing geometry to a liquid recirculation zone that filled the packing cavity, as observed in Figure 2-10. This transition was found to depend on liquid load and packing corrugation height.

Subramanian and Wozny utilized a three-dimensional VOF model to examine how fluid properties, packing perforations, and contact between two sheets of packing would affect wetted area and liquid holdup.⁵⁴ Experiments were performed on Montz B1-300 packing, with simulation geometries that were analogous to experimental packings. In experiments and simulations, increased flow rates yielded increased wetted areas. Silicon oil, which had the lowest contact angle and surface tension of the fluid examined in this study, demonstrated better wetting performance when compared to water and a water-glycerol mixture. Perforations were found to increase wetting by allowing fluid to travel from the front of a packing sheet to the back side of the same sheet. When two corrugated sheets of packing were simulated, increased holdup was observed at the contact points between packing sheets. Only 55-60% of the packing was wetted at their highest simulated flow rates (corresponding to a liquid load of $79 \text{ m}^3/\text{m}^2\text{h}$) with silicon

oil. Liquid distribution from the inlets and choice of boundary conditions were most likely the cause of this poor wetting.

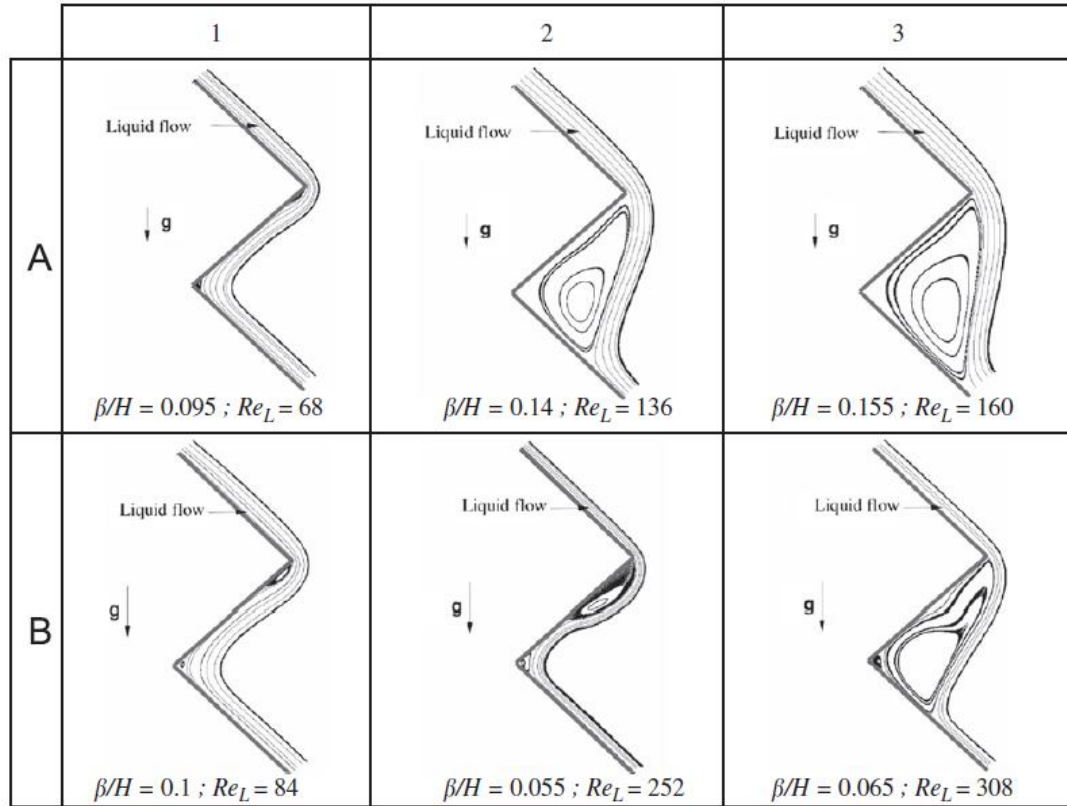


Figure 2-10: Examples of increasing liquid load causing the liquid profile to transition from a liquid film following the packing crimp to a liquid pool filling the packing cavity. Figure taken from Haroun *et al.*⁵³

Armstrong *et al.* performed simulations of dry pressure drop on periodic representative sections of packing of varying corrugation inclination angles.⁵⁵ Packing geometries with similar specific surface areas and channel opening angles to Montz-Pak B1-250.45 were generated with corrugation angles of 60°, 50°, 45°, 40°, and 30° as shown in Figure 2-11. The authors generated an empirical correlation using a genetic algorithm to create a correlation with a maximum error of 7.8% when compared to the

CFD simulations. The correlation was refined by utilizing the data of Said *et al.* to account for channel opening angle on pressure drop performance.⁴⁹ The final empirical correlation was able to predict pressure drop of all simulations with a mean relative error of 12.5% with corrugation angles ranging from 30-60° and channel opening angles varying from 30-120°.

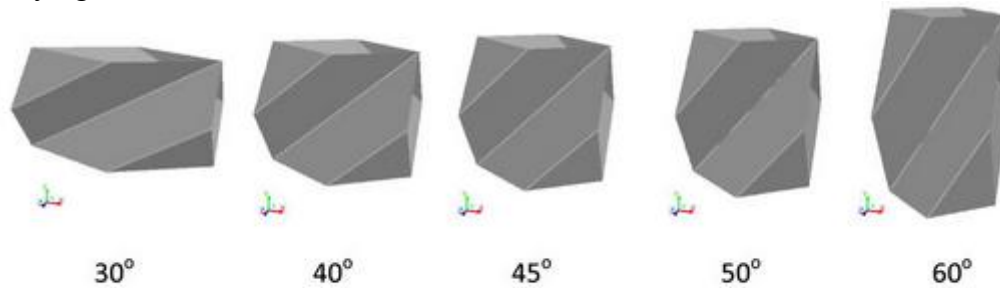


Figure 2-11: Periodic geometries examined by Armstrong *et al.*⁵⁵

Owens *et al.* performed single phase simulations through a bed of Mellapak N250.Y.¹⁰ Rather than simplify the geometry through utilization of periodic structures or a porous media approximation, a half element of Mellapak N250.Y (0.146m diameter x 0.155m height) was scanned using high-resolution computed tomography. The resulting slice images were converted into a Stereolithography format (STL) file, which was directly imported into CFD software. The resulting bed of packing was three half-elements tall (0.465m total) with a simulation diameter of 0.159m due to the wiper band not being properly constrained during imaging. CFD simulations compared favorably to experimental data. The two-layer, realizable k- ϵ turbulence model compared most favorably, yielding predictions that were on average 7.5% lower than experimental pressure drops. Increased negative velocities in the axial direction were present at the joints, which resulted in increased pressure drop when compared to the bulk of the

packing. This increased pressure drop was experimentally observed by varying the number of joints present in a bed of packing.

Zhang *et al.* performed single phase simulation and experiments to determine localized gas-phase mass-transfer coefficients.⁵⁶ Ammonia adsorption method (AAM) experiments utilized JKB-250Y structured packing coated with a piece of wet filter paper soaked in an aqueous solution of MnCl_2 with hydrogen peroxide. This compound reacts and changes colors in the presence of ammonia, and the degree of color-changing is related to the localized mass transfer coefficient. CFD simulations utilized a k- ϵ model. The turbulent diffusivity was related to the eddy viscosity by the turbulent Schmidt number. Simulation results showed an average deviation of 10% when compared to experimental results.

Brinkmann *et al.* performed single phase simulations in a small representative unit of packing to estimate the turbulence in the gas phase.⁵⁷ The turbulence, quantified as an volume-averaged eddy viscosity, was used to improve the predictions of a semi-empirical model. Agreement between the semi-empirical model and experimental data was observed when gas-phase turbulence was estimated via CFD. When turbulence was not accounted for (i.e. the eddy viscosity was set to 0), a significant deviation between experimental data and semi-empirical prediction was observed, validating the assumption of a turbulent gas phase through Mellapak 250.Y at an F-factor of $1.0 \text{ Pa}^{0.5}$.

Haroun *et al.* investigated wetting of an inclined plate and a single sheet of Mellapak 250.X using a three-dimensional VOF model.⁵⁸ Inclined plate results using a static contact angle of 70° compared favorably to experimental results. The CFD model was capable of predicting the various flow regimes experimentally observed: droplet flow, rivulet flow, and film flow. Countercurrent gas flow was simulated over a single sheet of Mellapak 250.X by imposing velocity conditions at the top of the packing sheet,

periodic conditions on the side, and a pressure outlet on the bottom. Contact angles of 0.1° , 10° , 30° , and 70° were examined at varying liquid flow rates. A contact angle of 10° was found to best predict the experimental data of Tsai *et al.* for wetted area.²⁹ Holdup results at a contact angle of 10° also compared most favorably to the simplified model of Raynal *et al.*⁴¹

SUMMARY

In the preceding research, concessions to available computing power were necessary. In the bulk of the research, the geometries had to be simplified in one of three ways: 1) REUs were studied, 2) packing was represented as a two-dimensional structure, or 3) the packed bed was approximated as a porous media. The use of REUs can be useful to study local small, local scale phenomena, but the use of such elementary geometries makes it impossible to accurately quantify any interactions between packing elements. In the case of using a two-dimensional geometry to quantify liquid holdup and wetted area, any impact from two corrugated sheets contacting each other is completely neglected, despite being a location where localized increased holdup has been observed in simulations and experiments.^{54,59} A porous media approximation requires significant data fitting is only valid for that particular system. This type of model will necessarily require the use of semi-empirical models to estimate wetted area. To capture all underlying physics that might impact packing performance, it is necessary to use an accurate geometry of a real system. Anything short of this will neglect details present under experimental conditions, which can impact hydraulic performance. Finally, any CFD predictions should be validated through the collection of experimental data.

Chapter 3: Simulation Details

This chapter is broken into eight sections detailing the different geometries, simulation settings, and mesh settings examined. The first two sections describe the geometry generation and simulation settings for single phase flows through a realistic packing representation generated via X-ray CT scans. The next two sections describe the generation and simulation settings for single phase flows through periodic geometries. The fifth and sixth sections detail the geometries and simulation settings for multiphase flows through small-scale geometries generated via SolidWorks. Finally, the last two sections cover geometry generation, mesh settings, and simulation settings for multiphase simulations on a packing geometry generated by X-ray CT scans. Full details for meshing and simulation settings can be found in Appendix A.

SINGLE PHASE FLOW GEOMETRY GENERATION – CT GEOMETRY

A half-element of Mellapak N250.Y placed inside an aluminum tube (ID 0.146 m) was initially scanned by the High-Resolution X-Ray Computed Tomography Facility at the University of Texas at Austin (UTCT). The scan was done using a 450kV, 1.3 mA unfiltered fan beam X-ray. A 512-channel cadmium-tungstate solid-state linear array detector was used. Slice thickness of 0.25 mm was used with an inter-slice spacing of 0.22 mm. A single ray was averaged (20 ms integration time) per view with 1400 views (angular positions) per slice. A source-to-object distance of 748 mm was used, yielding a maximum field of view of 158.3956 mm (155 mm field of reconstruction). Post-reconstruction ring correction was applied by UTCT staff. In total, 746 CT slices were generated as 16-bit TIFF images. The TIFF images were imported into Aviso 6.1. An isosurface was created with a threshold grayscale of 13500. The resulting isosurface was exported as an STL file for import into STAR-CCM+.

Due to the proximity of the wiper bands to the aluminum column wall, additional processing was needed in this region. The partial volume effect resulted in defects where the wiper bands contacted the column wall. The partial volume effect occurs as a result of representing the continuous, real geometry as discrete pixels. Some pixels may only be partly filled with plastic or metal, and this leads to errors in the geometric representation. In this case, pixels belonging to the column wall were extracted as part of the isosurface. These defects can be observed in Figure 3-1. These defects caused further problems by often extending the geometry beyond an ID of 0.14605 m. To eliminate these defects and generate a packing element with a total ID of 0.146 m, a square prism geometry with a cylinder cut from the center was generated in SolidWorks and exported as a Parasolid CAD file (.x_b). A top view of this geometry can be seen in Figure 3-2. The packing element was centered in the hollow cylinder, and then the hollow cylinder was subtracted from the packing element using a Boolean subtract operation in STAR-CCM+. This resulted in any features beyond a 0.146 m diameter being eliminated from the packing geometry. The effect of this on the wiper band regions is shown in Figure 3-3. The wiper band in the near-wall region is smoother, and no piece of the packing geometry extends beyond the desired diameter. Note, STAR-CCM+ handles Parasolid bodies as solids, not surfaces, making it ideal for this type of operation. The use of a surface format (e.g. .STL) for subtraction would not result in the desired final geometry.

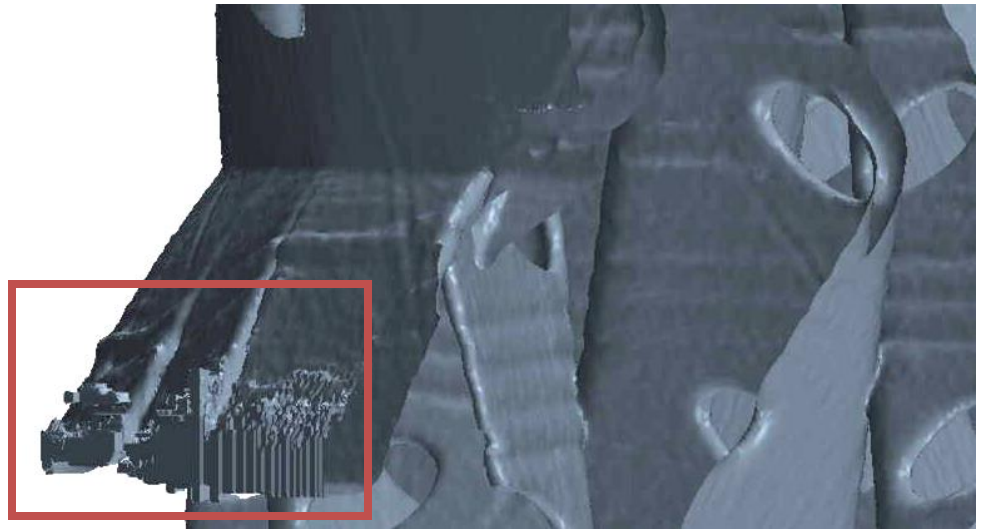


Figure 3-1: Example of the partial volume effect impacting the wiper band geometry.

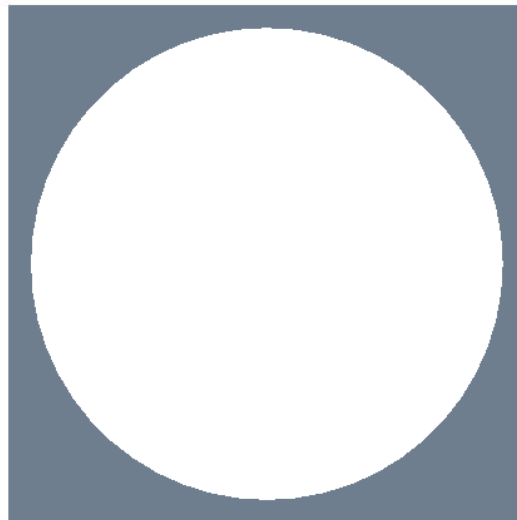


Figure 3-2: Geometry used to correct wiper band defects and generate a packing element with a uniform diameter.

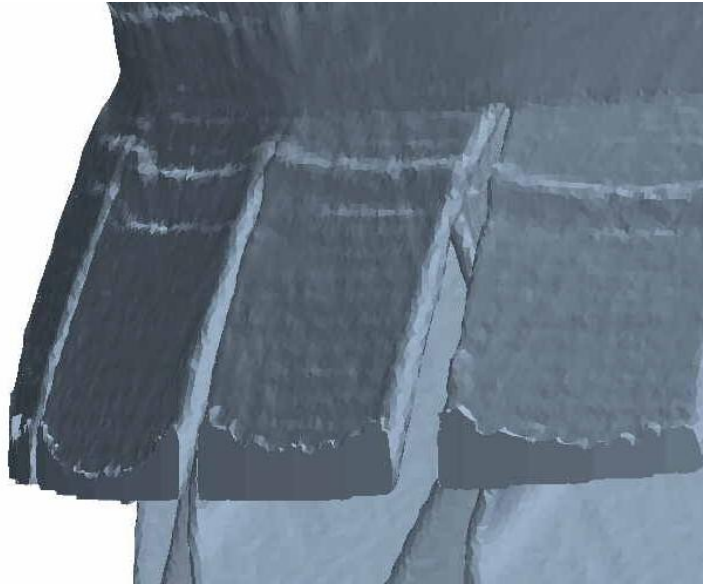


Figure 3-3: Wiper band section that has been corrected via Boolean subtraction.

The corrected packing geometry was then exported as an STL file. In a new simulation, the corrected geometry was imported three times. The packing elements were then arranged such that the bottoms of each element were placed at 0 m in the z-direction. This was the position for the first element. The second element was moved 0.1632 m in the positive z-direction. The third element was moved 0.3264 m in the positive z-direction. The distances moved ensured a 0.1 mm gap between packing elements. They were then rotated accordingly to produce the geometry desired. Table 3-1 summarizes the geometries examined and the placement of each element.

A 0.7985 m tube of diameter 0.1462 m was generated in SolidWorks and imported into STAR-CCM+. The simulation diameter was chosen to ensure a 0.0001 m gap was present between the tube wall. Such gaps are often used in geometry generation to prevent the creation of highly skewed and sliver elements, which can negatively impact simulation convergence and stability. The tube started at -0.190 m in the z-direction, giving the flow field generated from the mass flow boundary condition a small

section to develop naturally. The tube extended 0.119 m beyond the top of the third element to ensure any vortices from fluid exiting the packing would have a chance to dissipate before reaching the outlet, a pressure boundary condition. Figure 3-4 shows the final packed stack for the 90° rotation geometry (left) and a simulation schematic (right).

0° Rotation			
	Start Height (m)	End Height (m)	Rotation Relative to Bottom Element (°)
Bottom Element	0.0000	0.1631	0
Middle Element	0.1632	0.3263	0
Top Element	0.3264	0.4894	0

30° Rotation			
	Start Height (m)	End Height (m)	Rotation Relative to Bottom Element (°)
Bottom Element	0.0000	0.1631	0
Middle Element	0.1632	0.3263	30
Top Element	0.3264	0.4894	60

60° Rotation			
	Start Height (m)	End Height (m)	Rotation Relative to Bottom Element (°)
Bottom Element	0.0000	0.1631	0
Middle Element	0.1632	0.3263	60
Top Element	0.3264	0.4894	120

90° Rotation (Standard Practice)			
	Start Height (m)	End Height (m)	Rotation Relative to Bottom Element (°)
Bottom Element	0.0000	0.1631	0
Middle Element	0.1632	0.3263	90
Top Element	0.3264	0.4894	0

Table 3-1: Packed bed orientations examined for single phase nitrogen flow.

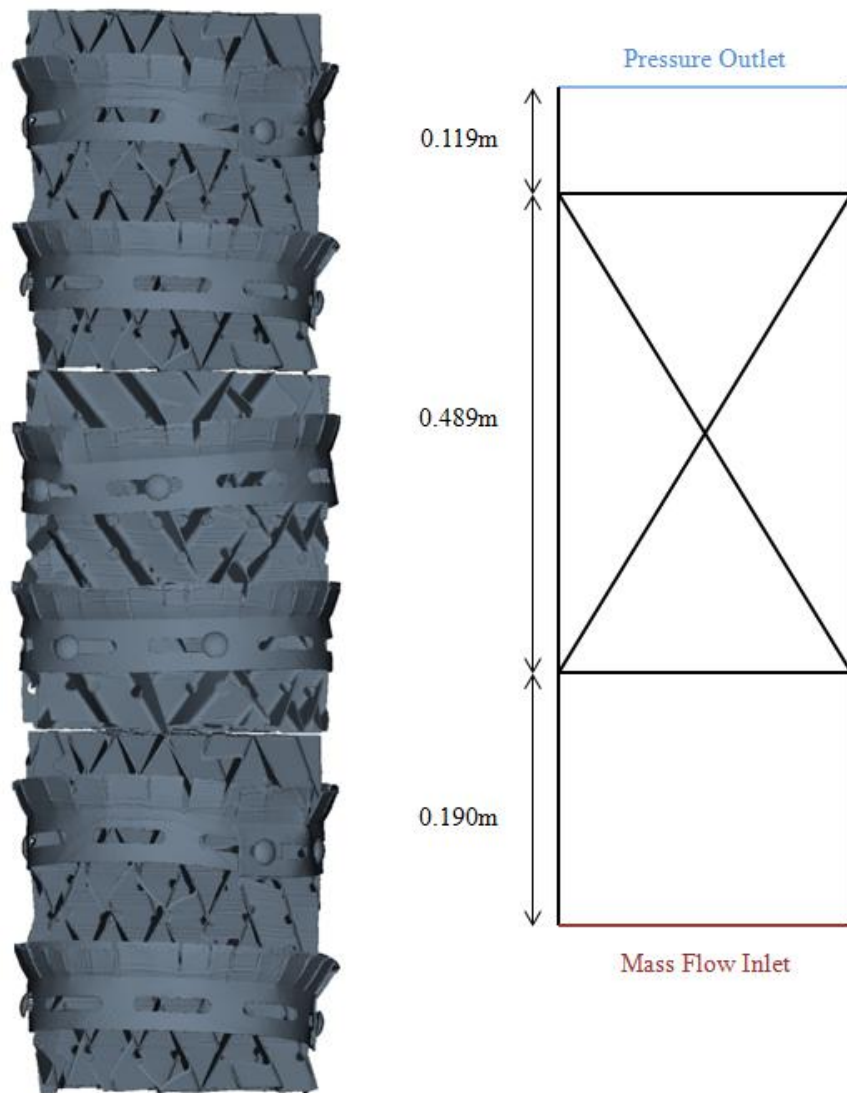


Figure 3-4: Final packed bed for simulations (left), and a simulation schematic (right) showing boundary conditions and packed bed placement.

SINGLE PHASE FLOW MESHING AND SIMULATIONS– CT GEOMETRY

Simulation Settings

Single phase simulations using the CT geometry were completed on the supercomputer Ranger (now decommissioned) in STAR-CCM+ 7.06.009. Simulations were for steady, turbulent flow of an incompressible gas with gravity effects enabled. The

continuity and Navier-Stokes equations were solved with the coupled implicit solver using a 2nd-order upwind discretization scheme. Details on the formulation can be found in the STAR-CCM+ user manual.¹⁴

Two turbulence models were examined as part of the simulations carried out on the CT geometry. The first was the SST k- ω model with an all y+ wall treatment. The second was the realizable k- ϵ model with a two-layer all y+ wall treatment. The default values for both turbulence models were used. The detailed physics continuum values and solver settings can be found in Appendix A. Figures A-1 and A-2 contain the physics continuum values and solver settings for the k- ω simulations. Figures A-3 and A-4 contain the physics continuum values and solver settings for the k- ϵ simulations. These two models are commonly applied to engineering applications and offer a satisfactory compromise between accuracy and computational speed.

Physical properties of the fluid were those of nitrogen at 25°C. Specifically, the density was 1.14527 kg/m³, and dynamic viscosity was 1.78837x10⁻⁵ Pa-s. The pressure outlet was set to 0.0 Pa. The mass flow inlet's flow direction was specified as the positive z-direction, and the mass flow magnitude varied depending on the flow-rate desired. The tube wall and packing elements were set as no-slip walls. Table 3-2 lists the mass flow rates examined and the corresponding F-factors for each flow.

Mass Flow Rate	F-Factor
(kg/s)	(Pa ^{0.5})
0.01096	0.61
0.02192	1.22
0.03288	1.83
0.04384	2.44
0.05480	3.05

Table 3-2: Flow rates examined using the CT geometry.

Initial simulations at the lowest mass rate were initialized with a constant pressure (0 Pa) and a uniform velocity in the z-direction (0.571 m/s). Pressure drop through the packing was monitored through the packing by calculating the area-weighted average at planes 0.02 m before the packing and 0.02 m after the packing. When pressure loss changed less than 0.001Pa per iteration, the simulation was deemed converged. At this point, the mass flow rate was changed to the next desired value, and the simulation was continued from the previously converged solution.

Mesh Settings

Three meshing models were used to generate the numerical grids used to solve the Navier-Stokes equations. The surface wrapper was initially called, followed by the surface remesher, and concluding with the polyhedral volume mesher. The surface wrapper and remesher act to locate and triangulate all solid surfaces present in the simulation. Volume meshing acts to fill the domain bounded by the surface mesh with volume elements (e.g. tetrahedrons, polyhedrons, hexahedrons, etc.).

The surface wrapper can be visualized as a balloon filling the flow geometry and re-skinning the surfaces it can contact. Any features this balloon cannot reach are deleted, removing any double surfaces and internal features. The surface wrapper acts to re-skin the entire geometry, filling any holes and gaps that may be present. It also acts to prevent contact between separate features in the geometry (e.g. the tube wall and the wiper bands). In the end, a closed, non-intersecting, manifold surface is produced. Meshing was performed on the decommissioned Spur visualization cluster. Meshing of this magnitude can be accomplished via the supercomputer Ranger by using a large memory (1 TB memory) node. The standard visualization nodes on Ranger did not possess enough

memory (32 GB) to perform the necessary meshing and visualization on the CT geometry examined.

The surface wrapper does not produce an optimal surface mesh, and the surface remesher is recommended to be used in combination with the surface wrapper. The surface remesher retriangulates the surface mesh in an effort to increase surface quality and optimize the surface for volume meshing. The size of triangles generated is based on user input. In these studies, a minimum surface size and target surface size were specified. The minimum surface size is the absolute smallest surface triangle allowed. The target size is the desired edge length produced in the absence of any curvature or proximity refinement. Because the quality of the tetrahedrons formed for volume meshing depends directly upon the surface mesh, it is important to ensure a high quality surface mesh is generated in this step.

The irregular nature of structured packing prohibits the use of structured meshes. Thus, an unstructured meshing routine was used. The polyhedral volume mesher begins by invoking the tetrahedral mesher. Tetrahedrons are grown from the triangular surface mesh, and new vertices are iteratively placed into the domain to generate high quality cells. At this point, the polyhedral mesher begins merging tetrahedral cells into arbitrary polyhedral-shaped cells. On average, polyhedral cells will have 14 cell faces and will result in a mesh with five times fewer cells than the tetrahedral equivalent.¹⁴

A mesh-independence study was performed examining the impact of minimum edge length and target size on pressure drop. Three meshes were generated with relevant parameters shown in Table 3-3. Full mesh details can be viewed in the Appendix in Figures A-5 (coarse), A-6 (medium), and A-7 (fine). The mesh independence study was carried out at an F-factor of $0.61 \text{ Pa}^{0.5}$ on the 90° packing element rotation geometry with the SST $k-\omega$ turbulence model.

Mesh	Polyhedral Cell Count	Target Cell Size (mm)	Minimum Cell Size (mm)
Coarse	5,761,281	35	1
Medium	30,266,917	35	0.45
Fine	41,088,812	20	0.4

Table 3-3: Mesh settings examined for the mesh independence study.

Impact of Prism Layers

The impact of prism layers was examined on a 35.78 mm section of packing (shown in Figure 3-5). Prism layer growth rate, thickness, and number of layers were examined. Prism layer growth used a geometric progression function to determine layer thickness. The stretching factor between adjacent layers is constant at the value defined in the simulation. For example, for a stretch factor of 1.5, if the first prism layer has a thickness of 0.5 units, the second layer will have a thickness of 0.75 units. Prism layer thickness controls the total distance from the surface the prism layer can extend. The number of layers sets how many prisms will be present in the near-wall region. By using prism layers, a high quality mesh near solid surfaces can be generated, and the wall distance can be readily controlled to ensure adequate resolution of the boundary layers.

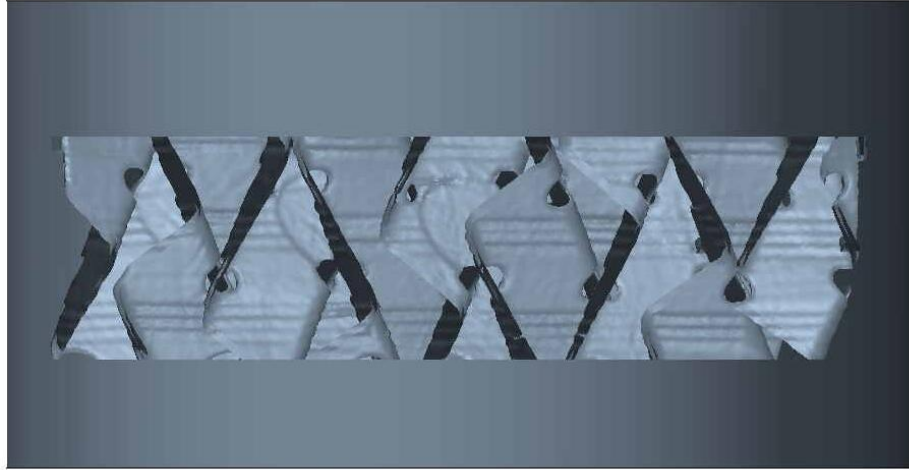


Figure 3-5: Cross-section of geometry to used examine the impact of prism layers on pressure drop and skin friction coefficient.

Pressure was measured 5 mm before the packing and 15 mm after the packing. The pressure drop difference was calculated to compare between different mesh settings. The locations of the packing relative to the inlet and outlet can be seen in the schematic presented in Figure 3-6.

SINGLE PHASE FLOW GEOMETRY GENERATION– PERIODIC GEOMETRY GENERATION

In addition to scanned geometries, a myriad of small-scale geometries were generated in SolidWorks to examine the impact of packing dimensions on packing pressure drop. One such geometry generated can be observed in Figure 3-7 with periodic boundaries indicated. The left and right sides were coupled as a periodic interface, meaning any flow leaving one side would be re-introduced to the computational domain on the other side. The top and bottom were coupled with a periodic interface, but a pressure drop was imposed to drive the fluid flow. In this manner, the periodic geometry could be considered an infinite sheet of structured packing. Table 3-4 summarizes the geometrical variables of the packing examined. Figure 3-8 shows a single sheet of

packing with the packing variables labeled, and Table 3-5 summarizes packing geometries examined. A 0.05 mm gap was present between sheets of packing to prevent the formation of highly skewed and sliver elements.

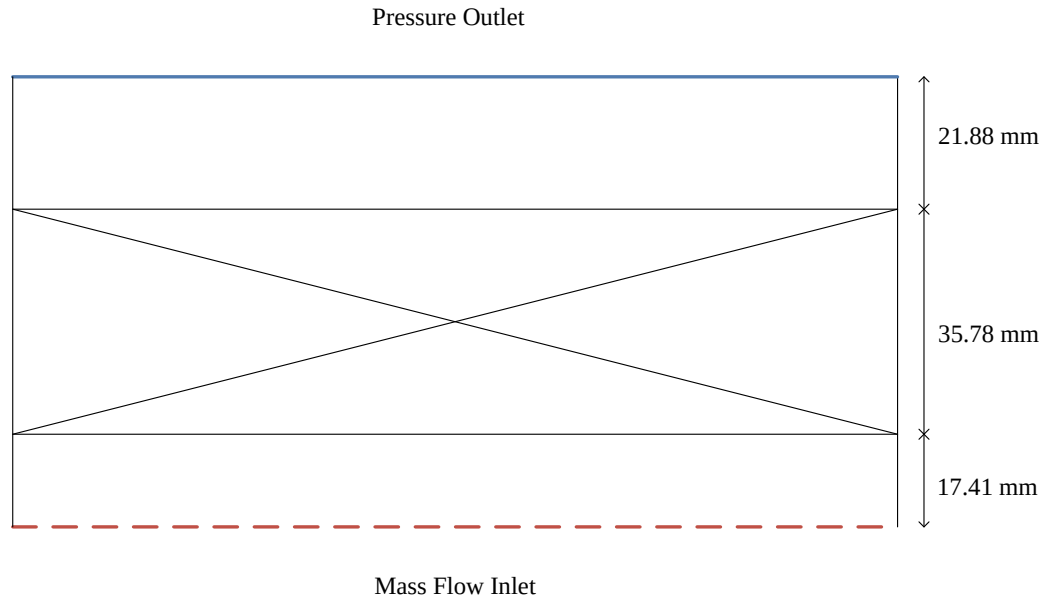


Figure 3-6: Schematic for prism layer studies geometry.

Packing Variable	Description	Dimensions
α	Packing corrugation angle (measured from the horizontal)	$^{\circ}$
a_p	Packing specific surface area (estimated by $4s/bh$)	m^2/m^3
b	Triangular channel base length	mm
s	Triangular channel side length	mm
h	Triangular channel height	mm
h_{ru}	Height of a repeating unit of packing	mm
L_c	Length of a flow channel = $h_{ru}/\sin(\alpha)$	mm
θ	Channel opening angle [$\tan(\theta) = (b/2)/h$]	$^{\circ}$

Table 3-4: Description of packing variables examined.

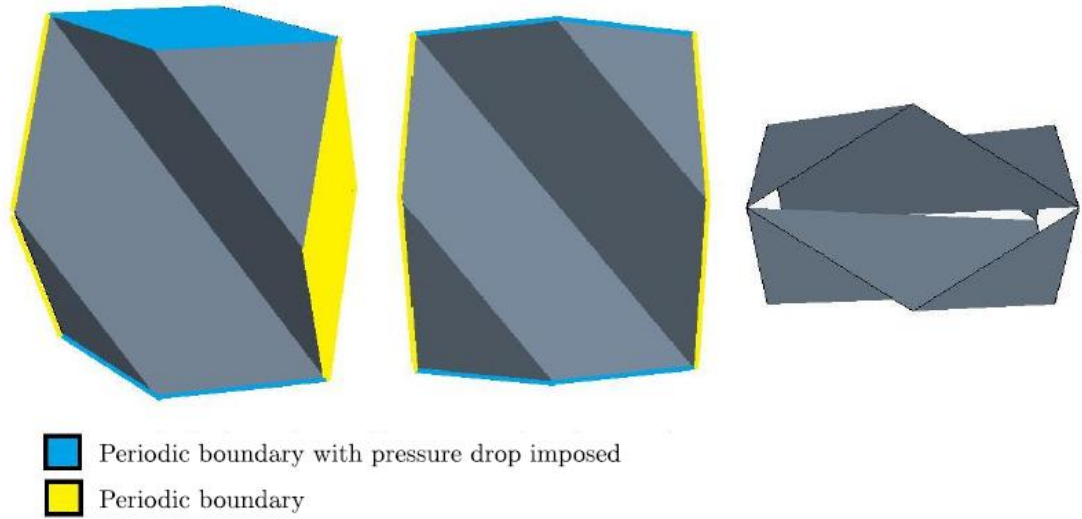


Figure 3-7: Example periodic geometry viewed from different angles with boundary conditions indicated. View showing 3D geometry (left), view of the packing element front (middle) and view from the top (right).

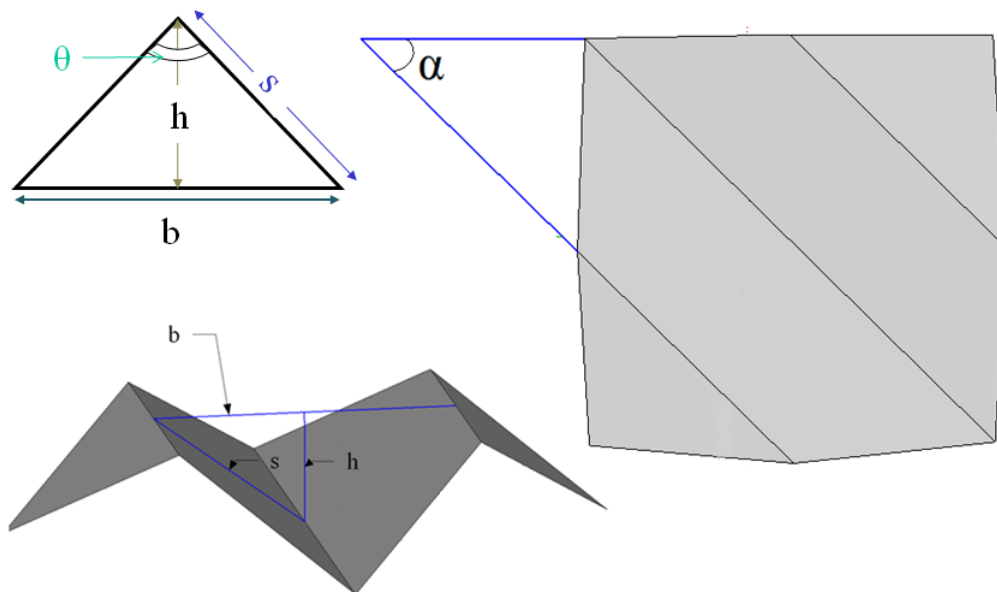


Figure 3-8: Packing sheet showing the main packing variables. Top left shows the triangular channel formed when looking down the corrugation angle. The right figure shows the definition of the corrugation angle. Bottom left shows a three-dimensional representation of the packing dimensions.

α °	h_{ru} mm	b mm	s mm	h mm	θ °	a_p m^2/m^3
40.00	34.00	26.05	16.75	10.53	102.1	244
45.00	36.83	26.05	16.75	10.53	102.1	244
50.00	40.52	26.05	16.75	10.53	102.1	244
55.00	45.41	26.05	16.75	10.53	102.1	244
60.00	52.09	26.05	16.75	10.53	102.1	244
65.00	61.63	26.05	16.75	10.53	102.1	244
70.00	76.15	26.05	16.75	10.53	102.1	244
75.00	100.63	26.05	16.75	10.53	102.1	244
40.00	28.53	21.85	15.18	10.53	92.1	264
45.00	34.00	24.04	15.98	10.53	97.6	252
55.00	48.56	27.85	17.46	10.53	105.8	238
60.00	58.90	29.44	18.10	10.53	108.9	233
65.00	72.92	30.81	18.66	10.53	111.3	230
70.00	93.41	31.95	19.13	10.53	113.2	228
75.00	126.94	32.84	19.51	10.53	114.7	227
50.00	20.26	13.02	8.37	5.27	102.1	489
50.00	40.52	26.05	18.15	12.64	91.7	221
50.00	40.52	26.05	20.47	15.80	79.0	199
50.00	81.04	52.09	33.49	21.06	102.1	122
50.00	25.00	16.07	15.90	13.72	60.7	289
50.00	60.00	38.57	21.62	9.77	126.3	229
50.00	35.97	23.12	16.38	11.60	89.8	244
50.00	60.29	38.75	21.38	9.03	130.0	244
45.00	30.00	21.21	27.16	25.00	46.0	205
45.00	9.00	6.36	12.41	12.00	30.0	650
70.00	18.62	6.37	12.41	12.00	30.0	650
45.00	33.61	23.77	12.30	3.18	150.0	650
70.00	69.49	23.77	12.30	3.18	150.0	650
45.00	12.30	8.70	6.15	4.35	90.0	650
70.00	25.43	8.70	6.15	4.35	90.0	650
45.00	24.60	17.39	12.30	8.70	90.0	325
45.00	49.20	34.79	24.60	17.40	90.0	163
60.00	25.00	12.50	12.25	10.53	61.4	372
60.00	90.00	45.00	24.84	10.53	129.8	210
60.00	42.00	21.00	14.87	10.53	89.8	269
45.00	16.00	11.31	8.00	5.66	90.0	500
60.00	83.17	41.57	24.00	12.00	120.0	192

Table 3-5: Periodic geometries examined for pressure drop studies. Geometries highlighted in blue were examined using the realizable k- ϵ , SST k- ω and LES turbulence models. Geometries highlighted in green were examined using the realizable k- ϵ and SST k- ω turbulence models. The remaining geometries were only examined with the realizable k- ϵ turbulence model.

SINGLE PHASE FLOW MESHING AND SIMULATIONS– PERIODIC GEOMETRY

Simulation Settings and Method

Steady-state simulations of turbulent, incompressible flow were carried out by imposing a pressure drop across the domain. The mass flow rate of gas across the top domain was monitored for convergence. When mass flow changed by less than 0.01% between iterations, the solution was deemed converged. At this point, a new pressure drop was chosen, and the solution was restarted from the prior solution. This process was repeated for at least five data points per simulation geometry with final F-factors ranging from 0.3-3.5 Pa^{0.5}. The two-layer realizable k- ϵ turbulence model was used for these simulations. Physics continuum and solver settings were those of the CT scan geometry (found in Figures A-3 and A-4). The one exception is the Courant number was set to 50 under the solver settings to allow for larger pseudo-time steps and faster convergence.

The impact of turbulence model choice was also examined on select geometries. The two-layer realizable k- ϵ model was compared to the all y+ SST k- ω model at various flow rates. The SST k- ω simulations are colored blue and green in Table 3-6. Solver and physics continuum settings matched those of the CT geometry (Figures A-1 and A-2) with the exception of the Courant number in the solver settings. It was set to 50 to allow for faster convergence.

Unsteady simulations for three geometries were carried out using the more computationally intensive large eddy simulation (LES) turbulence model. Due to the refined meshes and small time step required, only one flow rate was examined for comparison to the RANS turbulence model results. The LES simulation geometries examined are colored blue in Table 3-6. Default settings for the turbulence model are used. Specific physics continuum details can be found in Figure A-8, and specific solver settings can be found in Figure A-9. All scales of turbulence are modeled and assumed to

be isotropic when using a two-equation RANS turbulence model. This assumption can lead to inaccurate flowfield solutions in cases where turbulence is strongly anisotropic (e.g. cyclones). LES remedies this by directly solving for the large-scale structures of turbulence. Only the smallest scales, which are predicted to be more isotropic, are modeled. Simulation time step was chosen to keep the average CFL number below 0.5. Four inner iterations were used per time step; the STAR-CCM+ user manual recommends five or fewer inner iterations for a time accurate solution.¹⁴

Mesh Settings

Due to the small-scale of the simulations, a more refined mesh was used than for the CT-geometries. Detailed mesh settings for the bulk of the simulations can be found in Figure A-10 of Appendix A. The mesh settings presented are for steady-state RANS simulations only. Prism layers were used in all simulations when developing the non-dimensional model. Comparisons were made with polyhedral meshes in the absence of prism layers for select packing geometries. Simulations done via LES used a finer mesh. The base size (and thus minimum cell size and target cell size) was set at half the value used for RANS simulations (0.2 mm vs. 0.4 mm).

MULTIPHASE FLOW GEOMETRY GENERATION—SMALL-SCALE GEOMETRIES

For CFD simulations, best practices dictate evaluating the impact of boundary conditions on measured variables. To that end, three different small-scale geometries were examined: 1) Periodic Geometry, 2) Small Inlet Geometry, and 3) Large Inlet Geometry. The packing geometric parameter details can be found in Table 3-6.

α °	h_{ru} mm	b mm	s mm	h mm	θ °	a_p m^2/m^3
50.00	40.52	26.05	16.75	10.53	102.1	244

Table 3-6: Packing geometry parameters for multiphase simulations.

Periodic Geometry

The periodic geometry was generated in SolidWorks and imported into STAR-CCM+. Boundary conditions were placed around the domain in the exact same manner as for the single phase periodic geometry shown in Figure 3-7. After import and interface creation, the geometry was ready for meshing.

Small Inlet Geometry

This geometry was created by placing a small liquid inlet above the periodic packing element mentioned above. Figure 3-9 shows the geometry of the liquid inlet and overall geometry. The liquid velocity inlet was uniform thickness around the top of the boundary. A thin solid wall 2.0 mm in height surrounded the liquid inlet to isolate it from the pressure outlet. The sides of the geometry were periodic interfaces. The bottom geometry was similar to the periodic geometry (e.g. a 34 mm x 21 mm rhombus). Rather than a periodic interface, however, it was a pressure boundary condition. In this manner, it could serve as a liquid outlet and a gas inlet.

Large Inlet Geometry

This geometry consisted of the inlet created for the Small Inlet Geometry with four repeating units of packing placed below. Figure 3-10 shows the arrangement of the geometry. Again, a thin liquid inlet was surrounded by a thin wall 2.0 mm in height, which isolated the liquid inlet from the pressure outlet. The sides of the geometry were periodic interfaces. The bottom was a pressure boundary condition.

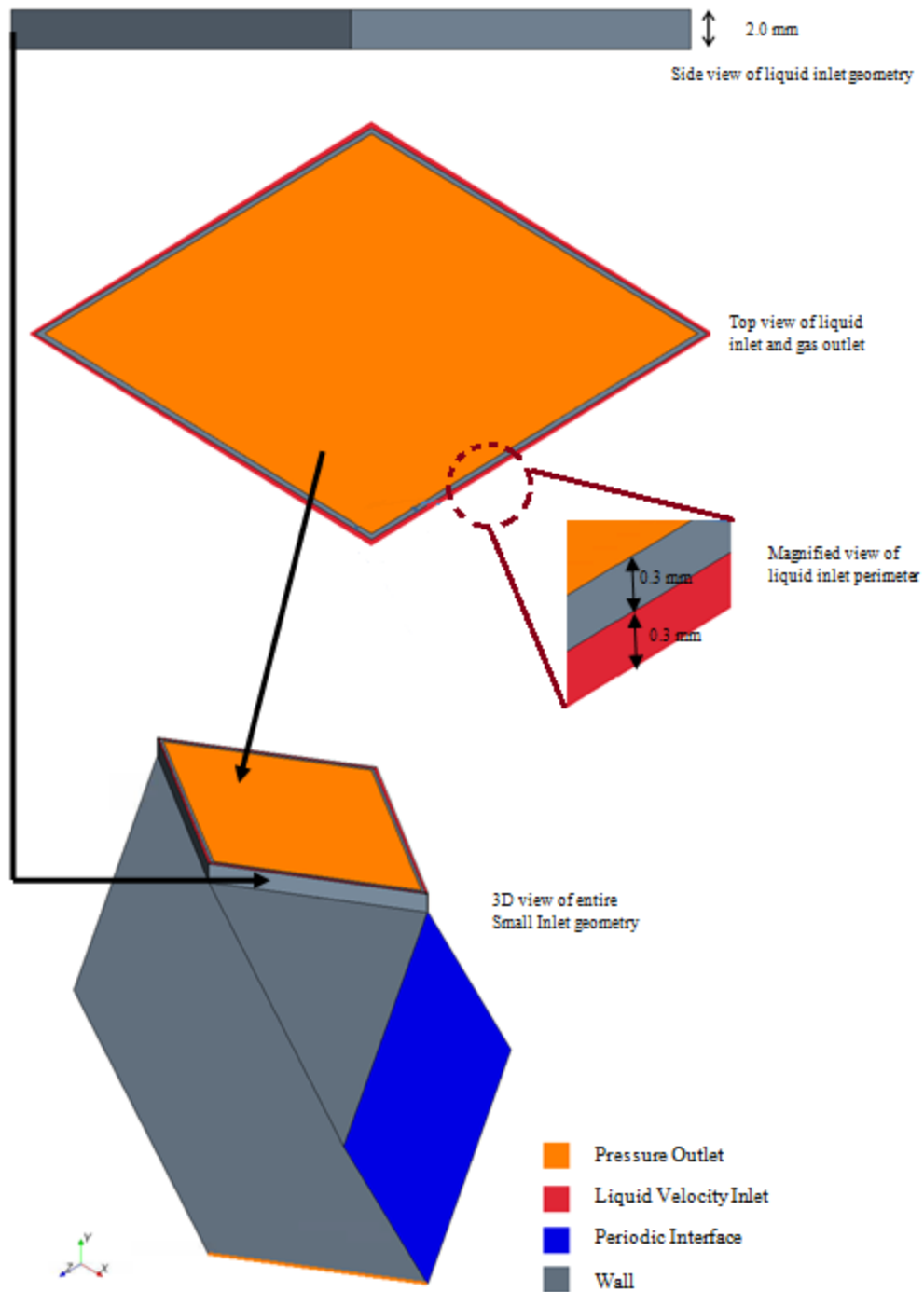


Figure 3-9: Small Inlet Geometry. Top shows the side view of the liquid inlet geometry. Middle shows the top view of the inlet geometry. The bottom shows a 3D representation of how the geometry is arranged.

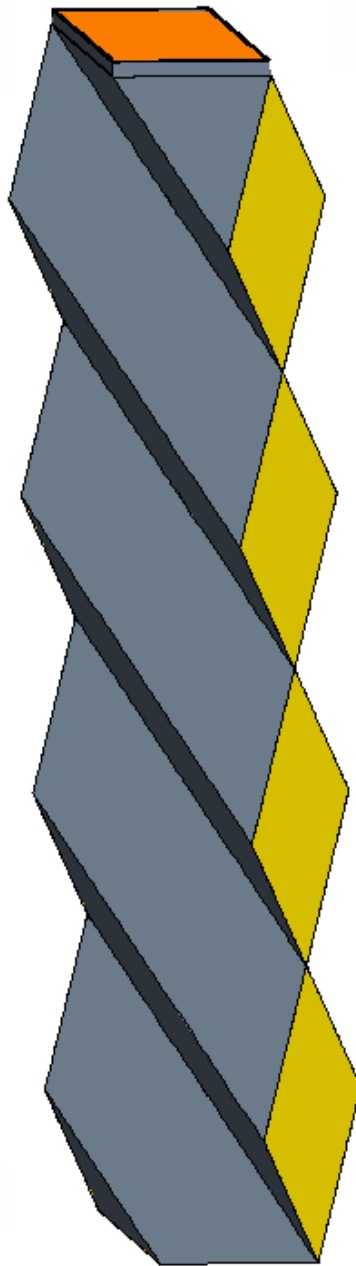


Figure 3-10: Large Inlet Geometry shown from an offset view.

MULTIPHASE MESHING AND SIMULATIONS— SMALL-SCALE GEOMETRIES

Simulation Settings and Method

Incompressible, multiphase flow was simulated using the volume of fluid (VOF) method implemented in STAR-CCM+ 7.06.009. Both laminar and turbulent (two-layer realizable $k-\epsilon$) simulations were examined for the periodic geometry. Detailed physics continuum and solver settings for multiphase turbulent flow can be found in Figures A-11 and A-12. Only laminar flow was examined for the Small Inlet Geometry and Large Inlet Geometry.

An additional boundary condition was required for VOF simulations to account for the wettability of the surface. This was done by prescribing a static contact angle on the boundaries designated as walls. Three static contact angles were examined: 0° , 30° , and 75° on all geometries. The complete wetting case ($\theta_c=0^\circ$) was chosen because experiments performed by Tsai *et al.* indicated Mellapak 125 and 250-series packings often achieve complete wetting.⁶⁰ Static contact angle of water on polypropylene has been observed to be $\sim 84^\circ$.⁶¹ The polypropylene sheets used to manufacture structured packing are textured to increase wettability. Thus, a slightly more wetting contact angle ($\theta_c=75^\circ$) was chosen for the weakly wetting simulations. The intermediate contact angle ($\theta_c=30^\circ$) was examined as a test case between the perfectly wetting and weakly wetting simulations. Wetted area was examined by monitoring the area of an isosurface defined at a liquid volume fraction of 0.5.

Three surface tensions were examined as part of these studies: 0.074, 0.037, and 0.018 N/m, yielding results for hypothetical fluids with surface tensions ranging from water to n-hexane. Gas density and viscosity were 1.14527 kg/m^3 and $1.78837 \times 10^{-5} \text{ Pa-s}$ for all simulations. Liquid density and viscosity were 997.561 kg/m^3 and $8.88714 \times 10^{-4} \text{ Pa-s}$ for all Large Inlet and Small Inlet geometry simulations. The periodic geometry was

used to examine the impact of liquid density and liquid viscosity on wetted area. Liquid densities examined were: 500, 997.561, and 1500 kg/m³. Liquid viscosities examined were 8.88714x10⁻⁴, 8.88714x10⁻³, and 0.01774 Pa-s. A summary of the hypothetical liquids examined for each geometry is shown in Table 3-7.

Geometry	Fluid Properties			
	Contact Angle	Surface Tension (N/m)	Liquid Density (kg/m ³)	Liquid Viscosity (Pa-s)
Periodic	0°, 30°	0.018, 0.037, 0.074	500	0.00088714
	0°, 30°, 75°	0.018, 0.037, 0.074	997.561	0.00088714
	0°, 30°	0.018, 0.037, 0.074	1500	0.00088714
	0°, 30°	0.018, 0.037, 0.074	997.561	0.00887140
	0°, 30°	0.018, 0.037, 0.074	997.561	0.01774000
Small Inlet	0°, 30°, 75°	0.018, 0.037, 0.074	997.561	0.00088714
Large Inlet	0°, 30°, 75°	0.018, 0.037, 0.074	997.561	0.00088714

Table 3-7: Summary of hypothetical fluids examined for all small-scale geometries utilized in multiphase fluid flow simulations.

Initial conditions were those of complete wetting of the liquid by some constant film thickness. To achieve this, it was necessary to make use of the wall distance solver. However, the wall distance solver is only available for turbulent simulations. Thus, a multi-step procedure was used to generate the initial wetting conditions. First, a turbulent simulation was initialized using the wall distance solver. Second, a table containing the volume fraction of each cell was created. Finally, the simulation solution was cleared, the physics continuum was changed from turbulent to laminar, and the initial condition for volume fraction was set to use the extracted table.

A field function was defined that returned a value of 1 if the wall distance was less than the prescribed film thickness, and 0 everywhere else. This field function was used for the initial conditions of the volume fraction, as shown in Figure 3-11. STAR-

CCM+. With the two-layer realizable k- ϵ turbulence model selected, the simulation was initialized.

After initialization was complete, a new xyz internal table was created within STAR-CCM+ under the Tools menu. This type of table records the cell centroids and the values for any scalar and vector fields the user chooses. In this case, the volume fraction of liquid was chosen as the scalar field. The table was then extracted, storing the volume fraction data in the table. At this point, the simulation's solution was cleared, and the physics continuum was changed from a turbulent simulation to a laminar simulation. The initial volume fraction options within the physics continuum tree were changed to those shown in Figure 3-12, to use a table as the initial condition.

🔍	Volume Fraction	
	Method	Composite
	Dimensions	Dimensionless
🔍	Composite	
🔍	Liquid	
	Method	Field Function
	Dimensions	Dimensionless
🔍	Field Function	
	Scalar Function	initial_vol_frac
🔍	Gas	
	Method	Constant
	Dimensions	Dimensionless
🔍	Constant	
	Value	0.0

Figure 3-11: Initial conditions to generate a uniform film thickness using a user-defined field function called initial_vol_frac.

Volume Fraction	
Method	Composite
Dimensions	Dimensionless
Composite	
Liquid	
Method	Table (x,y,z)
Dimensions	Dimensionless
Table (x,y,z)	
Table: X-Coordinate	X
Table: Y-Coordinate	Y
Table: Z-Coordinate	Z
Coordinate System	Laboratory
Table: Data	Volume Fraction of Liquid
Table	vol_frac_init
Gas	
Method	Constant
Dimensions	Dimensionless
Constant	
Value	0.0

Figure 3-12: Initial conditions to generate a uniform film thickness by using an extracted table called vol_frac_init.

For the Large Inlet Geometry and Small Inlet Geometry, the initial film thickness was always 0.3 mm. Liquid load for the Small Inlet and Large Inlet simulations was set by varying the velocity at the liquid inlet. Liquid loads of 36.7, 48.9, and 61.1 m³/m²-hr (15, 20, and 25 GPM/ft²) were simulated for the Small Inlet Geometry. Liquid loads of 48.9 and 61.1 m³/m²-hr (20 and 25 GPM/ft²) were simulated for the Large Inlet Geometry. Holdup was determined as a function of liquid load for these geometries. Experimentally, high liquid loads through structured packing lead to complete wetting. High liquid loads were used in the simulations to examine if complete wetting would be observed.

For the periodic geometries, the film thickness was varied to achieve the desired holdup within the geometry. Simulations were allowed to run until a pseudo-steady state was achieved. At this point, the liquid load could be determined from the average liquid phase mass flow through the vertical periodic boundaries. Fractional liquid holdup varied

from 5.5% to 8.0%. These values correspond to high liquid loads and were used to determine if CFD simulations could predict the complete wetting of the packing.

Meshing examined the impact of both the wall normal and wall tangent resolution on the periodic geometry. Wall normal resolution was examined by varying the number of prism layers in the near wall. It was set at 10, 15, and 20 prism layers with a total prism layer thickness of 1 mm. Resolution in the wall tangent direction was examined by changing the minimum cell size and target cell size. Minimum size varied from 0.09 to 0.034 mm. Target cell size varied from 1.0 to 0.38 mm. Time steps were chosen to ensure the average Courant number within the interfacial region was less than 0.5. This condition is necessary to achieve an accurate solution using the VOF model. In practice, it varied from 2.5×10^{-4} to 5×10^{-5} s, depending on mesh resolution. To ensure a time accurate solution, four inner iterations per time step were used. The STAR-CCM+ user manual recommends five or fewer inner iterations per time step for a time accurate solution.¹⁴

MULTIPHASE GEOMETRY GENERATION—CT GEOMETRY

The final geometry generated is shown in Figure 3-13. To create this geometry, the STL file generated after correcting the wiper band problems mentioned previously (i.e. Figure 3-1) was imported into STAR-CCM+. To generate a smooth interface between packing elements, roughly 4 mm was removed from each end of the packing geometry. This was accomplished via Boolean subtraction between the packing and a solid cylindrical geometry (5 mm tall x 146 mm diameter). This operation was performed on the top and bottom of the packing, yielding a packed element 155.2 mm tall. The element was copied two times. One copy was translated 155.3 mm upward. The other copy was translated -155.3 mm downward. At this point, the top half of the top element

and the bottom half of the bottom element were removed via Boolean subtraction. A liquid distributor was oriented 2.0 mm above the top half element. The liquid distributor's cross section is shown in Figure 3-14. It was generated by extracting the top surface of top element. The extracted surface was then translated 2.0 mm above the top element. It was then extruded 1.0 mm in the positive z-direction (upward) to generate a solid volume. At this point, the bottom faces were defined as the liquid inlet. The sides and top of the extruded volume were defined as walls. The corrugation angles were arranged perpendicular to those of the top element to simulate a joint (e.g rotated 90° from their starting condition). Only the middle element was monitored for pressure drop, wetted area, and liquid holdup. The bottom half element served to redistribute gas. The top half element served to redistribute the liquid. In this manner, the middle element could be thought of as an average packing element for comparison to experimental data.

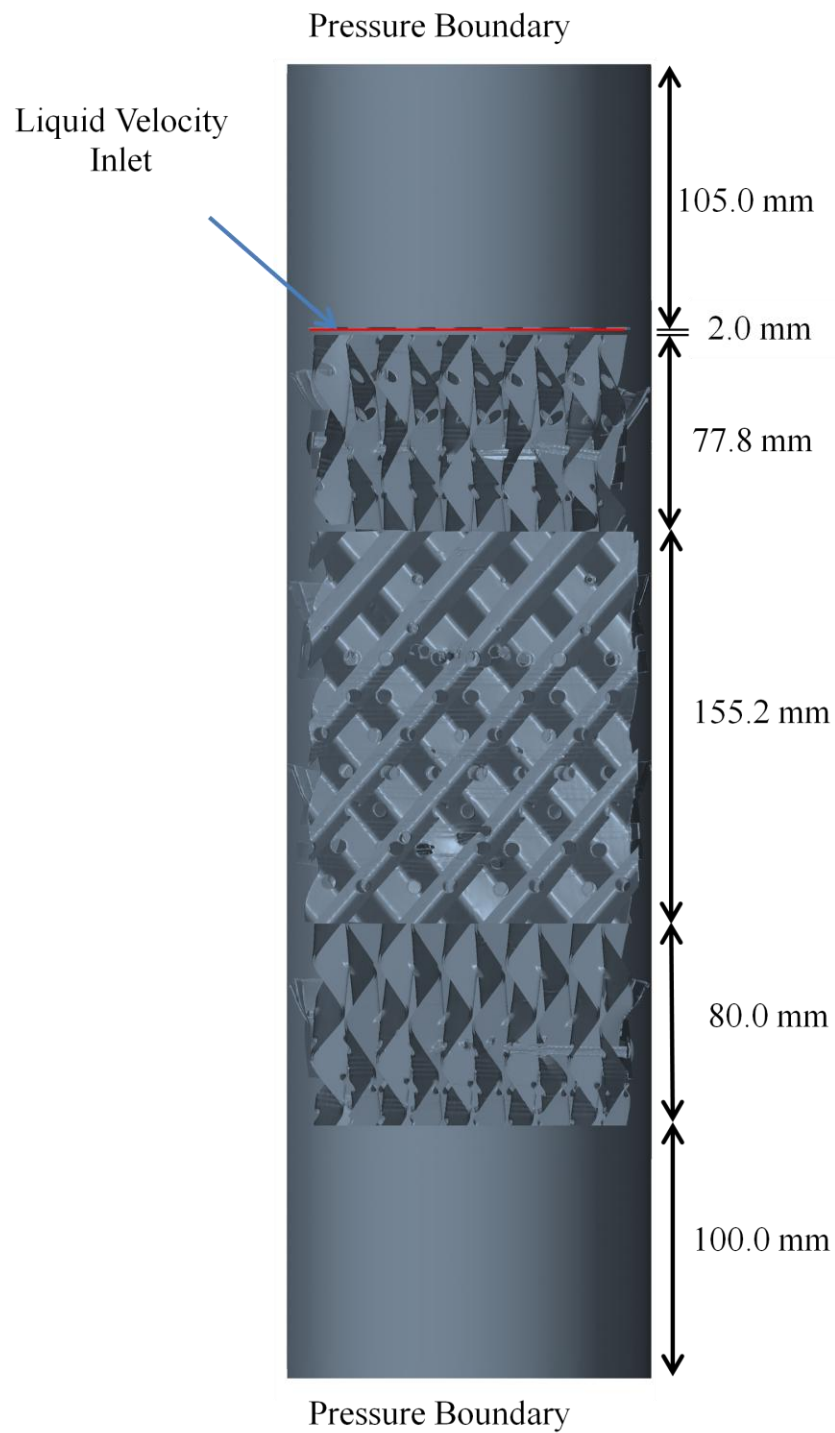


Figure 3-13: Multiphase CT Geometry used in present studies.



Figure 3-14: Top view of liquid velocity inlet geometry used in multiphase simulations.

MULTIPHASE MESHING AND SIMULATIONS– CT GEOMETRY

Irrigated pressure drop, wetted area, and liquid holdup were all monitored for the middle element. Irrigated pressure drop was monitored via plane-averaged pressures at the top and bottom of the middle element. Fractional liquid holdup was measured by integrating the volume fraction of liquid in all cells in the middle element region and normalizing by the empty column volume. Wetted area was measured by monitoring the area of an isosurface defined at a liquid volume fraction of 0.5. Turbulent, multiphase simulations were carried out using the realizable k - ϵ turbulence model. Turbulent, incompressible flow simulations were used in an effort to accurately predict irrigated pressure drop. Detailed physics continuum and solver settings are presented in Figures A-

11 and A-12. Detailed physical properties of the liquid and gas are presented in Table 3-8. The values were chosen to match the experimental conditions with a temperature of 15 °C.

Physical Property	Value
Gas Viscosity	1.73E-05 Pa-s
Gas Density	1.194 kg/m ³
Liquid Viscosity	0.00105 Pa-s
Liquid Density	997.561 kg/m ³
Surface Tension	0.074 N/m

Table 3-8: Physical properties for multiphase simulations on the CT geometry.

The bottom pressure boundary was set to a value of 25.0 Pa. The top boundary was set to a pressure of 0.0 Pa to yield a low F-factor. Liquid velocity at the inlet was set to achieve the desired liquid loads. Three liquid loads were examined: 24.4, 36.7, and 48.9 m³/m²-hr. Contact angles of 0° and 30° on the packing elements were examined. The tube wall contact angle was set at 0° for all simulation to eliminate any impact varying the wettability of the column wall had on predicted wetted area.

Detailed physics continuum and solver settings are presented in Figures A-11 and A-12. Detailed physical properties of the liquid and gas are presented in Table 3-8. The values were chosen to match the experimental conditions with a temperature of 15 °C. Meshing size was chosen based on the meshing studies carried out on the periodic geometry. The surface wrapper, surface remesher, prism layer mesher, and polyhedral mesher were used. The minimum mesh size was 0.068 mm. Target mesh size was 0.85 mm. Detailed mesh continuum settings are presented in Figure A-13.

Chapter 4: Experimental Methods

Several experimental campaigns were carried out to validate the CFD predictions of flow through half elements of Mellapak N250.Y. A sample piece of packing used in the experimental campaigns can be seen in Figure 4-1. The packing was made from corrugated sheets of polypropylene. Perforations, surface treatment/texture, and wiper bands (two per half element) were present on all pieces of packing utilized. Single phase pressure drop experiments were carried out in a bed of three half elements, exactly matching the simulation CT geometry shown in Figure 3-4. Irrigated pressure drop, wetted area, and liquid holdup experiments utilized a bed of 19 half elements with a total height of 3.12 m in an effort to obtain results for an average packing element.



Figure 4-1: Sample half element of Mellapak N250.Y used in experimental work.

SINGLE PHASE PRESSURE DROP EQUIPMENT AND INSTRUMENTATION

Dry pressure drop was measured through a bed of three half elements of Mellapak N250.Y. Total bed height was 480 mm. An experimental schematic and picture are

presented in Figure 4-2. The column consisted of an aluminum base and three polycarbonate tube sections (ID = 146.05 mm) with flanges on each tube end. For each upper flange was grooved to accept an O-ring to form an air-tight seal.

Gas entered the column through a 1.27 mm tubing process connection where it connected to a sparger 88.9mm in diameter. The sparger had a total of 57 holes distributed uniformly in the radial and angular directions. Each hole was 1.5875 mm in diameter. The top of the sparger is shown in Figure 4-3. The sparger was located 101.6 mm above the bottom of the first polycarbonate section.

The bottom polycarbonate section was an empty tube 0.7464 m in length. This section was meant to allow the flow field to develop naturally before encountering the packed bed. The second polycarbonate section was 0.966 m in length. Pressure ports were located 0.127 m, 0.6993 m, and 0.8295 m above the start of this section. Pressure ports were uniformly distributed around the column (i.e. at 0°, 90°, 180° and 270°). The packed bed started 0.1865 m above the start of second column section. At this point, two 1.56 mm wires were present to serve as the packed bed support. The packing support is shown in Figure 4-4. The top polycarbonate section was an empty section 0.254 m in length. This section served to lengthen the column and reduce the impact any local changes in lab air flow would have on the pressure measurements.

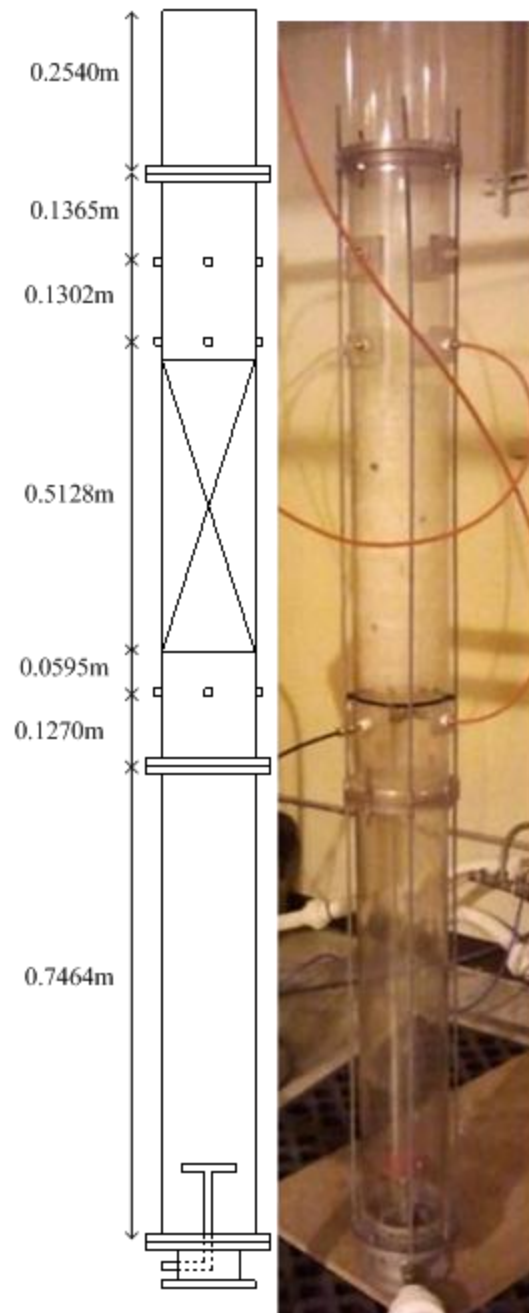


Figure 4-2: Schematic (left) and picture (right) of experimental test system used for dry pressure drop validation experiments.



Figure 4-3: Top view of the vapor distributor used in dry pressure drop studies.



Figure 4-4: Packing support used in single phase dry pressure drop studies. Figure taken from Owens.⁶²

Nitrogen flows were measured using two Micro Motion F050 flow meters arranged in parallel. Pressure drop measurements were made by four MKS 226A differential pressure sensors. All monitoring equipment output 4-20 mA signals. The signals were converted into 1-5V DC by placing high accuracy ($\pm 0.1\%$) 250- Ω resistors in the signal loops. This signal was read by a National Instruments USB-6008 data acquisition card. A LabVIEW virtual instrument (VI) converted the voltage signal into

process outputs (i.e. flow rates and differential pressures) for real-time process monitoring and data acquisition.

SINGLE PHASE PRESSURE DROP METHOD

The process flow diagram is shown in Figure 4-5. Prior to startup, the LabVIEW VI was started, allowing real-time monitoring of process variables. Building-supplied nitrogen was controlled via a gate valve. Pressure drop was measured across a stack of three half elements of Mellapak N250.Y. The pressure ports utilized were found 0.127 m and 0.6993 m above the start of the middle polycarbonate tube. All other pressure ports were capped for data measurement. Temperatures were monitored via a thermometer, and were found to vary between 20.8-22.9°C.

Nitrogen flow rates were varied from 0.62-2.75Pa^{0.5} by increments of 0.305Pa^{0.5}. Experimental order was randomized and repeated at least twice for each experimental run. After three minutes of steady operation at a given flow rate, data recording was initiated. Flow rates and pressure drop were recorded for a total of three minutes. At this point, data recording was stopped. This experimental procedure was repeated for the next nitrogen flow rate until all data was collected. At this point, the pressure drop and flow rate data for each flow rate was averaged over the span of three minutes in an Excel spreadsheet. Two packing orientations were examined. The first was packing elements oriented with the standard 90° rotation between layers. The second had no rotation between successive packing layers (i.e. 0° rotation).

IRRIGATED PRESSURE DROP AND WETTED AREA EQUIPMENT AND INSTRUMENTATION

The experimental setup for the irrigated pressure drop and wetted area experiments can be seen in Figure 4-6. Existing SRP infrastructure was used as the column base and sump. The sump consisted of a 1.038 m section of PVC pipe with an ID

of 0.57 m. A 0.632 m section of 0.427 m ID of PVC was attached to the sump. In this middle section, the nitrogen line (0.203 m OD) was introduced to the column. One additional 0.427 m ID PVC was used, totaling a length of 0.610 m. All sections had flanges utilizing an 18 in. ASME Class 150 flange bolt pattern. The lower flange connections had grooves to accept O-rings. The upper flange connections were flat-faced. In total, the height of the existing SRP column and sump used was 2.28m.

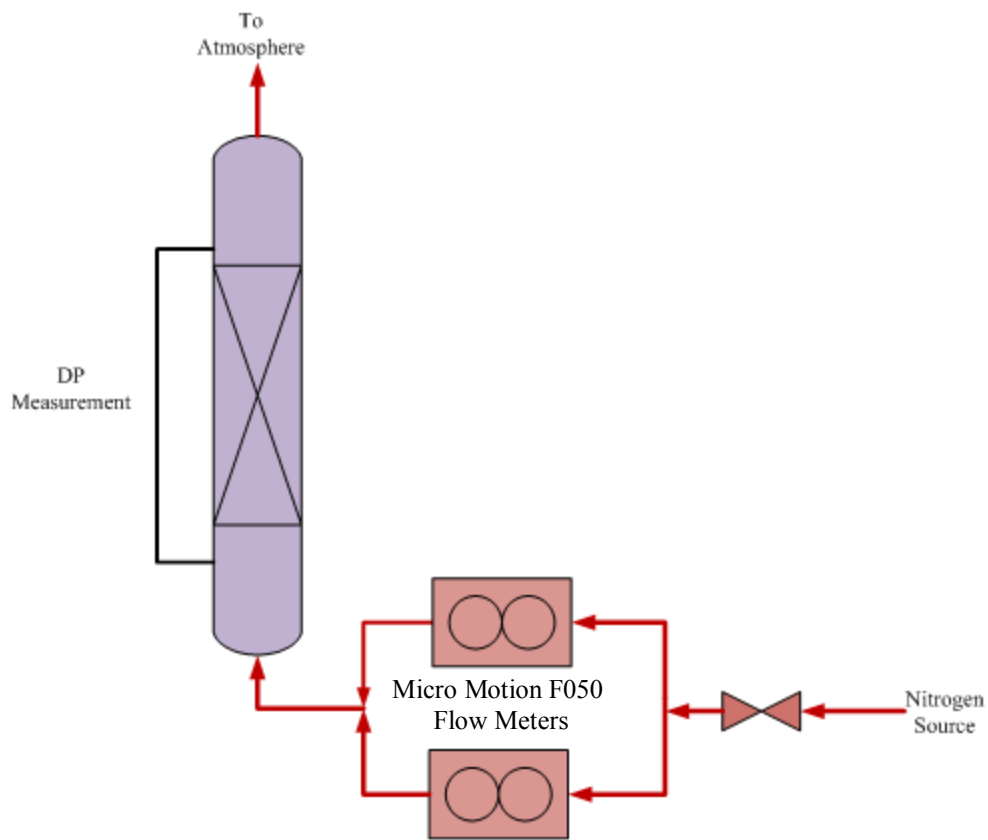


Figure 4-5 Process flow diagram for single phase nitrogen validation experiments.

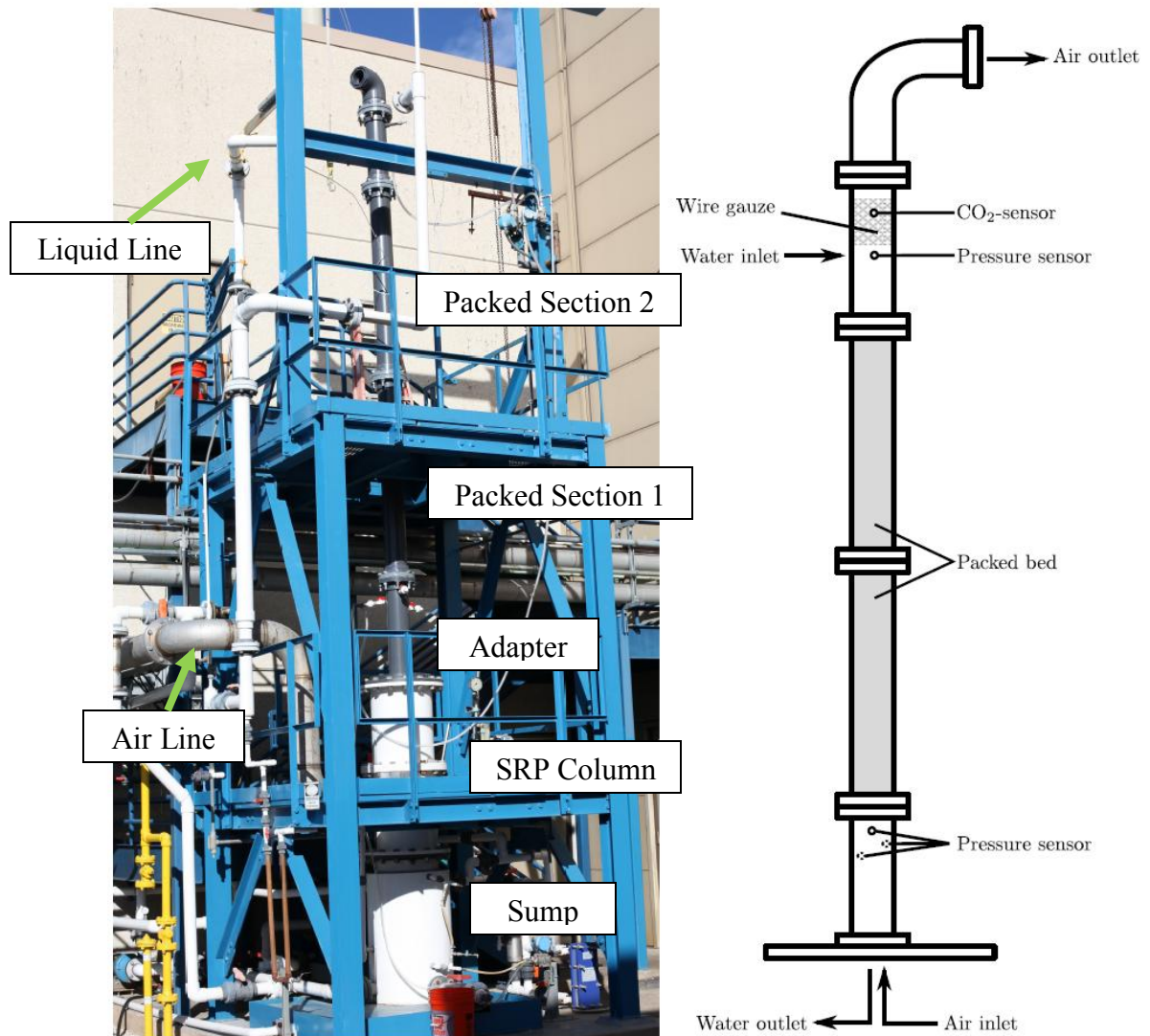


Figure 4-6: Picture (left) and experimental schematic (right) of column used in wetted area and irrigated pressure drop experiments. Figure from Waas.⁶³

An adapter was made to transition from the existing SRP column to 6 in. schedule 80 PVC pipe of ID 0.146 m (OD = 0.1683 m). The adapter was 0.787 m tall. The bottom was a 25.4 mm thick PVC plate with an 18 in. ASME Class 150 flange bolt-hole pattern. A 0.1683 m hole was drilled through the center of the plate, and the 0.146m ID pipe was centered and triple-welded to ensure a water-tight seal. A Schedule 80 Van Stone flange

was installed at the top of the adapter. Three couplings (0.5 in. NPT) were welded into the adapter at heights of 0.578 m, 0.629 m, and 0.679 m. They were located at angles of 0°, 120°, and 240°. These couplings served as process connections to allow for pressure drop measurements. Three connections at varying heights and angles were installed to ensure flexibility in the event of a liquid film covering one process connection, inhibiting accurate measurements pressure. A 3.175mm OD (0.125 in.) piece of stainless steel tubing was bent into a V shape. This V-shape was placed on the top lip of the pipe (roughly 50.8 mm from the top of the flange) and served as a packing support.

The packed bed consisted of two 6 in. Schedule 80 PVC sections, each being 1.524 m in length. This allowed for a total packed bed height of roughly 3.048 m. Van Stone flanges were used for all process connections. EPDM gaskets were installed to create water-tight seals.

A 0.610 m section of pipe was placed above the packed bed sections. A 1 in. NPT coupling was welded into the pipe 0.223 m above the start of this section. This coupling served as the liquid inlet. A 0.5 in. NPT coupling was welded into the column 90° from the liquid inlet. This coupling served as a process connection for the differential pressure instrumentation. One final 0.5 in. NPT coupling was welded into this section at a height of 0.475 m to serve as a process connection for the CO₂ analyzer. The top of the column consisted of an elbow fitted with a bushing (0.146x0.1016m). This allowed the gas flow to accelerate as it vented to atmosphere, minimizing the risk of ambient air impacting CO₂ concentration measurements.

The packed bed consisted of 19 half elements of Mellapak N250.Y. They were oriented in the column with corrugations aligned in the north-south and east-west directions, alternating from one piece of packing to the next. The liquid distributor had a drip point density of 720 points/m². It was oriented less than 25.4 mm from the top of the

packed bed. Above the liquid distributor, a 0.2286 m bale of stainless steel and Teflon co-knit served as a demister.

Carbon dioxide content was measured via a Horiba VIA-510 CO₂ analyzer. Differential pressure was measured via two Rosemount pressure transmitters. One was calibrated for low pressure (up to 750 Pa). The other was calibrated for high pressure (up to 6215 Pa). Water flow was measured via a MicroMotion F200 series flow meter. This flow meter also monitored water temperature. A centrifugal pump equipped with a variable speed drive was used to control water flow. Nitrogen flow was monitored via a MicroMotion F100 series flow meter. All process variables were measured in DeltaV. Water flow could be controlled directly via DeltaV. Nitrogen flow was controlled by hand through the use of a gate valve. CO₂ flow was controlled manually via a rotameter.

IRRIGATED PRESSURE DROP METHOD

A process flow diagram can be seen in Figure 4-7. Initially, 757 L of water was fed into the column sump and tank. Nitrogen flow was then set at the desired flow rate, and water flow is set at the maximum flow rate achievable before pressure drop through the column was above 1230 Pa/m of packing (0.5 in. H₂O/ft. of packing). After wetting the packing at these conditions for at least ten minutes, the pressure drop was monitored for steady state. When steady state was achieved, data was recorded for at least one minute. After recording the data, the liquid load was reduced to the next flow rate. Pressure drop readings were allowed to stabilize to a steady state for at least five minutes at the new liquid load. At this point, the data recording procedure was repeated, and the next liquid load was set. When all liquid loads were completed, the entire procedure could be repeated for the next nitrogen flow rate. A summary of experimental conditions achievable can be found in Table 4-1.

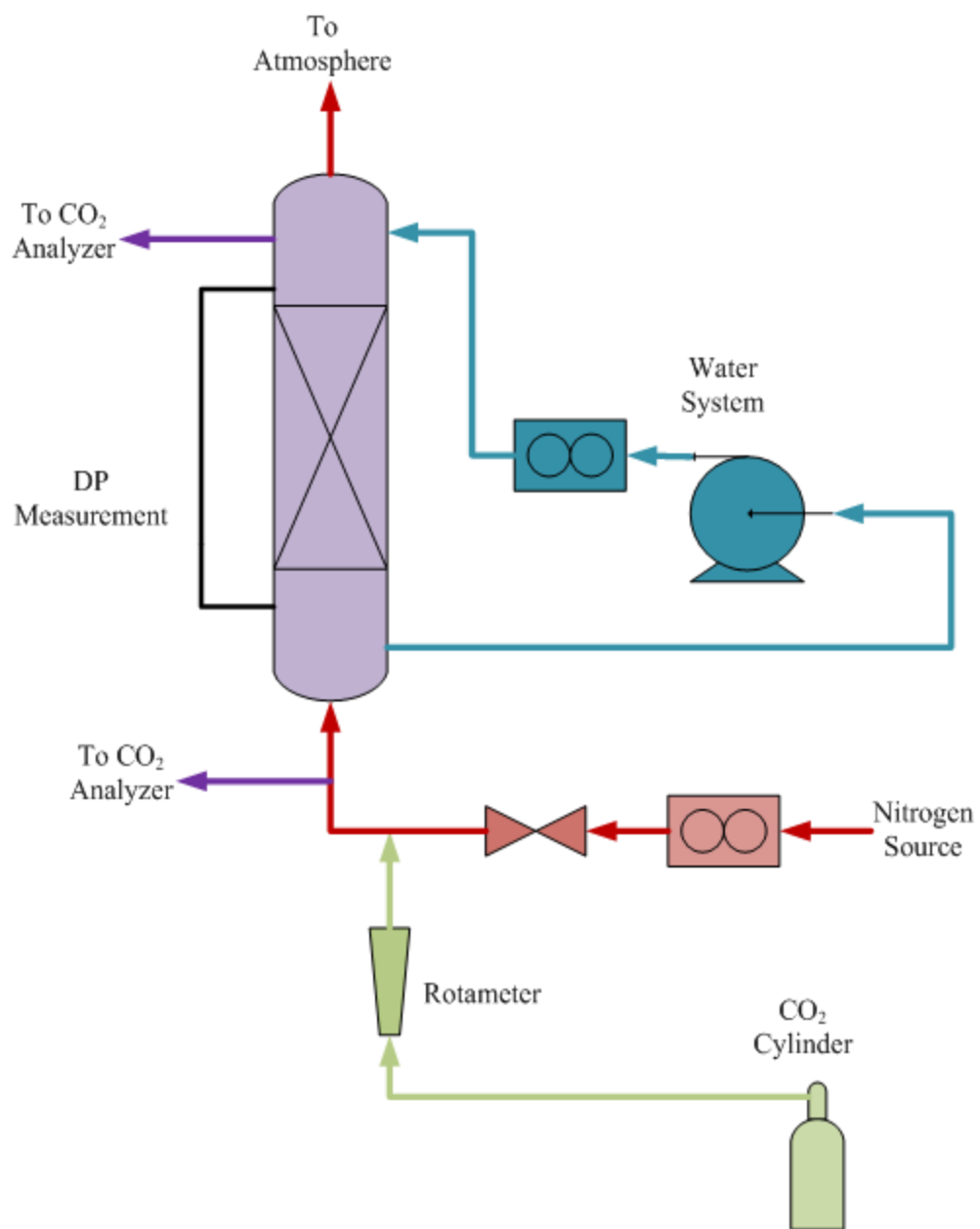


Figure 4-7: Process flow diagram for irrigated pressure drop and wetted area measurements.

Gas Rates			Liquid Loads Examined					
m ³ /min	ft ³ /min	F-factor (Pa ^{0.5})	m ³ /m ² -hr (GPM/ft ²)					
0.566	20	0.61	73.3 (30)	61.1(25)	48.9(20)	36.7(15)	24.4(10)	12.2(5)
1.133	40	1.23		61.1(25)	48.9(20)	36.7(15)	24.4(10)	12.2(5)
1.699	60	1.85				36.7(15)	24.4(10)	12.2(5)

Table 4-1: Summary of experimental conditions examined for irrigated pressure drop and wetted area experiments.

WETTED AREA METHOD

Initially, 757 L of water was fed into the system. Approximately 3 kg of caustic pellets are then added to the tank to yield a ~0.1M caustic solution. The pump was then turned on, and water was allowed to circulate between the column sump and holding tank. The solution was allowed to mix for approximately 45 minutes. At this point, it was possible to begin the titration process. Liquid samples from the column sump were gathered. A sample weighing approximately 10 g was then titrated against a 0.1N solution of HCl using phenolphthalein as an indicator. This procedure was repeated every five minutes until the NaOH concentration no longer varied. The concentration of NaOH was averaged from the last three samples taken and used as the initial concentration for wetted area experiments.

Nitrogen flow was then set at the desired flow. CO₂ flow was started, and the inlet CO₂ concentration was monitored via the Horiba VIA-510 CO₂ analyzer. The CO₂ rotameter was adjusted until the inlet concentration was between 300-400ppm_v CO₂. The inlet concentration was recorded in DeltaV, and the CO₂ analyzer was set to monitor the outlet gas concentration. At this point, the pump's set point was adjusted to yield the maximum liquid load achievable at a given nitrogen flow. The packing was wetted at these conditions for at least ten minutes before data was recorded. At this point, the liquid load was reduced by ~12.2 m³/m²-hr (5 GPM/ft²). The pressure drop and CO₂

concentration were monitored for steady state. After holding steady for at least three minutes, the process was repeated for each liquid load. At the end of a series of liquid load experiments, the CO₂ inlet concentration was measured again to ensure there was no significant experimental drift. This overall procedure was repeated for the next gas rate. The standard operation procedure (SOP) can be found in Appendix B.

LIQUID HOLDUP EQUIPMENT AND INSTRUMENTATION

An experimental schematic can be seen in Figure 4-8. The column consisted of an aluminum base, a 0.746 m section of polycarbonate tube, two 1.521 m sections of PVC pipe, and a 0.610 m section of PVC pipe. The aluminum base had a 1 in. NPT process connection drilled perpendicular to the base's axis. The process connection intersected a conical throat drilled along the central axis of the base. The polycarbonate tube was attached to the aluminum section via a flange. The flange was grooved to allow the installation of an O-ring, which was used to create a water-tight seal.

While the ID of the PVC and polycarbonate sections was the same (0.146 m), the flanges were incompatible. Joining the polycarbonate tube to the PVC was accomplished via silicone caulk (GE Silicone II Clear Kitchen and Bath Caulk). The PVC pipe connections were Van Stone flanges with EPDM gaskets placed between to create water-tight seals. Water entered the column through a 1 in. NPT connection placed in the 0.610 m section of PVC pipe. This connection was located 0.223m above the start of this section.

The packed bed consisted of 19 half elements of Mellapak N250.Y. They were oriented in the column with corrugations aligned in the north-south and east-west directions, alternating from one piece of packing to the next. The liquid distributor had a

drip point density of 720 points/m². It was oriented less than 25.4 mm from the top of the packed bed.

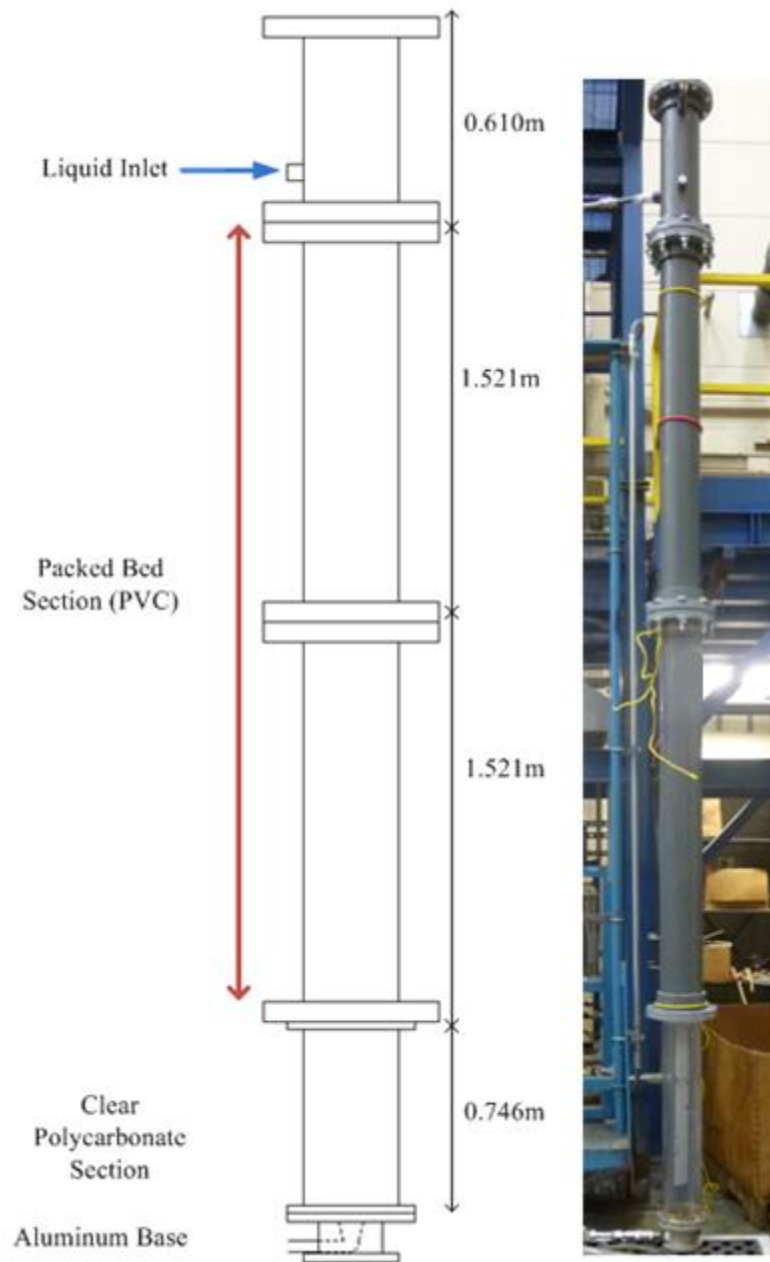


Figure 4-8: Experimental schematic (left) and apparatus (right) for liquid holdup experiments.

Liquid flow was monitored via a MicroMotion Basis F050 flowmeter. The 4-20mA signal was converted to a 1-5V DC via a high accuracy ($\pm 0.1\%$) 250- Ω resistor. This signal was read by the computer via a National Instruments USB-6008 into a LabVIEW VI created to monitor the liquid load. The pump was a 3-HP FHP Performa+ centrifugal pump controlled with a variable speed drive. No gas flow was used in these experiments, but prior research found little to no variation in liquid holdup in the pre-loading regime of structured packing.^{7,8}

LIQUID HOLDUP METHOD

A process flow diagram can be seen in Figure 4-9. Water was added to the column through the open top with a bucket. Under normal column operation, water was pumped from the column base, through the pump and flow meter, past a ball valve, and to the top of the column.

Initially, water was pumped through the column at $73.3 \text{ m}^3/\text{m}^2\text{-hr}$ (30 GPM/ft²) for at least three minutes to achieve total wetting of the packing. The liquid load was then adjusted to the desired liquid load by changing the set point on the variable speed drive. The chosen liquid load was randomly chosen from those listed in Table 4-2. Liquid load was monitored via LabVIEW. The flow rate was allowed to stabilize for at least one minute. After achieving flow stabilization for three minutes, the liquid level was marked on the polycarbonate section. If this indicated level did not change over the next 2-3 minutes, the indicated line was considered to be the steady state line. If the level did change, a new line was marked. This procedure was repeated until steady-state had been reached.

When steady-state had been reached, the ball valve immediately after the flow meter was closed, and the pump was turned off. Liquid was allowed to drain out of the

packing. The change in liquid height was measured with a ruler. At this point, the ball valve was opened. This entire procedure was repeated, starting with the pre-wetting of the packing (i.e. liquid flow at $73.3 \text{ m}^3/\text{m}^2\text{-hr}$ to achieve complete wetting of the packing). Each flow rate was examined two times each day of experiments.

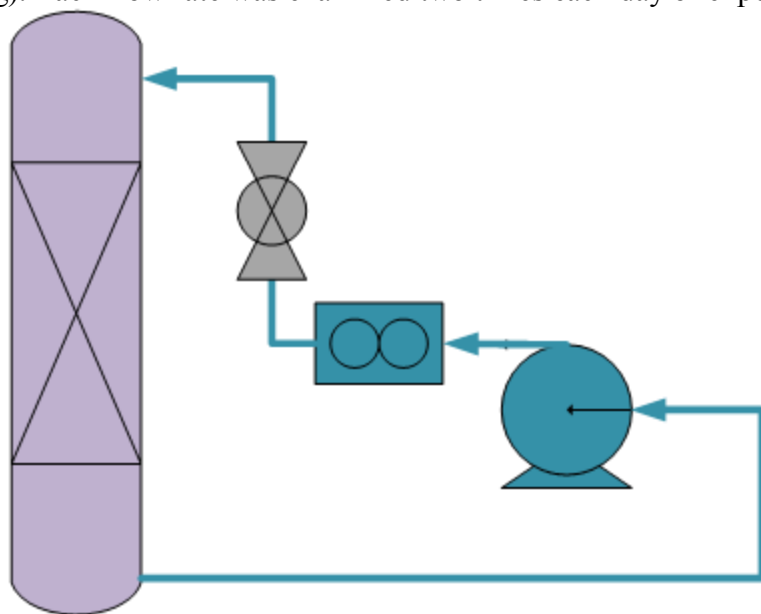


Figure 4-9: Process flow diagram for liquid holdup experiments.

Liquid Loads Examined					
$\text{m}^3/\text{m}^2\text{-hr}$ (GPM/ft ²)					
12.2 (5)	24.4 (10)	36.7 (15)	48.9 (20)	61.1 (25)	73.3 (30)

Table 4-2: Summary of experimental conditions examined for irrigated pressure drop and wetted area experiments.

To account for the liquid holdup in the packing distributor and associated piping, a separate series of experiments was performed using the column base and clear polycarbonate tubing. Liquid was pumped through the distributor at the desired liquid

load. Upon reaching steady state, a steady state line was marked on the column wall, the ball valve was shut, and the pump was turned off. Liquid was allowed to drain out of the distributor, and the difference in heights was measured to determine liquid volume.

Chapter 5: Single Phase Results

This chapter is broken into two main sections. The first deals with the validation of the CFD predictions. This is accomplished through comparisons of CFD results to experimental data with a bed of packing composed of three half elements of Mellapak N250.Y. The impacts of joint rotation angle, turbulence model choice, and prism layer meshing were examined. The second section of this chapter deals primarily with demonstrating the capabilities of CFD in the area of packing design. Variations in pressure drop through small periodic geometries with fully developed flow were examined by changing the geometric packing parameters. A new non-dimensionalization is proposed. Functional comparisons are made to the Rocha-Bravo-Fair and Delft semi-empirical models for dry pressure drop.

MESH INDEPENDENT SOLUTION

Best practices for CFD require a grid dependency study be used to analyze the quality of the mesh and ensure all relevant flow features are being properly captured.⁶⁴ This is generally done by running a simulation on a coarse mesh, refining the mesh, and reaching a new converged state. To maximize computational efficiency, the coarse solution should be used as the starting point for the fine-mesh simulation. Roache recommends the use of a Grid Convergence Index (GCI) for measuring the relative errors.⁶⁵ The fine grid GCI is defined as:

$$GCI[*fine grid*] = F_s \frac{|\varepsilon|}{r^p - 1} \quad \text{Equation 5-1}$$

where F_s is a factor of safety ($F_s = 3$ is recommended), ε is the relative error between the fine grid solution and another solution, p is the order of the basic numerical method ($p = 2$ for 2nd order methods), and r is the grid refinement ratio. For unstructured meshes, Roache recommends the use an effective r defined in three dimensions as:

$$r_{effective} = \left(\frac{N_1}{N_2}\right)^{\frac{1}{3}} \quad \text{Equation 5-2}$$

where N_1 is the number of cells in the fine grid, and N_2 is the number of cells in the coarse grid. The use of only the relative error, ε , to estimate grid convergence is not recommended. The relative error, ε , does not take into account the grid refinement level or the order of the numerical method. Furthermore, ε can be made arbitrarily small by simply using a grid refinement ratio very near unity.⁶⁵ The GCI can be considered a measure of uncertainty in the grid index and is generally a conservative estimate of how close to the asymptotic solution a given solution is.

The results of the mesh independence are presented in Table 5-1. Calculated values for relative error, grid refinement ratio, and fine-grid GCI are calculated using the mesh indicated in the row and one level coarser (i.e. Medium-Coarse and Fine-Medium). The flow rate was equivalent to an F-factor of $0.61 \text{ Pa}^{0.5}$, and the simulation tube inner diameter was 146.2 mm. A stack of three half-elements of Mellapak N250.Y were used with the joint rotation of 90° . The shear stress transport (SST) $k-\omega$ turbulence model was used in these studies. The fine-grid GCI of the Fine-Medium mesh is 1.37%, indicating the pressure drop through this stack of packing is 8.894 Pa with an error band of 1.37%. The large relative error between the Medium-Coarse grids indicates the Coarse grid results are not within the asymptotic region, making the fine grid GCI calculation for the Medium-Coarse mesh suspect. In this case, the coarse grid GCI (and thus error band) for Medium-Fine can be estimated by:

$$GCI[coarse\ grid] = GCI[fine\ grid]r^p \quad \text{Equation 5-3}$$

For the Medium-Fine mesh, this yields a coarse-grid GCI of 1.67%, allowing the pressure drop to be 8.884 Pa with an error band of 1.67%. This residual error was considered acceptable, considering the Medium mesh required only 75% of the calculation time as

the Fine mesh. Average iteration time was 12 s on the Medium Mesh and 16 s on the Fine Mesh when using 448 processors on the now-decommissioned Ranger computing cluster.

Mesh	Polyhedral Cell Count	Target Cell Size (mm)	Minimum Cell Size (mm)	Pressure Drop (Pa)	$ \varepsilon $	$r_{\text{effective}}$	Fine Grid GCI
Coarse	5,761,281	35	1	8.094773	xx	xx	xx
Medium	30,266,917	35	0.45	8.884974	8.89%	1.7384	13.20%
Fine	41,088,812	20	0.4	8.894122	0.10%	1.1073	1.37%

Table 5-1: Pressure drop results for the three meshes examined.

Figure 5-1 show cross-sections of the meshes generated for the grid convergence studies for a region immediately preceding the packing. The mesh is coarse far away from the packing elements. Flow through an empty tube is not expected to be complex, and thus a coarse mesh is acceptable in this region. This is also where the target cell size will have the most impact. Near the packing itself, the minimum cell size will come into effect. The automatic meshing tools will refine the mesh near the packing surface due to automatic proximity and curvature refinement. The impact of the minimum cell size can be most easily observed in Figure 5-2. The Coarse mesh had a minimum cell size over twice that of the Medium and Fine meshes. This difference is observed as significantly larger polyhedral cells found in the coarse mesh picture. In all cases, the mesh is noticeably less refined in the near-wall region when compared to the bulk of the packing. Again, this is due to lack of features activating automatic mesh refinement.

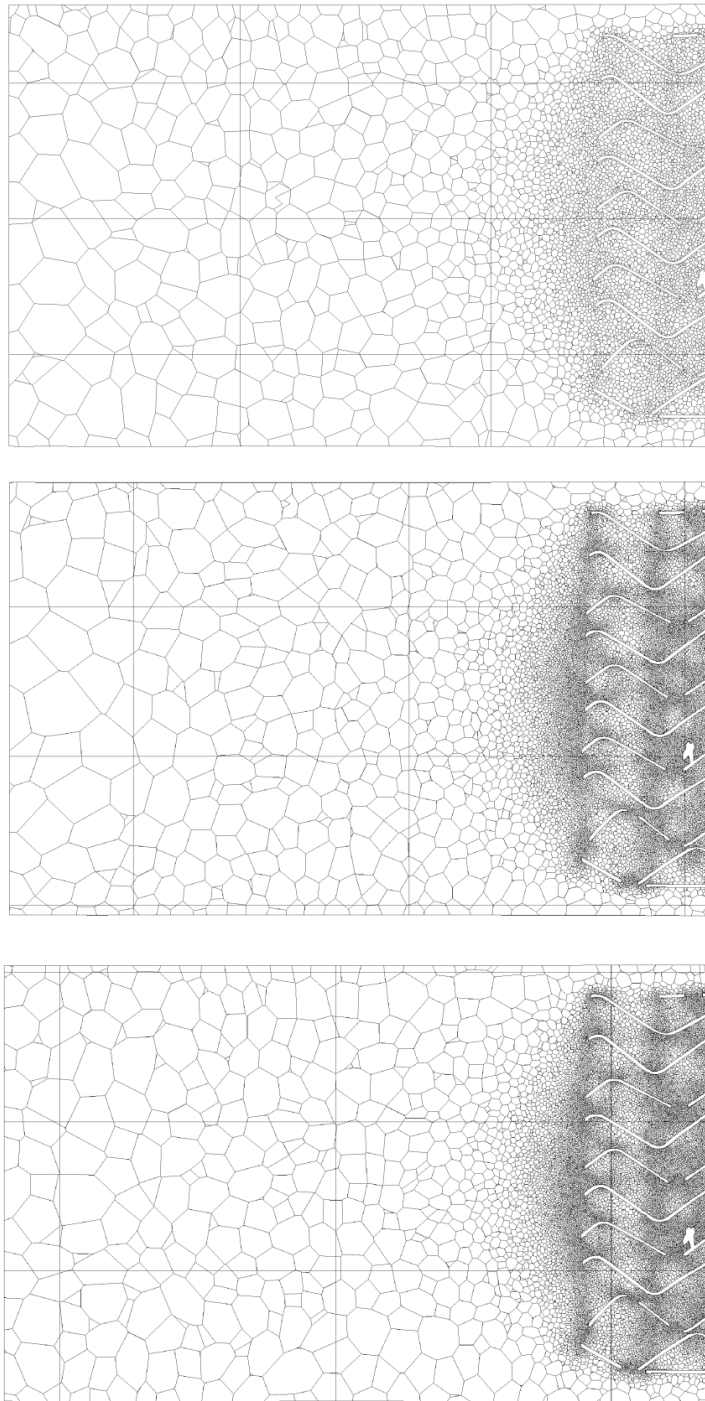


Figure 5-1: Meshes generated for the grid convergence studies. The Coarse mesh is shown at the top, Medium mesh at center, and Fine mesh at bottom. Flow is directed from left to right.

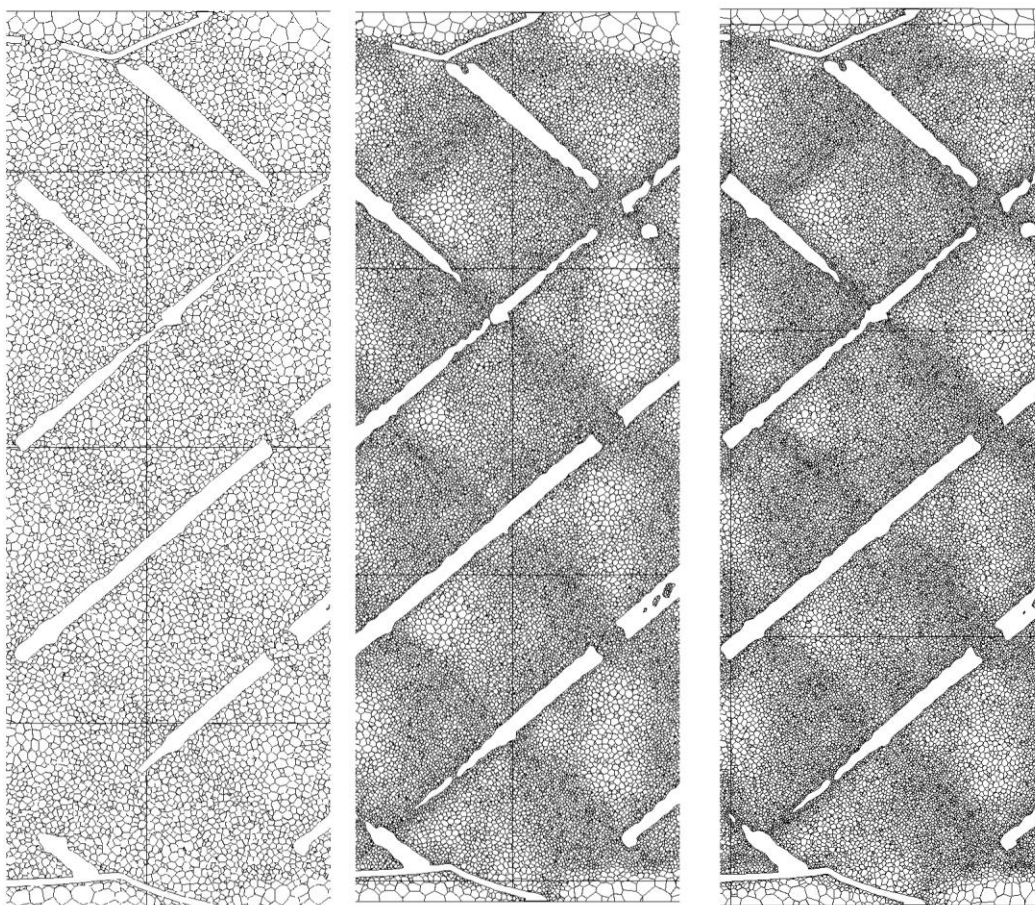


Figure 5-2: Meshes generated for the grid convergence studies. The Coarse mesh is shown at left, the Medium mesh at center, and the Fine mesh at right.

JOINT ROTATION COMPARISONS

It is common industrial practice to rotate successive packing elements 90° to ensure satisfactory liquid and vapor redistribution in the packing. Increased pressure drop is associated with these interfaces between packings—commonly referred to as joints. To examine the impact the joint rotation angle had on pressure drop, four distinct geometries were examined via CFD simulations. Three half elements of Mellapak N250.Y were used

in all studies with joint rotation angles of 0° , 30° , 60° , and 90° . Figure 5-3 shows the joint rotation angles examined moving from one element to the next. In all cases, the packing is viewed from the top of the element. The goal of this work was to determine if any significant additional capacity could be realized by using a different joint rotation angle. A sample stack of packing can be observed in Figure 3-4.

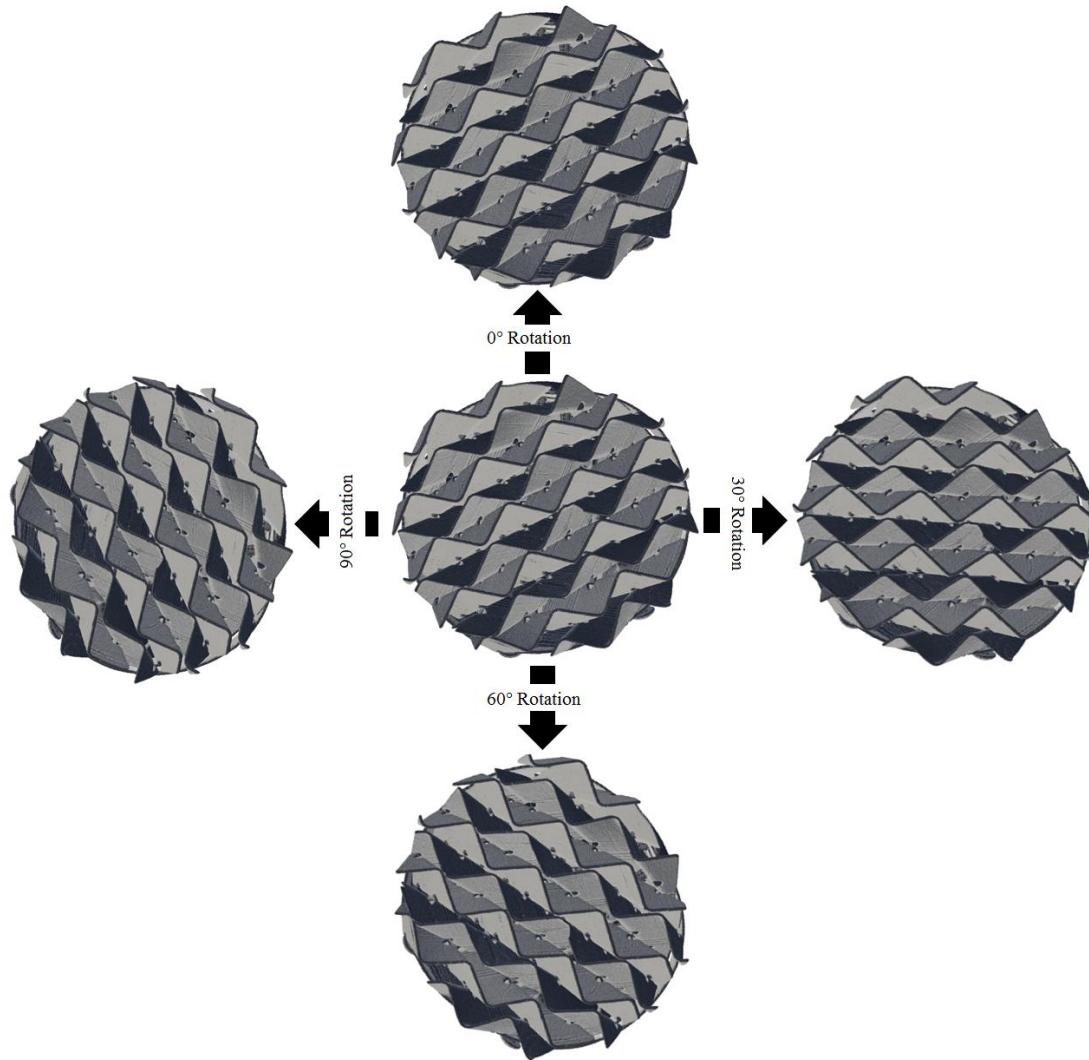


Figure 5-3: Joint rotation angles examined to determine the impact on pressure drop. The central element is the first element viewed from the top. An element shown after an arrow is the view from the top of the second (rotated) element.

F-factors ranging from $0.62 \text{ Pa}^{0.5}$ to $3.05 \text{ Pa}^{0.5}$ (superficial velocities from 0.58-2.85 m/s) were examined with the SST k- ω turbulence model. This turbulence model was chosen for initial studies based on literature recommendations.^{49,55,66} Pressure drop simulation results are summarized in Figure 5-4. At all flow rates, the predicted pressure drop for a joint rotation of 0° is the lowest, and the pressure drop at 90° is the highest. This is to be expected because there is no significant direction change at the joint the flow must overcome when the packing elements have a 0° rotation. The predicted pressure drops between the 30° , 60° , and 90° cases were similar. When compared to the 0° case, the 30° , 60° , and 90° cases had average pressure drops that were 5.8%, 7.3%, and 8.4% greater. On average, the 30° and 90° pressure drops were predicted to be within 3%, leaving little room for an optimization about the joint rotation angle, especially considering the lower degree of mixing that might be present at the joint due to a smaller joint rotation angle.

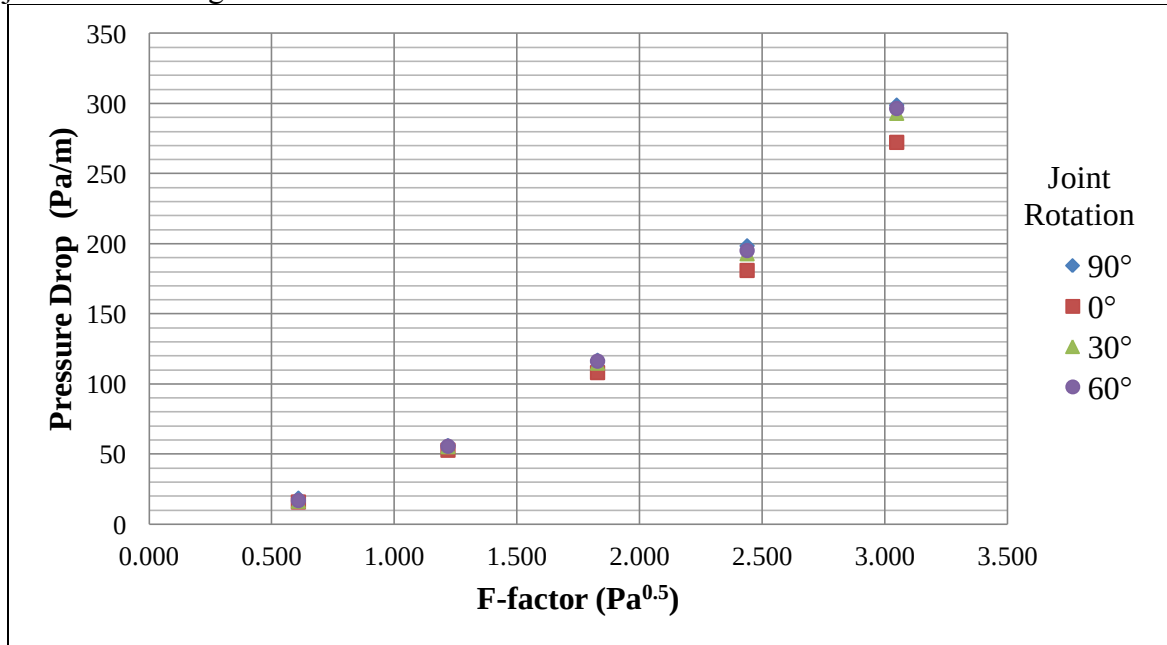


Figure 5-4: Simulated pressure drop through a bed of three Mellapak N250.Y half elements with varying joint rotation angles.

In an effort to explain why the pressure drop was higher with a non-zero joint rotation angle, area-averaged pressure was calculated in 1mm increments through the height of the packing. The results for the 0° and 90° cases are presented in Figure 5-5 for an F-factor of 3.05 Pa^{0.5}. The packing starts at a height of 0mm. Upon the gas entering the packing, pressure drops rapidly, even when compared to the bulk of the packing. In the first 40 mm of the packing pressure drops by 18.9 and 18.8 Pa in the 0° and 90° cases respectively. This 40 mm of length was chosen because it is roughly the height of a repeating unit of packing. The pressure profile in the first element of packing in both cases is very similar. The first element pressure drop is 49.3 and 49.0 Pa in the 0° and 90° cases respectively. From this, the first 40 mm (or 24.5% of the element height) corresponds to 38.3 and 38.4% of the total pressure drop in the first element for the 0° and 90° cases respectively.

After the first joint, the behavior of the two geometries is significantly different. In the 0°, another entrance region is not noticeable based on the pressure drop profile. In the 90° case, another entrance region can be distinguished by the rapid decrease in the pressure immediately following the joint. The pressure drop through the second packed element is 41.2 and 47.8 Pa for the 0° and 90° cases respectively. Following a similar calculation procedure as above, it is found that the first 24.5% of the second element accounts for 11.4 Pa (27.6% total element DP) in the 0° case and 16.7 Pa (34.9% total element DP) in 90° case. Furthermore, this difference in the entrance regions alone accounts for 64.5% of the total pressure drop difference in the second element between the 0° and 90° cases. The final element demonstrates similar behavior to this second element.

Although the total pressure drops between the two cases are similar (130.4 Pa for 0° rotation and 143.1 Pa for 90° rotation), it should be noted that this sort of estimate is

under the best possible conditions. When liquid is introduced, an increase in holdup will be observed immediately above a joint, which is where the rate of pressure drop is at a maximum. The increased liquid holdup will serve to decrease the cross-sectional area available for gas flow, thus increasing pressure drop. This will result in back-mixing of the liquid and premature flooding at the joint.

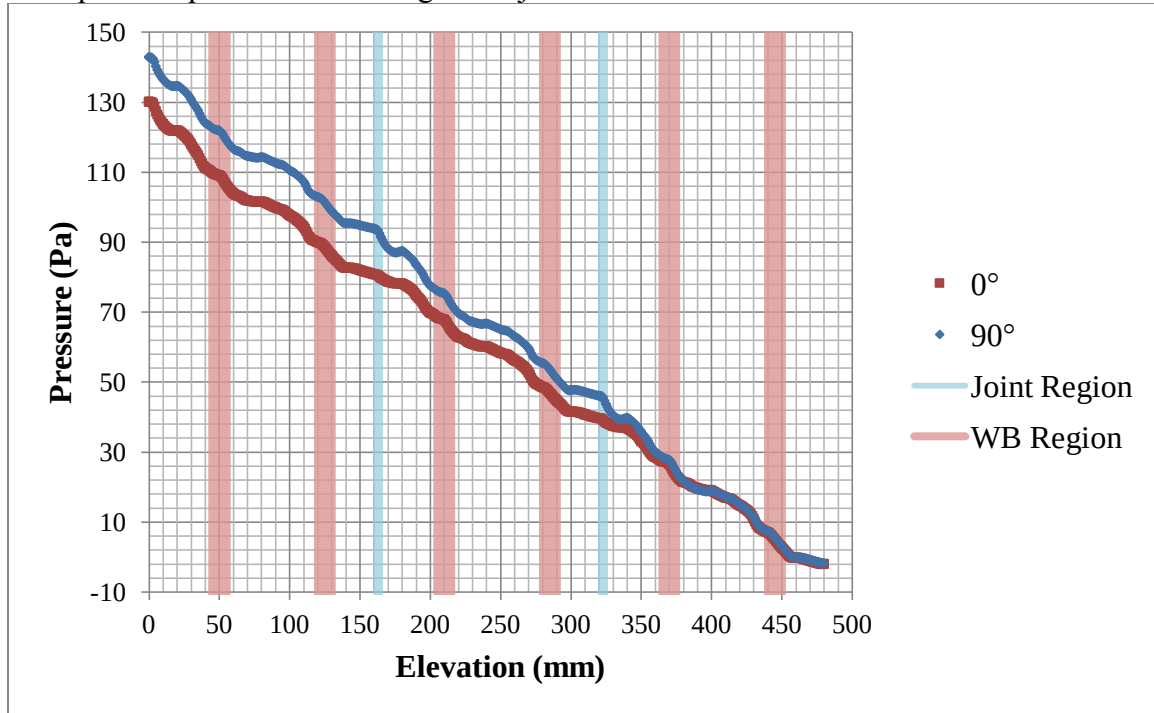


Figure 5-5: Area-weighted pressures for the 0° rotation and 90° rotation cases. F-factor was $3.05 \text{ Pa}^{0.5}$, and simulations were carried out using an SST k- ω . Joints are at 163 and 326 mm. There were two wiper bands per half element located at roughly.

The wiper bands (an example wiper band is indicated in Figure 1-2) also have an observable effect on the pressure in the packing. As the fluid moves past the wiper band (i.e. the regions labeled WB Region in Figure 5-5), it undergoes acceleration due to a decrease in cross sectional area available for gas flow. This causes an increase in pressure drop. Upon passing the wiper bands, the fluid decelerates, and there is a pressure

recovery section, much like the behavior observed for flow through an orifice plate. Figure 5-6 shows a cross section of the pressure map of the middle packing element. In the annular region leading up to the wiper band, the pressure is significantly higher than in the packing itself due to fluid stagnation. Immediately after the wiper bands, pressure drops significantly in the annular region to a level comparable to the packing pressure itself. This constriction and expansion cause significant disturbances in the flow field. When coupled with gas exiting the packing and impacting the column wall (i.e. the fluid undergoes a rapid change in preferred flow direction), zones of recirculation are created in this annular region, increasing total pressure drop through the packed bed.

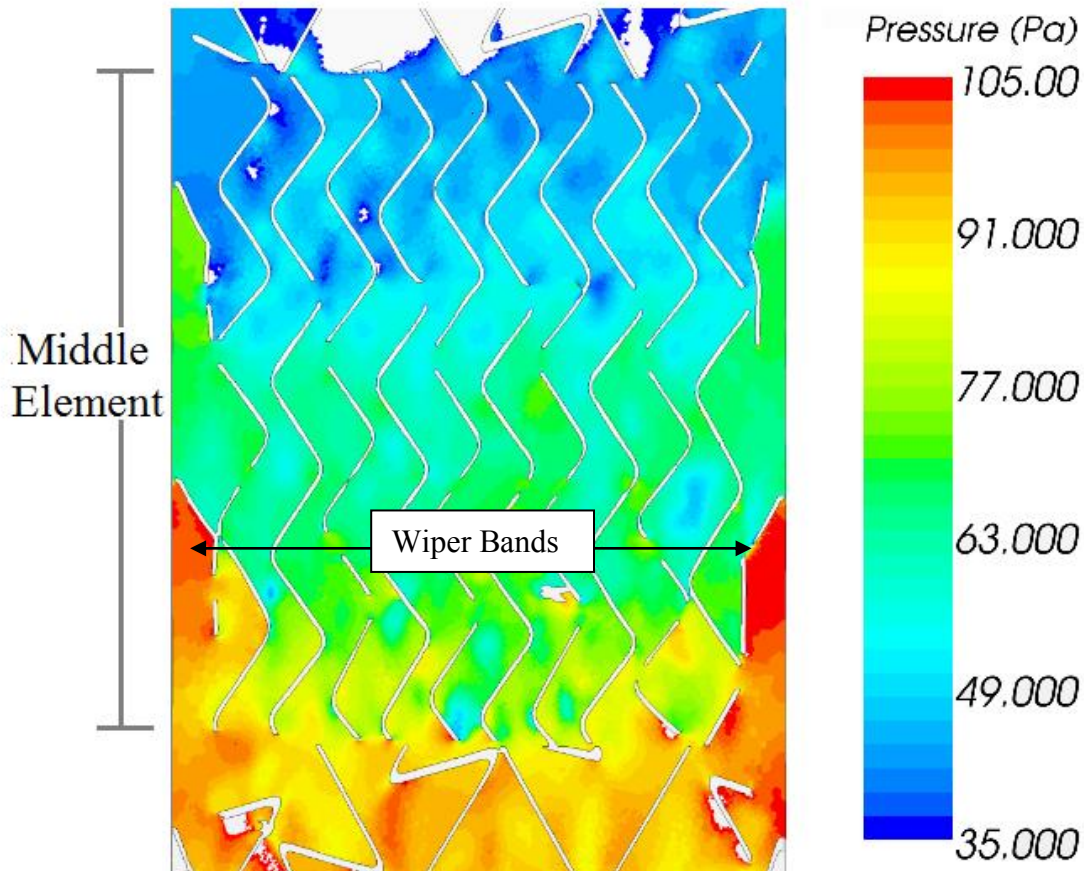


Figure 5-6: Cross-section of middle packing element showing the variation in pressure. Indicated regions are the wiper bands.

The increased pressure drop at the joint for the 30°, 60°, and 90° rotation angles can best be explained by examining the velocity field before and after the joint. In particular, Figure 5-7 shows areas where the z-direction of the velocity is negative at varying heights for the 0° and 90° geometries. The 30° and 60° geometries present behavior similar to the 90° case. Prior to the joint in both cases (i.e. at -5 mm in Figure 5-7), there is very little negative velocity, and it is largely confined to the region near the wall. This is due to vortices being shed and the influence of the wiper bands. Immediately following the joint, negative velocities are present in a large portion of the flow field in the 90° case. These eddies dissipate energy, and cause an increase in pressure drop until they have dissipated within the packing. In the 0° case, the flow channels are aligned from one element of packing to the next. Minimal negative z-velocities are found in the bulk of the packing. Rather, the negative velocities are largely confined to the region near the tube wall.

The 90° and 0° cases were compared to experimental work. The results are summarized in Figure 5-8. CFD predictions for the 0° and 90° joint rotation geometries are an average of 22% and 17% low when compared to the experimental data. If we consider pressure drop at an F-factor of $\sim 2.44 \text{ Pa}^{0.5}$, the difference in pressure drop for the two geometries is 7.7 Pa in the experiments and 8.4 Pa in the simulations. This is a 9.1% difference, indicating the CFD predictions can capture the difference in joint orientation. Sources of further discrepancies include choice of turbulence model and resolution of the boundary layer, which will be discussed in subsequent sections.

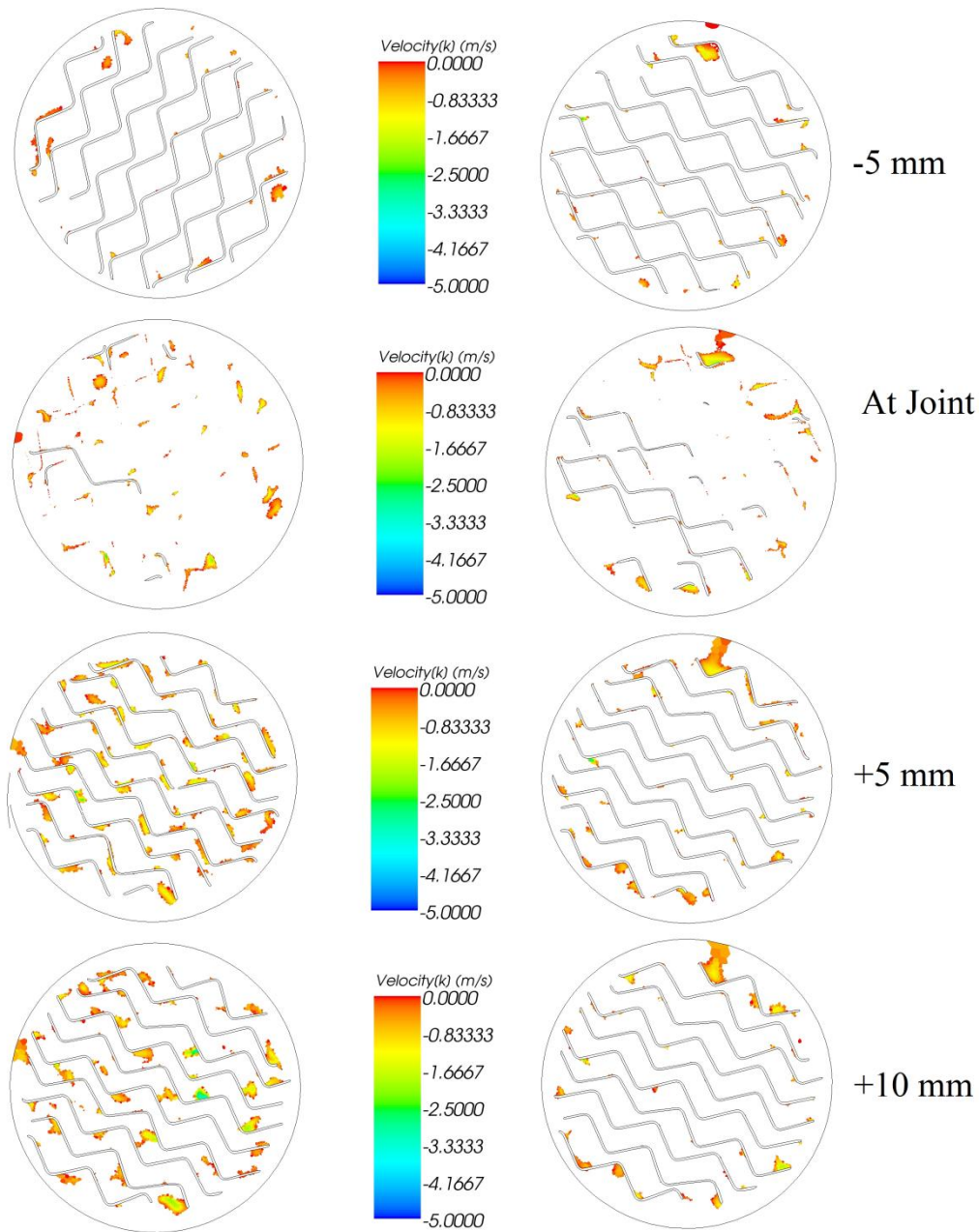


Figure 5-7: Negative z-direction velocities for the 90° (left) and 0° (right) joint rotation cases. Flow rate is an F-factor of $3.05 \text{ Pa}^{0.5}$. Vertical positions are indicated relative to the joint on the right side.

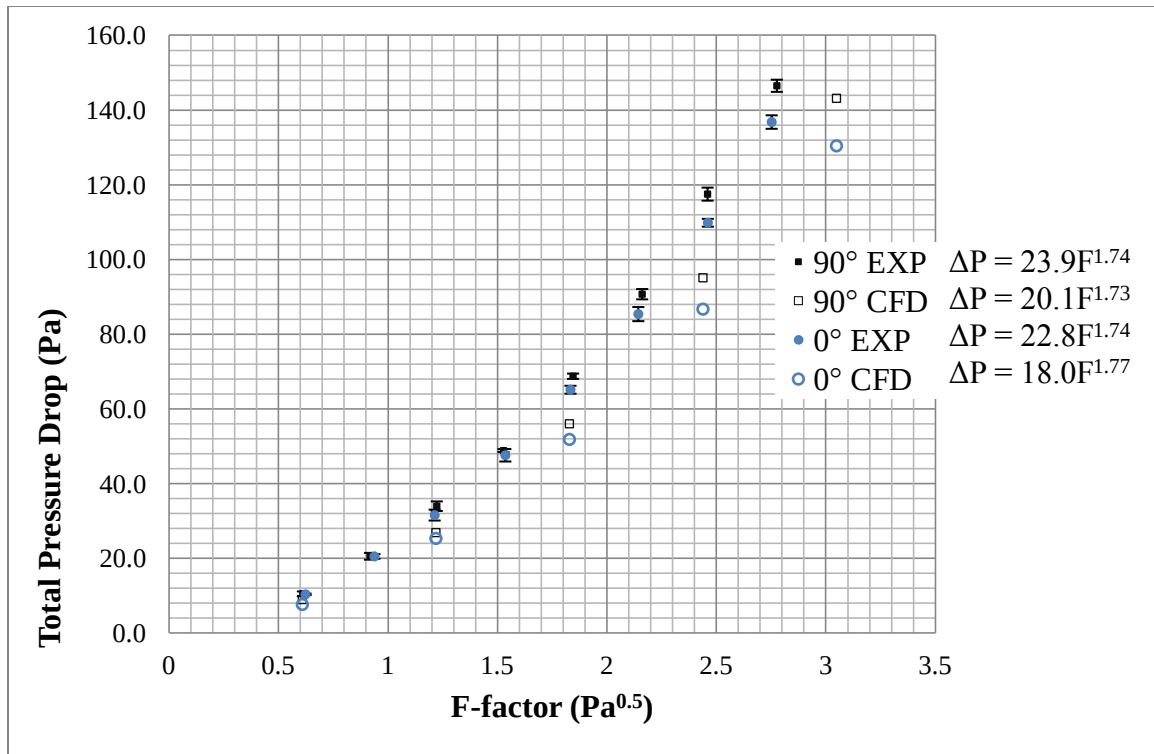


Figure 5-8: Simulated pressure drop vs. experimental pressure drop for the 90° and 0° joint rotation geometries. Error bars indicate 95% confidence interval. Turbulence model used was the SST k- ω model.

TURBULENCE MODEL COMPARISONS

Two turbulence models were compared in the 90° rotation geometry. Specifically, the all y^+ SST k- ω turbulence model and the two-layer realizable k- ϵ turbulence model were examined. Comparisons to experimental results are shown in Figure 5-9. Also shown in Figure 5-9 are predicted pressure drops using the semi-empirical Stichlmair model.⁶⁷ Simulation and semi-empirical predictions are lower than observed experimental pressure drops. However, the CFD predicted pressure drops perform better than the Stichlmair model. In particular, the realizable k- ϵ model had predictions that were 14.8% lower on average. The SST k- ω turbulence model yielded predictions that were 18.3%

low, and the Stichlmair model yielded results that were 30.7% low. The CFD simulations also captured the power law dependence of the pressure drop on the F-factor. The predicted realizable k- ϵ model predicted an exponent of 1.7464. Regressed experimental data showed an exponent of 1.7537. All regressed equations demonstrated R^2 values greater than 0.998.

Stichlmair parameters were taken from the Aspen Plus v7.3 data banks ($C_1=1$, $C_2=3$, $C_3=0.35$, $a_p=250 \text{ m}^2/\text{m}^3$, $\epsilon=0.85$). It should be noted that while the specific area and porosity used in the Stichlmair calculation differs from the vendor-listed values, the coefficients given above were most likely regressed using an $a_p=250 \text{ m}^2/\text{m}^3$ and $\epsilon=0.85$. By doing so, a_p and ϵ are merely additional coefficients used in the semi-empirical model, and they are not necessarily based on actual packing geometry. The Stichlmair model is given by:⁶⁷

$$\begin{aligned} d_p &= \frac{6(1-\epsilon)}{a_p} \\ Re_g &= \frac{d_p U_{SG} \rho_G}{\mu_G} \\ f_0 &= \frac{C_1}{Re_g} + \frac{C_2}{Re_g^{0.5}} + C_3 \\ \Delta P_{dry} &= \frac{3}{4} f_0 \left(1 - \frac{\epsilon}{\epsilon^{4.65}} \right) \rho_G \left(\frac{Z}{d_p} \right) U_{GS}^2 \end{aligned}$$

where U_{GS} is the superficial gas velocity and Z is the total bed height.

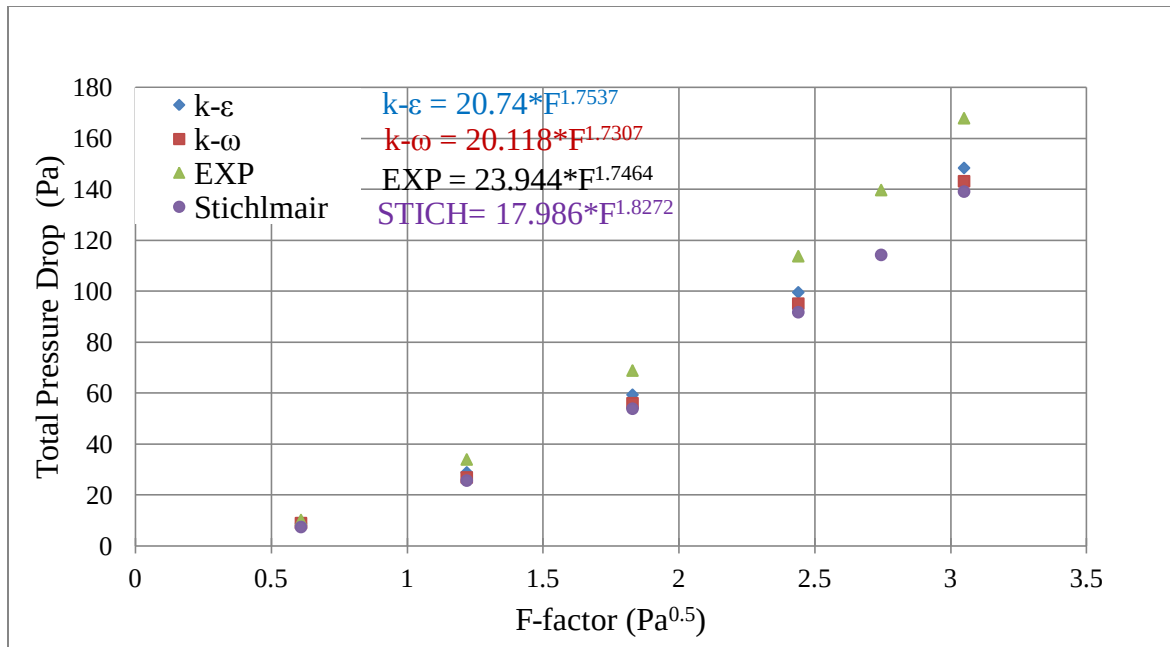


Figure 5-9: Experimental and predicted pressure drops through a bed of packing with a joint rotation angle of 90°.

IMPACT OF A BOUNDARY LAYER MESH

Total column pressure drop can be thought of in terms of three mechanisms. The first is the direction change, which accounts for pressure drop due to regions near the column wall and the joints. This was observed in the prior section. The second mechanism is an interaction between criss-crossing gas streams in the bulk of the packing. This will be considered in a later section. The final mechanism for pressure drop is friction between the gas and the packing surface (or liquid film in the case of countercurrent flow). In an effort to increase simulation accuracy, it was desired to mesh the boundary layer using prism layers. Per the Star-CCM+ user manual, it is necessary to resolve the boundary layer using a prism mesh to achieve accurate results for the skin friction (i.e. wall shear stress).¹⁴

As examining the effects of accurately resolving the boundary layer required many simulations to examine the various parameters available, a smaller, representative geometry was chosen for the bulk of the analysis. Full geometry details are presented in Chapter 3. In short, the geometry consisted of a 35.78 mm section of packing in a 75.07 mm tube. F-factor was set at 3.05 Pa^{0.5}. The realizable k-ε model was used because it proved to be the most accurate model examined for predicting pressure drop. Pressure drop and the skin friction coefficient were monitored as a function of prism layer thickness, stretching ratio, and number of prism layers. The skin friction coefficient is defined as:

$$C_f = \frac{\tau_w}{0.5\rho_{ref}U_{ref}^2} \quad \text{Equation 5-4}$$

where τ_w is the wall shear stress, ρ_{ref} is a reference density (1.0 kg/m³ was used here), and U_{ref} is a reference velocity (1.0 m/s was used in present studies). The necessity of the prism layers is best shown by Figure 5-10, where an example prism layer mesh is shown. By examining the velocity magnitude, it can be observed that the gradients normal to the packing surface are significantly larger than gradients in the wall-tangent direction. The accuracy of the wall shear stress calculation necessarily depends on the accuracy of the flow field and velocity gradients in the near wall region, requiring the use of fine mesh in the wall normal direction to accurately calculate the wall shear stress.

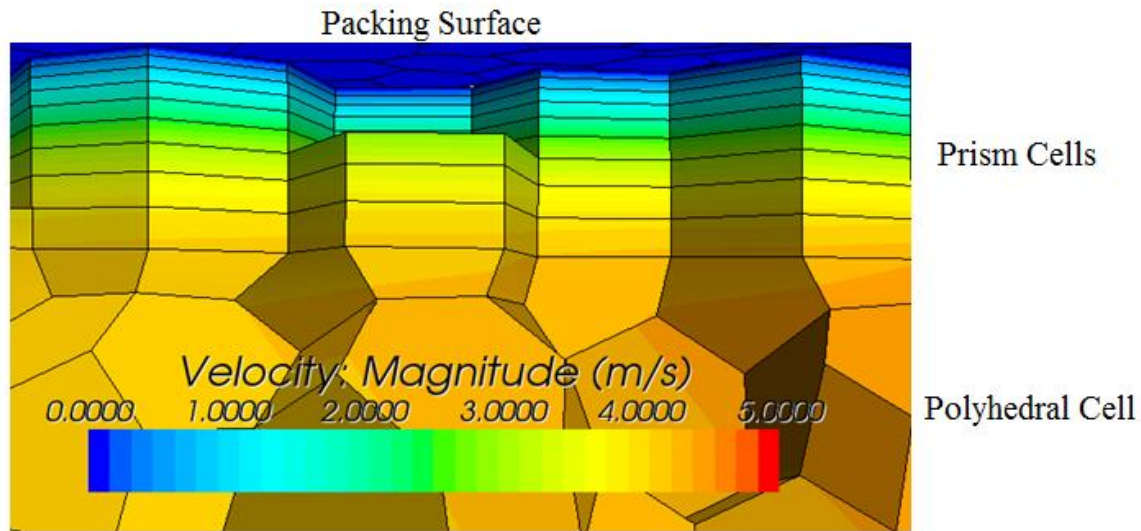


Figure 5-10: Example volume mesh with a prism layer near the wall.

The results of the mesh independence study are shown in Table 5-2. The pressure drop and skin friction coefficient predictions are lowest when only the polyhedral mesher with the Medium mesh settings (Figure A-6) is used. As the number of prism layers increases for a constant prism layer thickness, the average y^+ decreases. As the y^+ value decreases, C_f and the pressure drop increase until $y^+ \leq 1$. Prism layer thickness (0.5 mm vs. 1.0 mm) did not have a significant impact the value of C_f and pressure drop, provided the average y^+ value was low enough. Finally, the prism layer stretching factors examined (1.05 and 1.2) had very little impact on the values of the pressure drop and skin friction coefficient. Increasing the stretching factor further would require additional analysis of the pressure drop and skin friction coefficient. The results shown in Table 5-2 demonstrate that an ~8% increase in pressure drop can be observed by merely ensuring the boundary layer is adequately resolved.

Number of Prism Layers	Prism Layer Thickness (mm)	Pressure Drop (Pa)	Average y^+	C_f	Prism Layer Stretching Factor
0	N/A	11.81	5.2	0.47	1.05
2	0.5	12.27	3.24	0.56	1.05
5	0.5	12.60	1.36	0.62	1.05
9	0.5	12.65	0.70	0.63	1.05
9	0.5	12.71	0.37	0.63	1.2
12	0.5	12.75	0.49	0.64	1.05
12	1	12.84	0.92	0.64	1.05
12	1	12.81	0.37	0.64	1.2

Table 5-2: Impact of prism layer on pressure drop predictions on a small-scale CT geometry at an F-factor of $3.05 \text{ Pa}^{0.5}$ using the two-layer realizable k- ϵ turbulence model. Shaded prism layers were used in the full-scale CT geometry of three half elements.

A simulation at an F-factor of $3.05 \text{ Pa}^{0.5}$ was carried out on the full CT geometry (i.e. 3 half elements of Mellapak N250.Y) using the realizable k- ϵ turbulence model. Results are summarized in Table 5-3. The use of a prism layer mesh increases the pressure drop by 5% when compared to the base polyhedral mesh. This brings the difference between experimental data (predicted from a regressed power law) and the CFD simulations to less than 10%. Future studies on pressure drop should use prism layers to yield a more accurate pressure drop prediction. Additional tuning of skin friction via surface roughness would further enhance the CFD predictions.

Case	Pressure Drop	Experimental Percent Difference (%)
Medium Polyhedral Mesh	148.34	-11.64
Prism Mesh	156.07	-7.03
Extrapolation of Experimental Data	167.87	N/A

Table 5-3: Pressure drop as a function of prism layers in a packed bed of three half-elements at an F-factor of $3.05 \text{ Pa}^{0.5}$. The experimental extrapolation was produced using the power law regression of experimental data shown in Figure 5-9.

WIPER BANDS AND PRESSURE DROP

In columns less than 1 m in diameter, the walls and wiper bands have a noticeable impact on the pressure drop.¹¹ This was observed in the present studies when compared to the work of Owens *et al.*¹⁰ Figure 5-11 shows the different packings used in present studies and those used by Owens *et al.* Present studies used packings with two wiper bands per half element, resulting in increased pressure drop observed experimentally. Experimental comparisons of the total pressure drops are shown in Figure 5-12 for packed beds of equivalent height. Pressure drop for elements with two wiper bands per half element were roughly 35% higher than the elements with one wiper band per half element. Comparisons between experiments and simulations must take care to account for this behavior in small diameter columns. Packing characterization studies undertaken in the lab should also ensure the full details of the packing (including the number of wiper bands per element and element height) are well-documented to ensure fair comparison between packings of different types.

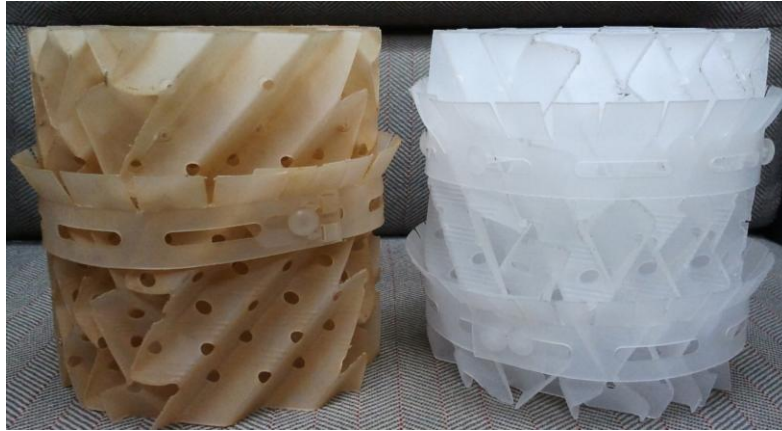


Figure 5-11: Packing used by Owens *et al.* shown at left. Packing used in present studies shown at right. Current studies have two wiper bands per half element. Owens *et al.* used one wiper band per half element.

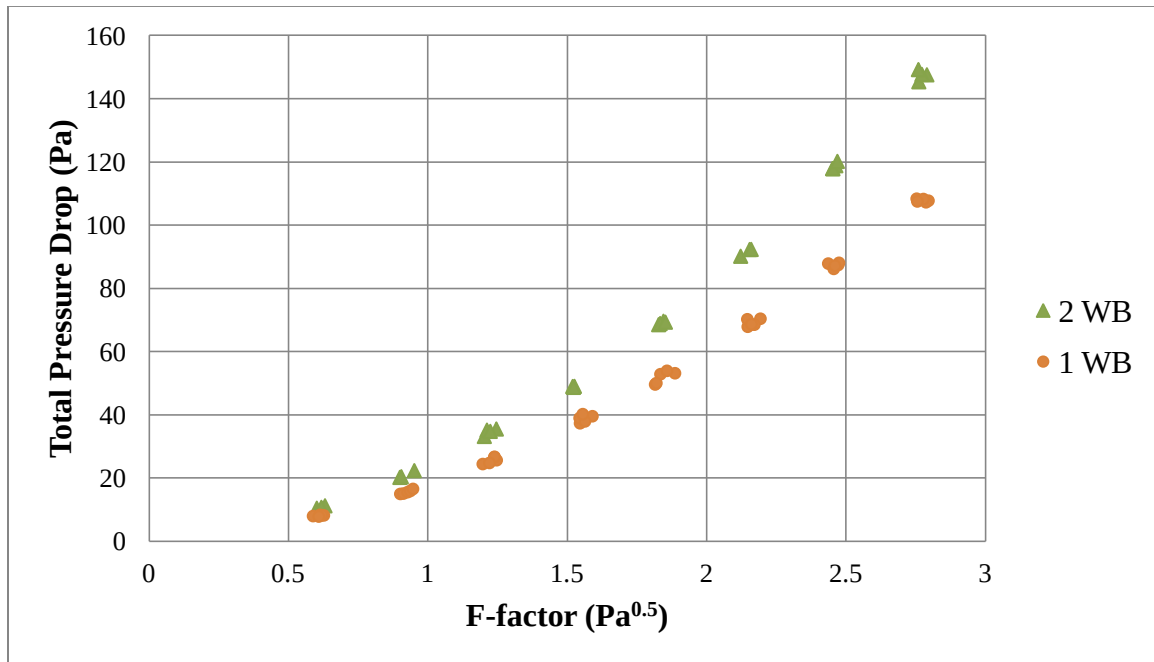


Figure 5-12: Comparisons between two beds of equivalent height of Mellapak N250.Y. One wiper band pressure drop data (1 WB) taken from Owens *et al.*¹⁰

DEVELOPMENT OF PRESSURE DROP MODEL

A large variety of periodic packing geometries was examined in an effort to understand the relevant velocity and length-scales for non-dimensionalization of the

pressure drop. The flow field in the packing was initially considered to be analogous to a mixing (or shear) layer, shown in Figure 5-13. In the turbulent mixing layer, the difference in velocities (i.e. the shear velocity) is the relevant velocity scale for non-dimensionalization.¹⁶ In the case of structured packing, the difference between velocities of gas in criss-crossing channels is given by twice the horizontal gas velocity. For simplicity, only the horizontal velocity is used for scaling:

$$U_{GH} = \frac{U_{GS}}{\epsilon(1-h_L)\tan(\alpha)} \quad \text{Equation 5-5}$$

where U_{GS} is the superficial velocity, ϵ is the packing porosity h_L is the liquid holdup, and α is the corrugation angle (measured from the horizontal). For single phase flow, h_L is 0. All packing parameters are defined in Figure 3-8.

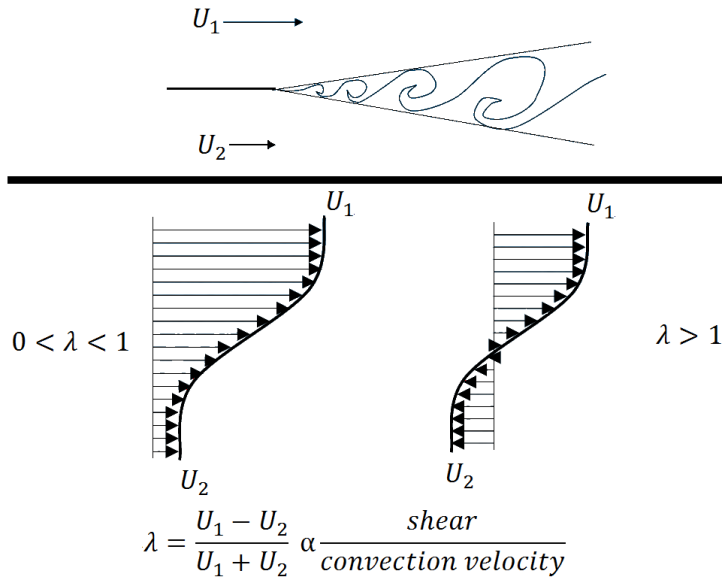


Figure 5-13: Two-dimensional mixing layer.

In the Rocha-Bravo-Fair model, the channel side length, s , is used as a length-scale for the Reynolds number.²³ This allows a Reynolds number based on the horizontal velocity to be written as:

$$Re_{GH} = \frac{\rho_G U_{GH} s}{\mu_G} \quad \text{Equation 5-6}$$

The pressure drop can be computed via analog to pressure drop in a pipe:⁶⁸

$$\frac{\Delta P_{shear}}{\frac{1}{2} \rho_G U_{GH}^2 \left(\frac{L_c}{s} \right)} = f_H \quad \text{Equation 5-7}$$

where ΔP_{shear} is the pressure drop due to the horizontal velocity, f_H is a friction factor that will depend on the horizontal gas Reynolds number, and L_c is the channel length given by:

$$L_c = \frac{h_{ru}}{\sin \alpha} \quad \text{Equation 5-8}$$

where h_{ru} is the height of a repeating unit in structured packing. This non-dimensionalization for a series of packings with packing parameters $b=26.05$ mm, $h=10.53$ mm, and $s=16.75$ mm is shown in Figure 5-14. The pressure drops were computed using the two-layer realizable $k-\epsilon$ turbulence model on periodic geometries. As the corrugation angle α increases, the non dimensionalization performs worse, indicating the pressure drop due to turbulence generated by the horizontal velocity is inadequate to describe the full pressure drop in the packing itself. Thus, it is necessary to account for another mechanism of pressure drop. Specifically, the friction between the gas and packing surface must be taken into account.

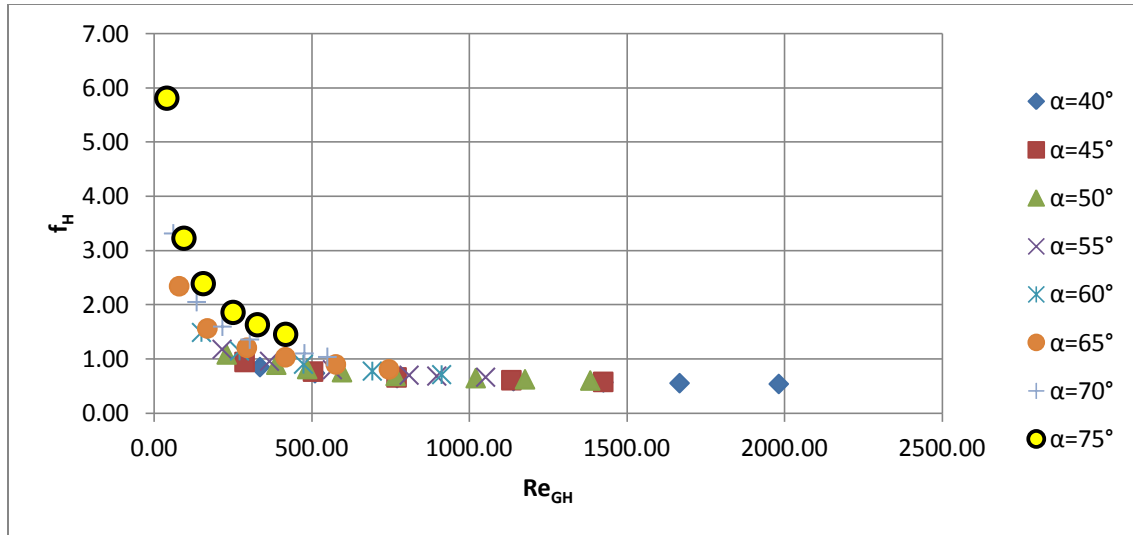


Figure 5-14: Initial non-dimensionalization of the pressure drop using only the horizontal gas velocities. Corrugation angles for each packing examined are given in the legend. All packings examined had packing parameters of $b=26.05$ mm, $h=10.53$ mm, and $s=16.75$ mm.

Pressure Drop due to Friction between the Gas and Packing Surface

To eliminate the effect of the horizontal velocity, flow through vertical channels with a rhomboid cross section were simulated. This would represent a packing with a corrugation angle of 90° . A sample geometry cross-section is shown in Figure 5-15. This cross-section was extruded 20 mm to generate the different vertical channels examined. Table 5-4 summarizes the packing parameters examined in the vertical channel simulations. Pressure drop was imposed across the domain, and simulations were continued until mass flow was converged. The relevant velocity scale chosen for this pressure drop was the effective gas velocity given by:

$$U_{GE} = \frac{U_{GS}}{\epsilon(1-h_L)\sin(\alpha)} \quad \text{Equation 5-9}$$

In the vertical channel simulations, U_{GE} simplifies to U_{GS} . Various length scales were examined, and the most appropriate was determined to be the hydraulic diameter of a rhombus given by:

$$d_{h,rhombus} = \frac{bh}{s} \quad \text{Equation 5-10}$$

As an aside, the hydraulic diameter of these rhombus channels can be related to the packing specific surface area as:

$$a_p = \frac{4s}{bh} = \frac{4}{d_{h,rhombus}} \quad \text{Equation 5-11}$$

in the case of extremely thin sheets (e.g. stainless steel sheets that are ~0.1 mm in thickness). The Reynolds number and friction factor can then be defined by:

$$Re_{G,rhombus} = \frac{\rho_G U_{GE} d_{h,rhombus}}{\mu_G} \quad \text{Equation 5-12}$$

$$\frac{\Delta P_{friction}}{\frac{1}{2} \rho_G U_{GE}^2 \left(\frac{L_c}{d_{h,rhombus}} \right)} = f_E \quad \text{Equation 5-13}$$

where f_E is the friction factor that depends on $Re_{G,rhombus}$. Results of this non-dimensionalization are shown in Figure 5-16. From the plotted data, it can be seen that a power law regression adequately represents the friction factor by:

$$f_E = 5.698 Re_{G,rhombus}^{-0.597} \quad \text{Equation 5-14}$$

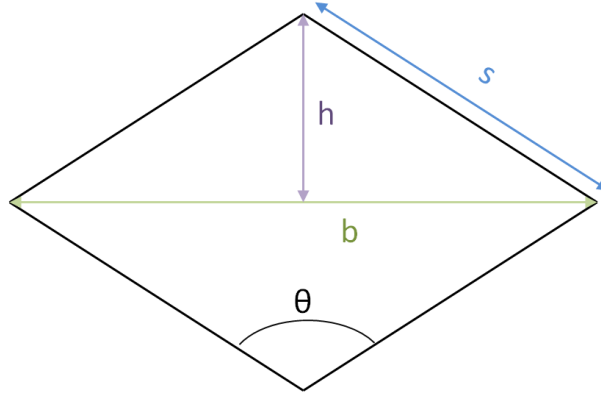


Figure 5-15: Cross-section of vertical channels used to determine pressure drop due to friction of the gas and packing surface.

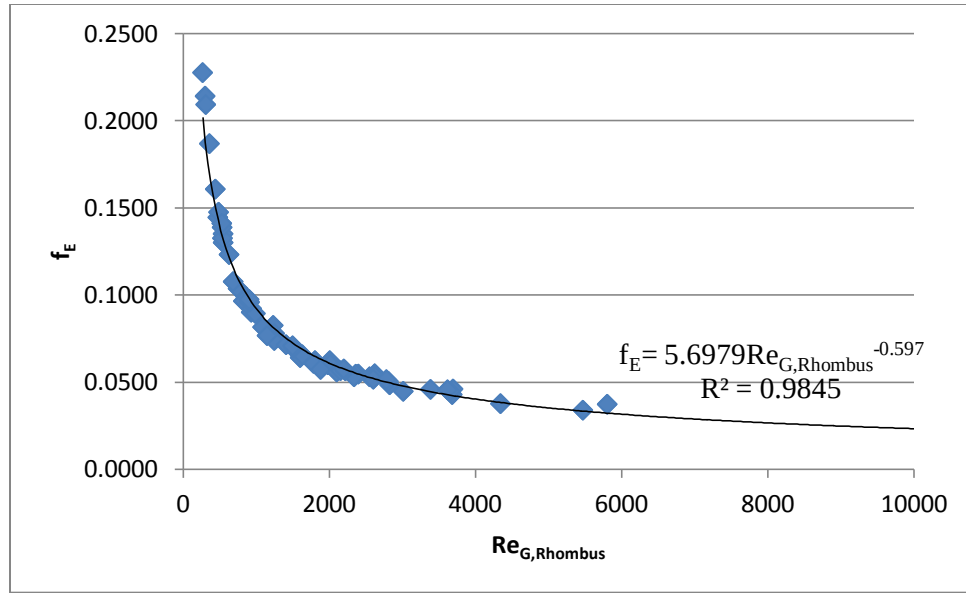


Figure 5-16: Results of non-dimensionalization of pressure drop in vertical channels.

b (mm)	s (mm)	h (mm)	θ (°)
26.1	16.7	10.5	102.1
52.1	33.5	21.1	102.1
13.0	8.4	5.3	102.1
19.5	15.4	11.9	79.0
14.6	16.9	15.3	51.3
16.8	15.6	13.2	65.0
31.6	18.7	10.1	115.0
41.6	22.9	9.7	130.0
21.0	19.6	16.5	65.0
25.1	17.7	12.5	90.0
25.1	48.4	46.8	30.0
21.1	16.7	13.0	77.9
42.1	33.5	26.1	77.9
10.5	8.4	6.5	77.9
23.7	15.4	9.8	101.0
30.5	16.9	7.3	128.7
26.4	15.6	8.4	115.0
20.1	18.7	15.8	65.0
19.4	22.9	20.8	50.0
33.0	19.6	10.5	115.0
25.1	17.7	12.5	90.0
93.5	48.4	12.5	150.0

Table 5-4 Vertical rhombus channel dimensions examined to determine pressure drop due to friction between the gas and packing surface.

Final Model Proposal

Dry pressure drop can now be calculated as the sum of two different contributions. The first is the pressure drop due to friction between the gas and packing surface. The second is the pressure drop due to the horizontal velocity, which will be termed the shear pressure drop. In a periodic element, the total pressure drop is given by:

$$\Delta P_{total} = \Delta P_{friction} + \Delta P_{shear} \quad \text{Equation 5-15}$$

From the CFD simulations, the total pressure drop is known. From Equations 5-14 and 5-13, $\Delta P_{friction}$ can be calculated. Calculating $\Delta P_{shear} = \Delta P_{total} - \Delta P_{friction}$ and non-dimensionalizing as before using Equations 5-6 and 5-7 yields Figure 5-17. The high corrugation angle data now fall on the same line as the other geometries. This improvement comes solely from accounting for the pressure drop due to the gas interacting with the packing surface. Once again, these data are for the channels with packing dimensions $b=26.05$ mm, $h=10.53$ mm, and $s=16.75$ mm.

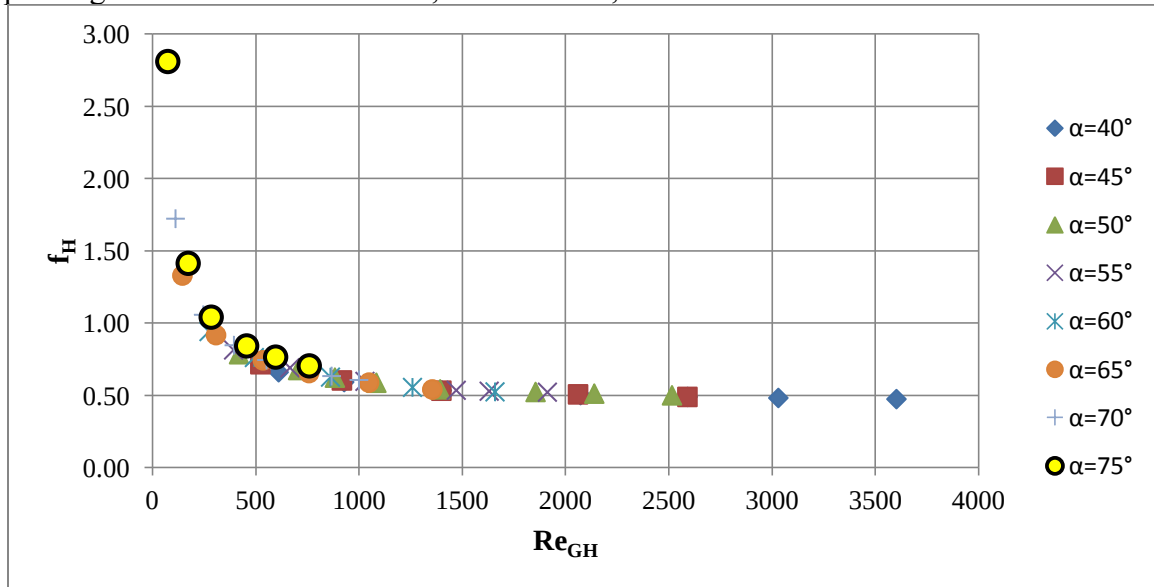


Figure 5-17: Results of the non-dimensionalization of shear pressure drop. Corrugation angles for each packing examined are given in the legend. All packings examined had packing parameters of $b=26.05$ mm, $h=10.53$ mm, and $s=16.75$ mm.

When all packing geometries simulated (geometry details shown in Table 3-6) are included in the non-dimensionalization, Figure 5-18 is generated. The bulk of the data appears to follow a power-law regression. A non-linear least squares regression was performed to yield:

$$f_H = 4.671Re_{GH}^{-0.291} \quad \text{Equation 5-16}$$

This regression yields a percent error of 4.5% on the predicted pressure drop when compared to the CFD results. The maximum percent error is 27.2%. The quality of the fit can be observed in a parity plot shown in Figure 5-19. Fewer than 16% of the model predictions deviate from the CFD simulated pressure drops by more than 10%. Fewer than 7% deviate by more than 20% with the deviations scattered randomly in the geometries examined. This semi-empirical model accurately predicts CFD pressure drops for a wide range of packing geometries. Specific surface areas range from 122 to 650 m^2/m^3 , corrugation angles range from 40° to 75° , and the channel opening angle from 30° to 150° .

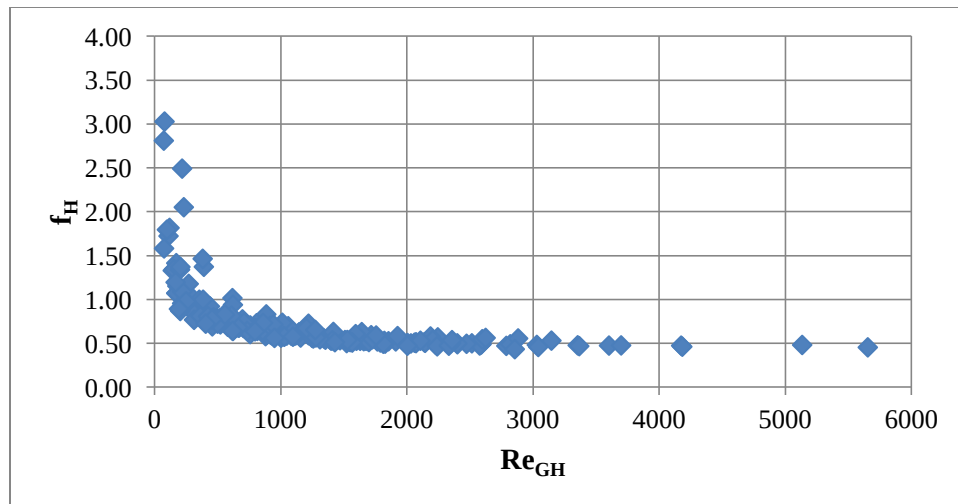


Figure 5-18: Non-dimensionalization of the shear pressure drop for all periodic geometries examined.

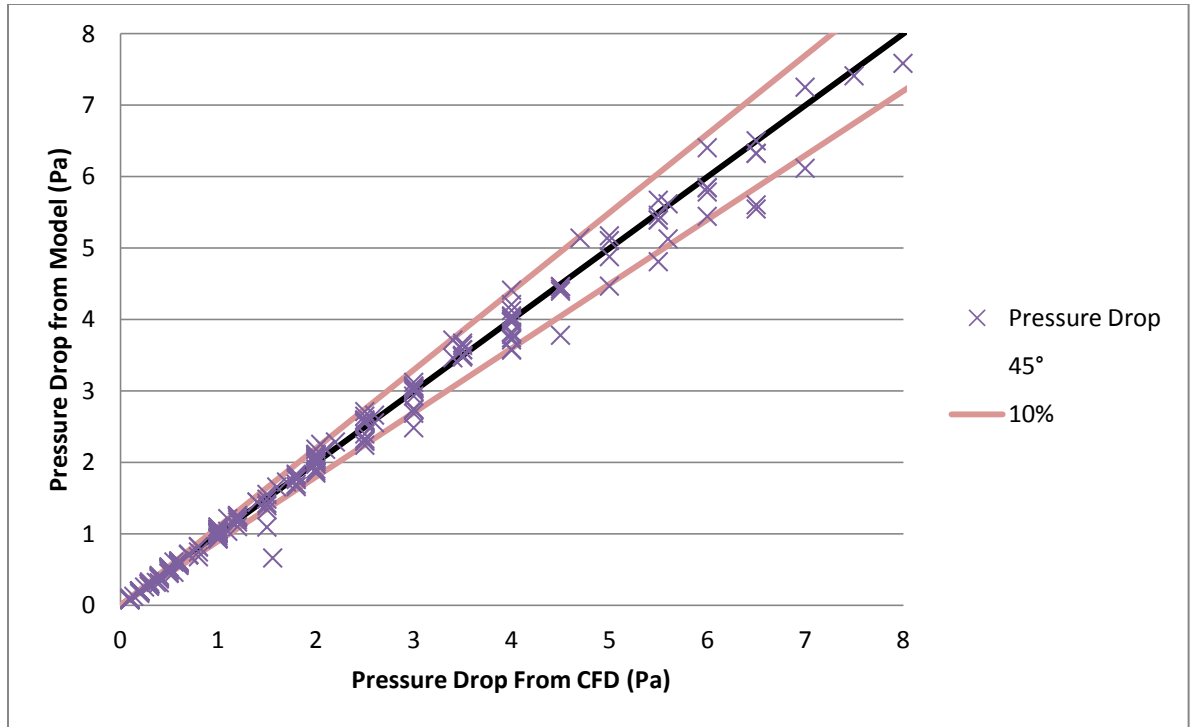


Figure 5-19: Comparison of simulated pressure drop vs. predicted pressure drop from the proposed non-dimensionalization.

It should be noted that while the choice of the channel side length, s , at the beginning was arbitrary, it proved to be the most appropriate channel dimension to use for the non-dimensionalization of the shear pressure drop. The pressure drop per unit height can be written by dividing by h_{ru} :

$$\left(\frac{\Delta P}{\Delta z}\right)_{dry} = \left[\left(\frac{\rho_G U_{GE}^2}{2}\right) \frac{f_E}{d_{h,rhombus}} + \left(\frac{\rho_G U_{GH}^2}{2}\right) \frac{f_H}{s} \right] \frac{1}{\sin \alpha} \quad \text{Equation 5-17}$$

$$f_H = 4.671 \text{Re}_{GH}^{-0.291}$$

$$f_E = 5.698 \text{Re}_{G,rhombus}^{-0.597}$$

To ensure the non-dimensionalization was correct, simulations of water and nitrogen were carried out on a geometry with $b=26.05$ mm, $h=10.53$ mm, $s=16.75$ mm, and $\alpha=50^\circ$. Results are presented in Figure 5-20. The data points fall directly on top of

each other, indicating the effect of fluid properties has been captured correctly by the proposed model.

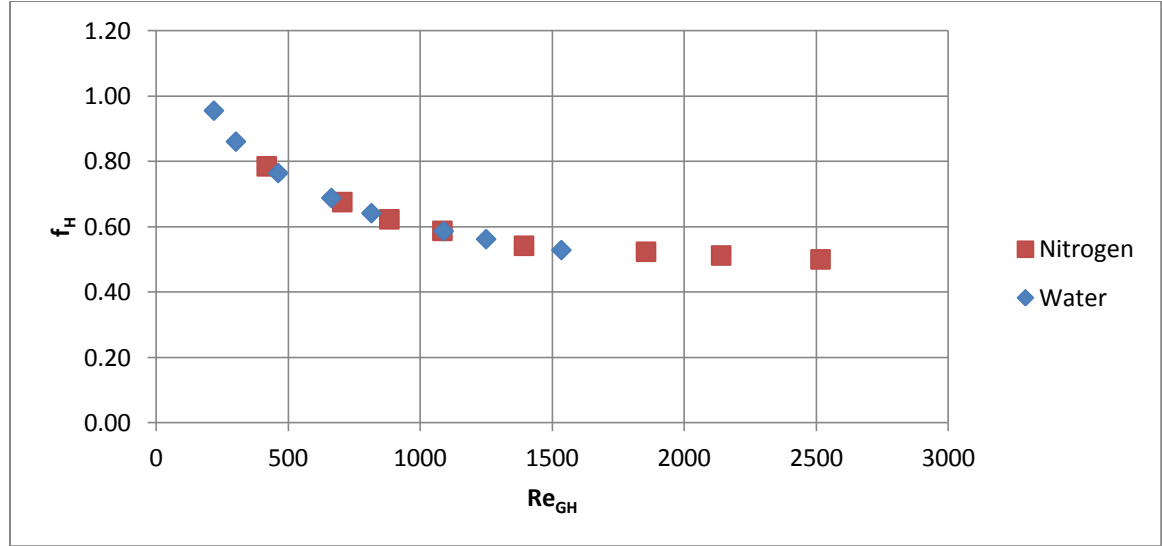


Figure 5-20: Comparisons between water and nitrogen using the proposed non-dimensionalization.

Packing Analysis

Using Equation 5-17, it is possible to examine the impact of a wide-variety of packing parameters on total pressure drop. It should be noted that there are three degrees of freedom when dealing with structured packing geometry. For the following studies, α and a_p were always chosen as independent variables. The third variable was either the packing channel height, h , or the channel opening angle, θ . Packing specific area was chosen as an independent variable because it is directly related to material costs. Channel corrugation angle was a natural choice for an easy-to-manipulate variable in structured packings (e.g. Mellapak 250.Y at $\alpha=45^\circ$ vs. Mellapak 250.X at $\alpha=60^\circ$). Packing channel height or channel opening angle were chosen mainly due to convenience in the geometric formulation.

Figure 5-21 shows the impact of varying the channel height h while holding the packing specific area and corrugation angle constant at $250 \text{ m}^2/\text{m}^3$ and 45° . Nitrogen properties were used with $\rho_G = 1.14527 \text{ kg/m}^3$ and $\mu_G = 1.78837 \cdot 10^{-5} \text{ Pa}\cdot\text{s}$. Superficial gas velocity was set at $U_{GS} = 1 \text{ m/s}$. As channel height varies from 9 mm to 20 mm, the shear pressure drop and the total pressure drop undergo a maximum near $h=11.3 \text{ mm}$. The friction pressure drop remains flat as the rhombus hydraulic diameter and effective gas velocity do not vary. Shear pressure drop varies from 73% of the total pressure drop at $h=20 \text{ mm}$ to 80% of the total pressure drop at $h=11.3 \text{ mm}$.

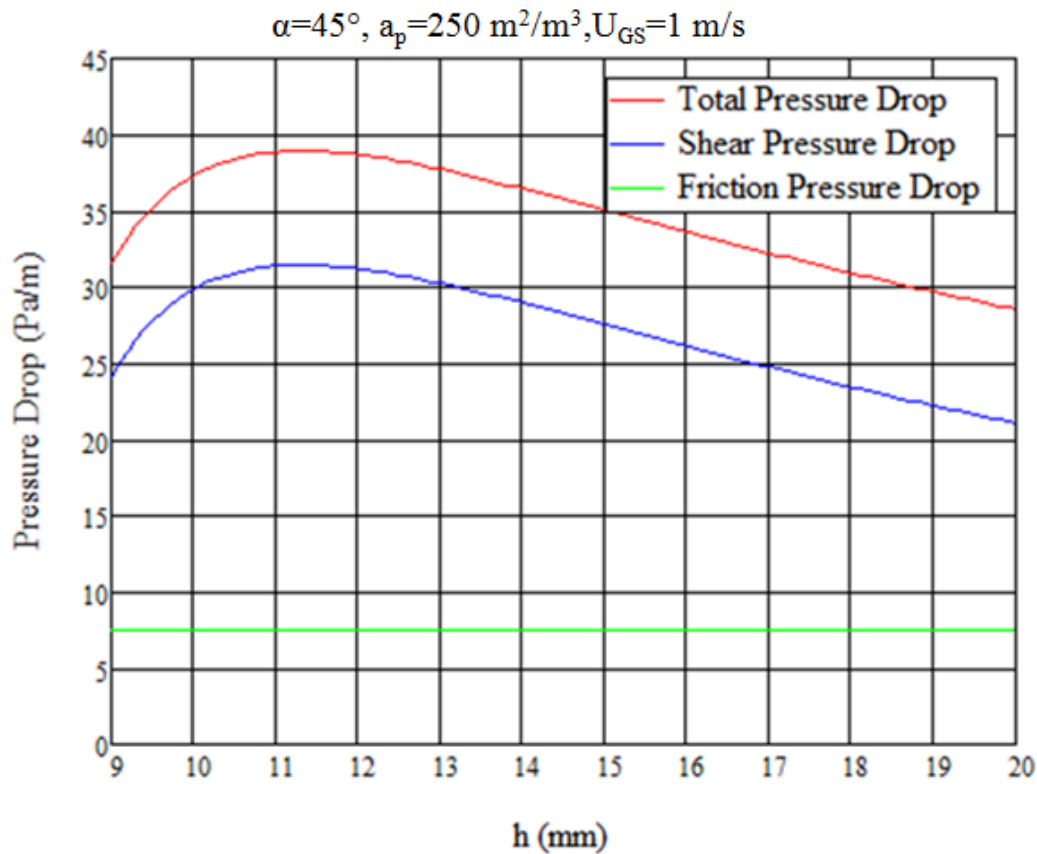


Figure 5-21: Pressure drop in a hypothetical packing as a function of the channel height, h , with constant corrugation angle and packing specific area. Superficial gas velocity was 1 m/s.

Figure 5-22 plots the pressure drop in a hypothetical packing ($\alpha=45^\circ$, $a_p=250 \text{ m}^2/\text{m}^3$) as a function of the channel opening angle, θ . As with the channel height, there is a maximum pressure drop. This is achieved at $\theta \sim 90^\circ$. This opening angle also happens to be what Mellapak, Flexipac, and Gempak type structured packings use for a channel opening angle.¹ Based on the CFD simulations, the pressure drop of these packings is actually being maximized. Thus, it should be possible to decrease column pressure drop by utilizing a different channel opening angle.

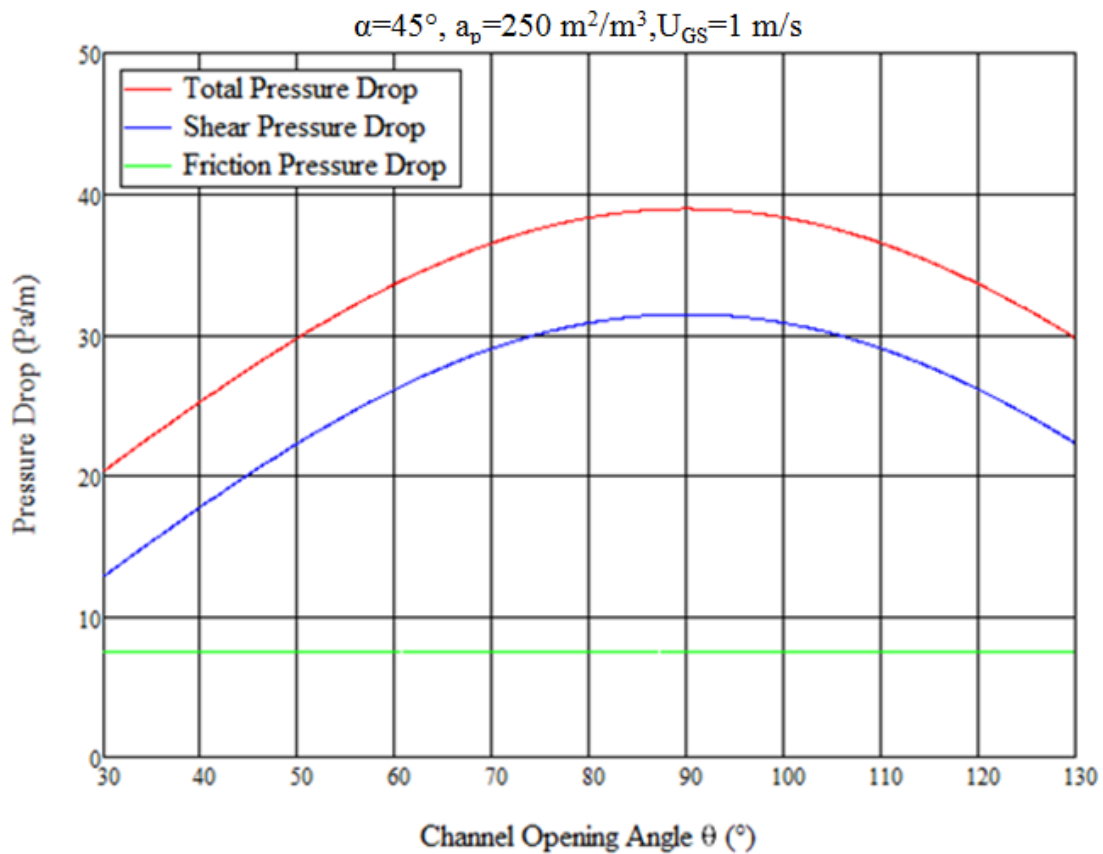


Figure 5-22: Pressure drop in a hypothetical packing as a function of the channel opening angle, θ with constant channel corrugation angle and packing specific area. Superficial gas velocity was 1 m/s.

Figure 5-23 shows the impact of increasing the channel corrugation angle. As expected, as corrugation angle increases, total pressure drop decreases for a constant superficial velocity. This effect is caused largely by the reduction in the horizontal velocity. The effective velocity also decreases with increasing corrugation angle, leading to a reduction in the friction pressure drop as well. At a corrugation angle of 40° , the shear pressure drop accounts for 83% of the total pressure drop in the packing. At a corrugation angle of 75° , the shear pressure drop only accounts for 40.7% of the total pressure drop.

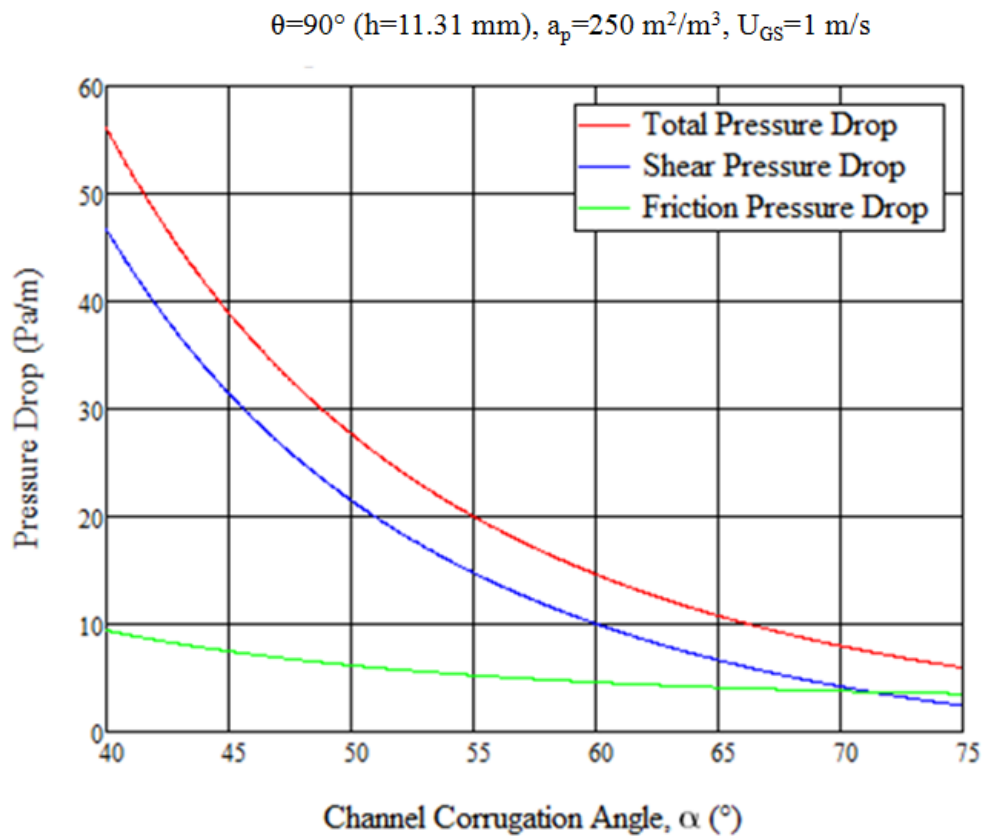


Figure 5-23: Pressure drop in a hypothetical packing as a function of the packing corrugation angle, α , with constant channel opening angle and specific surface area. Superficial gas velocity was 1 m/s.

Figure 5-24 shows pressure drop as a function of increasing packing specific area. Channel corrugation angle and channel opening angle were held constant at 45° and 90° respectively. As packing specific area increases, total pressure drop increases. The friction pressure drop becomes slightly more important as a_p increases. At $a_p=125 \text{ m}^2/\text{m}^3$, the shear pressure drop accounts for 83.9% of total pressure drop. At $a_p=250 \text{ m}^2/\text{m}^3$, the shear pressure drop accounts for 80.8% of total pressure drop.

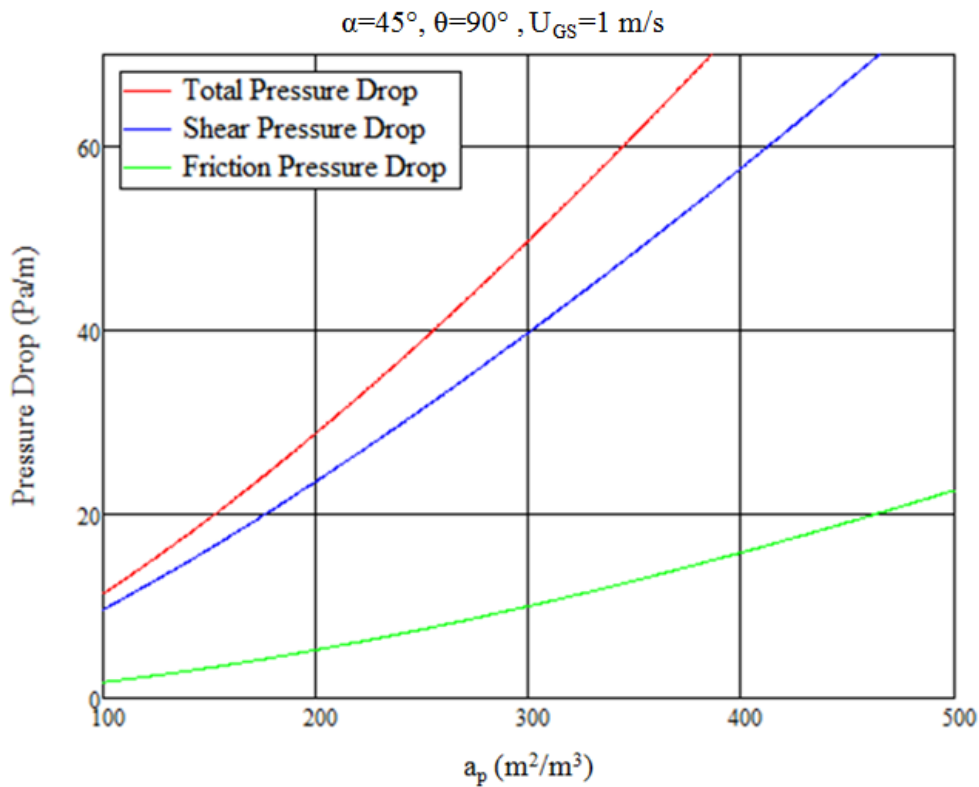


Figure 5-24: Pressure drop in a hypothetical packing as a function of the packing specific area, a_p , with constant corrugation angle and channel opening angle. Superficial gas velocity was 1 m/s.

Functional Comparison to Semi-Empirical Models

The Delft and Rocha-Bravo-Fair models were used for comparison to the current proposed model for functional similarities. Simplifying the equations of the Delft model for dry pressure drop and neglecting pressure drop due to the joints and column wall yields:²³

$$\begin{aligned}\Delta P_{dry} &= (\zeta_{GL} + \zeta_{GG}) \frac{\rho_G U_{GE}^2}{2} \\ \zeta_{GL} &= \psi \xi_{GL} \frac{h_{pb}}{d_{hG} \sin(\alpha)} \\ \xi_{GL} &= \left\{ -2 \log \left[\frac{\left(\frac{k_i}{d_{hG}} \right)}{3.7} - \frac{5.02}{Re_{Ge}} \log \left(\frac{\left(\frac{k_i}{d_{hG}} \right)}{3.7} + \frac{14.5}{Re_{Ge}} \right) \right] \right\}^{-2} \\ \zeta_{GG} &= (1 - \psi) \xi_{GG} \frac{h_{pb}}{d_{hG} \sin(\alpha)} = (1 - \psi) 0.722 (\cos \alpha)^{3.14} \frac{h_{pb}}{d_{hG} \sin(\alpha)} \\ d_{hG} &= \frac{2bh}{b+2s} \\ \psi &= \frac{2s}{b+2s} \\ Re_{Ge} &= \frac{\rho_G U_{GE} d_{hG}}{\mu_G}\end{aligned}$$

where k_i is the roughness of the packing surface, h_{pb} is the packed bed height, d_{hG} is the hydraulic diameter of the triangular channels, and ψ is the fraction of the cross-section of the triangular channel occupied by the packing surface. Substituting in the expressions for d_{hG} and ψ yields:

$$\begin{aligned}\zeta_{GL} &= \xi_{GL} \frac{h_{pb}}{\sin(\alpha)} \frac{s}{bh} \\ \zeta_{GG} &= 0.722 (\cos \alpha)^{3.14} \frac{h_{pb}}{\sin(\alpha)} \frac{1}{2h} \\ \Delta P_{dry} &= \left[\xi_{GL} \frac{s}{b} + \frac{0.722}{2} (\cos \alpha)^{3.14} \right] \frac{\rho_G U_{GE}^2}{2} \frac{h_{pb}}{\sin(\alpha)h} \\ &= \left[\xi_{GL} \frac{1}{d_{h,rhombus}} \left(\frac{\rho_G U_{GE}^2}{2} \right) + \frac{0.722}{2h} (\cos \alpha)^{1.14} \left(\frac{\rho_G U_{GH}^2}{2} \right) \right] \frac{h_{pb}}{\sin(\alpha)}\end{aligned}$$

Dividing by h_{pb} :

$$\left(\frac{\Delta P}{\Delta z} \right)_{dry} = \left[\frac{\xi_{GL}}{d_{h,rhombus}} \left(\frac{\rho_G U_{GE}^2}{2} \right) + \frac{0.722}{2h} (\cos \alpha)^{1.14} \left(\frac{\rho_G U_{GH}^2}{2} \right) \right] \frac{1}{\sin(\alpha)}$$

For a given roughness (k_i), ξ_{GL} can be adequately represented by a power law function yielding:

$$\left(\frac{\Delta P}{\Delta z}\right)_{dry} = \left[\frac{C_1 Re_{Ge}^{n_1}}{d_{h,rhombus}} \left(\frac{\rho_G U_{GE}^2}{2} \right) + \frac{0.722}{2h} (\cos \alpha)^{1.14} \left(\frac{\rho_G U_{GH}^2}{2} \right) \right] \frac{1}{\sin(\alpha)}$$

for $k_i=0$, $C_1 = 0.543$ and $n_1 = -0.314$ for $Re_{Ge} < 11000$. Rewriting the above yields:

$$\begin{aligned} \left(\frac{\Delta P}{\Delta z}\right)_{dry} &= \left[\frac{f_{E,Delft}}{d_{h,rhombus}} \left(\frac{\rho_G U_{GE}^2}{2} \right) + \frac{f_{H,Delft}}{s} \left(\frac{\rho_G U_{GH}^2}{2} \right) \right] \frac{1}{\sin(\alpha)} \quad \text{Equation 5-18} \\ f_{H,Delft} &= \frac{0.722}{2h} (\cos \alpha)^{1.14} \\ f_{E,Delft} &= \left(\frac{d_{hG}}{d_{h,rhombus}} \right)^{n_1} C_1 Re_{G,rhombus}^{n_1} \end{aligned}$$

$f_{H,Delft}$ accounts for the gas-gas interaction in the Delft model, and $f_{E,Delft}$ accounts for the gas-liquid/solid interaction in the Delft model. The Rocha-Bravo-Fair (RBF) model for dry pressure drop is given by:²³

$$\begin{aligned} \left(\frac{\Delta P}{\Delta z}\right)_{dry} &= f \left(\frac{\rho_G}{s} \right) (U_{GE})^2 \\ f &= A + \frac{B}{(Re_{GS})} \\ Re_{GS} &= \frac{\rho_G U_{GS} s}{\mu_G} \end{aligned}$$

where A and B are packing specific constants needed to calculate the friction factor.

Substituting f into the model equation and substituting in velocity terms yields:

$$\left(\frac{\Delta P}{\Delta z}\right)_{dry} = \left[A + \frac{B}{\epsilon \sin \alpha} \left(\frac{bh}{s^2} \right) \left(\frac{1}{Re_{G,rhombus}} \right) \right] \left(\frac{\rho_G}{s} \right) (U_{GE})^2$$

As B is a packing specific constant, and the constants arranged near B are also packing specific constants, it's convenient to write:

$$\left(\frac{\Delta P}{\Delta z}\right)_{dry} = \left[A + \frac{B}{\epsilon \sin \alpha} \left(\frac{bh}{s^2} \right) \left(\frac{1}{Re_{G,rhombus}} \right) \right] \left(\frac{\rho_G}{s} \right) (U_{GE})^2$$

This model is similar to a porous media approximation. Specifically, it is analogous to the Darcy-Forcheimer law. The term involving A is meant to represent inertial effects and the term involving B is meant to represent viscous effects. The RBF model can be rewritten as:

$$\left(\frac{\Delta P}{\Delta z}\right)_{dry} = \left[\frac{2A}{s(\cos \alpha)^2} \left(\frac{\rho_G U_{GH}^2}{2} \right) + \left(\frac{2\tilde{B}}{s} \right) Re_{G,rhombus}^{-1} \left(\frac{\rho_G U_{GE}^2}{2} \right) \right]$$

$$\begin{aligned}
&= \left[\frac{f_{H,RBF}}{s} \left(\frac{\rho_G U_{GH}^2}{2} \right) + \frac{f_{E,RBF}}{d_{h,rhombus}} \left(\frac{\rho_G U_{GE}^2}{2} \right) \right] \frac{1}{\sin(\alpha)} \quad \text{Equation 5-19} \\
f_{H,RBF} &= \frac{2A \sin \alpha}{(\cos \alpha)^2} \\
f_{E,RBF} &= \left(\frac{2B}{\epsilon} \left(\frac{bh}{s^2} \right)^2 \right) Re_{G,rhombus}^{-1}
\end{aligned}$$

Table 5-5 summarizes the results of these transformations. In all cases, the pressure drop due to friction between the gas and packing surface (f_E) share a power law functional dependence. All depend on the fluid properties and the packing dimensions. The gas-gas interaction, however, differs significantly between the CFD-derived model and the two semi-empirical models. Namely, the CFD-derived model depends on packing dimensions, the gas flow rate, and the fluid properties. The two semi-empirical models only depend on the packing type/dimensions. In other words, the two semi-empirical models are assuming a fully turbulent flow regime where the friction factor due to the horizontal gas velocity no longer depends on the horizontal Reynolds numbers. When compared to the proposed model derived from CFD (Equation 5-17), assuming a constant value for f_H would fail to predict pressure drops at low values of the horizontal Reynolds number (i.e. Re_{GH}) as shown in Figure 5-17. This failure of the RBF and Delft model would thus be most pronounced in packings where the channel corrugation angles are high, thus reducing the horizontal component of the gas velocity.

It is possible to simplify the proposed model based on CFD predictions to a functional form more closely resembling the semi-empirical models. Namely, as Re_{GH} increases, f_H approaches an asymptote as shown in Figure 5-17. Using this knowledge, and limiting the data set to $Re_{GH} > 500$ and regressing the data with a constant value for f_H yields:

$$\left(\frac{\Delta P}{\Delta z}\right)_{\text{dry}} = \left[\left(\frac{\rho_G U_{GE}^2}{2} \right) \frac{f_{E,500}}{d_{h,rhombus}} + \left(\frac{\rho_G U_{GH}^2}{2} \right) \frac{f_{H,500}}{s} \right] \frac{1}{\sin \alpha} \quad \text{Equation 5-20}$$

$$f_{H,500} = 0.5075$$

$$f_{E,500} = 28.073 Re_{G,rhombus}^{-0.775}$$

where the friction factors have the forms indicated above. The average percent error is 5.79% with a maximum absolute percent error of 17.84%. A parity plot showing the comparison between Equation 5-20 and the CFD data is shown in Figure 5-25. The CFD data is only for $Re_{GH} > 500$. By doing this, the gas-gas interaction friction becomes a constant, similar to the Rocha-Bravo-Fair and Delft models. However, like the semi-empirical models, this simplification would not be able to adequately predict pressure drops when the Reynolds number based on the horizontal gas velocity (Re_{GH}) is low. In the case of low Re_{GH} , the assumption of a constant gas-gas interaction friction factor, f_H , fails.

Model	Gas-Gas Interaction (f_H)	Functional Dependence	Gas-Solid Friction Factor (f_E)	Functional Dependence
CFD-Derived	$4.671 Re_{GH}^{-0.291}$	Fluid properties, packing dimensions, and flow rate	$5.698 Re_{G,rhombus}^{-0.597}$	Fluid properties, packing dimensions, and flow rate
Delft	$\frac{0.722 s}{2h} (\cos \alpha)^{1.14}$	Packing dimensions	$\left(\frac{d_{hG}}{d_{h,rhombus}} \right)^{n_1} C_1 Re_{G,rhombus}^{n_1}$	Fluid properties, packing dimensions, and flow rate
RBF	$\frac{2A \sin \alpha}{(\cos \alpha)^2}$	Packing type and dimensions	$\left(\frac{2B}{\epsilon} \left(\frac{bh}{s^2} \right)^2 \right) Re_{G,rhombus}^{-1}$	Fluid properties, packing dimensions, and flow rate

Table 5-5: Summary of functional forms of friction factors between CFD- derived pressure drop model and two semi-empirical models.

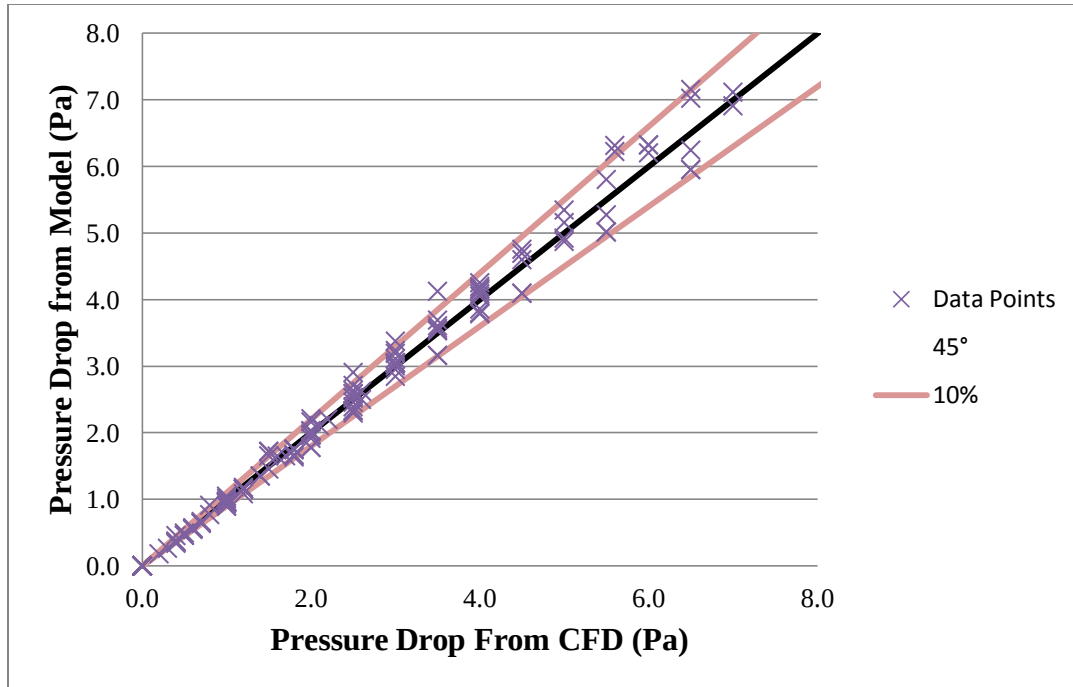


Figure 5-25: Parity plot showing calculated CFD pressure drops vs. model predictions of asymptotic model (i.e. a constant value of f_H) generated with $Re_{GH} > 500$.

One other key difference between the Delft model and the CFD-derived model is the influence of packing geometry. Namely, as the channel opening angle increases beyond 90° (i.e. h/b reduced below 0.5), the Delft model shows an increase in pressure drop as shown in Figure 5-26.²⁶ The CFD predictions indicated a maximum pressure drop at a channel opening angle of 90° ($h/b=0.5$), with pressure drop per unit height decreasing when the channel opening angle was reduced or increased. This difference in behavior between the two models cannot be rectified and possibly indicates a failure in the Delft model at capturing the relevant physics.

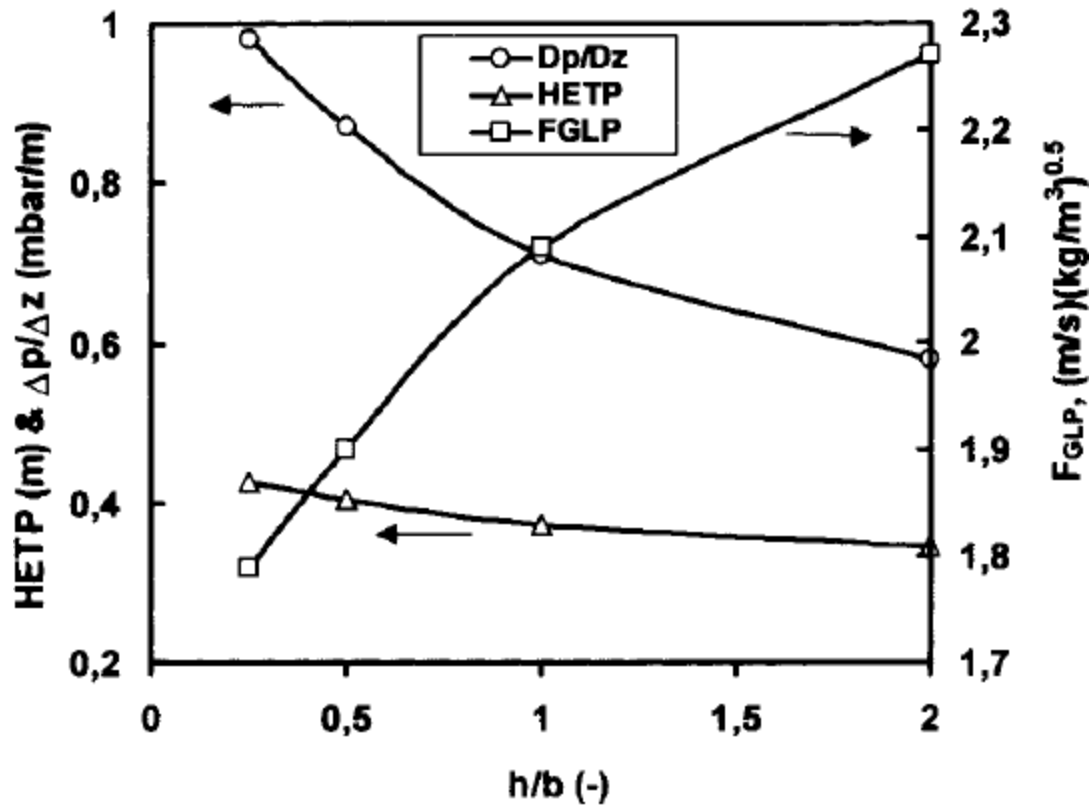


Figure 5-26: Impact of changing the channel height-to-base on structured packing performance in the Delft model. Figure taken from Olujić *et al.*²⁶

Turbulence Model Comparisons

Several different geometries were examined using both the SST $k-\omega$ and realizable $k-\epsilon$ turbulence models. For convenience, the subset from Table 3-6 is shown again here in Table 5-6. Packing designation is used to describe the geometries in figures shown below. It is coded by the values of relevant packing parameters separated by a hyphen. Specifically, the packing designation is packing specific area-channel corrugation angle-channel opening angle (i.e. $a_p-\alpha-\theta$).

Packing Designation	α °	h_{ru} mm	b mm	s mm	h mm	θ °	a_p m ² /m ³
650-45-30	45.00	9.00	6.36	12.41	12.00	30.0	650
650-70-30	70.00	18.62	6.37	12.41	12.00	30.0	650
650-45-150	45.00	33.61	23.77	12.30	3.18	150.0	650
650-70-150	70.00	69.49	23.77	12.30	3.18	150.0	650
500-45-90	45.00	16.00	11.31	8.00	5.66	90.0	500
192-60-120	60.00	83.17	41.57	24.00	12.00	120.0	192

Table 5-6: Packing examined with different turbulence models. Blue shaded packings were used in LES simulations in addition to the SST k- ω and realizable k- ϵ turbulence models.

Figure 5-27 shows the effect of turbulence model on predicted F-factors for the 650-45-150 and 650-70-150 geometries. The three turbulence models give similar results at all pressure drops examined. The predicted F-factors using the SST k- ω are an average of 2.5% higher than the realizable k- ϵ for the 650-45-150 packing. Predicted F-factors are 1.7% higher for the 650-70-150 packing. When compared to the LES, the realizable k- ϵ model performs best. The predicted LES F-factor is 1.36% lower than the realizable k- ϵ prediction.

Figure 5-28 shows the effect of turbulence model on predicted F-factors for the 650-45-30 and 650-70-30 packings. The SST k- ω predicts greater F-factors (or lowest pressure drops) on both geometries. Predicted F-factors using the SST k- ω are 9.5% and 3.4% higher than the realizable k- ϵ turbulence model for the 650-45-30 and 650-45-70 geometries respectively. The realizable k- ϵ again matches the LES predictions with the F-factor predicted via LES being 7.4% lower than the realizable k- ϵ prediction.

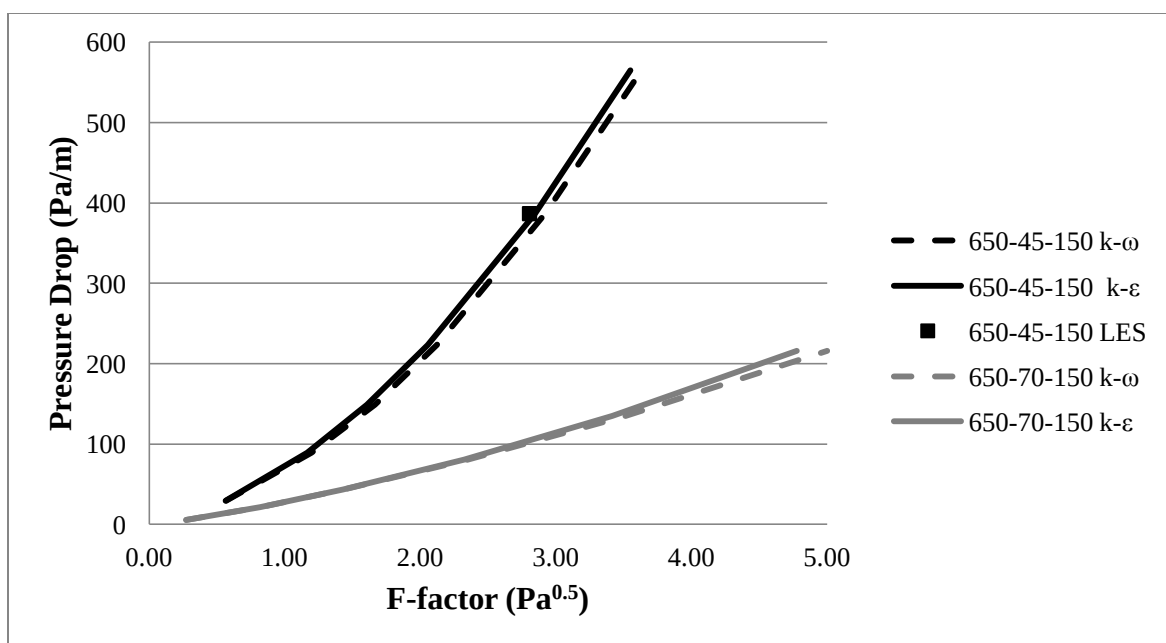


Figure 5-27: Effect of turbulence model choice on calculated flow rates for packings designated by 650-45-150 and 650-70-150.

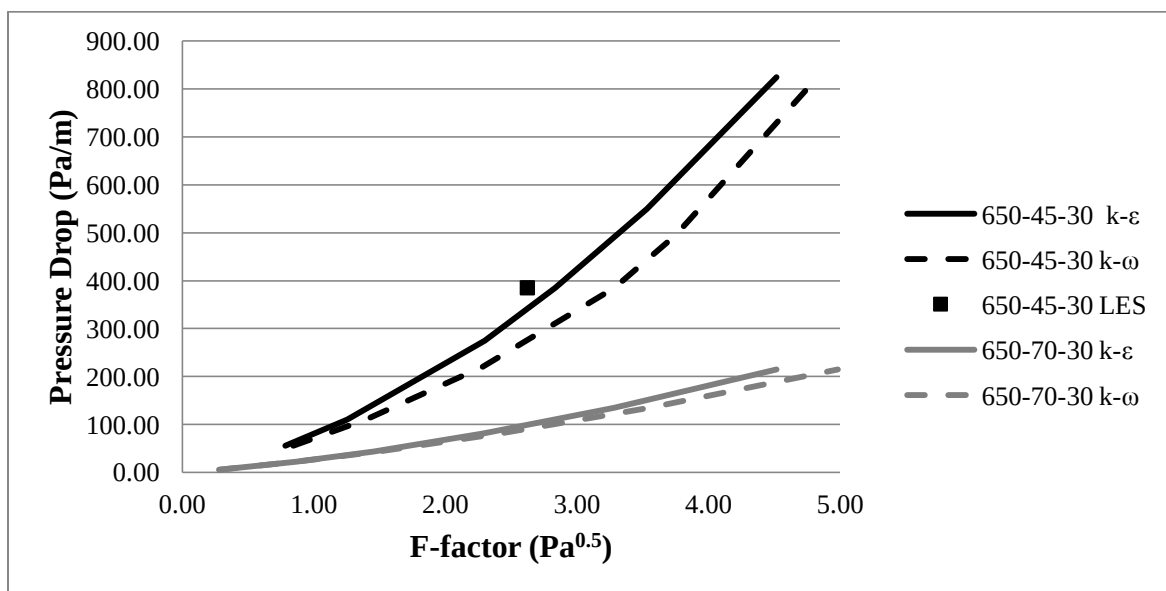


Figure 5-28: Effect of turbulence model choice on calculated flow rates for packings designated by 650-45-30 and 650-70-30.

Figure 5-29 shows the effects of turbulence model choice on the 500-45-90 packing. The SST $k-\omega$ once again predicts the highest F-factor for a given pressure drop. On average, predicted F-factors are 14.6% greater than the realizable $k-\epsilon$ model. The LES prediction is closest the realizable $k-\epsilon$. The LES predicted F-factor is 10.0% lower when compared to the realizable $k-\epsilon$ model.

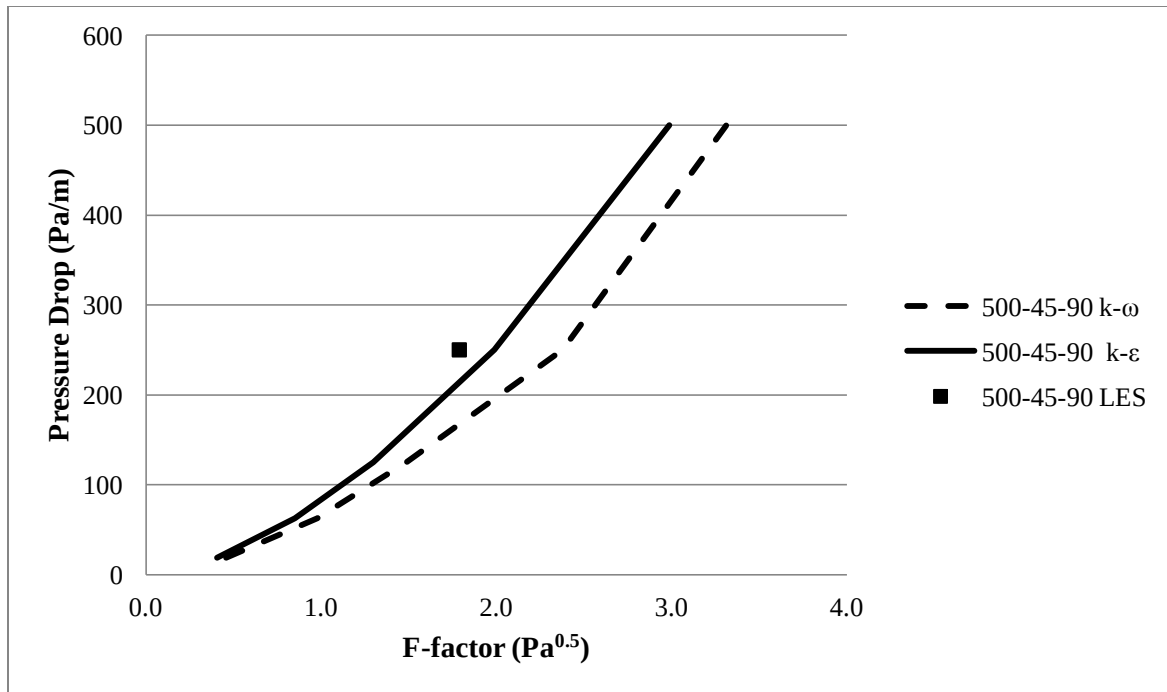


Figure 5-29: Effect of turbulence model choice on calculated flow rates for packings designated by 500-45-90.

From the above figures, we can conclude that the SST $k-\omega$ model predicts higher F-factors for a given pressure drop when compared to the realizable $k-\epsilon$ model. In other words, for a given flow rate, the SST $k-\omega$ model will yield a lower pressure drop per unit height. When compared to the LES simulations, the realizable $k-\epsilon$ model matched most

closely. For the geometries examined, the LES model yielded the highest pressure drop per unit height at a given flow rate.

Effect of Geometry and Flow Field

In an effort to understand why pressure drop depends on the geometry, the velocity field was examined in three geometries using LES simulations. The three geometries are designated: 650-45-30, 500-45-90, and 650-45-150. In the first set of images shown in Figure 5-30, the flow field observed at the top of the periodic element is shown. When comparing the 650-45-30 and 500-45-90 geometries, key differences in the velocity field can be observed. Most noticeable is the size of the vortex present. In the 650-45-30 geometry, the vortex is confined to the center of the channel. Toward the sharp apexes of the rhombus, core regions of gas flow in the preferred flow direction (i.e. 45° from the horizontal). From the top of the packing, the preferred flow directions are toward the observer and to the right (top apex) and toward the observer and to the left (bottom apex). In the case of the 500-45-90 geometry, the vortex is not confined by narrow channel walls and influences the entire velocity field. This behavior would maximize the shear pressure drop (and thus the total pressure drop), as seen in Figure 5-22 at the channel opening angle of 90° .

The behavior of the ultra-wide channel opening angle geometry (650-45-150) is more complex and varies significantly with time. The large central swirl observed in the other two geometries is not persistent in the 650-45-150 geometry. At $t=0.041470s$, the velocity is largely directed toward the observer and to the right. At $t=0.061352s$, the velocity is largely directed toward the observer and to the left. The two channels are so narrow that neither is capable of generating significant flow along the corrugation angle. Rather, the mixing layer where the horizontal velocities are in direct competition with is

spread from the top vertex to the bottom vertex. This region is unpredictable, and the horizontal velocities take turns “winning” the observed flow direction.

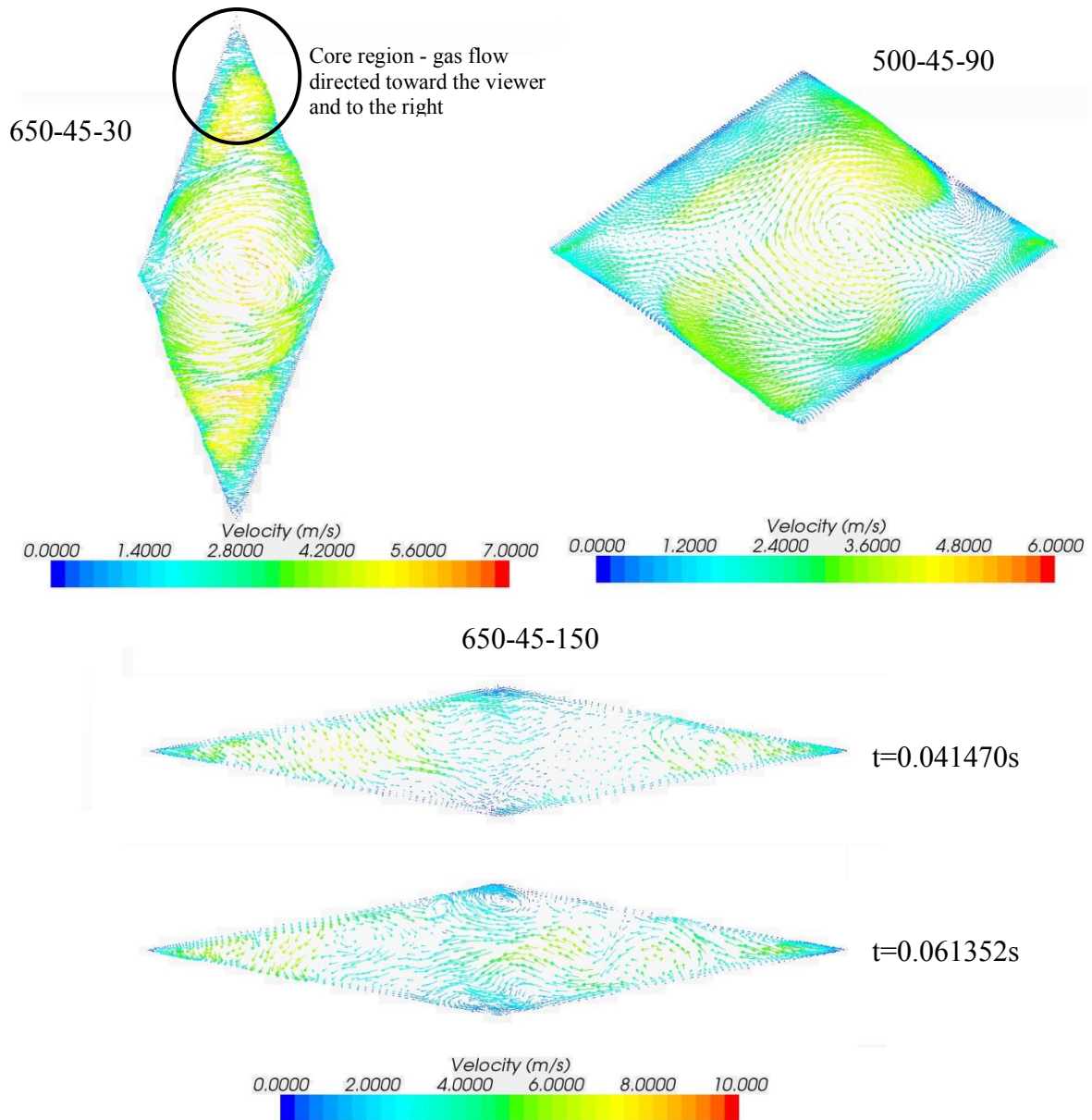


Figure 5-30: Velocity field at the top of the packing element. Top left is geometry 650-45-30. Top right is 500-45-90. Bottom is 650-45-150 at 0.04147s and 0.066552s.

In the second set of figures, a view perpendicular to the preferred flow direction is shown. Figure 5-31 shows the way this view was generated.

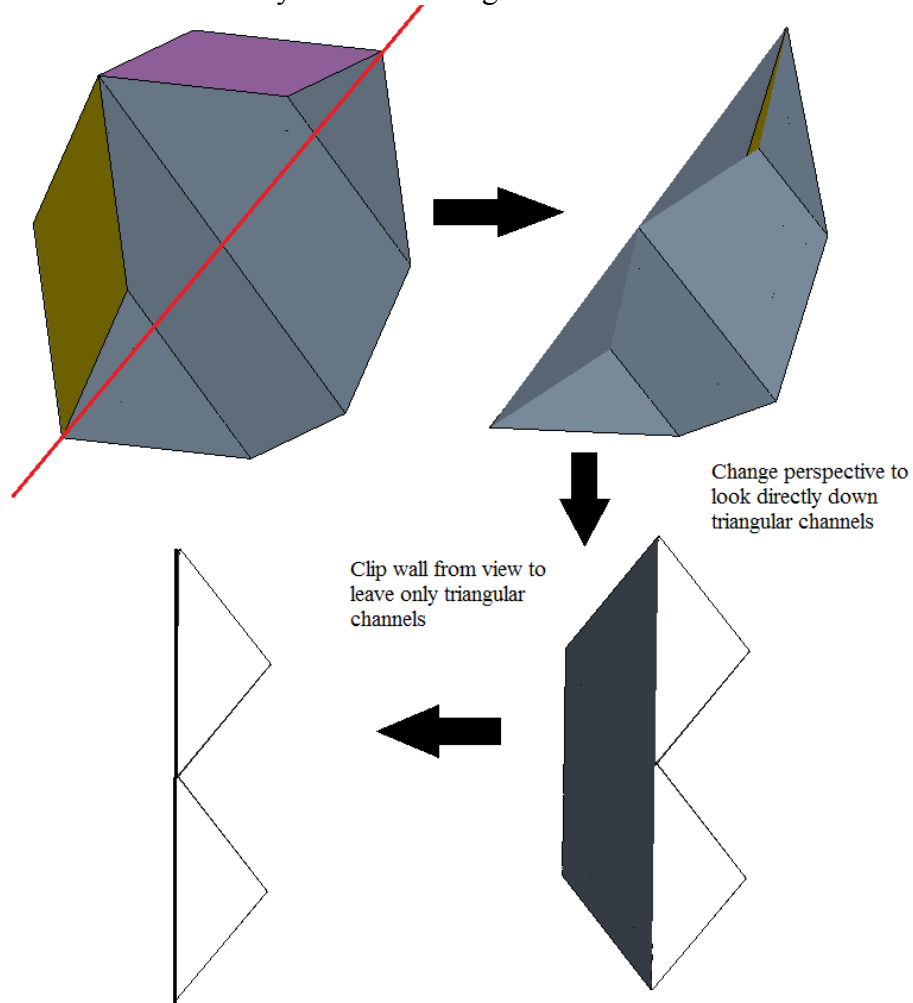


Figure 5-31: Perpendicular view to the preferred flow direction of one set of triangular channels.

Figure 5-32 shows a comparison of the three different geometries. When comparing the 650-45-30 and 500-45-90 geometries, key differences in the flow field can again be observed. Namely, the sharp channels of the 650-45-30 confine the size of the

vortex present. This allows a portion of gas flow near the triangular point to be directed directly at the observer, and consequently in the preferred flow direction along the corrugation angle. This portion of gas appears to be largely unaffected by the vortices generated by the interaction of intersecting gas jets flowing up the opposite channel. This helps to reduce the impact of the shear pressure drop. In the 500-45-90 geometry, the vortex is present in the entire gas channel, which would explain the maximized pressure drop observed in Figure 5-22 at the channel opening angle of 90°. In both the 650-45-30 and 500-45-90 geometries, the observed flow fields are average in that the vortices and flow behavior do not deviate significantly with time.

The 650-45-150 geometry was too tall to show a snapshot of both channels in one figure with adequate resolution of the velocity vectors. Thus, only one channel is shown. There was strong transient behavior observed, so two snapshots are shown for two different times. At $t=0.040940s$, the velocity direction is not directed at the viewer, indicating flow is not directed through the packing parallel to the corrugation angle (i.e. in the preferred flow direction). At $t=0.061352s$, the flow is directed toward the viewer, indicating the flow at that point in time is directed along the corrugation angle. This is best explained by how “flat” the triangular channels produced by this geometry are. Persistent vortices cannot be generated due to the geometry configuration. Rather, the entire channel is dominated by the mixing layer generated between the two sheets.

To examine this mixing region where the horizontal velocities are in direct competition, the x-velocities in a central vertical plane were examined. Figure 5-33 shows the plane that was cut from the packing. In this case, the x-velocity is the horizontal gas velocity present.

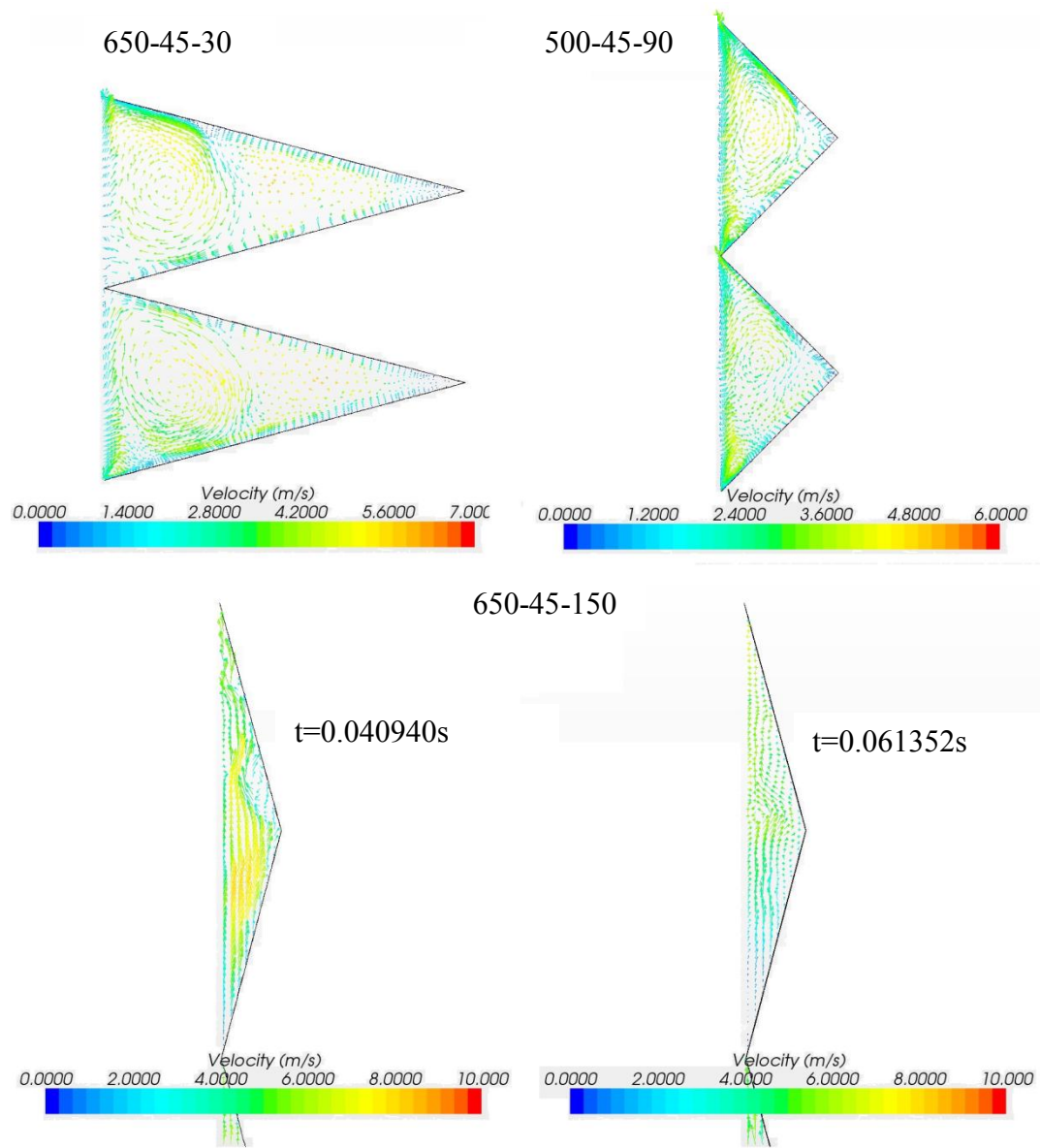


Figure 5-32: Velocity field perpendicular to preferred flow direction for the three different packings. Top left is geometry 650-45-30. Top right is 500-45-90. Bottom left is 650-45-150 at 0.040940s. Bottom right is 650-45-150 at 0.061352s.

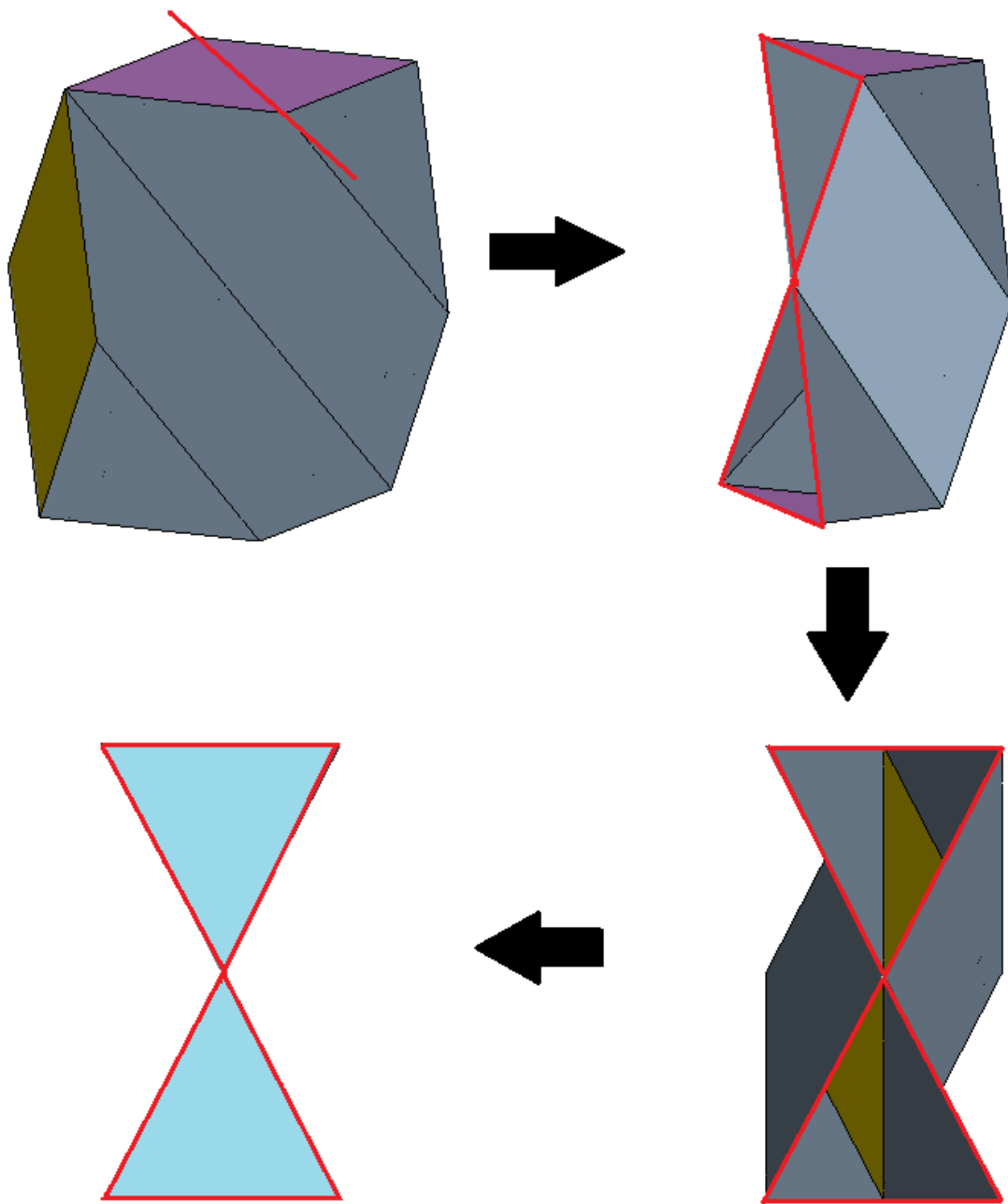


Figure 5-33: Central vertical plane cut from the packing to examine the x-velocity magnitude.

Figure 5-34 shows a comparison of the x-velocity magnitude between the packings 500-45-90 and 650-45-130. The top half shows the x-velocities at 500-45-90 at two different moments in time. At both instants, on either the left or right sides, the preferred horizontal velocity is easily observed being of similar magnitude, but in opposite directions. In the center of the packing, a region where the x-velocity is near zero can be observed. The horizontal velocities are in direct competition in this mixing layer and induce swirl in the flow through the packing. Furthermore, this region can be observed to vary significantly with time as evidenced by the variation observed between the two snapshots.

The bottom half of Figure 5-34 shows the x-velocity of the 650-45-130 geometry. Unlike the 500-45-90 packing, no clear region of preferred flow direction is observed on the left and right sides. Instead, the velocities are in direct competition in the entire cross section. At $t=0.041147\text{s}$, the preferred horizontal velocity is in the positive x-direction in the bottom half of the packing and in the negative x-direction in the top half of the packing. At $t=0.059352\text{ s}$, the preferred x-velocities have been reversed. The snapshot at $t=0.0504657\text{ s}$ shows the velocity field in transition between these two extremes. The channels are too narrow for a persistent, preferred flow direction to be induced in either side of the packing. Rather, the turbulent mixing layer as shown in the center of the 500-45-90 packing dominates the entire cross-section of the 650-45-150 packing.

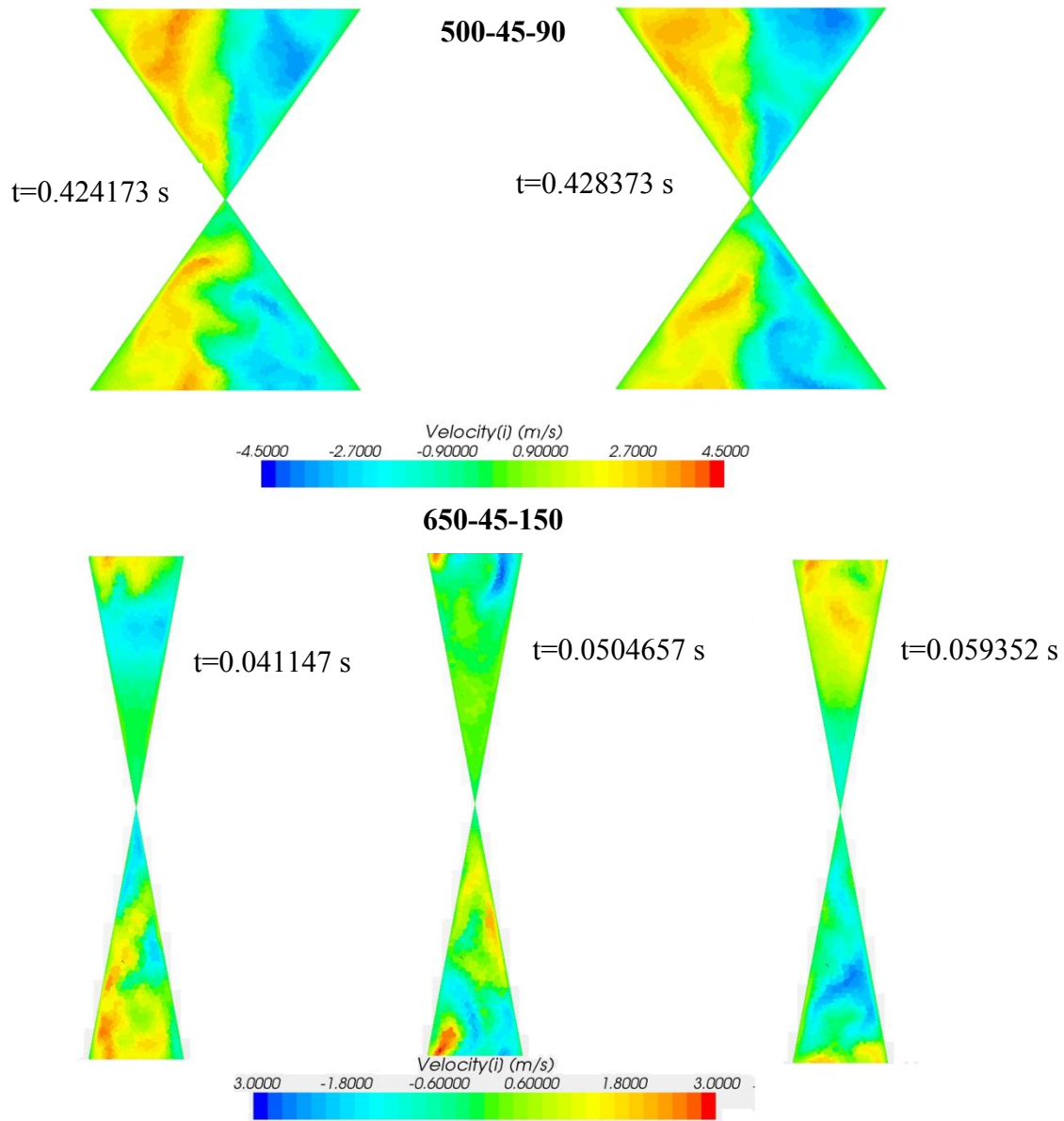


Figure 5-34: X-velocities in the vertical plane at the center of the packing. Top figures are for packing 500-45-90 at $t=0.424173$ s (left) and $t=0.428373$ s (right). Bottom figures are for packing 650-45-150 at $t=0.041147$ s (left), $t=0.0504657$ s (middle), and $t=0.059352$ s (right).

Chapter 6: Evaluation of CFD to Simulate Multiphase Flow

This chapter is separated into two main sections. The first deals with the use of small-scale simulations where a wide variety of physical properties and boundary conditions were examined. The use of small-scale geometries allowed for more physical properties to be examined. It also allowed for more computational grids to be examined to aid in the determination of appropriate mesh settings for the pilot-scale (i.e. CT geometry) simulations. The second section of this chapter compares CFD predictions to experimental data collected via CO₂ absorption experiments. Fractional liquid holdup, wetted area, and irrigated pressure drop predictions are compared to experimental data.

SMALL-SCALE SIMULATIONS

Small-scale simulations were broken down into three geometries as detailed in Chapter 3. There was a periodic geometry, the Small Inlet geometry, and the Large Inlet geometry. All three geometries had channel dimensions of $b=26.05$ mm, $s=16.75$ mm, and $h=10.53$ mm. Channel corrugation angle was 50° . The Small Inlet geometry and Large Inlet geometry had a thin strip around the perimeter of the top of the packing that served as a liquid velocity inlet, introducing an ideal liquid distribution to the packing surface. Below the liquid velocity inlet, one repeating unit of packing was present in the Small Inlet geometry. Four repeating units of packing were present in the Large Inlet Geometry. The nature of Small Inlet geometry and Large Inlet Geometry allowed for liquid load to be controlled directly by changing the liquid velocity. The periodic geometry had a constant liquid holdup for each simulation, allowing liquid load to be determined as a function of liquid holdup.

Grid Sensitivity – Periodic Simulations

The first aspect of the grid sensitivity examined the effect of the total number of prism layers present in the near wall region. Prism layers were used to ensure adequate resolution of the thin film present on the packing surface while minimizing the need for extreme mesh refinement within the whole of the computational domain. In the following cases, a prism layer growth rate of 1.07 and a total prism layer thickness of 1.0 mm were used. Three meshes with 10, 15, and 20 prism layers were examined. All meshes had a minimum cell size of 0.072 mm and target cell size of 0.8 mm. Simulation fluid properties are presented in Table 6-1. Predicted liquid load and fractional wetted area were the variables of interest for the grid sensitivity. Fractional wetted area for the periodic simulations is defined as the area of the liquid film (defined at $\alpha_L=0.5$) divided by the simulation surface area (3543 mm²). Results for liquid load are presented in Figure 6-1. The total number of prism layers has very little effect on the predicted liquid load, with relative difference between predicted liquid loads at a given holdup varying by less than 4%.

Property	Value	Units
Liquid Density	997.561	kg/m ³
Liquid Viscosity	8.8710E-04	Pa-s
Gas Density	1.14527	kg/m ³
Gas Viscosity	1.78837E-05	Pa-s
Surface Tension	0.074	N/m
Contact Angle	0	°

Table 6-1: Physical properties used for grid convergence study.

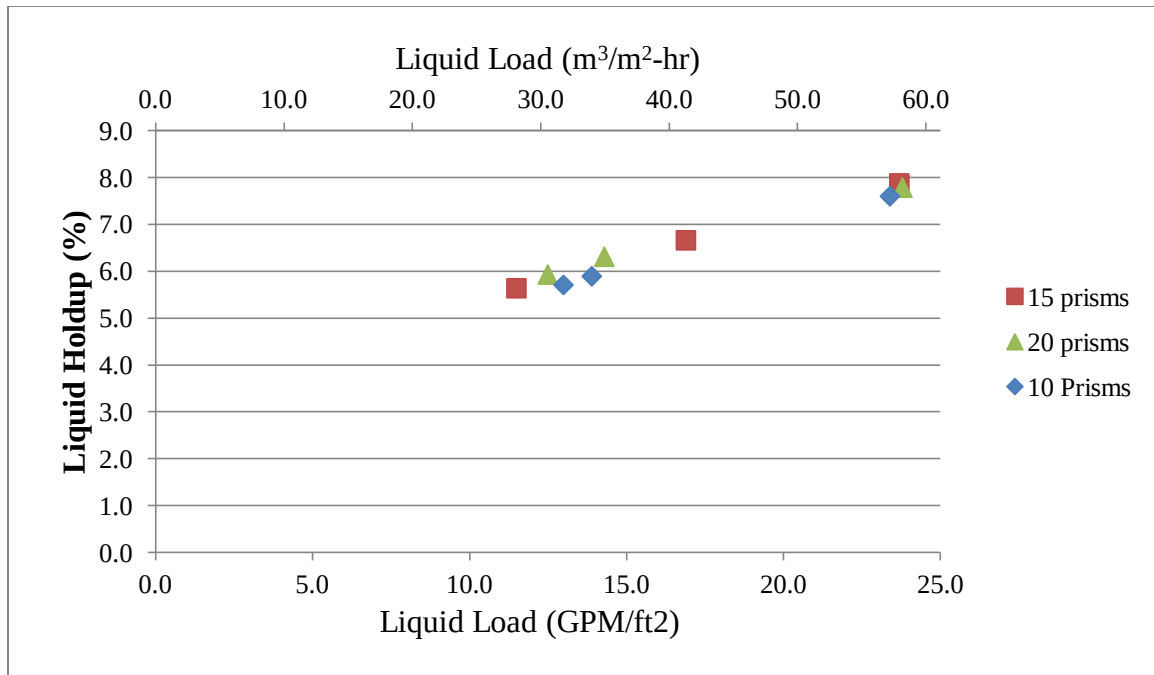


Figure 6-1: Impact of number of prism layers on predicted liquid load.

Figure 6-2 shows fractional wetted area as a function of liquid holdup and total number of prism layers. At the lowest liquid holdups examined, the number of prism layers has the strongest impact. At a fractional liquid holdup of 5.9%, the 10 prism layer mesh has a fractional wetted area of 0.816. This is 8.2% lower than the fractional wetted area of 0.889 of the 20 prism layer mesh. The 15 prism layer mesh predicts a fractional wetted area of 0.87 (generated from linear interpolation), which is within 2% of the value predicted using 20 prism layers. At a liquid holdup of ~7.8%, fractional wetted areas are within 1.5% regardless of the number of prism layers. From Figures 6-2 and 6-1, 15 prism layers represent an adequate level of accuracy for the range of conditions simulated in these studies.

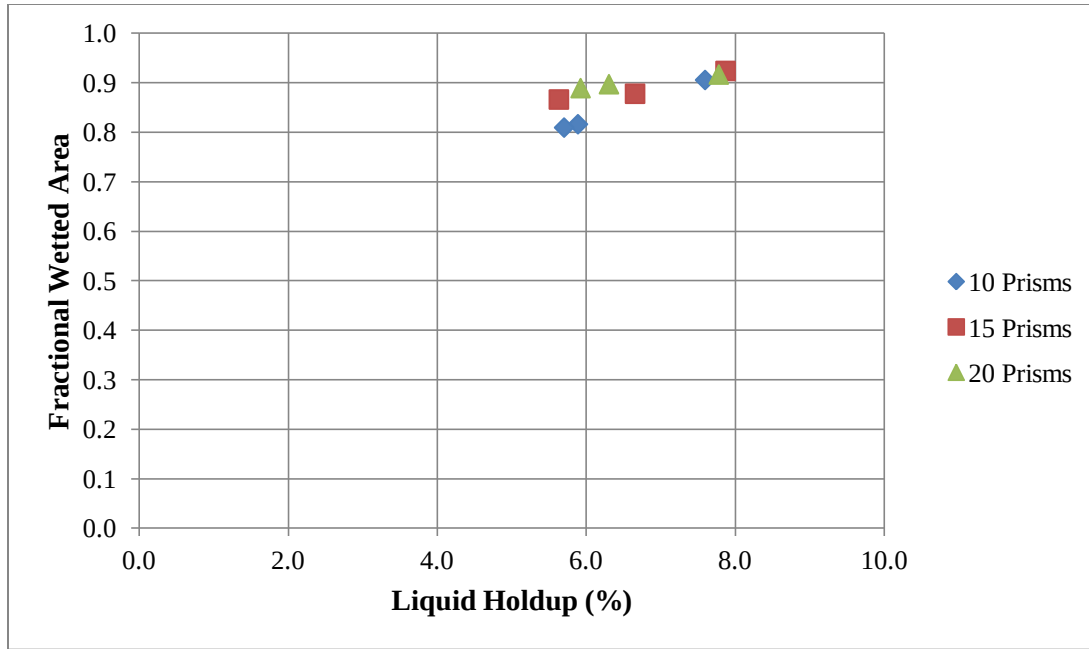


Figure 6-2: Effect of number of prism layers on fractional wetted area predictions.

With the wall-normal direction adequately resolved, the rest of the domain was examined for grid sensitivity by changing the mesh base size. The base size controls the minimum and target size of the mesh cells. Table 6-2 details the three meshes examined for a liquid holdup near 6.6%. The coarse grid simulation liquid mass flow rate and fractional wetted area deviate by 11% and 5% respectively when compared to the medium grid. The medium mesh and fine mesh are very similar with a 0.2% difference in liquid mass flow and 1.0% difference for wetted area. When the $GCI[\text{Coarse Grid}]$ (details of the calculation can be found in Chapter 5) is computed, a 3.18% error on the fractional wetted area and a 0.72% error on the liquid flow rate is found for the Medium mesh. With an eye toward significantly larger simulations, the use of the medium mesh settings is used for the remainder of the simulations. This allows for lower computational time per iteration and larger time steps without violating stability criteria for the numerical methods.

Mesh	Min	Target	Base	Total	Holdup	Liquid Flow Rate	Fractional Wetted Area	r	GCI[Coarse Grid]	
	Size	Size	Size	Cells					Fractional Wetted Area	Liquid Flow Rate
	(mm)	(mm)	(mm)		(%)	(kg/s)				
Coarse	0.0900	1.00	1.00	147230	6.58	0.00500	0.918		29.68%	67.26%
Medium	0.0720	0.80	0.80	207306	6.64	0.00450	0.875	1.41	3.18%	0.72%
Fine	0.0342	0.38	0.38	739067	6.64	0.00451	0.866	3.57		

Table 6-2: Results summary for the grid sensitivity study for multiphase simulations.

Impact of Contact Angle – Periodic Simulations

This introduction to the contact angle is merely meant to introduce the reader to the definition and significance of the contact angle and its relationship to the surface tension. The main goal of the present research was to determine the effect of the contact angle as an independent boundary condition between the liquid and packing surface. Specifically, it was desired to determine if experimentally measured static contact angles were the appropriate choice to prescribe as the boundary condition in multiphase CFD simulations. In reality, the contact angle and surface tension are inherently coupled.

The contact angle is the angle formed by a liquid at a three-phase boundary (e.g. liquid, gas, and solid). It is typically measured from inside the liquid as shown in Figure 6-3. It is a measure of the wettability of a solid by some liquid. A contact angle of 0° indicates the liquid will completely wet the solid. A contact angle of 180° indicates the liquid will not wet the solid. Intermediate contact angles result in partial wetting of the surface.

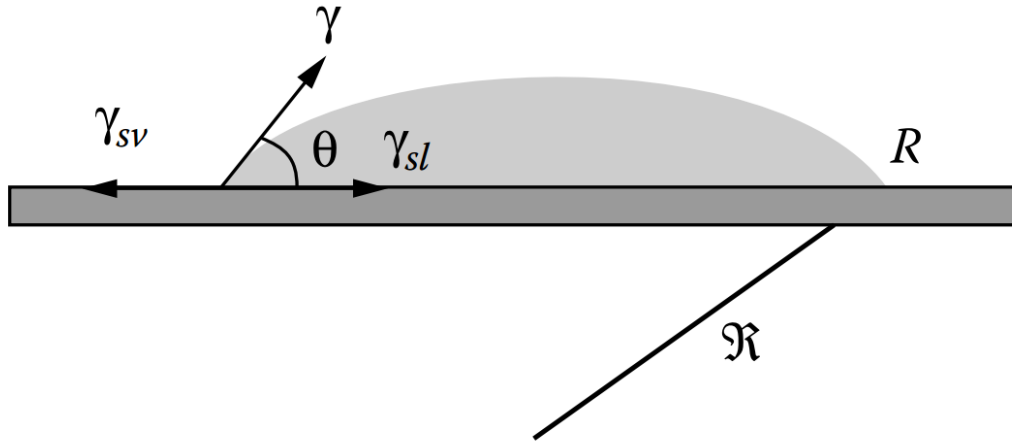


Figure 6-3: Definition of the contact angle. Figure taken from Starov *et al.*⁶⁹

Using a force balance, a relationship between the contact angle and interfacial tensions of the three phases can be derived:⁶⁹

$$\gamma \cos \theta_c = \gamma_{sv} - \gamma_{sl} \quad \text{Equation 6-1}$$

where θ_c is the static contact angle, γ is the liquid-vapor surface tension, γ_{sv} is the solid-vapor interfacial tension, and γ_{sl} is the solid-liquid interfacial tension. If the right-hand side of Equation 6-1 remains constant, any changes in the surface tension must be met with corresponding changes in the contact angle. Tsai *et al.* found that for a given system (stainless steel-dilute caustic-air), a reduction in surface tension via surfactants was met with a corresponding decrease in contact angle.⁶⁰ Nicolaiewsky and Fair conducted an extensive study of contact angles with different liquids and packing surfaces and concluded reduced surface tensions were generally correlated with lower contact angles.⁷⁰ However, it should be noted that for all systems examined, contact angles measured were considered to be wetting (i.e. measured contact angles were less than 90°).

Present studies examined the impact of varying only the contact angle while holding all other simulation parameters constant. Figure 6-4 demonstrates the effect of contact angle on a series of simulations where surface tension was held constant at 0.074 N/m. The density and viscosity of the gas and liquid are shown in Table 6-1. Figures presented show the wetted area (blue) on the “back” packing sheet shown in Figure 3-7. From Figure 6-4, the contact angle primarily determines if the liquid flows as a film or a rivulet. In the completely wetting contact angle scenario (0°), liquid flows primarily as a film. For a weakly wetting case (75°), the liquid flows primarily as a rivulet, leading to very little wetted area. At the contact points between packing sheets (i.e. the corners and center of the pictures), a liquid droplet has formed. This droplet serves to allow liquid flowing on opposite sheets to contact and redistribute from the packing ridge into the “valley” below. The rivulet flow of the weakly wetting case also serves to increase the predicted liquid load for similar liquid holdups.

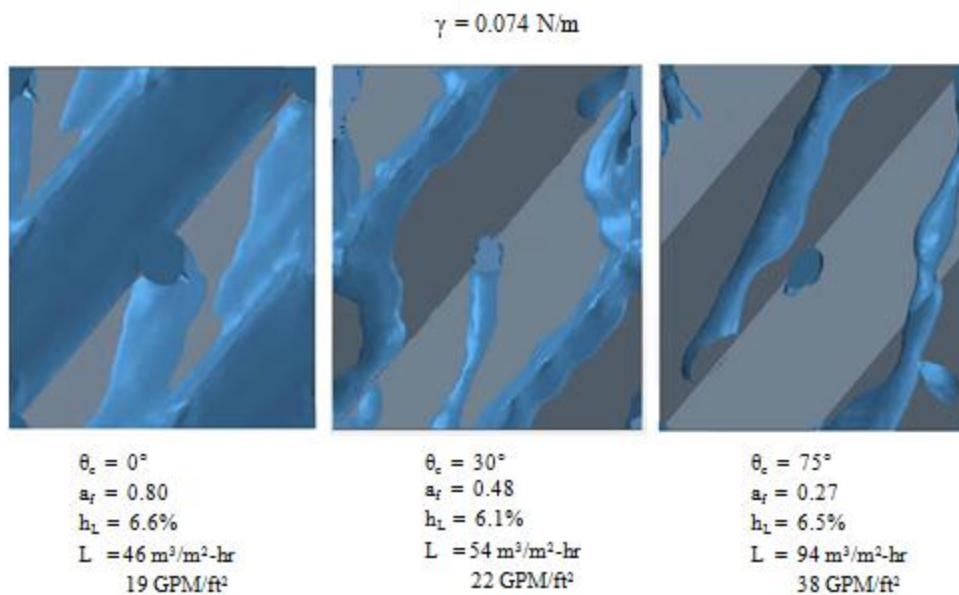


Figure 6-4: Impact of changing the contact angle on periodic simulations.

Figure 6-5 summarizes the impact of varying contact angle and liquid holdup on predicted fractional wetted area and liquid load. As liquid holdup is increased, fractional wetted area and predicted liquid load increase. When liquid holdup is regressed as a power-law function of liquid load, the 0° and 30° cases demonstrate exponents of 0.49 and 0.716 respectively. Semi-empirical models have shown exponents ranging from 0.333 (e.g. Olujic²⁴) to 0.718 (e.g. Tsai⁷¹), placing the CFD predictions within the same range as that observed experimentally.

Impact of Surface Tension – Periodic Simulations

Tsai *et al.* showed that a reduction in surface tension leads to an increase in wetted area.⁶⁰ CFD simulations were performed using three different surface tensions. The wetted area predictions for a contact angle of 0° are shown in Figure 6-6. At the highest surface tension, the lowest fractional area is observed. This is due to the liquid being unable to spill over the packing ridge at all points. This is one limitation of the geometry examined. The geometry had sharp angles at the packing ridges and valleys. Most structured packings have rounded edges, which allow liquid to spill over much more easily. As surface tension is reduced, more liquid is able to spill over the packing ridge. This can be noticed by the increase in wetted area and the increase in liquid load observed at the lowest surface tension. In general, gravity and surface tension are in direct competition with each other for area generation. Gravity serves to spread the liquid by pulling it toward and over the packing ridge while surface tension acts to prevent the liquid from spilling over the packing ridge.

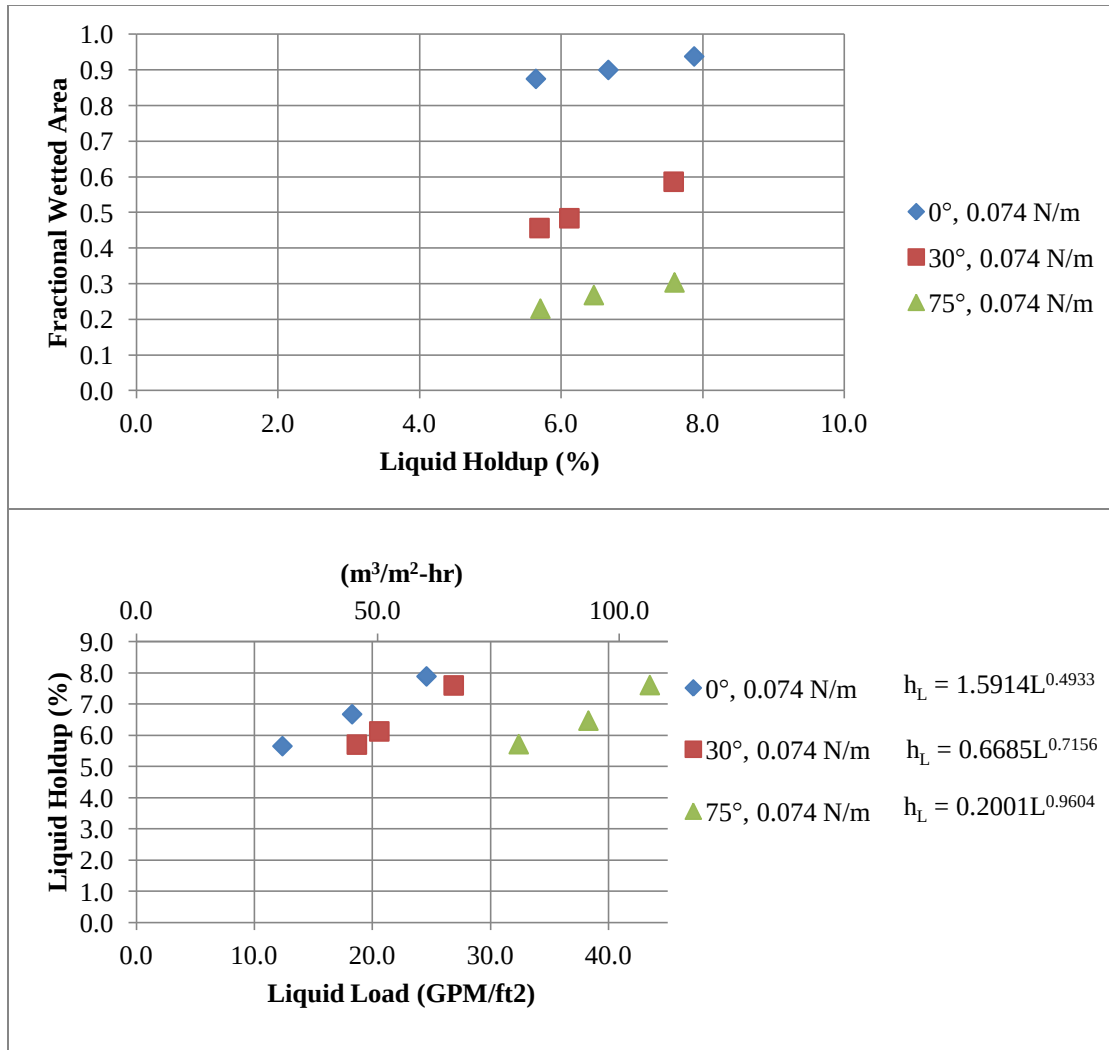


Figure 6-5: Impact of varying simulation contact angle and liquid holdup on fractional wetted area (top) and liquid load (bottom). Surface tension was constant at 0.074 N/m.

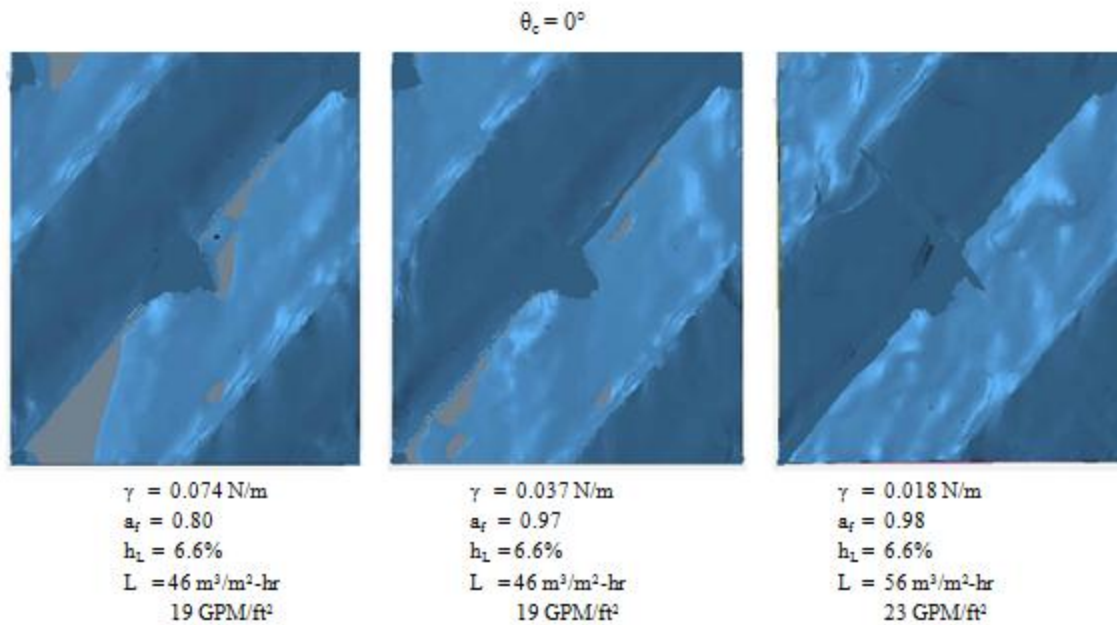


Figure 6-6: Influence of surface tension on wetted area predictions with a static contact angle of 0° .

Figure 6-7 shows the impact of reducing surface tension at a contact angle of 30° . At the highest surface tension, rivulet flow is observed. As the surface tension is reduced, the flow transitions to film flow. This transition results in significant increase in predicted liquid area. At a surface tension of 0.074 N/m , the fractional wetted area is 0.48 . At a surface tension of 0.018 N/m , the fractional wetted area is 0.80 . Furthermore, at the lowest surface tension, it can again be observed that the liquid is spilling over the packing ridge. Again, gravity and surface tension are in direct competition with each other to create wetted area. At the lowest surface tension, the weight of the fluid is dominant as evidenced by the high wetted areas predicted.

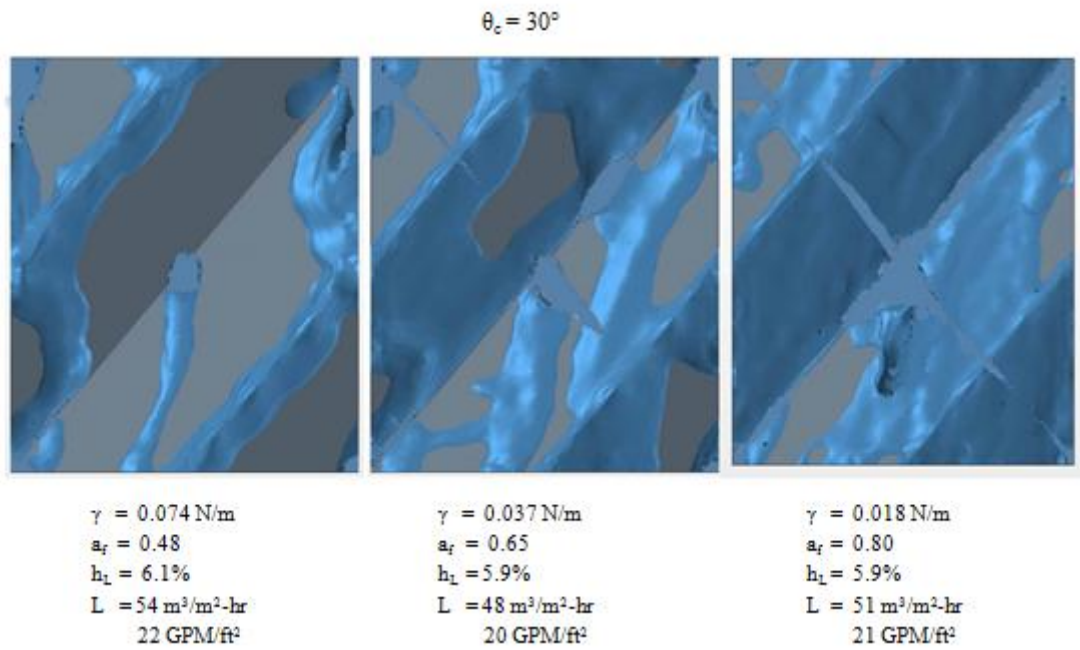


Figure 6-7: Influence of surface tension on wetted area predictions with a static contact angle of 30° .

Results for simulations varying surface tension and contact angle are summarized in Table 6-3. In general, the lowest wetted areas are observed at the highest surface tensions and highest contact angles. As the surface tension is reduced, fractional wetted area is increased. Similarly, as the simulation contact angle is reduced, fractional wetted area is increased for a given liquid holdup.

Contact Angle	Liquid Load (GPM/ft ²)	Liquid Load (m ³ /m ² -hr)	Fractional Wetted Area	Liquid Holdup (%)	Surface Tension (N/m)
0°	22.8	55.7	0.99	6.69	0.018
0°	13.6	33.3	0.98	5.67	0.018
0°	33.5	81.9	0.99	7.90	0.018
30°	20.9	51.1	0.80	5.91	0.018
30°	19.7	48.2	0.77	5.72	0.018
30°	36.0	88.0	0.94	7.61	0.018
75°	45.6	111.5	0.35	6.48	0.018
75°	56.8	138.9	0.42	7.62	0.018
75°	38.0	92.9	0.34	5.72	0.018
0°	18.7	45.7	0.97	6.68	0.037
0°	13.5	33.0	0.96	5.66	0.037
0°	26.7	65.3	0.97	7.89	0.037
30°	19.6	47.9	0.65	5.90	0.037
30°	18.1	44.3	0.63	5.71	0.037
30°	29.6	72.4	0.78	7.60	0.037
75°	44.7	109.3	0.30	6.47	0.037
75°	51.2	125.2	0.38	7.61	0.037
75°	37.0	90.5	0.29	5.72	0.037
0°	18.7	45.7	0.90	6.67	0.074
0°	12.9	31.5	0.87	5.65	0.074
0°	25.3	61.9	0.938	7.88	0.074
30°	22.2	54.3	0.48	6.12	0.074
30°	19.9	48.7	0.46	5.70	0.074
30°	29.8	72.9	0.59	7.59	0.074
75°	38.3	93.6	0.27	6.47	0.074
75°	43.5	106.4	0.30	7.61	0.074
75°	32.4	79.2	0.23	5.71	0.074

Table 6-3: Summary of the impact of contact angle and surface tension.

Impact of Density – Periodic Simulations

The impact of density can be observed in Figure 6-8 for a contact angle of 30°. Three densities were examined varying from 500-1500 kg/m³. Liquid viscosity, gas

density, and gas viscosity are shown in Table 6-1. At similar liquid holdup, as liquid density increases, fractional wetted area increases. This is most easily explained by surface tension and the fluid weight competing. As the density of the fluid increases, so does its weight. This serves to increase the force directing the fluid toward and over the packing ridge, allowing for increased wetted area generation. At the lowest densities, it can be observed the weight of the fluid is insufficient to spill the liquid over the packing ridge. Thus, a liquid rivulet stays inside the packing valley and flows at the corrugation angle of 50° .

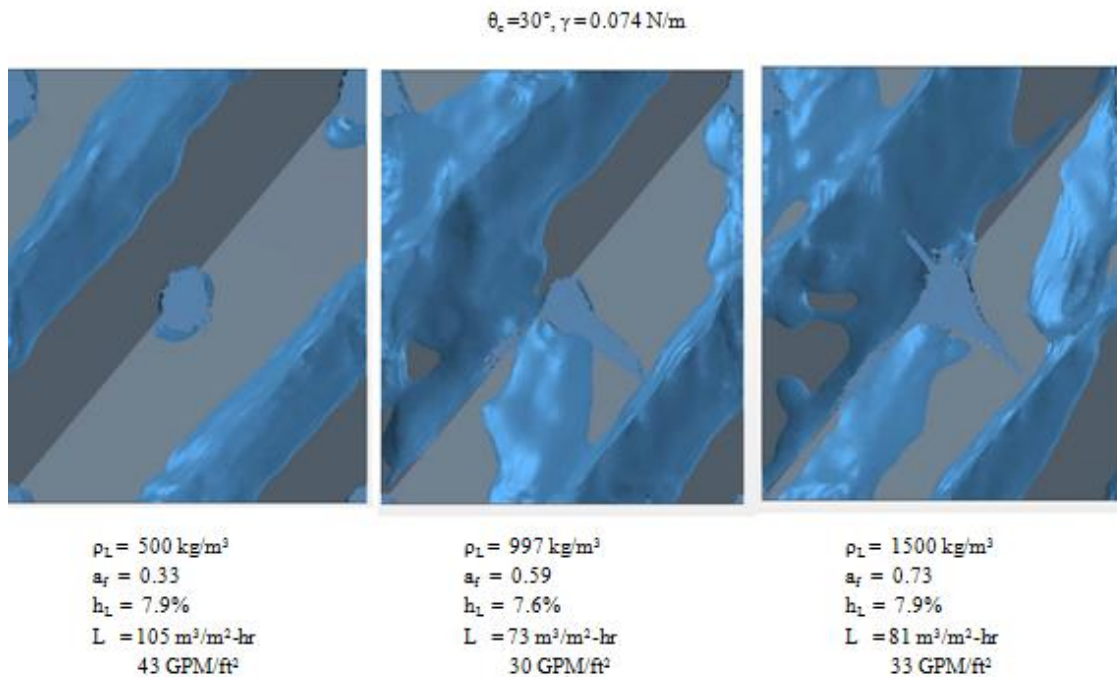


Figure 6-8: Impact of varying density at constant surface tension (0.074 N/m) and contact angle (30°). Liquid holdup was 7.6-7.9%.

Figure 6-9 summarizes the impact of increasing density and surface tension on wetted area for contact angles of 0° and 30° . At a given holdup, the higher density fluid

results in increased wetted area. Lower surface tension once again results in increased wetted area for both contact angles examined at a constant liquid holdup.

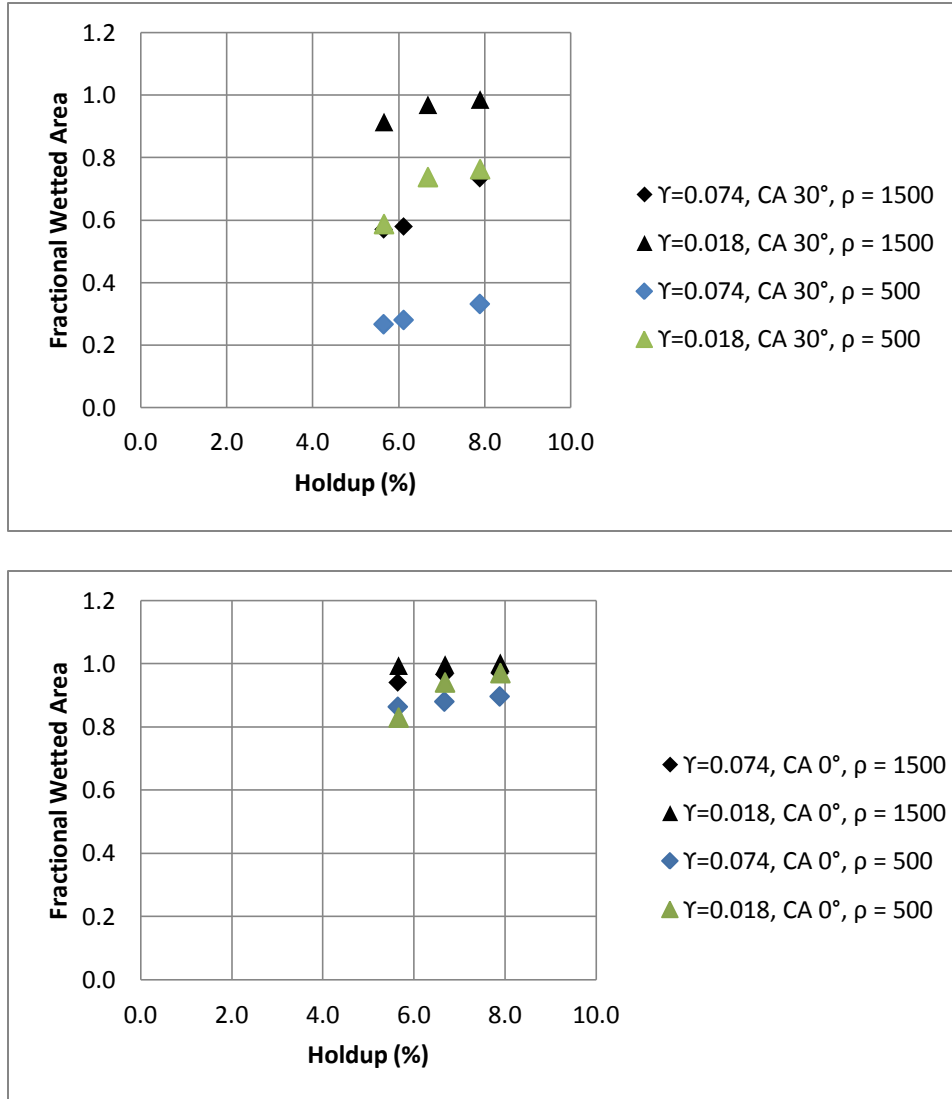


Figure 6-9: Impact of density and surface tension on periodic simulations using a contact angle of 30° (top) and 0° (bottom). Black markers are simulations with liquid a liquid density of 1500 kg/m³. Colored markers have a density of 500 kg/m³. Triangle markers have a surface tension of 0.018 N/m. Diamond markers have a surface tension of 0.074 N/m.

It should be noted, however, that the increase in wetted area can also be attributed to an increase in predicted liquid load as shown in Figure 6-10. In the majority of cases, the higher density fluid demonstrates significantly higher liquid loads. The exceptions are the simulations using $\theta_c=30^\circ$ and a surface tension of 0.074 N/m. In this case, the two densities demonstrate similar liquid loads, but vastly different wetted areas. This is best explained by considering the image shown at left in Figure 6-8. The low density fluid forms a rivulet in the channel valley, flowing at the corrugation angle of 50° . This behavior results in the low fractional areas predicted. This rivulet would be expected to have a relatively high average velocity due to the small area with which the liquid contacts the packing surface. With the increased density, the liquid is able to escape the channel valley and spread out. This results in a thinner film which covers a larger area. This thin film has a lower average velocity than the rivulet present in the low density simulations. In all other cases (i.e. the low surface tension and simulations with $\theta_c=0^\circ$), the low density liquid is already capable of spilling over the edge, as demonstrated by fractional wetted areas above 0.5. Thus, the slight increase in wetted area generated at higher densities does not serve to lower the average film velocity enough to offset the increased weight of the fluid.

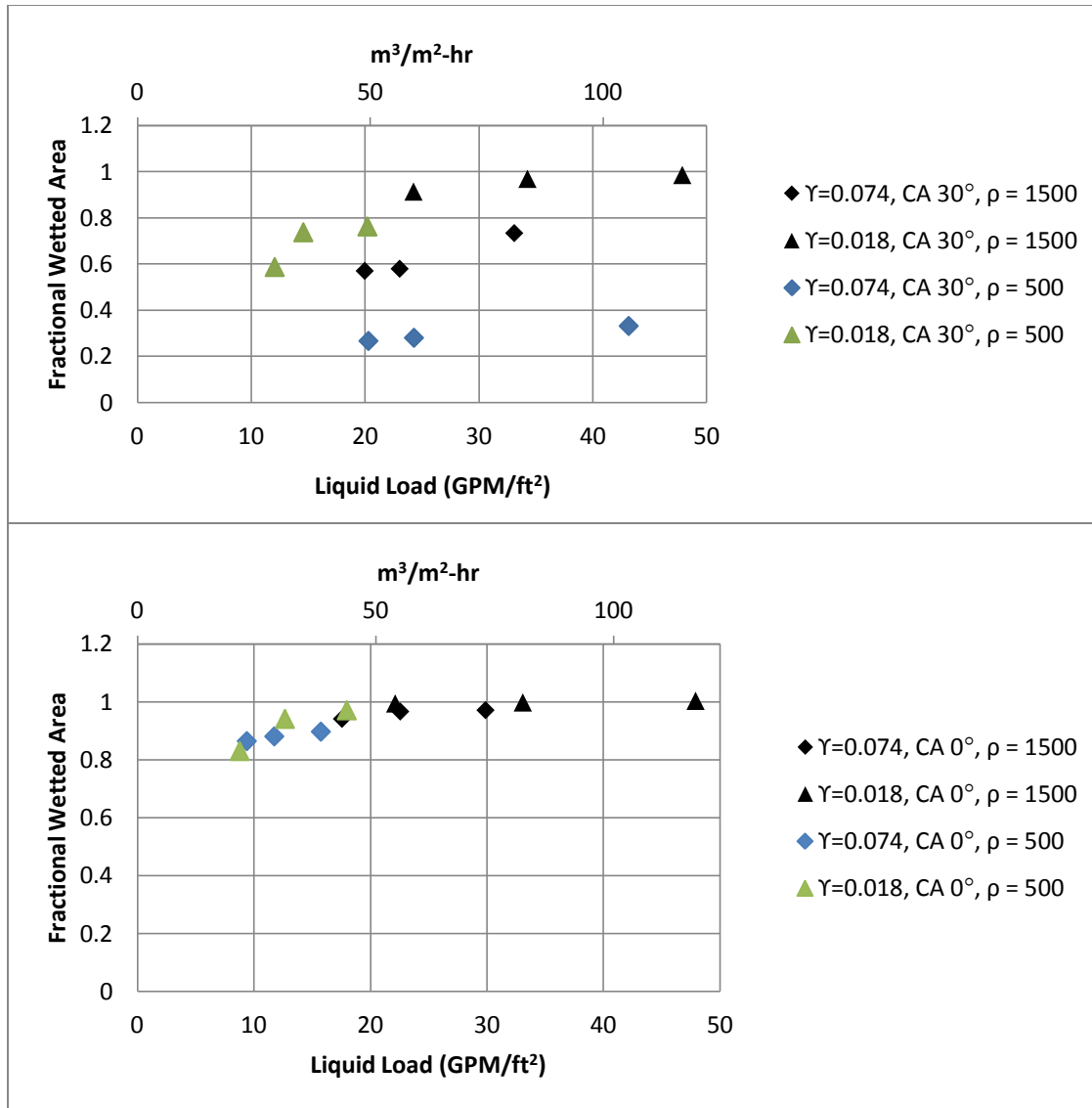


Figure 6-10: Impact of predicted liquid load on fractional wetted area for simulations of different densities. Contact angle of 30° shown at top. Contact angle of 0° shown at bottom. Black markers are simulations with liquid a liquid density of 1500 kg/m³. Colored markers have a density of 500 kg/m³. Triangle markers have a surface tension of 0.018 N/m. Diamond markers have a surface tension of 0.074 N/m.

Impact of Viscosity – Periodic Simulations

Figure 6-11 shows the impact of increasing viscosity. Gas properties are shown in Table 6-1. Liquid density was 997.561 kg/m^3 , surface tension was 0.074 N/m , and contact angle was 0° . For a given liquid holdup, increased liquid viscosity resulted in drastically lower liquid load. A 20-fold increase in liquid viscosity resulted in a 12.5-fold reduction in predicted liquid load. Wetted area was reduced slightly at increased viscosities. Increased viscosities also significantly smoothed the gas-liquid interface. This would be expected due to the significantly reduced Reynolds number due to both the lower liquid velocity and increased viscosity.

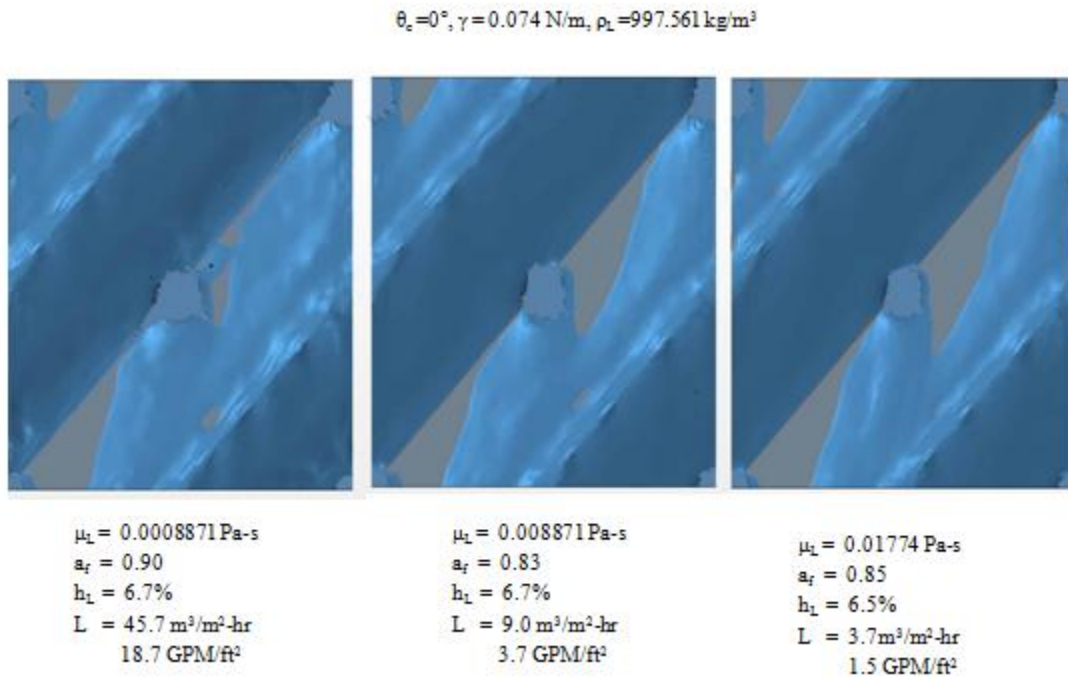


Figure 6-11: Impact of increasing liquid viscosity for periodic simulations. Contact angle was set at 0° , surface tension was 0.074 N/m , and liquid density was 997.561 kg/m^3 .

Figure 6-12 summarizes the impact of viscosity on fractional wetted area and liquid load for $\theta_c = 0^\circ$. For a surface tension of 0.074 N/m , viscosity slightly lowers the

predicted wetted areas for a given liquid holdup. At a low surface tension, however, viscosity has a more pronounced effect. The wetted area shows very little dependence on the liquid load at the lowest viscosity examined. At increased viscosities, however, there is a strong dependence of fractional wetted area on liquid load. This dependence could be due to two different mechanisms. First, at low viscosities, the surface is wavier, causing gradients in curvature and film height. These disturbances would allow liquid to more easily spill over the packing ridge, completely wetting the packing at all liquid loads. Second, liquid spilling down from the contact points would be expected to have increased momentum at low viscosities. It would crash into the film in the packing valley, causing the film to spill over the channel ridge.

Figure 6-13 demonstrates the impact of increasing viscosity when the contact angle is set at 30° and the surface tension is 0.018 N/m. Again, a lower liquid load is observed in the increased viscosity case. Furthermore, the high viscosity case has a fractional wetted area of 0.68, which is 15% lower than the low viscosity case ($a_f=0.80$). The decrease in wetted area is due to the liquid being unable to spill over the packing ridge at high viscosities. At the high viscosity, the liquid film present is uniform and smooth. At the low viscosity, the liquid film appears significantly more disturbed with variations in curvature and film height. These variations would serve to help drive flow over the packing ridge. At high viscosities, the disturbances are damped by viscous forces.

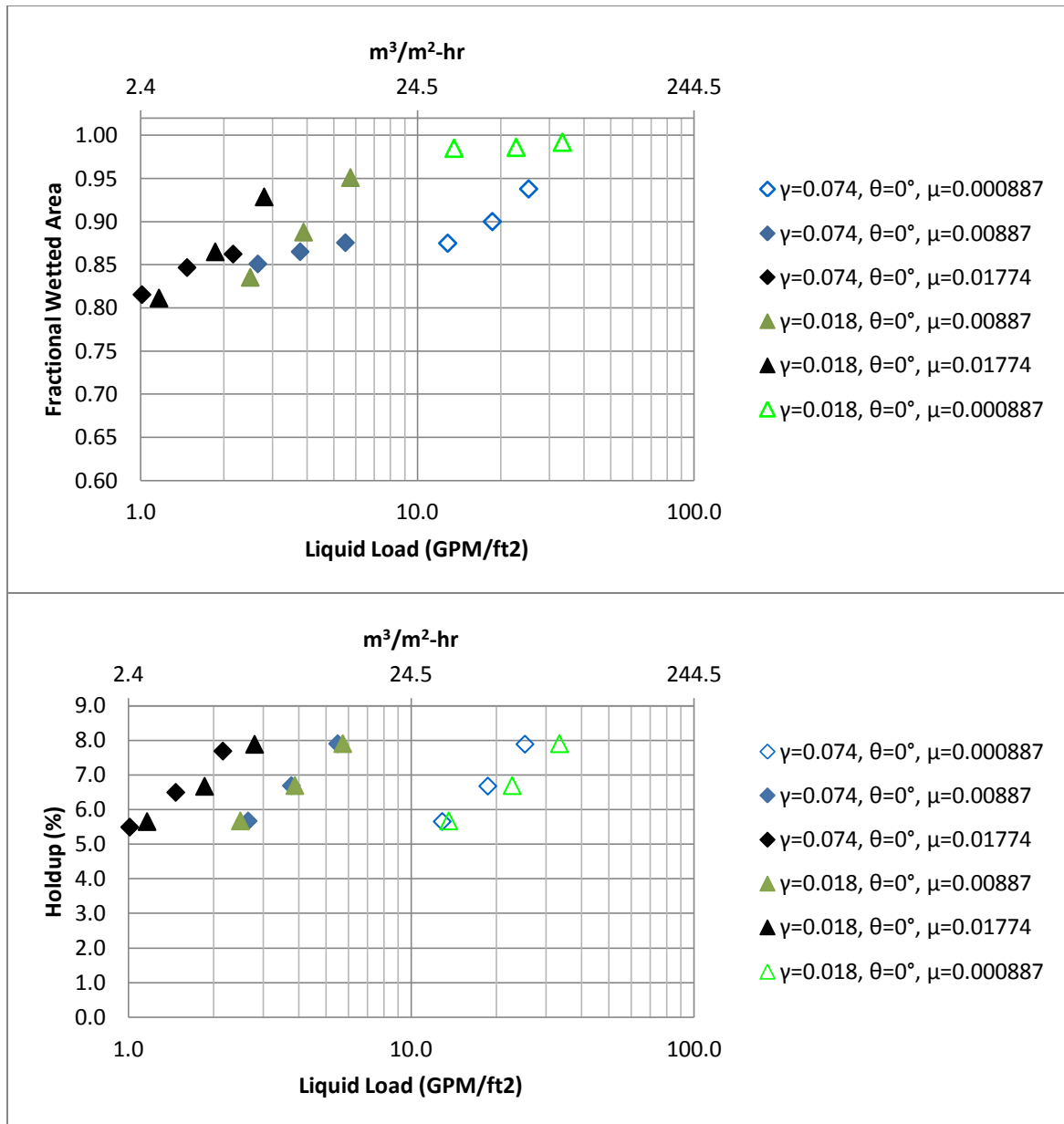
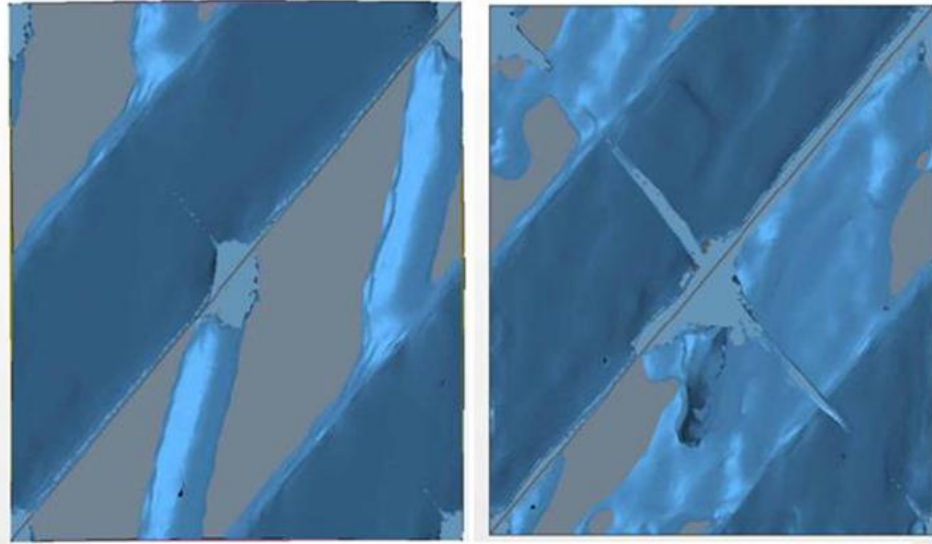


Figure 6-12: Summary of the increased viscosity results for a contact angle of 0° . Black markers are 20x base viscosity, solid colored markers are 10x base viscosity, and hollow markers are base viscosity. Diamonds are the high surface tension case. Triangles are the low surface tension case. Top shows the impact of liquid load on fractional wetted area. Bottom shows the impact of holdup on predicted liquid load.

$$\theta_c = 30^\circ, \gamma = 0.018 \text{ N/m}, \rho_L = 997.561 \text{ kg/m}^3$$



$$\mu_L = 0.01774 \text{ Pa-s}$$

$$a_f = 0.68$$

$$h_L = 6.7\%$$

$$L = 5.9 \text{ m}^3/\text{m}^2\text{-hr}$$

$$2.4 \text{ GPM/ft}^2$$

$$\mu_L = 0.0008871 \text{ Pa-s}$$

$$a_f = 0.80$$

$$h_L = 5.9\%$$

$$L = 51.1 \text{ m}^3/\text{m}^2\text{-hr}$$

$$20.9 \text{ GPM/ft}^2$$

Figure 6-13: Liquid film showing the impact of increased viscosity on predicted wetted area for a contact angle of 30° and a surface tension of 0.018 N/m . High viscosity shown at left. Base viscosity shown at right.

Figure 6-14 summarizes the effects of increased viscosity on wetted area and liquid load. At high surface tensions, viscosity plays very little role in wetted area generation for a given liquid holdup. This is because at no point is the liquid capable of spilling over the channel ridge. Only the contact points serve to distribute the liquid from a ridge into a packing channel valley below. At the low surface tension cases, increased viscosity serves to inhibit the liquid from spilling over the channel ridge to completely wet the packing.

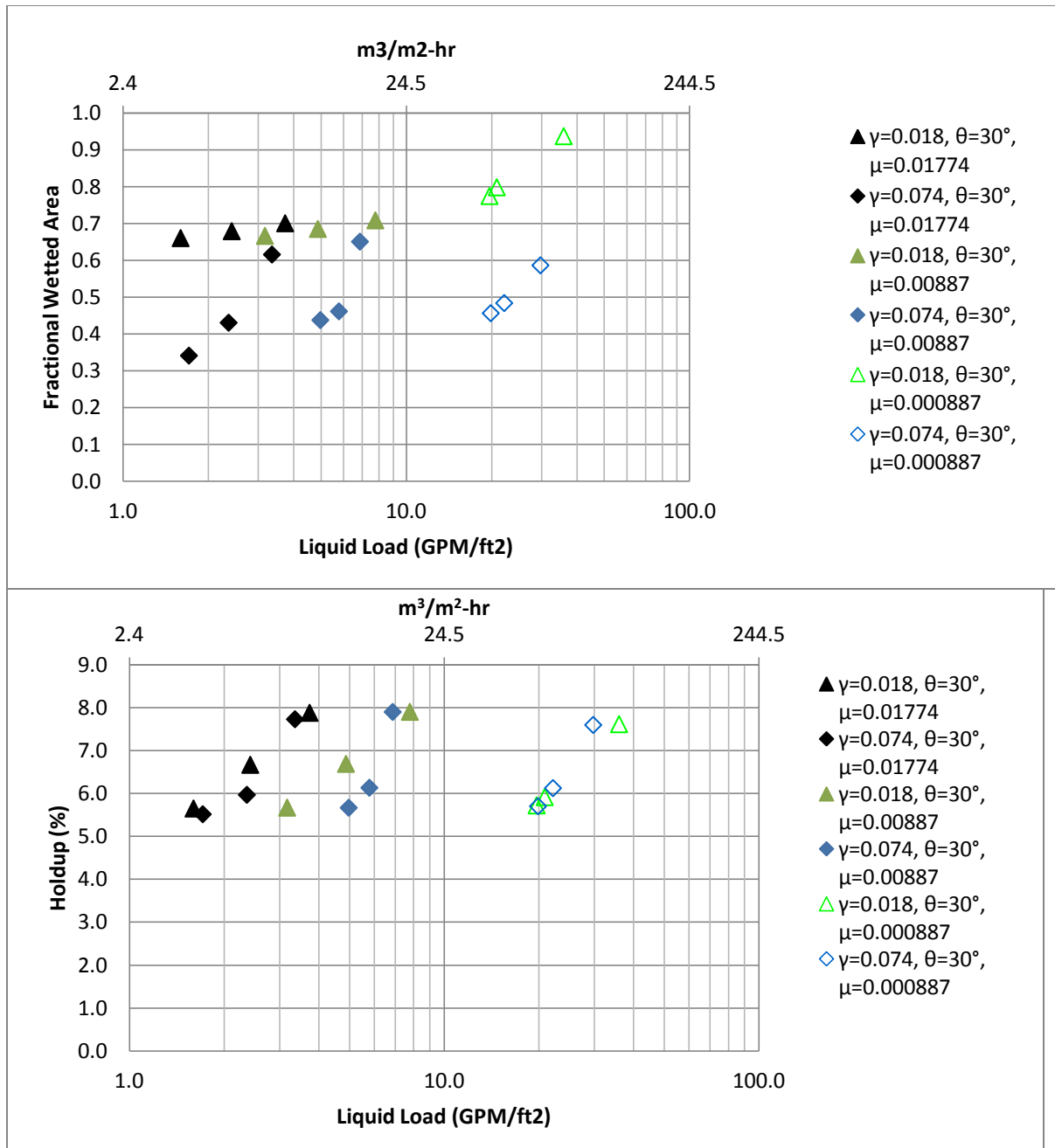


Figure 6-14: Summary of the increased viscosity results for a contact angle of 30° . Black markers are 20x base viscosity, solid colored markers are 10x base viscosity, and hollow markers are base viscosity. Diamonds are the high surface tension case. Triangles are the low surface tension case. Top shows the impact of liquid load on fractional wetted area. Bottom shows the impact of holdup on predicted liquid load.

Impact of Boundary Conditions

Three geometries were examined: a periodic geometry, the Small Inlet geometry, and the Large Inlet geometry. The Small Inlet geometry consisted of one unit of the repeated packing element with a thin liquid velocity inlet around the packing perimeter. The Large Inlet geometry consisted of the Small Inlet geometry with three additional repeating packing units below. Figure 6-15 shows the differences in predicted wetted area and liquid hold for the Small Inlet and periodic geometries. Three different contact angles are shown with the remainder of physical properties matching those of Table 6-1. The Small Inlet geometry demonstrates higher wetted areas and liquid holdups when compared to the periodic geometry. The higher wetted area is explained due to the perfect distribution of liquid onto the packing surface. Essentially, the liquid is not relying on the contact points and ability to spill over the ridge to wet the top half of the packing geometry. Rather, the liquid is perfectly distributed around the entire perimeter.

Figure 6-16 shows how contact angle affects the predicted flow pattern in the Large Inlet geometry. Like in the periodic geometry, as contact angle is increased, the flow transitions from film flow to rivulet flow. In this case, at a contact angle of 75° , the liquid rivulet prefers to flow at the channel corrugation angle of 50° . The liquid rivulet is largely confined to the channel valley. For comparisons between the three geometries, “Unit” is used to refer to which repeating unit the data was harvested from in the Large Inlet geometry as shown in Figure 6-16. They are labeled numerically with Unit 1 being the first repeated packing unit below the liquid distributor.

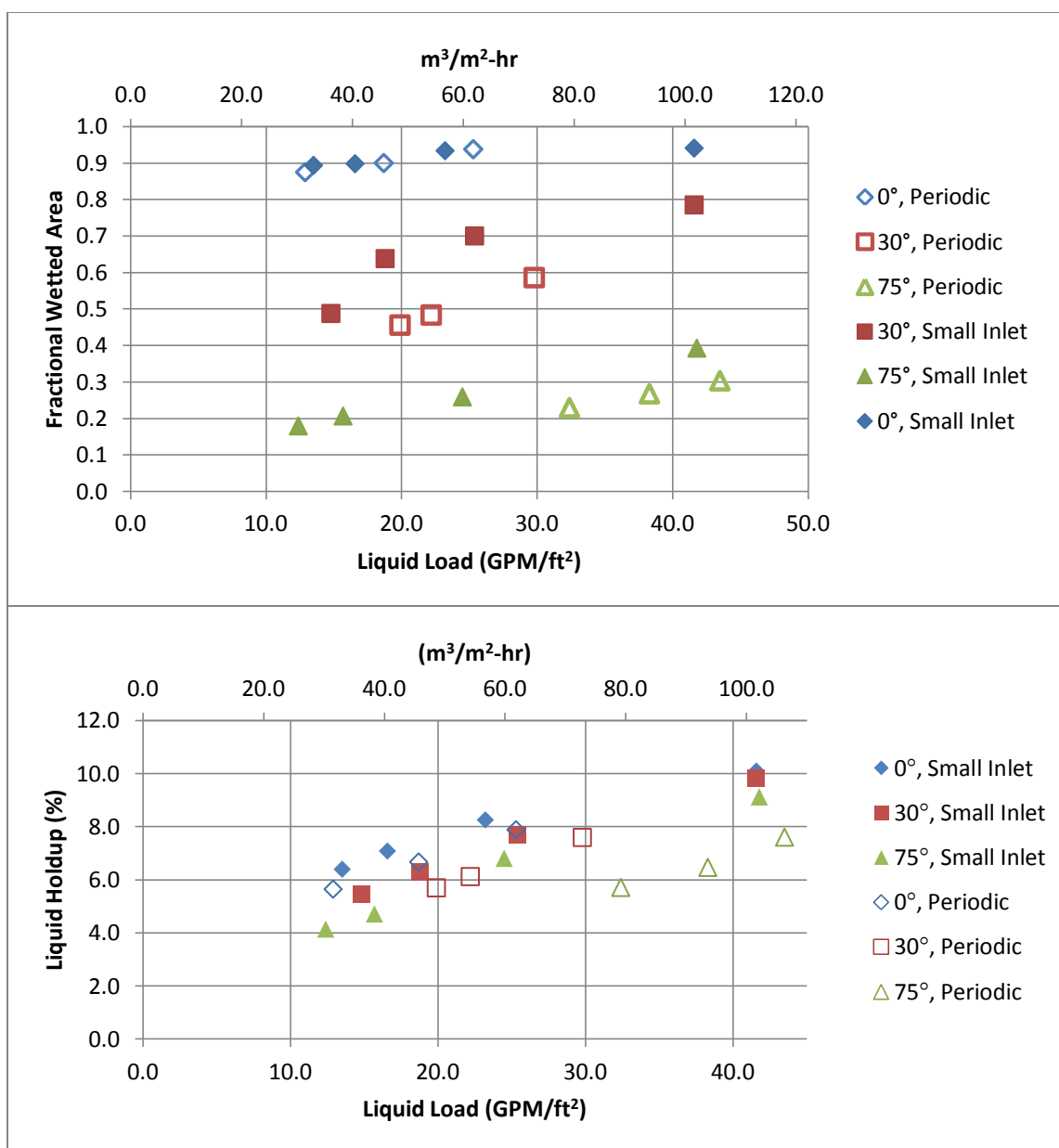


Figure 6-15: Periodic geometry vs. the Small Inlet geometry. Top shows the predicted wetted areas for three contact angles. Bottom shows the liquid holdup vs. liquid load for three different contact angles. Hollow markers are the periodic geometry.

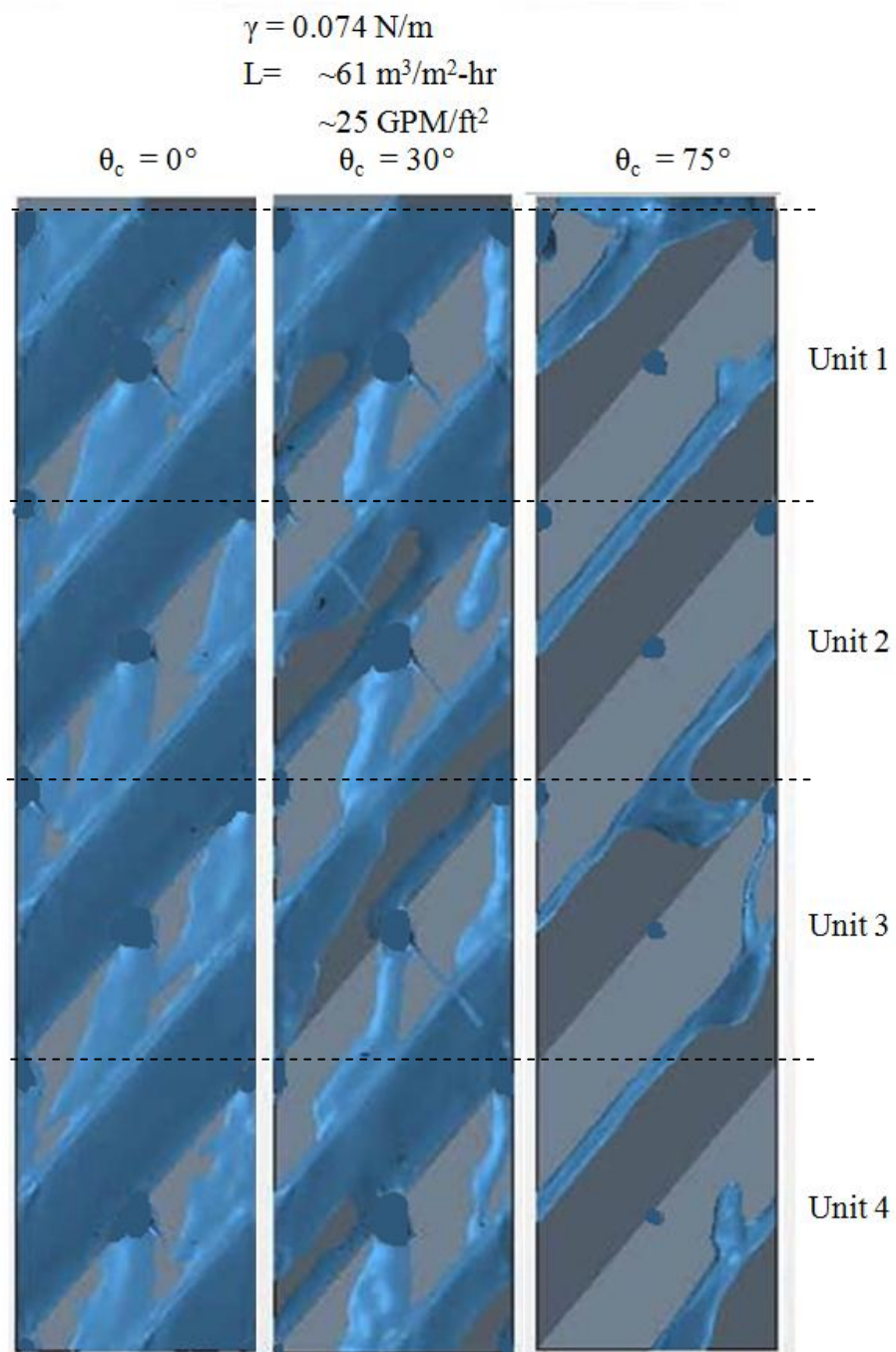


Figure 6-16: Effect of contact angle on Large Inlet geometry flow field.

The results for geometry comparisons for contact angles of 0° , 30° , and 75° are shown in Figure 6-17, 6-18, and 6-19 respectively. Average liquid loads are indicated in the legend for the three geometries. Fluid physical properties are shown in Table 6-1. In all cases, excellent agreement is observed between the Small Inlet geometry and the first repeating unit of the Large Inlet geometry for both holdup and fractional wetted area. In the case of the Large Inlet geometry, a maximum liquid holdup and fractional wetted area are observed in the first repeating unit. Past the first unit, the liquid holdup and wetted area decrease sharply. At a contact angle of 0° , the periodic geometry exhibited a higher degree of wetting and increased holdup when compared to the bottom repeating unit of the Large Inlet geometry. For a contact angle of 30° , the liquid holdup and fractional wetted area were comparable between the periodic geometry and bottom unit of the Large Inlet geometry. The simulations using a contact angle of 75° deserve special mention because the predicted liquid load in the periodic geometry is significantly higher, which results in the increased fractional area and liquid holdup observed. From this comparison, it is clear care should be taken with multiphase CFD simulations when creating the geometry and boundary conditions. If a single repeating unit is used, with perfect liquid distribution, increased holdup and wetted area predictions will be observed when compared to a larger geometry or a periodic geometry.

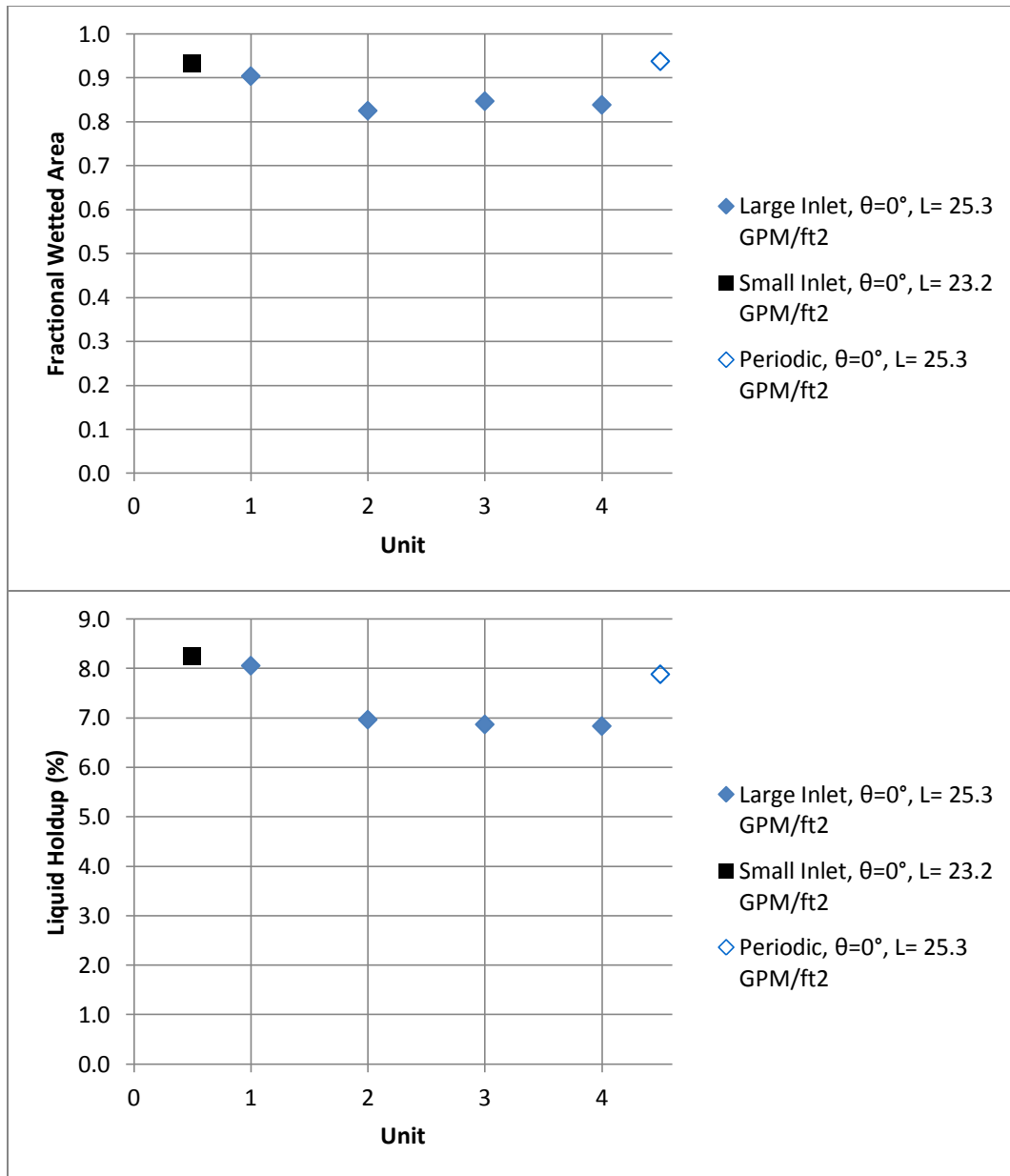


Figure 6-17: Impact of geometry and inlet conditions on fractional wetted area (top) and liquid holdup (bottom) with a contact angle of 0° and a surface tension of 0.074 N/m.

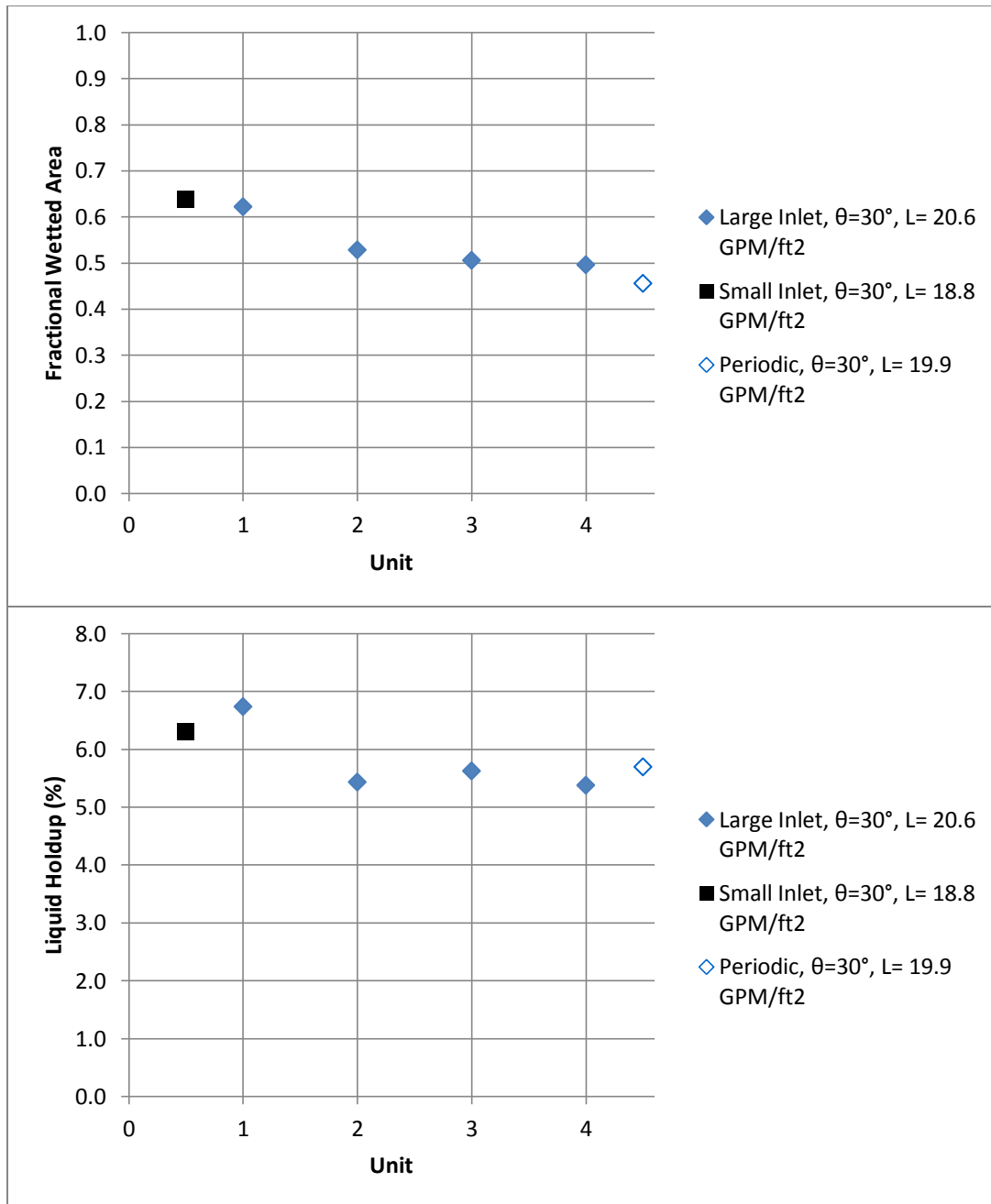


Figure 6-18: Impact of geometry and inlet conditions on fractional wetted area (top) and liquid holdup (bottom) with a contact angle of 30° and a surface tension of 0.074 N/m.

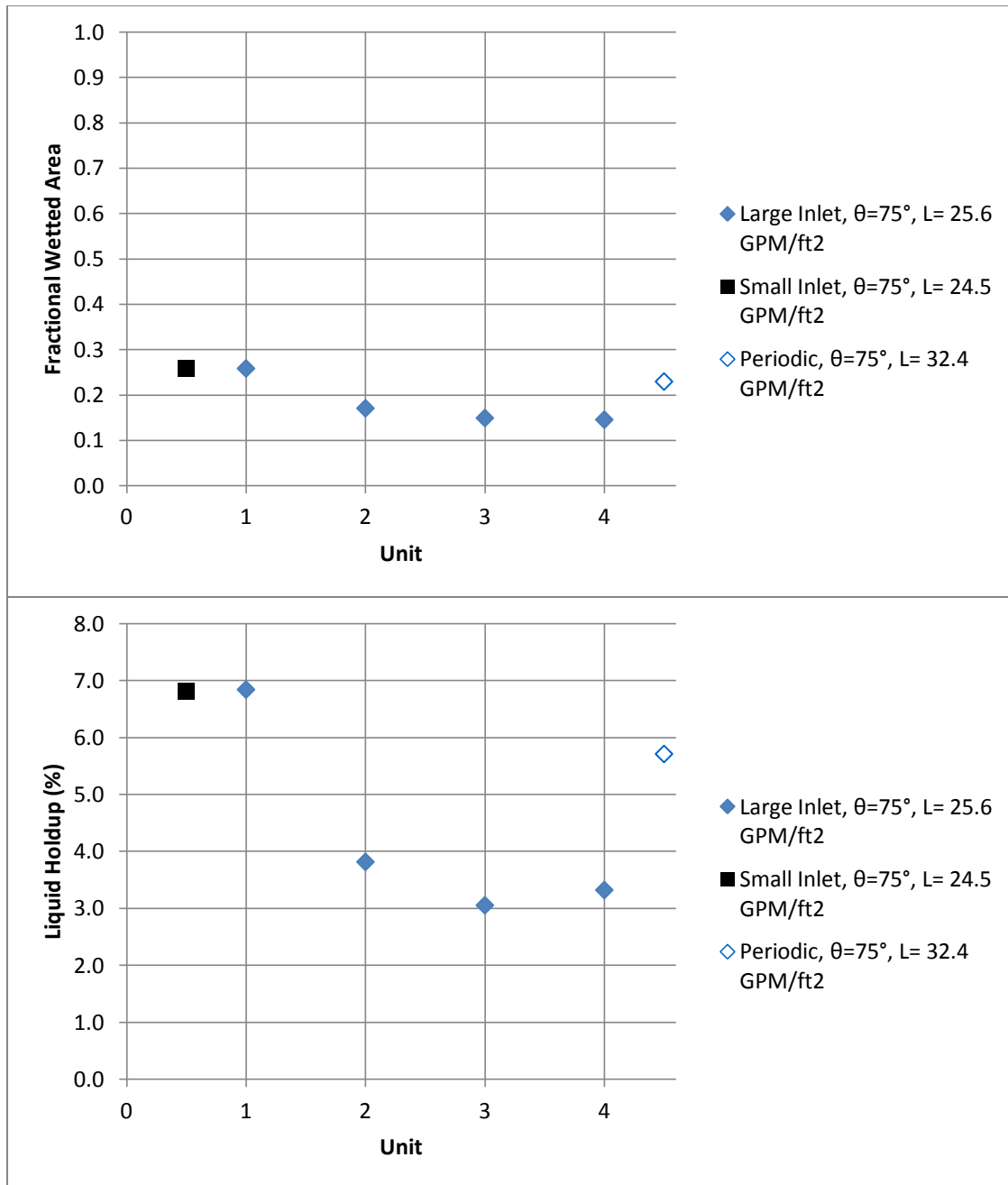


Figure 6-19: Impact of geometry and inlet conditions on fractional wetted area (top) and liquid holdup (bottom) with a contact angle of 75° and a surface tension of 0.074 N/m.

Effect of Turbulence Model – Periodic Geometry

Laminar and turbulent simulations on the periodic geometry were performed to determine if the use of a turbulence model had a significant effect on the wetted area and liquid load. Figure 6-20 shows parity plots comparing fractional wetted area predictions. Each data point in a series represents a different liquid holdup examined. For both the 0° and 30° cases, the fractional wetted area is largely unchanged when using the realizable $k-\epsilon$ turbulence model. The worst deviation is found in the high surface tension case with a contact angle of 0° . The predicted fractional wetted area for the turbulent simulations is 1-5% lower than the laminar simulations. This is most likely due to the turbulence model causing an increase in effective liquid viscosity.

Figure 6-21 shows the predicted liquid loads as a function of flow regime. In all cases, the liquid loads differ by less than 10%. The choice between laminar simulations and turbulent simulations appears to be insignificant when computing fractional wetted area and liquid loads in the range of simulations considered for these studies.

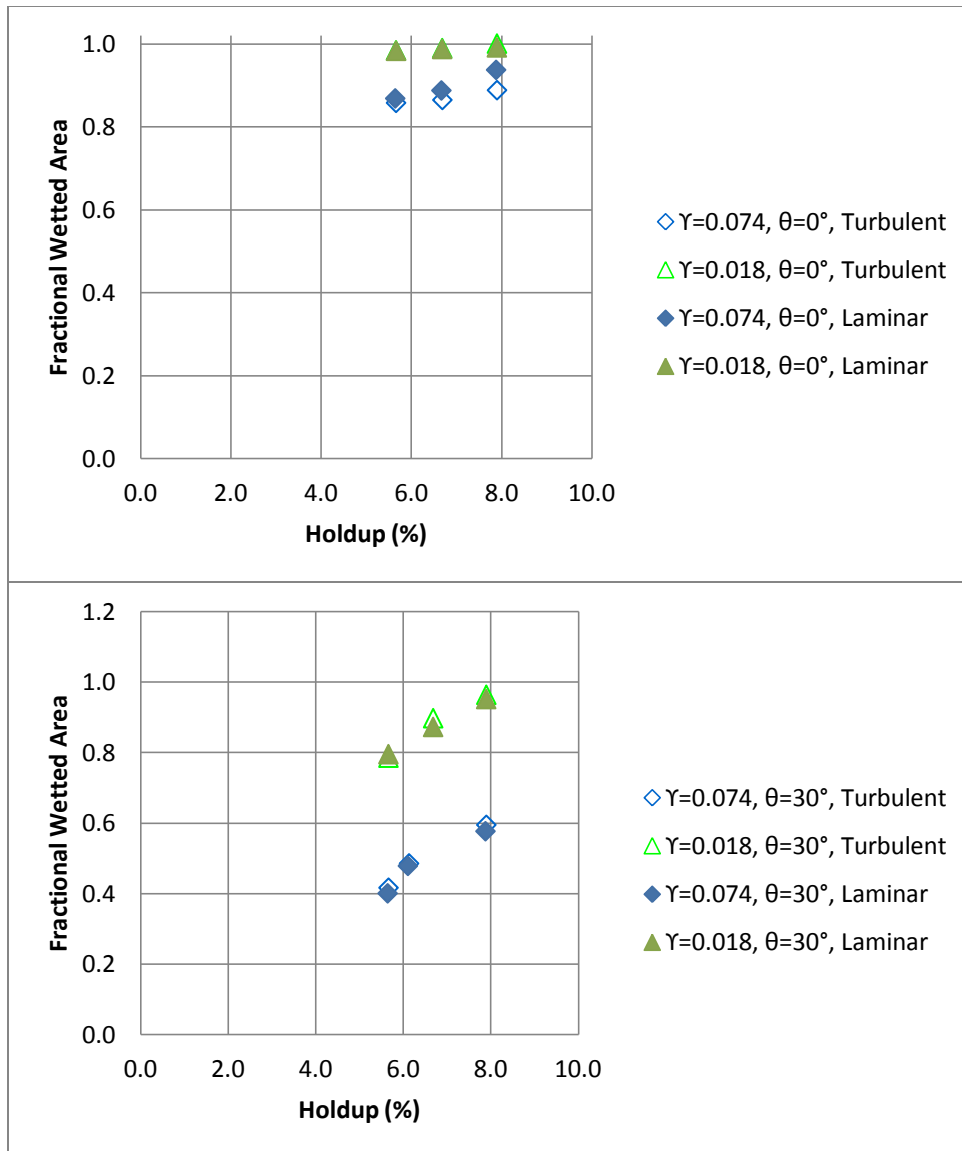


Figure 6-20: Fractional wetted area as a function of liquid holdup and flow regime choice. Laminar simulations are solid markers. Turbulent simulations are hollow markers. High surface tension simulations are diamonds. Low surface tension simulations are triangles. Results for a contact angle of 0° are shown at top. At bottom are results for a contact angle of 30° .

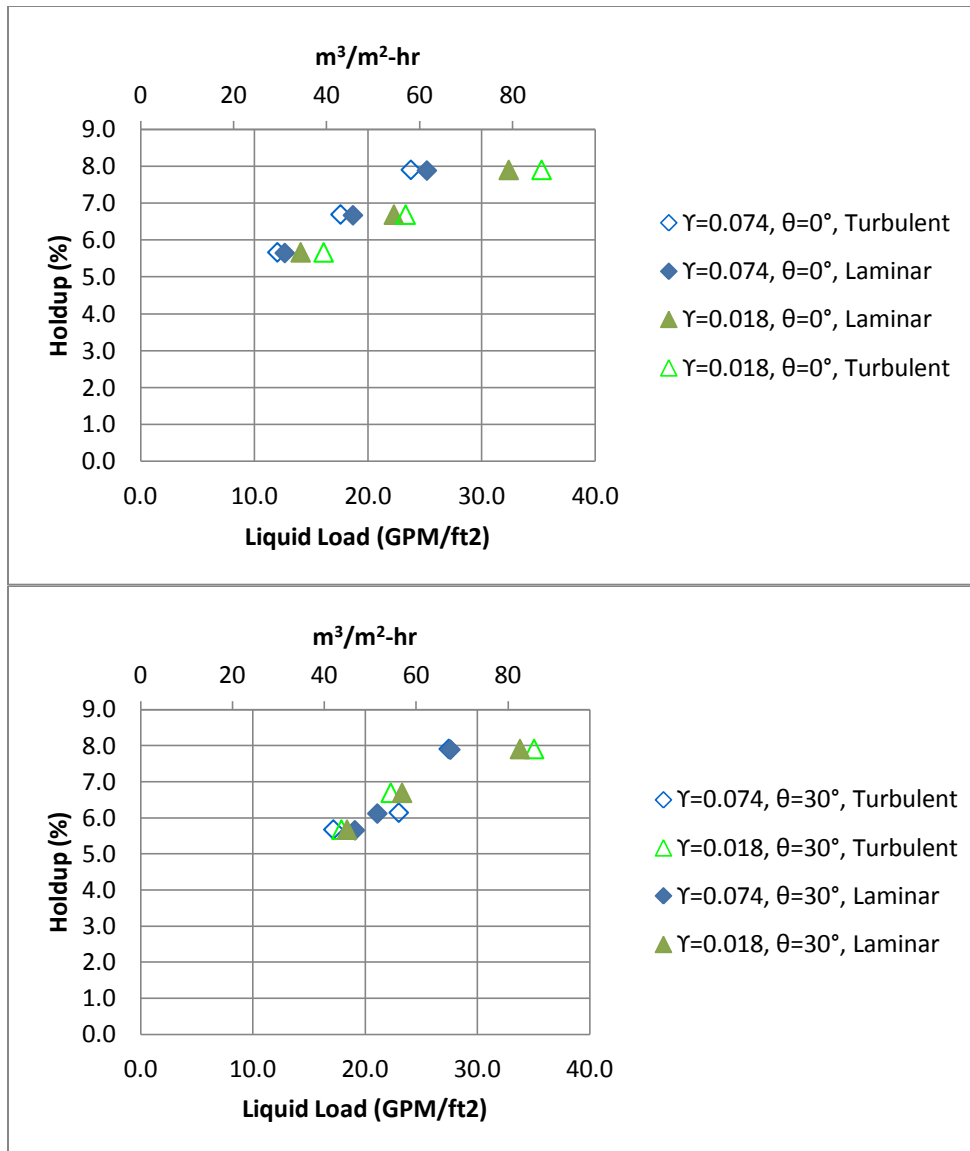


Figure 6-21: Predicted liquid loads as a function of liquid holdup and flow regime. Laminar simulations are solid markers. Turbulent simulations are hollow markers. High surface tension simulations are diamonds. Low surface tension simulations are triangles. Results for a contact angle of 0° are shown at top. At bottom are results for a contact angle of 30° .

Comparison to a Semi-Empirical Models

Liquid holdup was found to be a function of liquid density, viscosity, and liquid load. Specifically,

$$h_L \left(\frac{\rho_L}{\rho_{ref}} \right) \left(\frac{\mu_{ref}}{\mu_L} \right) = A_1(\theta_c) f(Re_L) \quad \text{Equation 6-2}$$

where ρ_L is the liquid density, ρ_{ref} is some reference density (1000 kg/m³ is used here), μ_L is the liquid viscosity, μ_{ref} is some reference viscosity (0.0001 Pa-s is used here), $A_1(\theta_c)$ is some constant that depends weakly on the static contact angle, and Re_L is the Reynolds number defined by Tsai as:⁷¹

$$Re_L = \frac{\rho_L Q}{\mu_L L_p} \quad \text{Equation 6-3}$$

where Q is the volumetric flow rate of the liquid and L_p is the wetted perimeter. L_p can be calculated with the following equation:

$$\frac{L_p}{A_c} = \frac{4s}{bh} \quad \text{Equation 6-4}$$

where A_c is the cross-sectional area of the column. Figure 6-22 shows the results of the above parameterization. Excellent fit of the data is produced with a power law dependence of the modified liquid holdup on the Reynolds number.

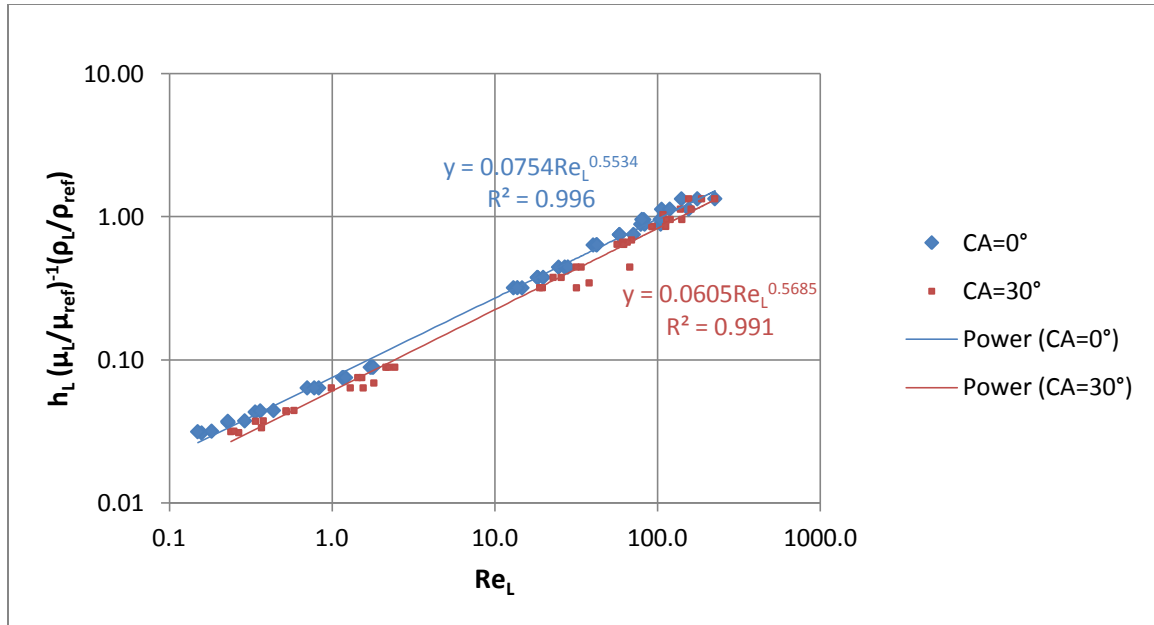


Figure 6-22: Scaled holdup as a function of the liquid Reynolds number.

Taking the exponent of Re_L to be 0.56 and manipulating equation 6-2 yields:

$$h_L = A_1(\theta_c) \left(\frac{Q}{L_p}\right)^{0.56} \left(\frac{\mu_L}{\rho_L}\right)^{0.44} \left(\frac{\rho_{ref}}{\mu_{ref}}\right) \quad \text{Equation 6-5}$$

Thus, it can be observed that the liquid holdup depends on the liquid load raised to a power of 0.56, the liquid viscosity raised to the power of 0.44, and the liquid density raised to the power of -0.44. The power on the viscosity and density term deviates significantly when compared to models developed by Olujic and Tsai.^{23,71} Tsai correlated the liquid holdup as:⁷¹

$$h_L = 21.84 \left[\frac{1}{s^2 g^{\frac{2}{3}}} \left(\frac{\mu_L}{\rho_L}\right)^{\frac{1}{3}} \left(\frac{Q}{L_p}\right) \right]^{0.718} \quad \text{Equation 6-6}$$

Thus, holdup depends on the liquid viscosity raised to the power of 0.24 and the liquid density raised to a power of -0.24. The Delft model from Olujic assumes a laminar liquid film. Specifically, the holdup in the Delft model is calculated as:²³

$$h_L = \delta_{Delft} a_p$$

$$\delta_{Delft} = \left(\frac{3\mu_L U_{LS}}{\rho_L g a_p \sin \alpha} \right)^{\frac{1}{3}} \quad \text{Equation 6-7}$$

where U_{LS} is the superficial liquid velocity. From Equation 6-6, the dependency of holdup on liquid viscosity raised to a term of 1/3. The density is raised to a power of -1/3. The CFD predictions qualitatively predict similar trends. An increase in density results in a decrease in holdup, and an increase in viscosity results in an increase in holdup. The exact dependence, however, deviates significantly. This might be explained due to the geometry chosen. The packing valley and ridge were sharp angles for these studies, inhibiting liquid flow over the channel ridge. In terms of the liquid load, the Delft model depends on the liquid load raised to a power of 1/3. Tsai's holdup model depends on the liquid load raised to a power of 0.718. This places the CFD predictions (liquid load raised to a power of 0.56) within the range observed experimentally. Structured packings have rounded edges, which would allow liquid to spill over more easily, leading to a different preferred flow direction when compared to the CFD simulations. Figure 6-23 compares the CFD model predictions for liquid holdup to the Tsai and Delft models. In most cases, the Tsai model predicts the lowest values for liquid holdup at a given liquid load, and the Delft model predicts the highest values for liquid holdup. The CFD predictions are found between these two models. The holdup values for a contact angle of 0° are always greater than the holdup predictions for a contact angle of 30°.

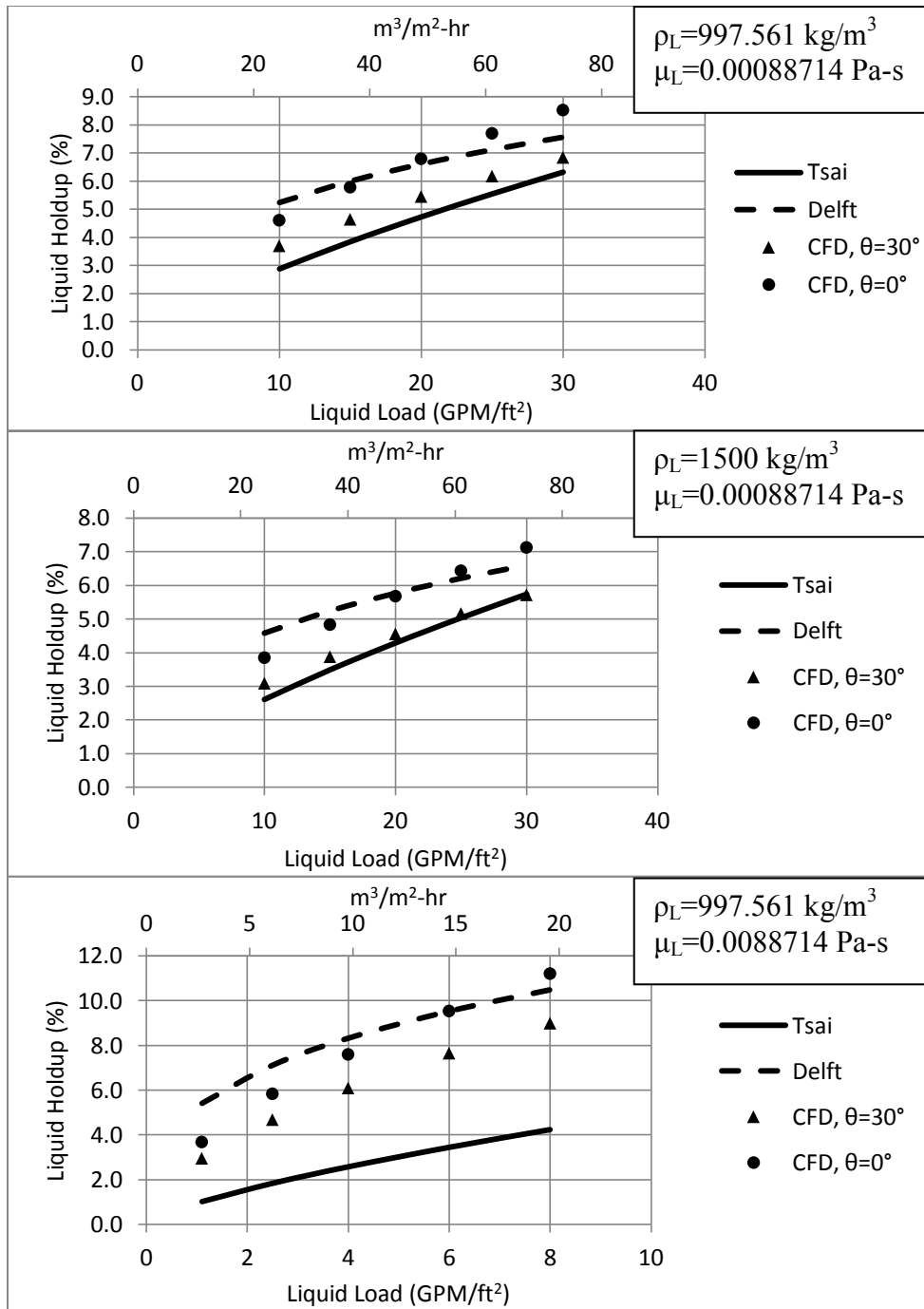


Figure 6-23: Comparison between CFD holdup predictions (at contact angles of 0° and 30°), the Tsai model, and the Delft model for different liquid physical properties. CFD model equations are shown in Figure 6-22. Top: $\rho_L = 997.561 \text{ kg/m}^3$, $\mu_L = 0.00088714 \text{ Pa-s}$. Middle: $\rho_L = 1500 \text{ kg/m}^3$, $\mu_L = 0.00088714 \text{ Pa-s}$. Bottom: $\rho_L = 997.561 \text{ kg/m}^3$, $\mu_L = 0.0088714 \text{ Pa-s}$.

Tsai *et al.* generated a correlation to predict fractional wetted area:²⁹

$$\frac{a_e}{a_p} = 1.34 \left[\left(\frac{\rho_L}{\gamma} \right) g^{\frac{1}{3}} \left(\frac{Q}{L_p} \right)^{\frac{4}{3}} \right]^{0.116} \quad \text{Equation 6-8}$$

Fractional wetted area is a function of liquid density, surface tension, the gravitational constant (9.81 m/s²), the volumetric flow rate, and the wetted perimeter defined by Equation 6-4. Figure 6-24 shows a comparison between the CFD predictions on the periodic geometry and Equation 6-8 for a surface tension of 0.074 N/m. Other liquid properties used are shown in Table 6-1. From this, it is clear the fully-wetting contact angle is the best fit to the semi-empirical model. The CFD predictions are, on average, 5.5% lower than the semi-empirical model, with the deviations growing at higher liquid loads. It should be noted that Equation 6-8 was developed using data for liquid loads less than 73 m³/m²-hr (30 GPM/ft²).

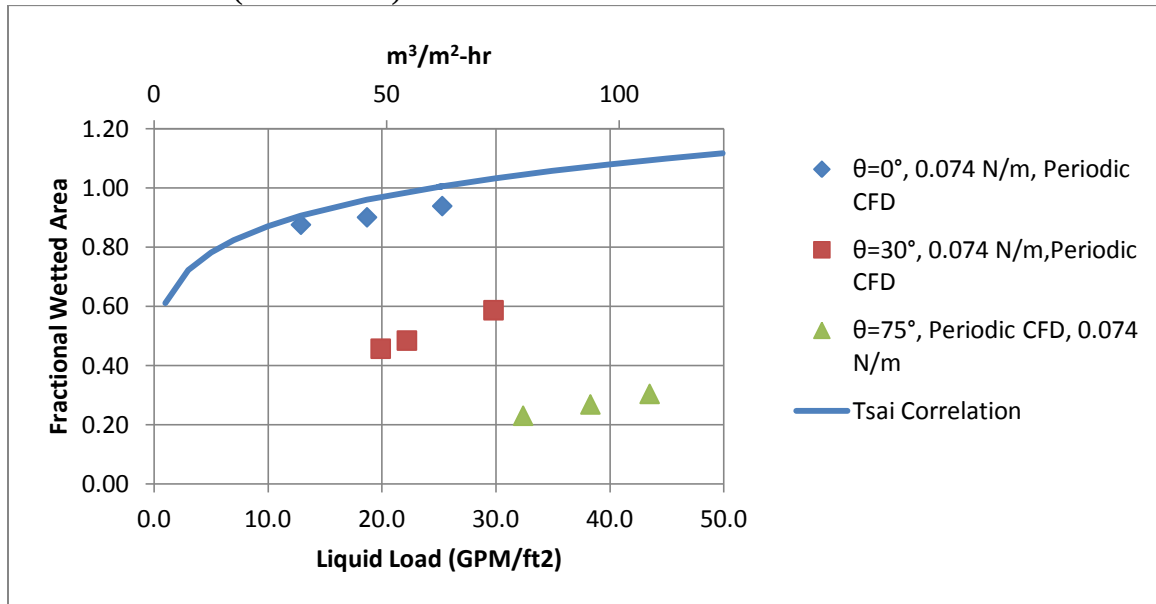


Figure 6-24: Periodic simulations compared to the Tsai correlation. Surface tension was set at 0.074 N/m.

Figure 6-25 shows periodic simulation predictions compared to Equation 6-8 for a surface tension of 0.037 N/m. Again, the fully wetting contact angle demonstrates the most accurate predictions with an average error of 6.8%. However, the CFD predictions are significantly less sensitive to the liquid load than Equation 6-8. This could be explained by the simulation limitations. Specifically, CFD predictions relied entirely on the isosurface created at a liquid volume fraction of 0.5 to compute wetted area. Any mist or satellite droplets formed, leading to enhanced wetted area, would not be captured with these simulations.

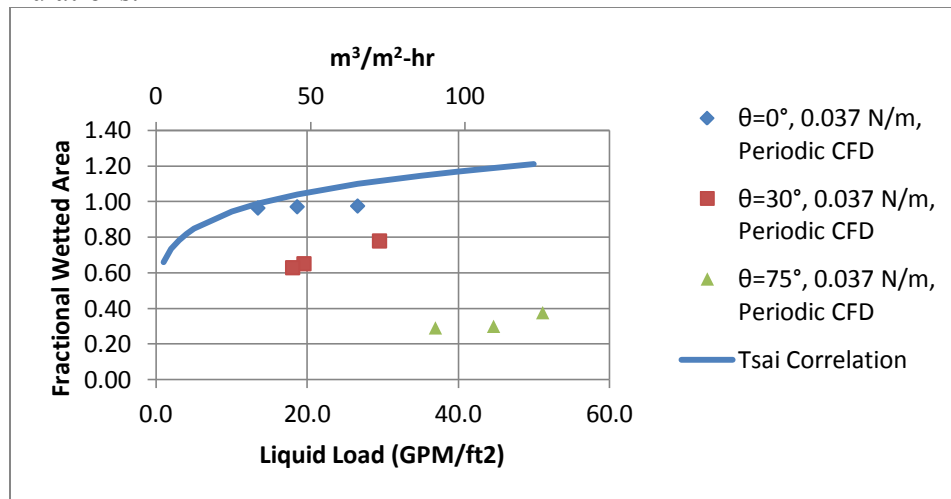


Figure 6-25: Periodic simulations compared to the Tsai correlation. Surface tension was set at 0.037 N/m.

Figure 6-26 compares the periodic simulations to Equation 6-8 at a surface tension of 0.018 N/m. The simulations using a contact angle of 0° again predict wetted areas closest to the correlation with an average error of 14.5%. The wetted area predicted via CFD is not sensitive to the liquid load at the fully wetted contact angle. In the case of the correlation, increased liquid loads always result in increased wetted areas. It should be noted that Equation 6-8 was generated using surface tensions from 0.030-0.072 N/m, which may lead to erroneous predictions at the present surface tension of 0.018 N/m.

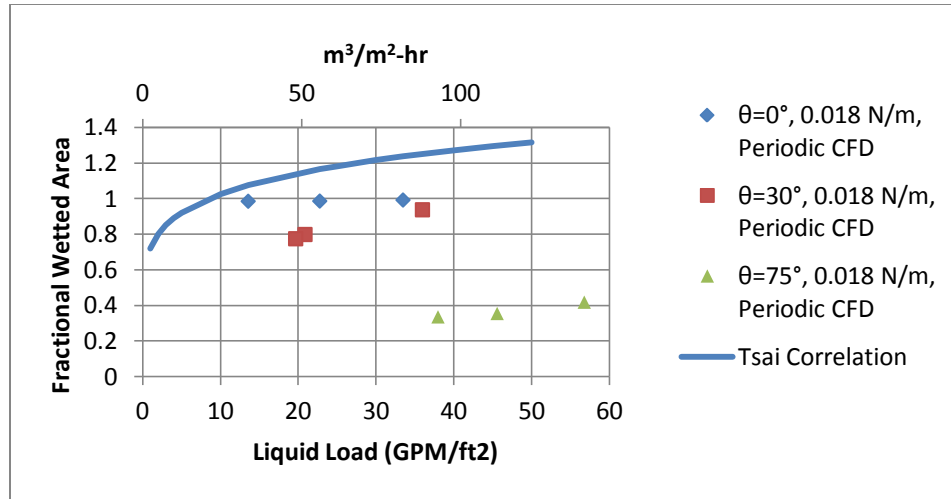


Figure 6-26: Periodic simulations compared to Tsai correlation. Surface tension was set at 0.018 N/m.

PILOT-SCALE SIMULATIONS AND EXPERIMENTAL RESULTS

This section focuses on the validation of CFD predictions as applied to multiphase simulations over a packing geometry generated via X-ray CT scans. Experimental liquid holdup, wetted area, and irrigated pressure drop were measured at the SRP pilot plant in a bed of Mellapak N.250Y consisting of 19 half-elements with a total packed bed height of 3.12 m and an inner column diameter of 0.146 m.

Experimental Data Analysis

The absorption of CO₂ into a dilute caustic solution as a method of determining effective interfacial area was studied by Tsai *et al.*⁶⁰ The authors calculated the effective interfacial area as:

$$a_e \cong \frac{U_{GS} \ln\left(\frac{y_{CO_2,in}}{y_{CO_2,out}}\right)}{Zk'_g RT} \quad \text{Equation 6-9}$$

where U_{GS} is the superficial gas velocity, $y_{CO_2,in/out}$ is the mole fraction of CO₂ in the gas phase at the inlet/outlet, Z is the total packed bed height, k'_g is the liquid phase mass

transfer coefficient, R is the ideal gas constant, and T is the absolute temperature. The liquid phase mass transfer coefficient (k'_g) can be calculated as:

$$k'_g \cong \frac{\sqrt{k_{OH^-} [OH]^- D_{CO_2,L}}}{H_{CO_2}} \quad \text{Equation 6-10}$$

where k_{OH^-} is the second order rate constant, $[OH]^-$ is the sodium hydroxide molarity, $D_{CO_2,L}$ is the diffusivity of CO_2 in the liquid phase, and H_{CO_2} is the Henry's Law constant for CO_2 . These parameters can be estimated as functions of the ionic strength of the solution and the temperature of the system. Full details can be found in the article by Tsai *et al.*⁶⁰ For convenience, a summary of the model is presented in Appendix C. Experimental conditions can be found in Table C-1.

Figure 6-27 shows the experimental results for fractional wetted area. The packing specific area of $215 \text{ m}^2/\text{m}^3$ was used for normalization. For the Tsai correlation, a liquid density of 998.38 kg/m^3 , a surface tension of 0.074 N/m , and a calculated wetted perimeter value of 4.09 m was used. The correlation matches the data very well with errors less than 6%. Increased gas flow rate results in slightly increased wetted areas. Superficial gas velocities ranged from 0.56 m/s to 1.69 m/s . Experiments also demonstrated excellent repeatability as demonstrated by the two sets of data collected at 40 ACFM. Average difference between the repeated runs was 3.0% with a maximum difference of 5.0%.

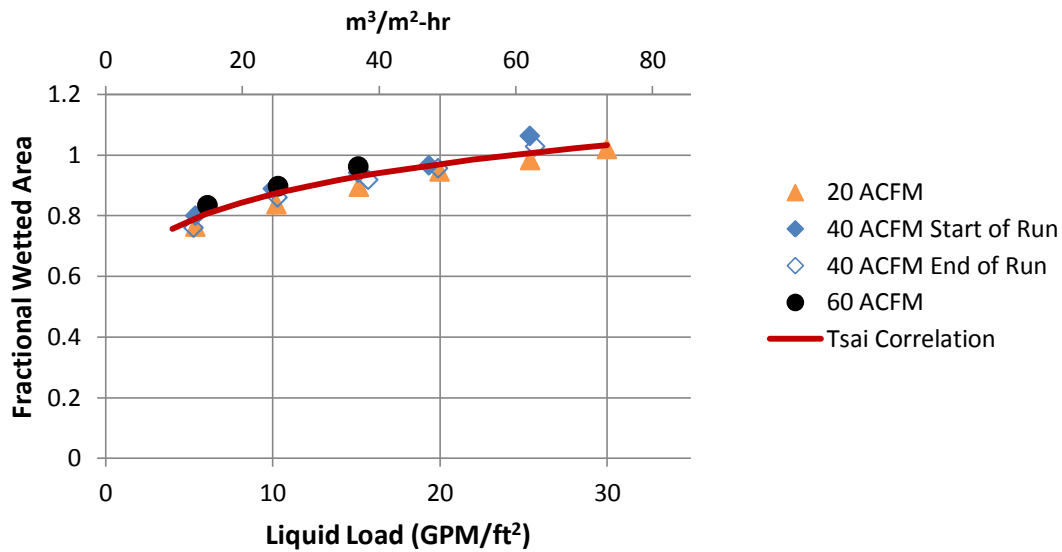


Figure 6-27: Summary of fractional wetted area experimental results.

Figure 6-28 shows the experimentally determined liquid holdup as a function of liquid load. Although these data were collected with a stagnant gas, the values should be applicable to countercurrent flow in the pre-loading regime. Several authors have noted that the liquid holdup does not depend on the superficial gas velocity in the pre-loading regime.^{7,8,72} Liquid holdup exhibits a power law dependence on the liquid load with an exponent of 0.56, which is in line with experimental observations made by the SRP for holdup within structured packing.

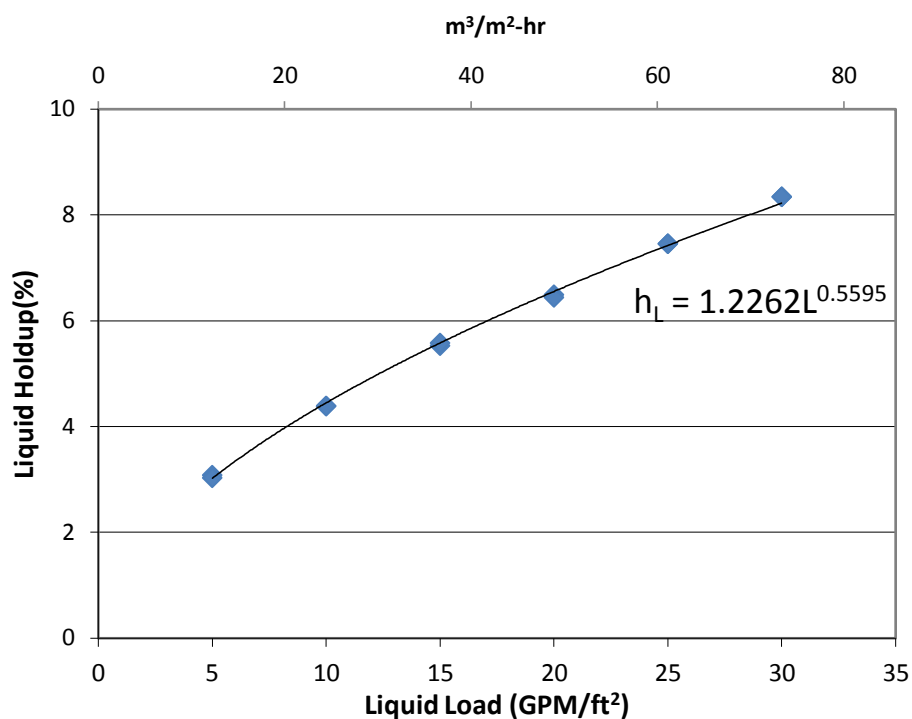


Figure 6-28: Experimental liquid holdup as a function of liquid load.

Simulation Results

Simulations using a CT geometry were performed using contact angles of 0° and 30°. The top pressure was set at 0.0 Pa. The bottom pressure was set at 25.0 Pa. Liquid loads were set at 24.5, 36.7, and 48.9 m³/m²-hr (10, 15, and 20 GPM/ft²). Physical properties used were chosen to be similar to the experimental conditions and are shown in Table 6-4.

Property	Value	Units
Liquid Density	997.561	kg/m ³
Liquid Viscosity	0.00105	Pa-s
Gas Density	1.194	kg/m ³
Gas Viscosity	1.725E-05	Pa-s
Surface Tension	0.074	N/m

Table 6-4: Liquid and gas physical properties used for multiphase CT geometry simulations.

Figure 6-29 shows the liquid surface generated with at a liquid load of $48.9 \text{ m}^3/\text{m}^2\text{-hr}$ (20 GPM/ft²) for a fluid with a contact angle of 0° . This figure was generated by clipping half the packing geometry to expose a single packing sheet. The packing sheets were not perfectly plum, leading to some artifacts of the adjacent packing sheet as indicated by the red arrows. The packing demonstrates nearly complete wetting. Of particular note are two features that can be observed. They are indicated with the green and purple arrows. The green arrow points to where the surface texture is present and influencing the liquid film. There are distinct variations in the liquid film that can be observed, demonstrating that these detailed packing features were captured via imaging and preserved during meshing. Furthermore, the texture has some effect on the predicted liquid flow as evidenced by the disturbances in the liquid film. The purple arrow indicates a perforation that has been completely covered with liquid. Experimentally, this has been observed with X-ray CT scans performed by Green on stainless steel packings as shown in Figure 6-30.⁷³ Like the periodic simulations, liquid accumulation is observed at the contact points between adjacent packing sheets in the multiphase CT geometry simulations. These contact points again serve to aid in liquid mixing and distribution, allowing liquid streams from adjacent sheets to come in direct contact with each other.

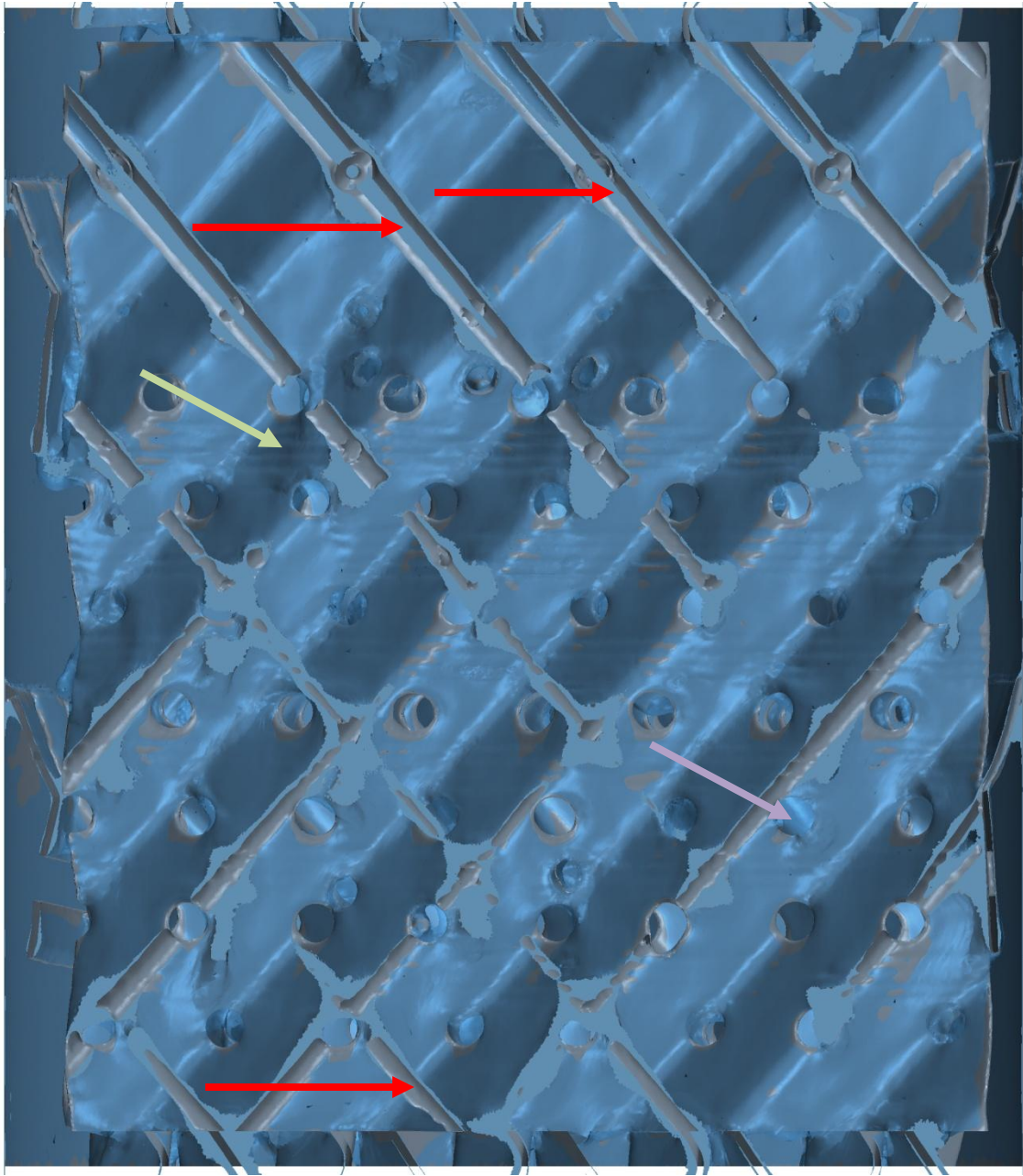


Figure 6-29: Liquid surface generated at a liquid load of $48.9 \text{ m}^3/\text{m}^2\text{-hr}$ ($20 \text{ GPM}/\text{ft}^2$) for a fluid with a contact angle of 0° . Red arrows indicate remnants of the adjacent packing sheet that were not clipped. The green arrow indicates the packing texture. The purple arrow indicates a perforation that has been completely covered by liquid.

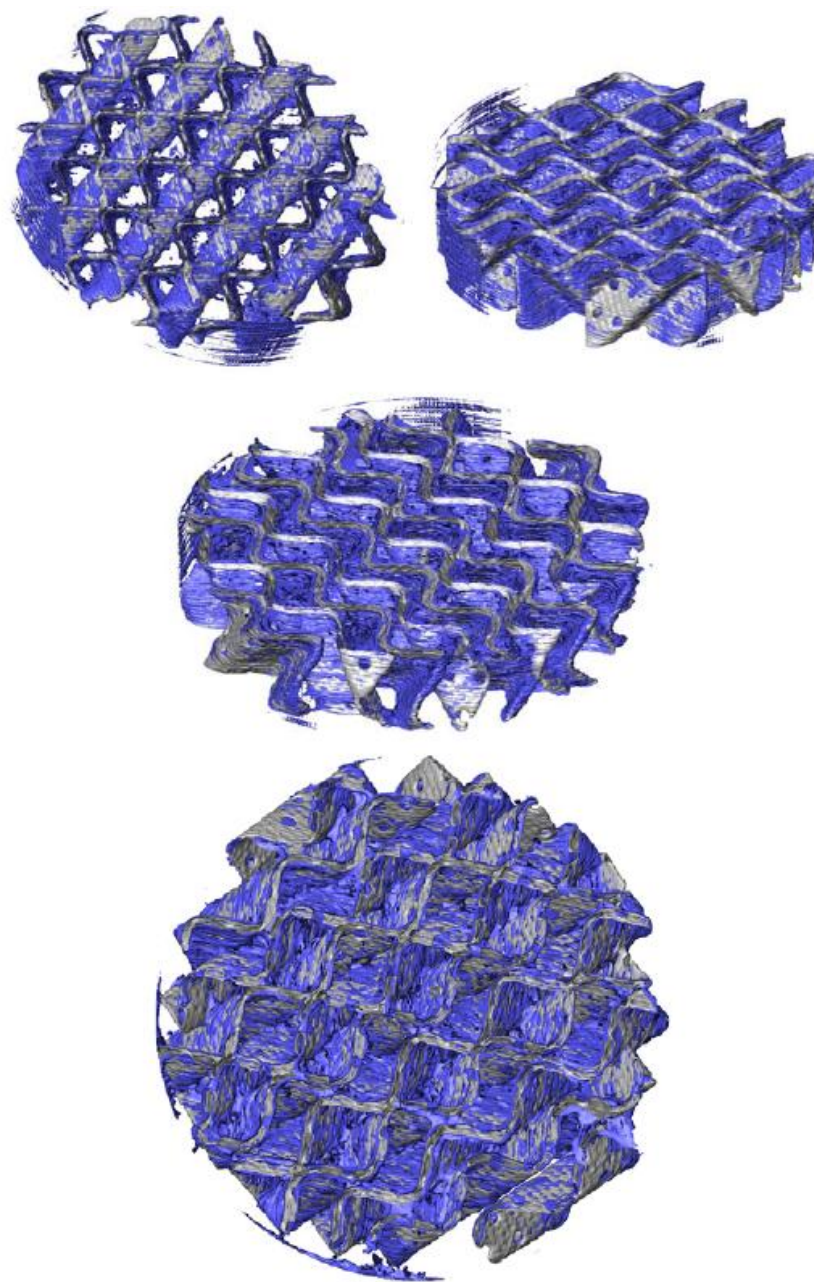


Figure 6-30: Liquid layer isosurface (blue) overlaid on a dry packing image (gray) as viewed from different angles. Images were generated via X-ray CT scans. Liquid load was $36.7 \text{ m}^3/\text{m}^2\text{-hr}$ ($15 \text{ GPM}/\text{ft}^2$). F-factor of the gas was $1.6 \text{ Pa}^{0.5}$. Figure taken from Green.⁷³

Figure 6-31 shows the liquid surface generated at a liquid load of $48.9 \text{ m}^3/\text{m}^2\text{-hr}$ (20 GPM/ft²) with a static contact angle of 30° . Significantly less wetting is observed than for the 0° contact angle case. The green arrow again indicates the packing texture influencing the liquid film. The purple arrow points to a contact point where liquid has accumulated, similar to the periodic geometries. These contact points allow liquid to mix and redistribute across adjacent packing sheets. The red arrow indicates how perforations enhance wetting by splitting rivulets.

When compared to the small-scale simulations, the liquid flow demonstrates a preferred flow direction significantly different than the channel corrugation angle as indicated by the black arrow. The physical properties are similar to those examined in the small-scale geometries, leading to the conclusion that it must be a difference in geometries causing the differences in preferred liquid flow direction observed in the simplified geometries vs. the CT geometry. One of the most significant differences between the simplified geometries and the CT geometry is the edge geometry for the channel valleys and ridges. In the simplified geometries, sharp edges were used. The CT geometry has rounded packing folds. The rounded edges allow the liquid to spill over channel ridges, yielding the preferred flow direction different from the channel corrugation angle. Figure 6-32 shows the liquid surface for a periodic geometry. It was created by “stitching” a periodic simulation result together to form a single packing sheet. In the case of the stitched geometries, a substantial amount of the flow prefers to travel at the channel inclination angle within the packing valley. Only at contact points is liquid observed to transition from the packing ridge to the packing valley below.

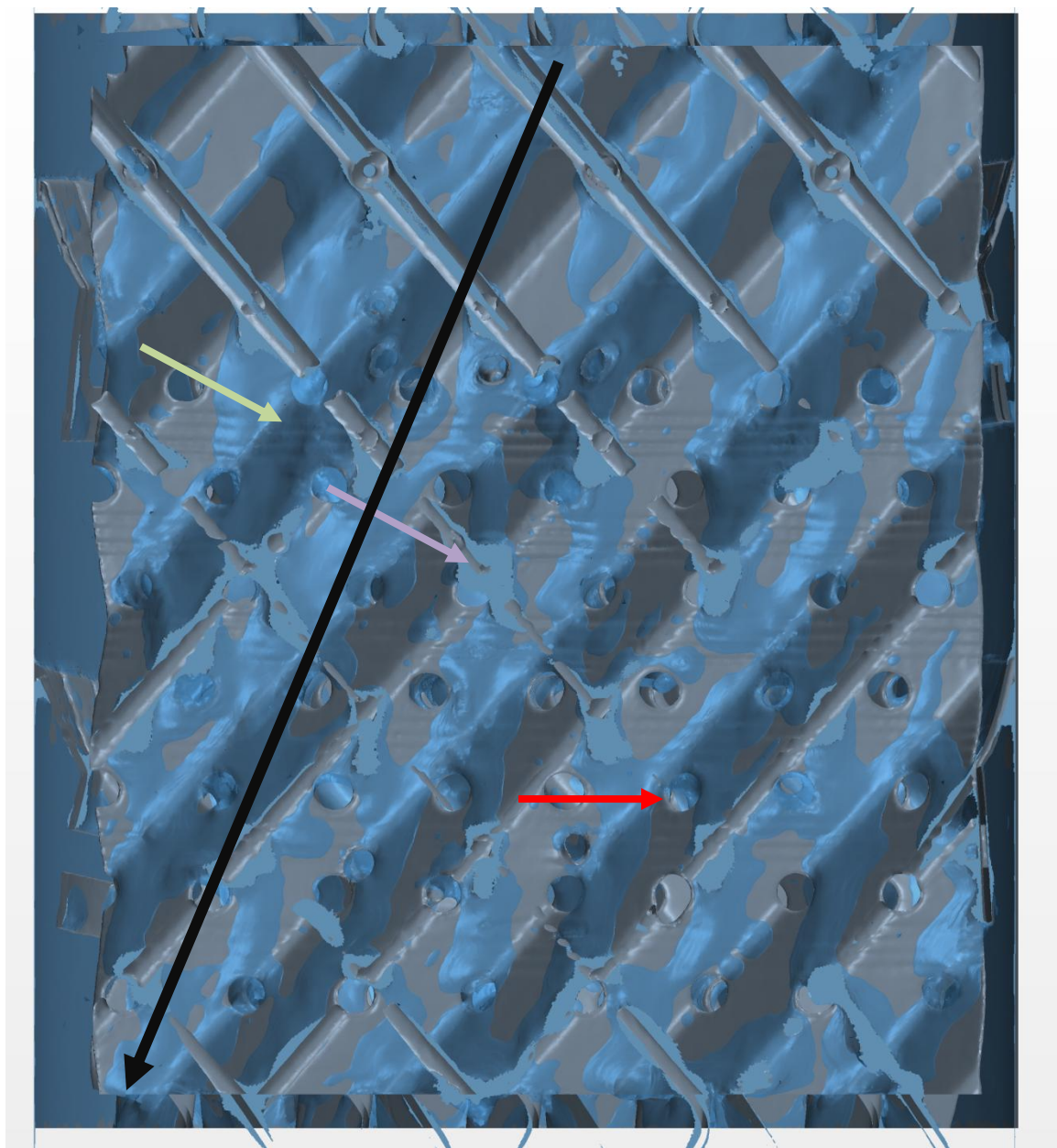


Figure 6-31: Liquid surface generated at a liquid load of $48.9 \text{ m}^3/\text{m}^2\text{-hr}$ ($20 \text{ GPM}/\text{ft}^2$) for a fluid with a contact angle of 30° . The red arrow indicates where perforations enhance wetting by splitting rivulets. The green arrow indicates where the surface texture influences the film. The purple arrow indicates a contact point between adjacent packing sheets. The black arrow indicates a preferred flow direction of the liquid.

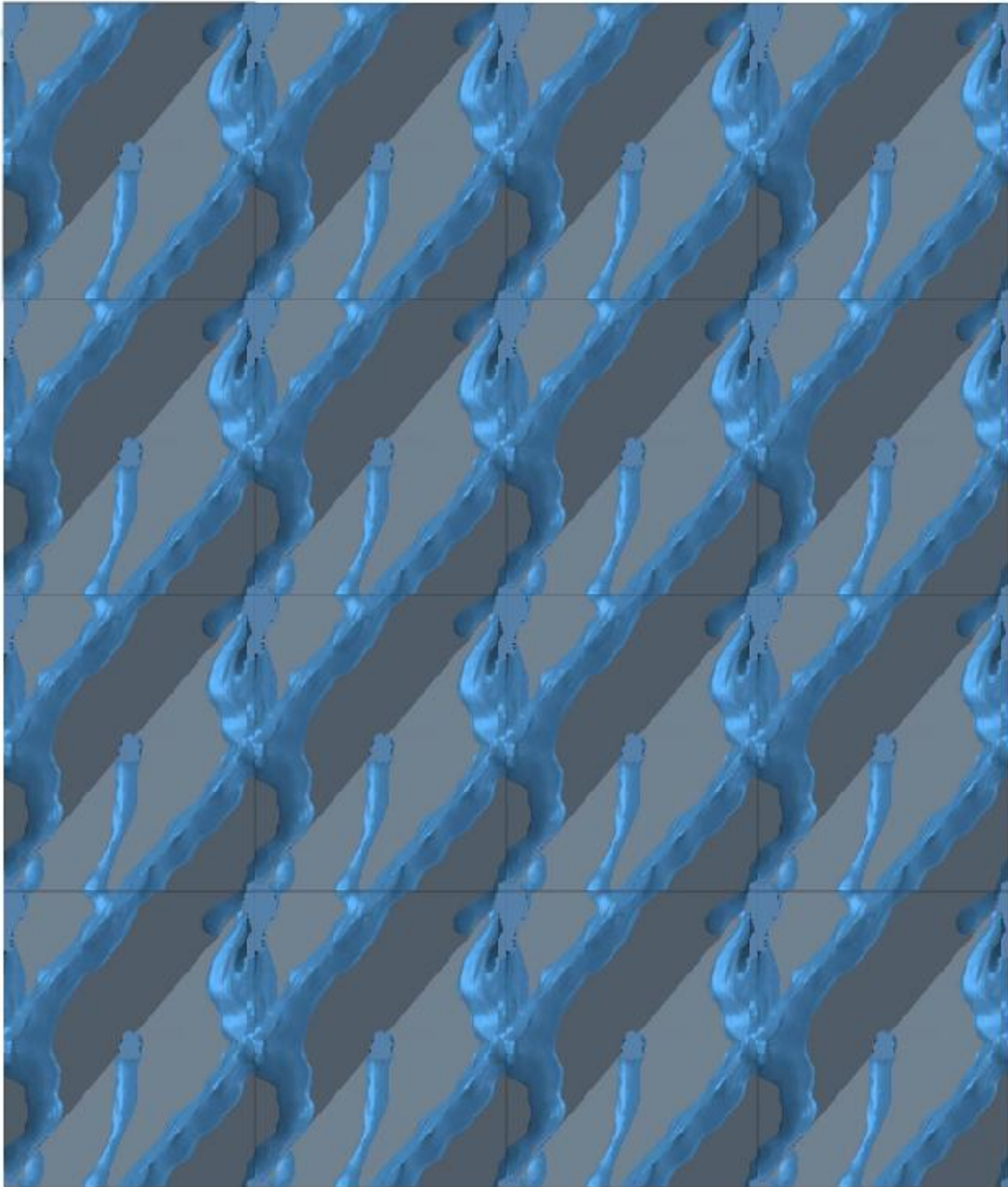


Figure 6-32: Liquid surface generated by stitching periodic packing geometries together. Contact angle was 30° , surface tension was 0.074 N/m , and predicted liquid load was $54 \text{ m}^3/\text{m}^2\text{-hr}$ (22 GPM/ft^2).

Figure 6-33 and Figure 6-34 show the velocity field at two vertical planes. Figure 6-33 shows the velocity field in a plane directly centered between two adjacent packing sheets. Figure 6-34 shows the velocity field at a plane oriented halfway within a packing channel. Figure 6-35 illustrates where the planes are defined relative to each other. In Figure 6-33, the preferred gas flow direction is largely in the vertical direction. Where packing sheets meet, there is a large amount of mixing and turbulence generated due to the differences in the competing horizontal velocities. In Figure 6-34, gas flow is largely along the packing corrugation angle. This is consistent with single phase behavior observed in Chapter 5. Within a channel, a clear horizontal velocity is present. In Figure 6-34, it is clear the preferred horizontal direction is toward the right.

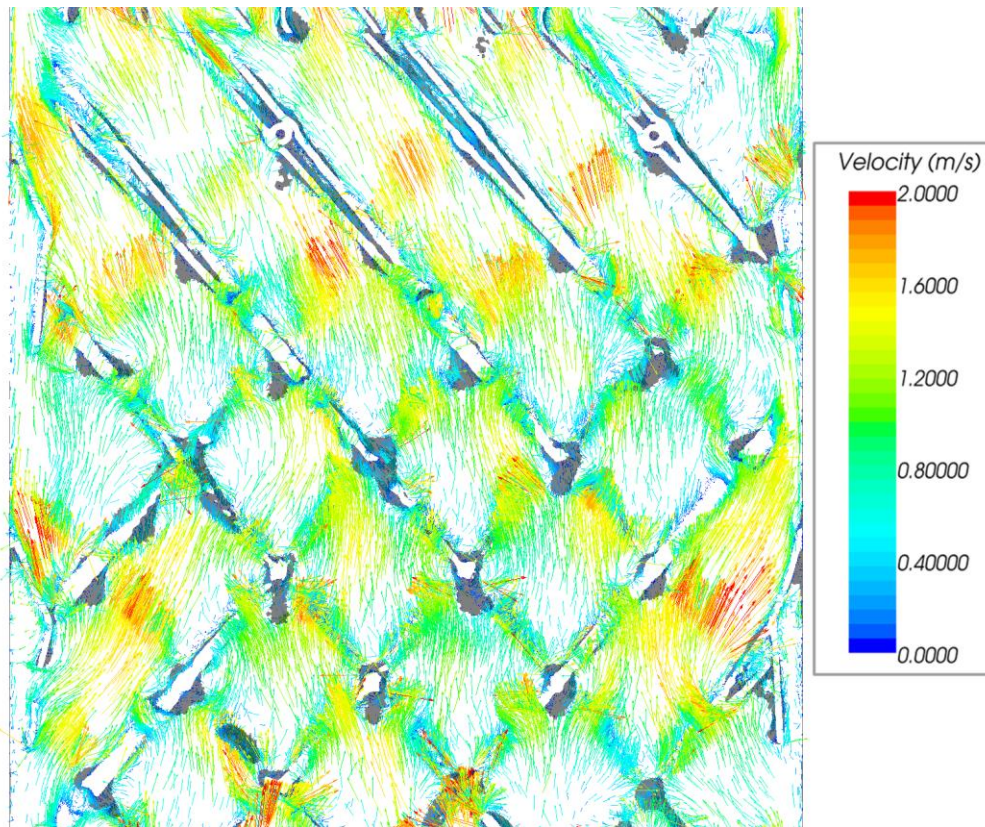


Figure 6-33: Velocity field in a vertical plane where two packing sheets meet.

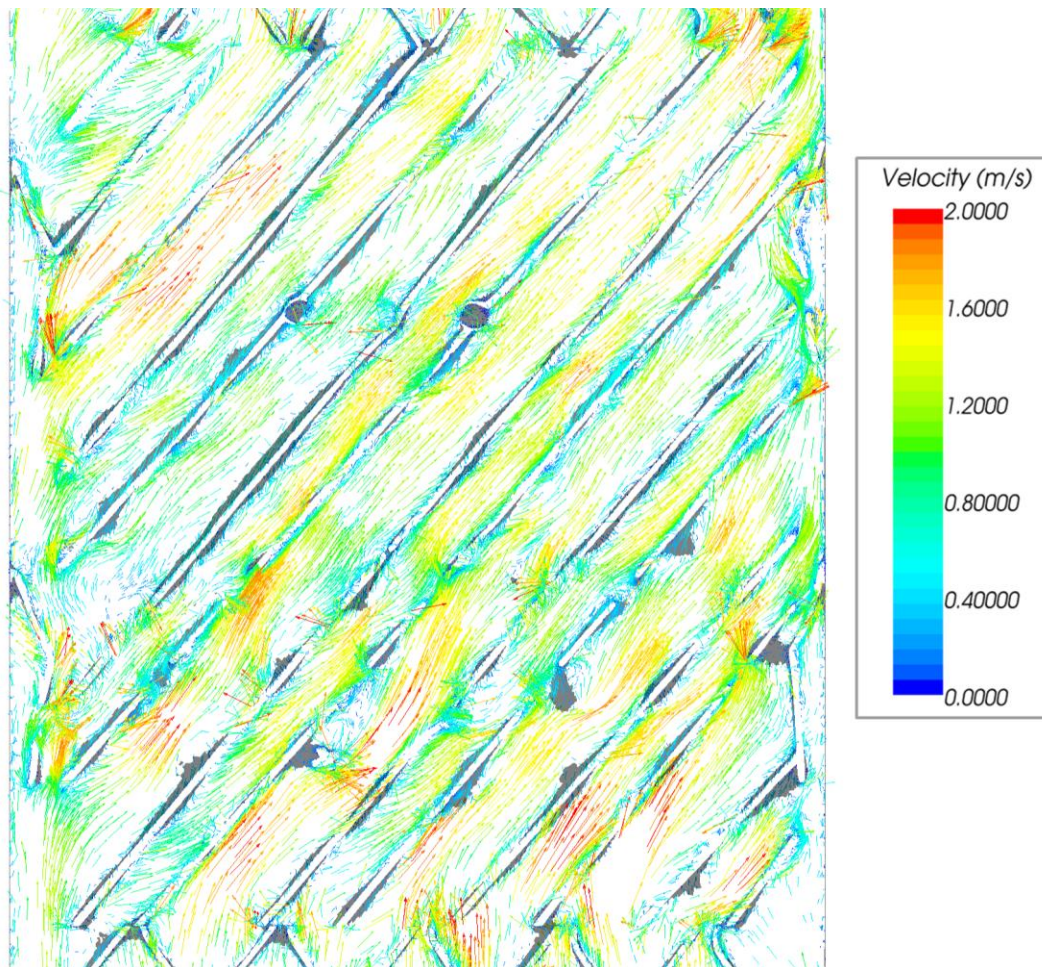


Figure 6-34: Velocity field at a plane halfway within a triangular channel.

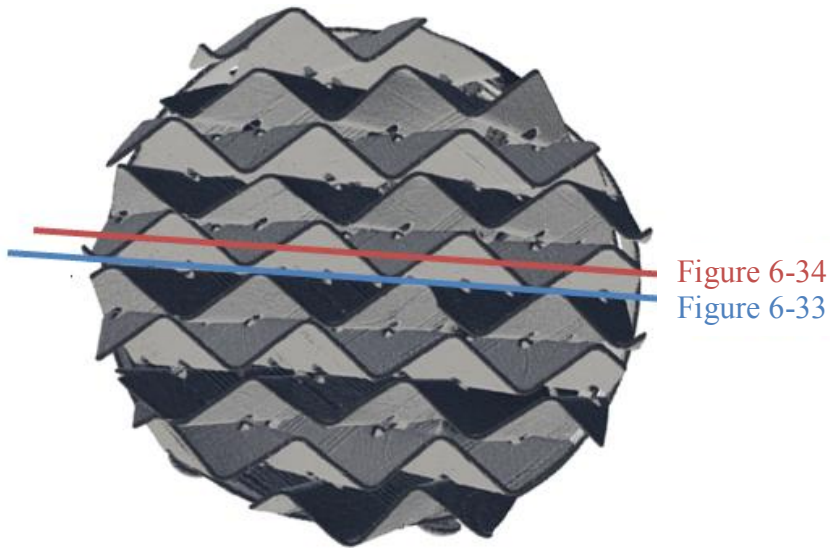


Figure 6-35: Illustration of where the two planes are located for the velocity fields shown in Figures 6-33 and 6-34.

Comparison Between Simulated Data and Experimental Data

Fractional wetted area, liquid holdup, and irrigated pressure drop were examined to determine the ability of CFD to predict experimental data. Figure 6-36 shows the comparison between the Tsai correlation and the CFD predicted fractional wetted area. The Tsai correlation was found to adequately predict the experimental data in a prior section. Thus, the semi-empirical was used to simplify the analysis. CFD simulations using a static contact angle of 0° were found to best represent the experimental predictions with an average error of 3.4%. Simulations using a contact angle of 30° exhibit a lower degree of wetting. On average, the predictions were 32.5% lower than the experimental model. The power law dependence of wetted area on liquid load is under predicted by the 0° simulations and over predicted by the 30° simulations. This is best observed by the regression of the data into a power law form as shown in Figure 6-36. For 0° , the liquid load is raised to a power of 0.080. For 30° , the liquid load is raised to a power of 0.245. For the model developed by Tsai *et al.*, the liquid load is raised to a

power of 0.1547.²⁹ This indicates a contact angle between 0° and 30° would be appropriate to capture the correct liquid load power law behavior. However, it should be noted that any increase in contact angle will result in decreased wetted area.

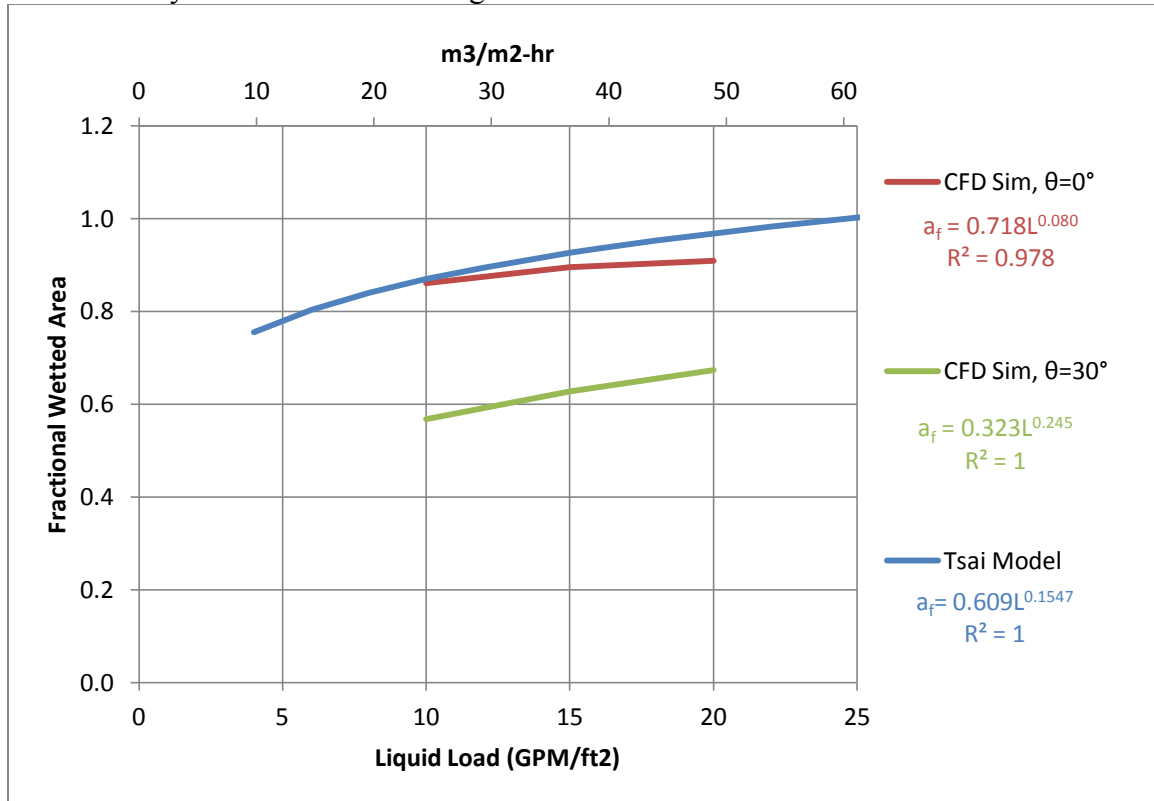


Figure 6-36: Comparison between experimental predictions and CFD simulations for fractional wetted area.

Figure 6-37 shows a comparison of liquid holdup between CFD simulations and experimental data. Liquid holdup was determined via CFD by integrating the liquid volume fraction in the geometric limits of the central packed element in the CT geometry (i.e. from $z=0$ -155.2 mm). In all cases, the CFD predictions over predict the experimental data. On average, the 0° predictions are 27.5% higher than the experimental data. The 30° predictions match better, being only 13.4% greater than the experimental data. Part of the error between the CFD simulations and the experimental data can be explained by the

method used to calculate the holdup in the CFD program. All liquid, even slight volume fractions that were entrained by the gas up the column were used to calculate the holdup. If only the liquid volume under the liquid film (i.e. a liquid volume fraction greater than 0.5) is used for the calculation of liquid holdup, the prediction is improved as shown by Figure 6-38. This is the method employed by Ataki and Bart.³⁸ In this case, the simulation holdup values using a contact angle of 0° are 21% higher than experimental data. The values using a contact angle of 30° are 7.2% higher than experimental data.

The discrepancy for the 0° data is best explained by a limitation of the VOF model implemented in this work. Namely, in the interfacial region, the viscosity is calculated with a simple average:

$$\mu = \alpha_L \mu_L + (1 - \alpha_L) \mu_G \quad \text{Equation 1-30}$$

This can lead to unphysical high viscosities in the interfacial region, allowing for significantly more momentum to be transferred from the gas to the liquid. A possible solution presented by Hashmi *et al.* is to prescribe the viscosity of the liquid as a function of volume fraction.⁷⁴ The authors also damped the turbulent viscosity in the interfacial region to prevent unphysical momentum transfer due to turbulence. In this manner, they were able to achieve significantly better fit with experimental data for shear-driven liquid wall films. These corrections are recommended for examination in future work.

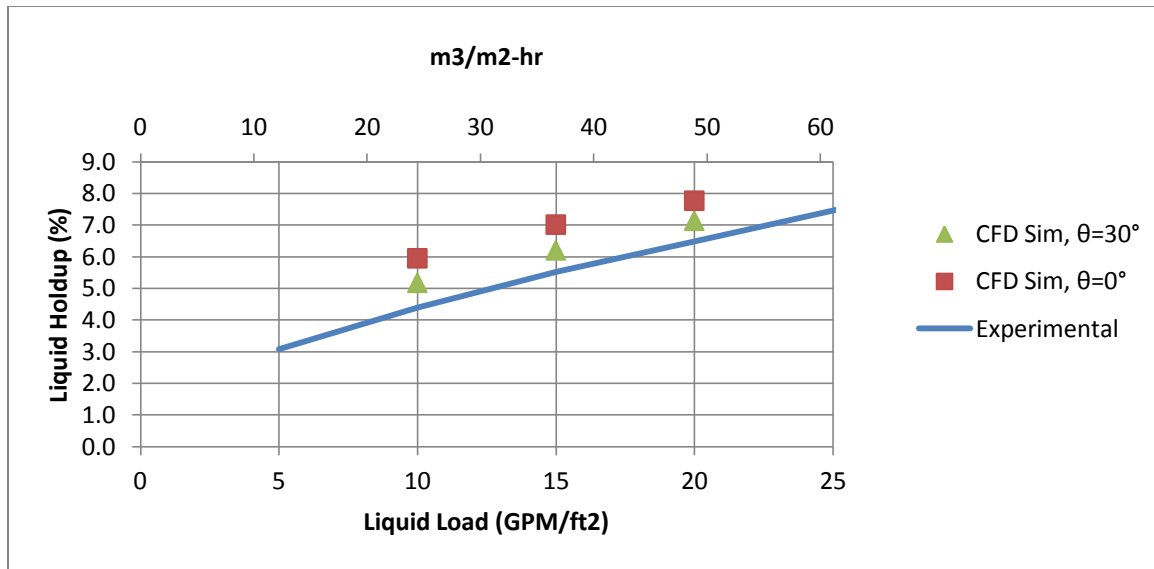


Figure 6-37: Comparison between experimental predictions and CFD simulations for liquid holdup. All liquid volume fraction was used to calculate the holdup in the CFD simulations.

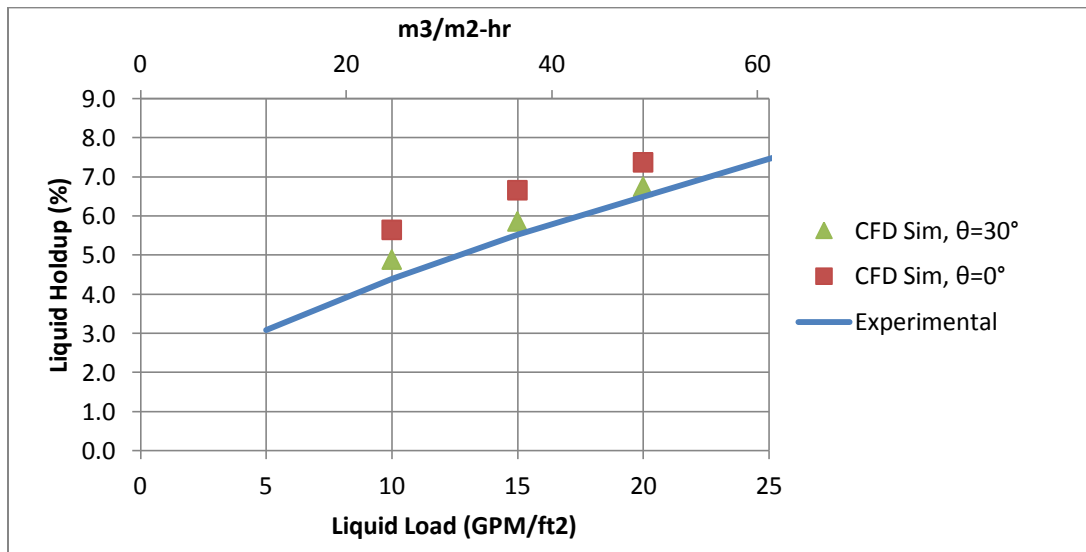


Figure 6-38: Comparison between experimental predictions and CFD simulations for liquid holdup. Only liquid volume fractions greater than 0.5 were used to calculate the CFD values.

Figure 6-39 shows a comparison of irrigated pressure drop data. Each plot represents a different liquid load. The top plot corresponds to a liquid load of $24.5 \text{ m}^3/\text{m}^2$ -

hr (10 GPM/ft²). The middle is 36.7 m³/m²-hr (15 GPM/ft²), and the bottom is 48.9 m³/m²-hr (20 GPM/ft²). CFD pressure drop was calculated in planes at the z=0.0 mm and z=155.3 mm, corresponding to the start and end of the central packing element. In all cases the CFD predictions overestimate the irrigated pressure drop. Using power law regressions to relate the experimental pressure drop to the F-factor, it is possible to estimate what the experimental pressure drop would be at the F-factors from the CFD simulations. The power law regressions are shown in each figure. The percent errors for the CFD predictions are shown in Table 6-5. The pressure drop is least accurate for a contact angle of 30°. The average percent errors are 37.0% for the 0° contact angle simulations and 47.4% for the 30° contact angle simulations. The predicted pressure drop is most accurate at increased liquid loads. The large discrepancy between experimental data and CFD predictions might again be due to limitations of the VOF model implementation for interfacial turbulence and shear. Specifically, the averaging of material properties in the interfacial region and false momentum transport across the interface due to the turbulent stresses are expected to cause inaccuracies in the gas flow field, and thus errors in pressure drop predictions. The corrections proposed by Hashmi *et al.* may correct the inaccurate predictions.⁷⁴

Contact Angle °	Liquid Load m ³ /m ² -hr	Liquid Load GPM/ft ²	CFD F-factor Pa ^{0.5}	CFD Pressure Drop Pa/m	Experimental Pressure Drop Pa/m	Percent Error
0	24.5	10	0.86	74.7	52.0	43.5%
0	36.7	15	0.77	74.4	52.1	42.7%
0	48.9	20	0.69	73.4	58.8	24.8%
30	24.5	10	0.82	73.1	47.6	53.6%
30	36.7	15	0.73	71.4	46.7	52.8%
30	48.9	20	0.66	73.5	54.1	35.8%

Table 6-5: Summary of irrigated pressure drop predictions.

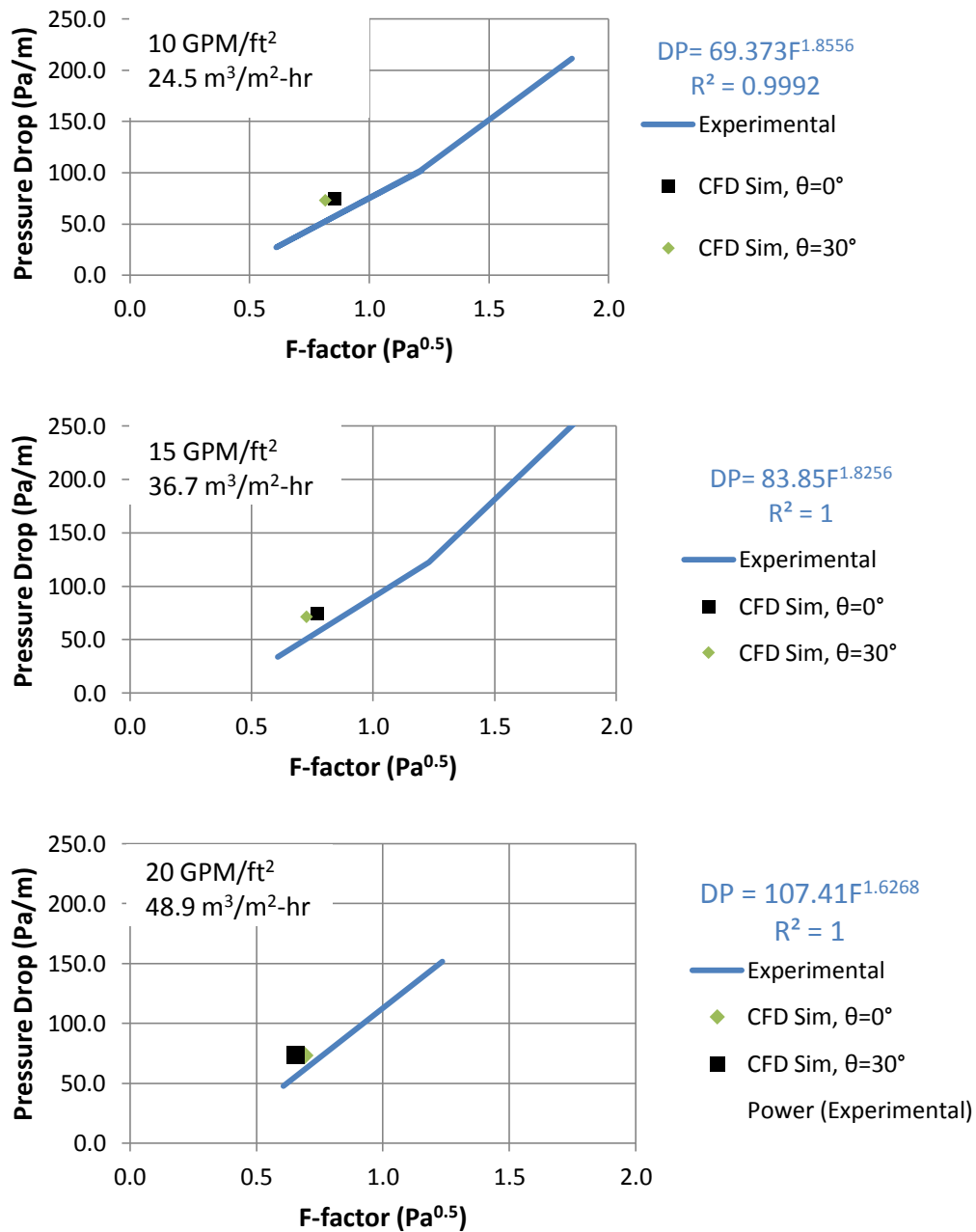


Figure 6-39: Comparison between experimental data and CFD simulations for irrigated pressure drop. Top is a liquid load of 10 GPM/ft², middle is 15 GPM/ft², and bottom is 20 GPM/ft² (24.5, 36.7, and 48.9 m³/m²-hr respectively).

Chapter 7: Conclusions and Recommendations

SUMMARY OF WORK AND CONCLUSIONS

The summary and conclusions are broken into two main sections. The first deals with the single phase simulations performed. Meshing enhancements, turbulent model recommendation, and the influence of channel geometrical parameters on the flow field and pressure drop are summarized. The second covers the multiphase simulations and experimental comparisons. The influence of boundary conditions and hydrodynamic properties are considered. Comparisons between experimental data and simulations using a detailed geometry created via X-ray CT are considered.

Single Phase Conclusions

A highly detailed packing geometry was created by performing X-ray CT scans. The packing element was placed in an aluminum tube for scanning. After reconstruction, a surface mesh file (.STL) was generated for import into STAR-CCM+. In regions where the wiper band contacted the wall, additional post processing was necessary. Defects in the geometry where the wiper bands contacted the aluminum wall during X-ray scanning were eliminated via Boolean subtraction using a CAD geometry designed to remove any features extending beyond the desired simulation geometry. This method of post processing could be applied to any other packing geometries generated, leaving a digital representation with the desired diameter.

Adjacent packing elements are usually rotated 90° relative to each other to redistribute gas and liquid. Single phase simulations and experiments demonstrated reduced pressure drop when the packing elements were not rotated relative to each other. Simulations demonstrated that this is due to significant back flow caused by the sudden direction change in the packing element when the elements were rotated. This back flow

was observed for all non-zero joint rotation angles examined (30°, 60°, and 90°). Comparisons to experimental data showed CFD under predicted the experimental data by roughly 20% using the SST k- ω model. The difference in pressure drop between the 90° and 0° geometries for experimental and simulations was within 10%, indicating CFD simulations can accurately predict the effect of modifying the bed geometry.

CFD simulations were performed using two well-known turbulence models. Specifically, the SST k- ω and the realizable k- ϵ were compared. The realizable k- ϵ performed best with average deviations between experimental data and CFD simulations being less than 15%. The SST k- ω performed slightly worse with average deviations less than 20%. Both CFD simulations performed better than the Stichlmair semi-empirical model. Furthermore, the CFD simulations were able to better capture the power law dependence of the pressure drop on the F-factor than the semi-empirical model. It should be noted, however, that the realizable k- ϵ model only performs best for Mellapak N250.Y simulations. Additional verification would need to be performed if a different packing were examined.

In an effort to increase the accuracy of CFD simulations, a prism layer meshing study was performed. Prism layers allow the boundary layer present near the packing surface to be accurately resolved, allowing for increased accuracy on the prediction of the wall shear stress. A study concluded that resolving the near-wall region leads to an increase in predicted skin friction, and thus an increase in pressure drop. At an F-factor of $3.05 \text{ Pa}^{0.5}$, the predicted pressure drop using the realizable k- ϵ turbulence model was 7% lower than experimental measurements when using prism layers. Without prism layers, the predicted pressure drop was 11.6% lower than experimental measurements.

Pressure drop in the packing bulk was examined through the use of periodic geometries. A wide range of corrugation angles, channel opening angles, and packing

specific surface areas were examined in an effort to determine how each parameter influences dry pressure drop within structured packing. Channel opening angles from 30-150°, corrugation angles from 40-75°, and packing specific areas from 122-650 m²/m³ were examined. A maximum pressure drop was found when the channel opening angle was 90°, which is the channel opening angle of many commercial types of packing

Two mechanisms were identified as key to developing a pressure drop model. The first was termed the shear pressure drop, which was caused by opposing horizontal velocities as gas moves up the triangular channels. This mechanism depended on the channel side length and the horizontal velocity. The second mechanism identified was skin friction. Skin friction depended on the effective gas velocity and packing specific area. CFD simulations and the regressed model showed that pressure drop depended strongly on the channel opening angle. For a given superficial gas velocity, pressure drop depended strongly on corrugation angle. Increased corrugation angle resulted in decreased pressure drop. Finally, increased packing specific area resulted in increased pressure drop due to both increased shear and friction pressure drops.

From a hydraulic view point, using a channel opening angle other than 90° would allow increased capacity for a given separation. However, the impact the channel geometry has on mass transfer remains unknown. Mass transfer results are expected to depend largely on the liquid/vapor system being examined. In the case of processes where the liquid side mass transfer resistance is dominant, the gas phase turbulence would have little effect. Thus, minimization of pressure drop should be attempted. If the gas side mass transfer resistance is dominant, the mass transfer would be coupled to the gas phase turbulence, and thus the pressure drop. Any geometry that reduces pressure drop may also result in decreased mass transfer. The impact of channel geometry on wetted area remains unknown. Because interfacial area is a key parameter influencing the

separation, it should be examined as part of any study optimizing a packing geometry for a specific separation.

The impact of the channel geometry on the velocity flow field was examined in an effort to understand how the channel opening angle influenced the total pressure drop. Geometries with channel opening angles of 30°, 90°, and 150° were examined using unsteady simulations by using large eddy simulations. At a channel opening angle of 90°, pressure drop was maximized due to swirling flow dominating the entire cross section. When a channel opening angle of 30° was used, the sizes of the vortices were confined by the narrow triangular channels. This led to a zone of flow that was directed up the corrugation angle with little to no swirl near the apex of the triangular channel. In the case of a channel opening angle of 150°, no persistent flow swirl or preferential horizontal velocity within the packing channels was observed.

Comparisons between turbulence models within the periodic geometries showed the SST k- ω model demonstrated the highest predicted gas velocities for a given pressure drop. The F-factors predicted were generally within 15% of the realizable k- ϵ model predictions. Large eddy simulations demonstrated F-factors that were slightly less than the values predicted by the realizable k- ϵ model.

Multiphase Conclusions

A wide range of hydrodynamic properties were examined on periodic geometries. The first step was evaluating appropriate mesh settings on the packing geometry. It was found that 15 prism layers within 1.0 mm of the packing surface were required to achieve grid independent results for the fluid simulations examined. An example of the mesh required is shown in Figure 7-1 with the volume fraction of liquid shown in red and the

gas is blue. When compared to single phase simulations, smaller minimum and target cell sizes were required for multiphase simulations.

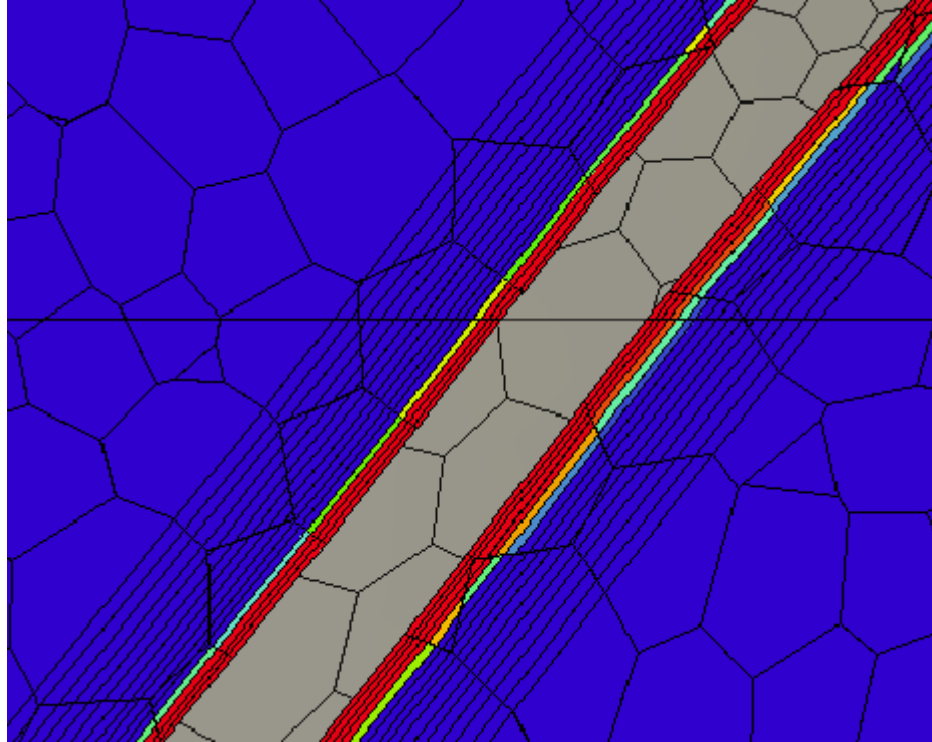


Figure 7-1: Example of prism layer mesh applied to the multiphase CT-generated geometry. Pure liquid is indicated by red shading. Pure gas is blue.

The prescribed static contact angle plays a significant role in determining the type of flow regime observed in the liquid. The three contact angles examined were all considered wetting. Contact angle values of 0° , 30° , and 75° were studied. At a contact angle of 0° , the liquid was a film covering nearly all the packing surface. When the contact angle was set at 75° , the liquid formed into a thin rivulet, leading to very little wetted area. Simulations with a contact angle of 30° exhibited intermediate behavior.

Three surface tensions were examined at each contact angle in the periodic simulations. For the 0° simulations, as surface tension was reduced, wetted area increased. This was due to the liquid being able to spill over the packing ridge at all

points. At high surface tensions, the liquid could only be distributed into the channel valley at contact points between adjacent packing sheets. At a contact angle of 30° , liquid was predominantly rivulet flow at the highest surface tension. When surface tension was reduced, the liquid transitioned into film flow, nearly wetting the entire packing surface. For a contact angle of 75° , lower surface tension only served to widen the rivulet. Film flow was never observed as evidenced by wettings always below 50%.

Next, the effect of density on wetted area was examined within periodic simulations at constant liquid holdup. Liquid densities of 500, 997.561, and 1500 kg/m^3 were examined. Higher densities were associated with increased wetted areas for a given liquid holdup. This was explained by the fact the liquid's weight (i.e. the gravitational force) acts to spread the liquid over the packing ridge to generate wetted area. As density increases, the weight of the liquid film increases, leading to more wetted area. This effect was observed for both the 0° and 30° contact angles. It should be noted that the non-dimensional model of Tsai *et al.* predicts an increase in liquid density will lead to an increase in wetted area.²⁹

Finally, the influence of liquid viscosity was examined. Liquid viscosities of 0.0008871, 0.008871, and 0.01774 Pa-s were examined. Wetted area proved to be a weak function of viscosity for a given liquid holdup. Highest wetted areas were observed at the lowest liquid viscosity. At the lowest viscosity, the liquid surface had noticeable disturbances with variations in film height. These variations would help to force fluid over the packing ridge, leading to increased wetted area. At high viscosities, the liquid film was uniform, and liquid could only be distributed into the packing valley at the contact points between adjacent packing sheets. If instead of constant liquid holdup, a constant liquid load was prescribed, it would be expected that the high viscosity fluids would demonstrate increased wetting. This is purely because increased viscosity will lead

to increased liquid holdup for a given liquid load. Thus, as demonstrated by the simulations, increased liquid holdup results in increased wetting until the surface is completely covered. If experiments are undertaken to study this behavior, it would be prudent to study the liquid loads in which incomplete wetting is observed for the low viscosity liquids.

Periodic simulations were then compared to two geometries with ideal liquid distribution (i.e. perfect liquid film being deposited around the packing perimeter). The first geometry (Small Inlet) had liquid inlet attached to one repeating packing unit. The second geometry (Large Inlet) had the liquid inlet with four repeating packing units below. When compared to the periodic simulations, the Small Inlet geometry demonstrated higher wetted areas and liquid holdups. The Small Inlet geometry simulation results compared favorably to the first repeating unit in the Large Inlet geometry. Subsequent repeating units of the packing demonstrated noticeably less liquid holdup and wetted area in the Large Inlet geometry. These results highlight the need to appropriately consider packing geometries and boundary conditions for comparison to experimental data.

A liquid holdup model was generated based on the periodic geometry results. When compared to semi-empirical models, the impact of liquid viscosity and liquid density were over estimated. This discrepancy was thought to be partly due to sharp angles used for the packing ridge and valley. In most commercial packings, the edges are rounded. Future simulations on these small scale geometries should modify the computational domain as necessary to more appropriately capture the actual packing geometry.

Wetted area results in the periodic geometry were compared to the model produced by Tsai *et al.*²⁹ At a surface tension of 0.074 N/m, the wetted areas predicted by

liquids with a contact angle of 0° were an average of 5.5% lower than the semi-empirical model predictions. As surface tension was reduced, the model predictions became worse. This was thought to be due to the CFD simulations not being able to account for any wetted area produced by mist or droplets being separated from the liquid film. Essentially, the maximum wetted area was limited by the available simulation surface area.

An experimental campaign was undertaken to collect wetted area, liquid holdup, and pressure drop data. Wetted area results compared favorably to the dimensionless model of Tsai *et al.*²⁹ CFD simulations performed using a full half element of Mellapak N250.Y generated via X-ray CT scans were compared to experimental data. For wetted area, the best fit of data was again found to be with a contact angle of 0° with an average error of 3.4%. CFD predictions with a contact angle of 30° were 32.5% lower than experimental data. Holdup predictions were 21% and 7.2% higher than experimental data for simulations with contact angles of 0° and 30° , respectively. Irrigated pressure drop predictions were 37% and 47% higher than experimental data for the 0° and 30° simulations. The poor performance of the holdup and irrigated pressure drop was believed to be an inherent limitation in the default formulation of the VOF model. Specifically, there are two problems with the formulation. First, simple averaging of the viscosity in the interfacial region will lead to a higher effective velocity than physically possible. Second, false momentum transfer due to turbulence will be present. Both of these will lead to increased pressure drop, and the increased viscosity would lead to increased liquid holdup.

FUTURE WORK

Future projects should focus on continued model refinements and validation. In particular, mass transfer data will need to be acquired and used to validate CFD predictions. To make use of the extensive SRP database, it would be wise to generate packing geometries similar to the experimental data SRP has already acquired for mass transfer coefficients. To this end, a new method of geometry generation is proposed to make this process easier.

Geometry Generation

While geometries generated via X-ray CT scans are very promising for CFD validations, they necessarily limit the data gathered to a very specific geometry. There is no way to easily decouple all pressure drop mechanisms from each other. To that end, it is recommended to generate packing geometries based on a CAD representation of a single sheet of packing. A schematic of the proposed geometry generation process is shown in Figure 7-2. This geometry generation process promises to be more robust, allowing for significantly more packing features to be examined and optimized, including perforation pattern, corrugation angle, channel opening angle, and surface texture. This procedure also lends itself to easily creating small periodic structures. Rather than stitching a large sheet together, the geometry from step 2 can be manipulated to generate periodic structures like those used in this work to examine pressure drop mechanisms and the impact of liquid properties. These periodic structures would be useful for performing mesh sensitivity analyses or examining the different choices of simulation settings. This procedure also has the benefit of being able to accurately represent packing sheets too thin to capture with X-ray CT scans (e.g. stainless steel packings with sheet thickness $\sim 0.1\text{mm}$)

Another benefit of this method is the scalability to larger columns. In columns with IDs less than 1m, pressure drop has been observed to be a function of column diameter.¹¹ As such, pressure drop results from the X-ray CT scan geometries are not directly applicable to larger columns. The geometry generation method proposed here, however, could be modified to generate a geometry approximating a large column, as shown in Figure 7-3. In this manner, the pressure drop due to the joint and packing geometry is still accounted for in an exact manner. Attempting to generate a periodic packing geometry in this manner using X-ray CT scans would be extremely difficult due to imperfections (e.g. slightly misaligned corrugated sheets) in the packing. These imperfections would make it difficult to create matching boundaries on all sides.

If a repeating square prism cannot be cut from the structured packing, a computational domain similar to that shown in Figure 7-4 could be used. In this case, sides of the domain would continue to be strictly periodic interfaces. The top interface would be located ~0.05 mm from the top of the packing. The bottom interface would be located ~0.05mm from the bottom of the packing. The top and bottom interface coupling would require using a transformation of the flow field to simulate the joint. At a minimum, a differential pressure would need to be imposed and the velocity field rotated 90° across the interfaces. To ensure complete matching between the top and bottom interfaces, the use of the periodic nature of the flow field in the x and y-directions would need to be used. It would also be possible to apply this periodic method to an actual cylindrical piece of packing in a tube.

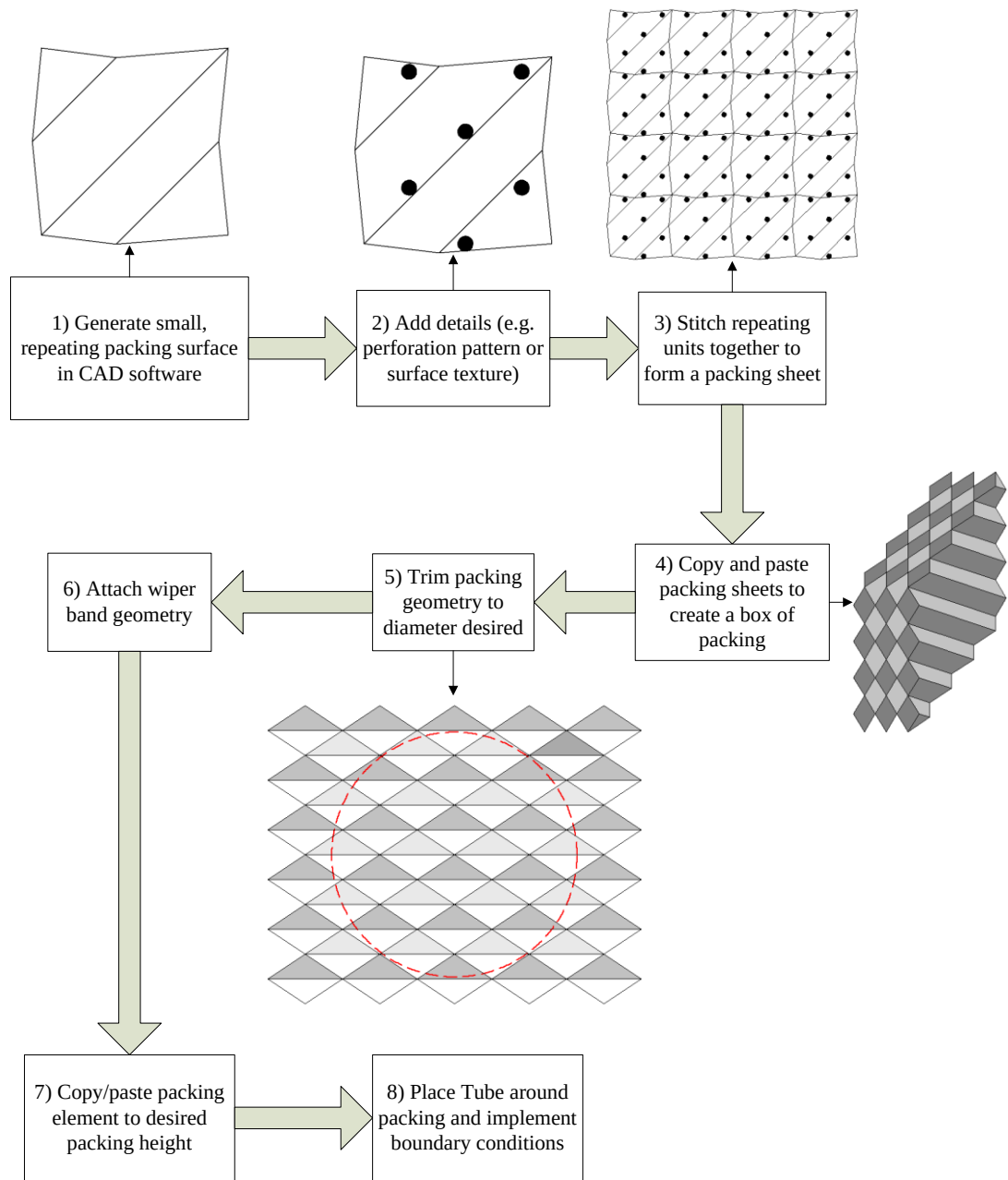


Figure 7-2: Schematic showing one possible method to generate novel packing geometries for CFD simulations.

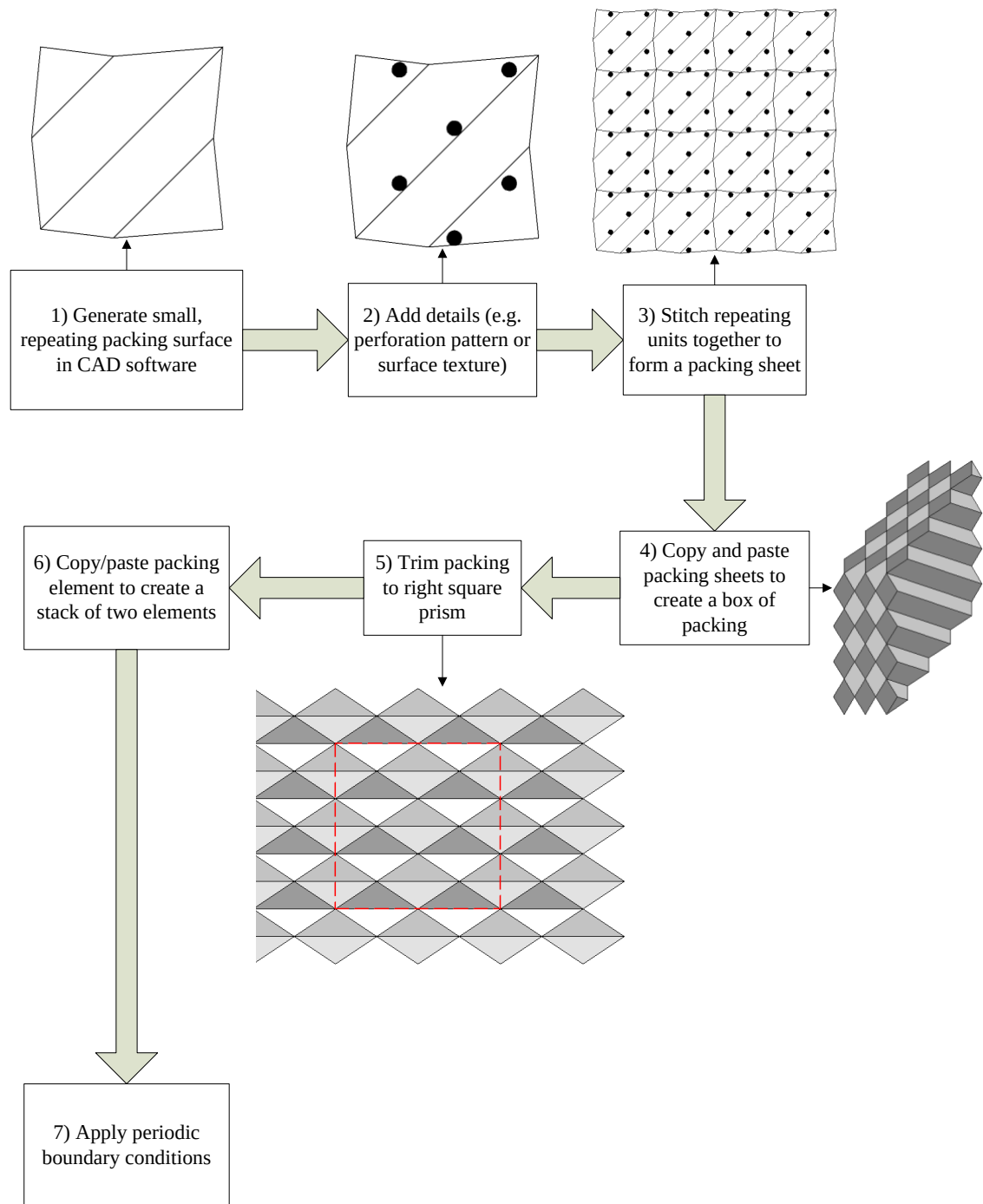


Figure 7-3: Schematic showing how to generate a packing geometry capable of simulating pressure drop in large columns

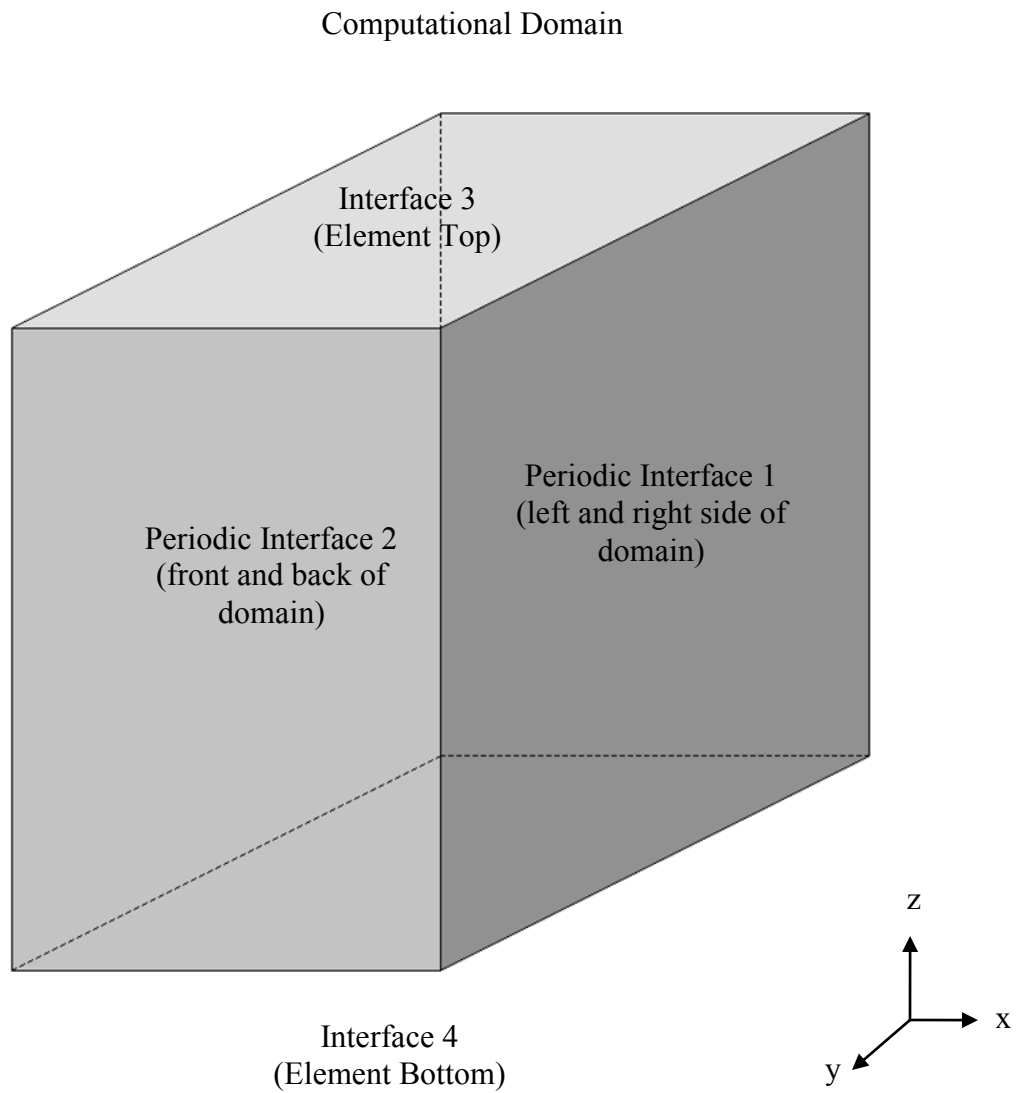


Figure 7-4: Possible geometric arrangement for arbitrary shaped packing element domain. Periodic interfaces are coupled with matching periodic boundaries. Interfaces 3 and 4 are coupled via a field function to mimic a joint.

Pressure Drop Mechanism Refinement

It is expected that perforations lower the expected pressure drop, unless they are completely covered by liquid during operation.⁷⁵ The impact of the perforation pattern and size should be examined to determine the impact on pressure drop. Additionally, the impact of the joint on pressure drop should be isolated using periodic simulations. At that point, it would be possible to isolate the pressure drop due to any outstanding wall effects from the other mechanisms.

Packing Design and Experimental Validation

CFD has been shown to accurately predict pressure drop in a packed bed. With a robust method of generating packing geometries, novel packing features could be examined with CFD to examine the impact on hydraulic capacity and pressure drop. The CFD predictions of the best novel features would then be tested in the pilot plant. With the advent of commercially available 3D printers, structured packing sheets of varying geometries could be printed, bundled together, and tested in the SRP pilot plant to compare to CFD predictions. Choice of turbulence model should continue to be examined to ensure the realizable k- ϵ model is a satisfactory choice for the novel geometries.

There is a need to capture localized velocity profiles through packing to further validate CFD. To that end, stereoscopic particle image velocimetry could be used. An example setup is shown in Figure 7-5. By using two radiation sources and detectors, it would be possible to trace the three-dimensional routes of neutrally buoyant particles through a bed of structured packing. Sufficient data collection would allow for mean flow fields to be quantified and turbulent fluctuations to be determined at varying flow rates.

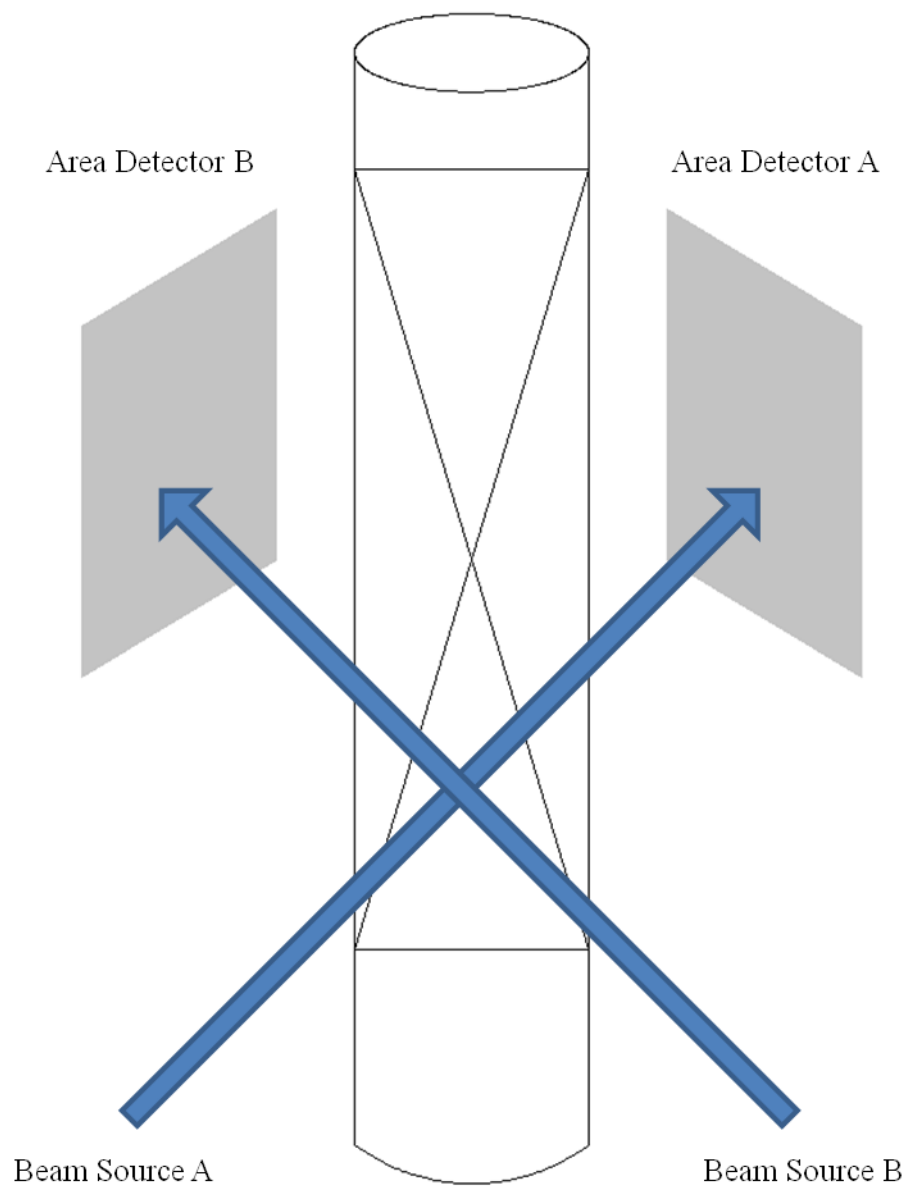


Figure 7-5: Hypothetical detector setup for stereoscopic particle image velocimetry.

Model Enhancement and Evaluation

The default formulation for the VOF model in STAR-CCM+ over predicts irrigated pressure drop and liquid holdup, which can be partly explained by two factors. The first is default averaging of fluid properties in the interfacial region (i.e. where $0 < \alpha_L < 1$). This leads to unrealistically high viscosities near the interface. The second factor is unphysical momentum transfer due to turbulence at the interface. Future research using the VOF model should attempt to implement the corrections of Hashmi *et al.* by damping turbulence near the interface and making the liquid viscosity a function of the liquid volume fraction.⁷⁴

Secondly, the Fluid Film model in STAR-CCM+ should be examined.¹⁴ The Fluid Film model rigorously calculates the gas phase velocities and approximates the liquid phase velocities using laminar film equations. There is no averaging of fluid properties and false momentum transfer due to turbulence should not be present in the Fluid Film model, eliminating the key weaknesses identified in the VOF simulations. To determine wetting, film height can be monitored in the simulation. One further advantage the Fluid Film model has is the ability to simulate droplet formation.

Gas and Liquid Phase Mass Transfer

CFD has proven capable of predicting hydraulic performance for liquid and gas flows. The next logical step is predicting and validating mass transfer performance in structured packing. To that end, experimental data on both the local and average mass transfer coefficients will need to be examined. The SRP has already examined mass transfer data for a variety of packing geometries where wetted area, gas phase mass transfer coefficients, and liquid phase mass transfer coefficients have been determined independently of each other.^{76,77} Localized gas phase mass transfer coefficients can be determined through ammonia absorption experiments.⁵⁶ A color change reaction occurs

between ammonia and an aqueous solution of MnCl_2 and hydrogen peroxide. This solution is soaked in filter paper, which is then attached to the packing surface. The degree of color change is related to the magnitude of the local gas phase mass transfer coefficient.

CFD predictions should be examined for sensitivity to various parameters required, including the turbulent Schmidt number and choice of turbulence model. It would also be prudent to determine the liquid phase and gas phase mass transfer coefficients separately for comparison to experimental results. As part of this study, the impact of different packing parameters should be examined (e.g. corrugation angle, perforation pattern, channel geometry, etc.). Once this has been accomplished, heat transfer would be the next logical step in predicting overall distillation performance. Temperature profiles in operating columns offer a method of data validation for any CFD simulations performed.

Appendix A: Simulation and Mesh Settings

Physics 1		Gravity	
Interfaces	[]	K-Omega Turbulence	
Regions	[Region 1]	Reynolds-Averaged Navier-Stokes	
Models		SST (Menter) K-Omega	
All y+ Wall Treatment		Convection	2nd-order
Cell Quality Remediation		Realizability Option	Durbin Scale Limiter
Constant Density		Compressibility Correction	☒
Coupled Flow		Low Re Damping Modification	☐
Integration	Implicit	a1	0.31
Discretization	2nd-order	Kappa	0.41
Positivity Rate Limit	0.2	BetaStar	0.09
Explicit relaxation	1.0	Beta1	0.075
Minimum Absolute Pressure	1000.0 Pa	Sigma_k1	0.85
Preconditioning Enabled	☒	Sigma_w1	0.5
Pressure difference scale factor	2.0	Beta2	0.0828
Minimum Reference Velocity	1.0E-10 m/s	Sigma_k2	1.0
Maximum Reference Velocity	1000000.0 m/s	Sigma_w2	0.856
Flow Boundary Diffusion	☒	Secondary Gradients	On
Secondary Gradients	On	Normal Stress Term	☐
Coupled Inviscid Flux	Roe FDS	Tke Minimum	1.0E-10
Gas		Sdr Minimum	1.0E-10
N2		Compressibility Parameters	
Database Material	Air (Air) [Standard/Gases]	Zeta_Star	1.5
Material Properties		Realizability Coefficient	
Density		Realizability Coefficient	0.6000000238418579
Dimensions	Mass/Volume	Steady	
Method	Constant	Three Dimensional	
Constant		Turbulent	
Value	1.14527 kg/m^3	Reference Values	
Dynamic Viscosity		Gravity	
Dimensions	Pressure-Time	Value	[0.0, 0.0, -9.81] m/s^2
Method	Constant	Reference Altitude	
Constant		Value	[0.0, 0.0, 0.0] m
Value	1.78837E-5 Pa-s	Minimum Allowable Wall Distance	
Gradients		Value	1.0E-7 mm
Verbose	☐	Reference Pressure	
Gradient Method	Hybrid Gauss-LSQ	Value	101325.0 Pa
Limiter Method	Venkatakrishnan		
Least-Squares Quality Criterion	☒		
Flat Cells Curvature Criterion	☒		
Cell Skewness Criterion	☒		
Chevron-Cell Criterion	☒		
Least-Squares Tensor Minimum Eigenvalues Ratio	0.1		
Normalized Flat Cells Curvature Factor	1.0		
Maximum safe (positive) skewness angle (deg.)	75.0		
Minimum unsafe (positive) skewness angle (deg.)	88.0		

Figure A-1: Physics continuum values for single-phase k- ω simulations on CT geometry.

Solvers		K-Omega Turbulence	
Wall Distance		Under-Relaxation Factor	0.8
Verbosity	0	Reconstruction Frozen	☐
Parallel memory optimization scaling factor	1.0	Reconstruction Zeroed	☐
Solver Frozen	☐	Temporary Storage Retained	☐
Coupled Implicit		Solver Frozen	☐
Courant Number	10.0	Under-Relaxation Factor Ramp	
Pressure Reference Location	Automatic Selection	Ramp Method	No Ramp
Reconstruction Frozen	☐	AMG Linear Solver	
Reconstruction Zeroed	☐	Verbosity	None
Temporary Storage Retained	☐	Max Cycles	30
Solver Frozen	☐	Convergence Tolerance	0.1
Courant Number Ramp		Cycle Type	Flex Cycle
Ramp Method	No Ramp	Parallel Migration Limit	25
AMG Linear Solver		Enable direct-solver	☐
Verbosity	None	Maximum direct-solver equations	32
Max Cycles	30	Epsilon	0.0
Convergence Tolerance	0.01	Group Size Control	Specified
Cycle Type	F Cycle	Group Size	2
Parallel Migration Limit	25	Relaxation Scheme	Gauss-Seidel
Enable direct-solver	☐	Acceleration method	None
Maximum direct-solver equations	32	Scaling	Disabled
Epsilon	0.0	Flex Cycle	
Group Size Control	Specified	Sweeps	1
Group Size	2	Restriction Tolerance	0.9
Relaxation Scheme	Gauss-Seidel	Prolongation Tolerance	0.5
Acceleration method	None	Group Size	
Scaling	Disabled	Group Size	2
F Cycle		K-Omega Turbulent Viscosity	
Pre-Sweeps	0	Under-Relaxation Factor	1.0
Post-Sweeps	1	Maximum Ratio	100000.0
Max Levels	50	Solver Frozen	☐
Group Size			
Group Size	2		
Expert Initialization			
Method	None		
Solution Driver			
Driver	None		
Convergence Accelerators			
Convergence Accelerators	None		

Figure A-2: Solver settings for single-phase k- ω simulations on CT geometry.

Physics 1		Gravity	
Interfaces		K-Epsilon Turbulence	
Regions	[Region 1]	Realizable K-Epsilon Two-Layer	
Models		Two-Layer Type	Shear Driven (Wolfstein)
Cell Quality Remediation		Convection	2nd-order
Constant Density		Normal Stress Term	
Coupled Flow		Two-Layer ReY*	60.0
Integration	Implicit	Two-Layer Delta ReY	10.0
Discretization	2nd-order	Secondary Gradients	On
Positivity Rate Limit	0.2	Buoyancy Production of Dissipation	Boundary Layer Orientation
Explicit relaxation	1.0	Cmu	0.09
Minimum Absolute Pressure	1000.0 Pa	C1e	1.44
Preconditioning Enabled	☒	C2e	1.9
Pressure difference scale factor	2.0	Ct	1.0
Minimum Reference Velocity	1.0E-10 m/s	Sigma_k	1.0
Maximum Reference Velocity	1000000.0 m/s	Sigma_e	1.2
Flow Boundary Diffusion	☒	Sarkar	2.0
Secondary Gradients	On	Tke Minimum	1.0E-10
Coupled Inviscid Flux	Roe FDS	Tdr Minimum	1.0E-10
Gas		Reynolds-Averaged Navier-Stokes	
N2		Steady	
Database Material	Air (Air) [Standard/Ga	Three Dimensional	
Material Properties		Turbulent	
Density		Two-Layer All y+ Wall Treatment	
Dimensions	Mass/Volume	Reference Values	
Method	Constant	Gravity	
Constant		Value	[0.0, 0.0, -9.81] m/s^2
Value	1.14527 kg/m^3	Reference Altitude	
Dynamic Viscosity		Value	[0.0, 0.0, 0.0] m
Dimensions	Pressure-Time	Minimum Allowable Wall Distance	
Method	Constant	Value	1.0E-7 mm
Constant		Reference Pressure	
Value	1.78837E-5 Pa-s	Value	101325.0 Pa
Gradients			
Verbose	☐		
Gradient Method	Hybrid Gauss-LSQ		
Limiter Method	Venkatakrishnan		
Least-Squares Quality Criterion	☒		
Flat Cells Curvature Criterion	☒		
Cell Skewness Criterion	☒		
Chevron-Cell Criterion	☒		
Least-Squares Tensor Minimum Eigenvalues Ratio	0.1		
Normalized Flat Cells Curvature Factor	1.0		
Maximum safe (positive) skewness angle (deg.)	75.0		
Minimum unsafe (positive) skewness angle (deg.)	88.0		

Figure A-3: Physics continuum values for single-phase k-ε simulations on CT geometry

Solvers		K-Epsilon Turbulence	
Wall Distance		Under-Relaxation Factor	0.95
Verbosity	0	Reconstruction Frozen	☐
Parallel memory optimization scaling factor	1.0	Reconstruction Zeroed	☐
Solver Frozen	☐	Temporary Storage Retained	☐
Coupled Implicit		Solver Frozen	☐
Courant Number	10.0	Under-Relaxation Factor Ramp	
Pressure Reference Location	Automatic Selection	Ramp Method	No Ramp
Reconstruction Frozen	☐	AMG Linear Solver	
Reconstruction Zeroed	☐	Verbosity	None
Temporary Storage Retained	☐	Max Cycles	30
Solver Frozen	☐	Convergence Tolerance	0.1
Courant Number Ramp		Cycle Type	Flex Cycle
Ramp Method	No Ramp	Parallel Migration Limit	25
AMG Linear Solver		Enable direct-solver	☐
Verbosity	None	Maximum direct-solver equations	32
Max Cycles	30	Epsilon	0.0
Convergence Tolerance	0.01	Group Size Control	Specified
Cycle Type	F Cycle	Group Size	2
Parallel Migration Limit	25	Relaxation Scheme	Gauss-Seidel
Enable direct-solver	☐	Acceleration method	None
Maximum direct-solver equations	32	Scaling	Disabled
Epsilon	0.0	Flex Cycle	
Group Size Control	Specified	Sweeps	1
Group Size	2	Restriction Tolerance	0.9
Relaxation Scheme	Gauss-Seidel	Prolongation Tolerance	0.5
Acceleration method	None	Group Size	
Scaling	Disabled	Group Size	2
F Cycle		K-Epsilon Turbulent Viscosity	
Pre-Sweeps	0	Under-Relaxation Factor	1.0
Post-Sweeps	1	Maximum Ratio	100000.0
Max Levels	50	Solver Frozen	☐
Group Size			
Group Size	2		
Expert Initialization			
Method	None		
Solution Driver			
Driver	None		
Convergence Accelerators			
Convergence Accelerators	None		

Figure A-4: Solver settings for single-phase k- ϵ simulations on CT geometry.

Nodes	Values		
Mesh 1			
Use Parallel Meshing		Surface Curvature	
Per-Region Meshing		Enable curvature deviation distance	
Interfaces		Basic Curvature	
Regions	[Region 1]	# Pts/circle	36.0
Verbose Output		Surface Growth Rate	
OOB translation		Surface Growth Rate	1.3
Interpolation Option	Nearest neighbor	Surface Proximity	
Models	# Points in gap 1.0		
Polyhedral Mesher	Search Floor 0.0 m		
Choose a Mesh Size Table	None	Surface Size	
Enable Mesh Expansion Control		Relative/Absolute	Relative to base
Run Optimizer		Size Method	Min and Target
Include Refinement		Relative Minimum Size	
Optimization Cycles	1	Percentage of Base	100.0
Quality Threshold	0.4	Absolute Size	1.0 mm
Surface Remesher	Relative Target Size		
Do curvature refinement		Percentage of Base	3500.0
Do proximity refinement		Absolute Size	35.0 mm
Do compatibility refinement		Tet/Poly Density	
Retain geometric features		Density	1.0
Create aligned meshes		Growth Factor	1.0
Minimum Face Quality	0.05	Tet/Poly Volume Blending	
Enable automatic surface repair		Blending Factor	1.0
Choose a mesh size table	None	Wrapper Feature Angle	
Surface Wrapper	Angle 30.0		
Do curvature refinement		Wrapper Scale Factor	
Do proximity refinement		Percentage	40.0
Do gap closure		Volumetric Controls	
Do wrapper mesh alignment			
Reference Values			
Base Size			
Value	1.0 mm		
Automatic Surface Repair			
Connected surface count limit	None		
Connected surface size limits	None		
Minimum Proximity			
Minimum Proximity	0.05		
Minimum Quality			
Minimum Quality	0.03		
CAD Projection			
Project to CAD			

Figure A-5: Mesh settings for “Coarse” CT geometry mesh

Nodes	Values		
Mesh 1			
Use Parallel Meshing	☐	Surface Curvature	
Per-Region Meshing	☐	Enable curvature deviation distance	☐
Interfaces	☐	Basic Curvature	
Regions	[Region 1]	# Pts/circle	36.0
Verbose Output	☐	Surface Growth Rate	
OOB translation	☐	Surface Growth Rate	1.4
Interpolation Option	Nearest neighbor	Surface Proximity	
Models		# Points in gap	1.0
Polyhedral Mesher		Search Floor	0.0 m
Choose a Mesh Size Table	None	Surface Size	
Enable Mesh Expansion Control	☐	Relative/Absolute	Relative to base
Run Optimizer	☒	Size Method	Min and Target
Include Refinement	☐	Relative Minimum Size	
Optimization Cycles	1	Percentage of Base	45.0
Quality Threshold	0.4	Absolute Size	0.45 mm
Surface Remesher		Relative Target Size	
Do curvature refinement	☒	Percentage of Base	3500.0
Do proximity refinement	☒	Absolute Size	35.0 mm
Do compatibility refinement	☐	Tet/Poly Density	
Retain geometric features	☐	Density	1.0
Create aligned meshes	☐	Growth Factor	1.0
Minimum Face Quality	0.05	Tet/Poly Volume Blending	
Enable automatic surface repair	☒	Blending Factor	1.0
Choose a mesh size table	None	Wrapper Feature Angle	
Surface Wrapper		Angle	30.0
Do curvature refinement	☒	Wrapper Scale Factor	
Do proximity refinement	☒	Percentage	75.0
Do gap closure	☐	Volumetric Controls	
Do wrapper mesh alignment	☐		
Reference Values			
Base Size			
Value	1.0 mm		
Automatic Surface Repair			
Connected surface count limit	None		
Connected surface size limits	None		
Minimum Proximity			
Minimum Proximity	0.05		
Minimum Quality			
Minimum Quality	0.03		
CAD Projection			
Project to CAD	☐		

Figure A-6: Mesh settings for “Medium” CT geometry mesh

Nodes	Values		
Mesh 1			
Use Parallel Meshing	☐	Surface Curvature	
Per-Region Meshing	☐	Enable curvature deviation distance	☐
Interfaces	☐	Basic Curvature	
Regions	[Region 1]	# Pts/circle	36.0
Verbose Output	☐	Surface Growth Rate	
OOC translation	☐	Surface Growth Rate	1.3
Interpolation Option	Nearest neighbor	Surface Proximity	
Models		# Points in gap	1.0
Polyhedral Mesher		Search Floor	0.0 m
Choose a Mesh Size Table	None	Surface Size	
Enable Mesh Expansion Control	☐	Relative/Absolute	Relative to base
Run Optimizer	☒	Size Method	Min and Target
Include Refinement	☐	Relative Minimum Size	
Optimization Cycles	1	Percentage of Base	40.0
Quality Threshold	0.4	Absolute Size	0.4 mm
Surface Remesher		Relative Target Size	
Do curvature refinement	☒	Percentage of Base	2000.0
Do proximity refinement	☒	Absolute Size	20.0 mm
Do compatibility refinement	☐	Tet/Poly Density	
Retain geometric features	☐	Density	1.0
Create aligned meshes	☐	Growth Factor	1.0
Minimum Face Quality	0.05	Tet/Poly Volume Blending	
Enable automatic surface repair	☒	Blending Factor	1.0
Choose a mesh size table	None	Wrapper Feature Angle	
Surface Wrapper		Angle	30.0
Do curvature refinement	☒	Wrapper Scale Factor	
Do proximity refinement	☒	Percentage	75.0
Do gap closure	☐	Volumetric Controls	
Do wrapper mesh alignment	☐		
Reference Values			
Base Size			
Value	1.0 mm		
Automatic Surface Repair			
Connected surface count limit	None		
Connected surface size limits	None		
Minimum Proximity			
Minimum Proximity	0.05		
Minimum Quality			
Minimum Quality	0.03		
CAD Projection			
Project to CAD	☐		

Figure A-7: Mesh settings for “Fine” CT geometry mesh

Physics 1			
Interfaces	[m_x_px_2, top_bot_2]	Large Eddy Simulation	
Regions	[Region 1]	Segregated Flow	
Models		Convection	Bounded-Central
All y+ Wall Treatment		Minimum Absolute Pressure	1000.0 Pa
Cell Quality Remediation		Flow Boundary Diffusion	☒
Constant Density		Secondary Gradients	On
Gas		Delta-V Dissipation	Off
N2		Bounded Differencing	
Database Material	N2 (Nitrogen) [Standard/Gase:	Upwind blending factor	0.15
Material Properties		Three Dimensional	
Density		Turbulent	
Dimensions	Mass/Volume	Wale Subgrid Scale	
Method	Constant	Cw	0.544
Constant		Ct	1.25
Value	1.225 kg/m^3	Kappa	0.41
Dynamic Viscosity		Limit Length Scale	☒
Dimensions	Pressure-Time	Reference Values	
Method	Constant	Gravity	
Constant		Value	[0.0, -9.81, 0.0] m/s^2
Value	1.7894E-5 Pa-s	Reference Altitude	
Gradients		Value	[0.0, 0.0, 0.0] m
Verbose	☐	Minimum Allowable Wall Distance	
Gradient Method	Hybrid Gauss-LSQ	Value	1.0E-6 m
Limiter Method	Venkatakrishnan	Maximum Number of Eddies	
Least-Squares Quality Criterion	☒	Value	1000.0
Flat Cells Curvature Criterion	☒	Reference Pressure	
Cell Skewness Criterion	☒	Value	101325.0 Pa
Chevron-Cell Criterion	☒		
Least-Squares Tensor Minimum Eigenvalues Ratio	0.1		
Normalized Flat Cells Curvature Factor	1.0		
Maximum safe (positive) skewness angle (deg.)	75.0		
Minimum unsafe (positive) skewness angle (deg.)	88.0		
Gravity			
Implicit Unsteady			

Figure A-8: Physics continuum values for periodic LES simulations.

Solvers			
Implicit Unsteady		Pressure	
Time-Step	1.0E-5 s	Under-Relaxation Factor	0.2
Freeze Time	☐	Pressure Reference Location	Automatic Selection
Temporal Discretization	2nd-order	Under-Relaxation Factor Ramp	
Solver Frozen	☐	Ramp Method	No Ramp
Wall Distance		AMG Linear Solver	
Verbosity	0	Verbosity	None
Parallel memory optimization scaling factor	1.0	Max Cycles	30
Solver Frozen	☐	Convergence Tolerance	0.1
Segregated Flow		Cycle Type	V Cycle
Reconstruction Frozen	☐	Parallel Migration Limit	25
Reconstruction Zeroed	☐	Enable direct-solver	☐
Temporary Storage Retained	☐	Maximum direct-solver equations	32
Solver Frozen	☐	Epsilon	0.0
Velocity		Group Size Control	Auto
Under-Relaxation Factor	0.8	Group Size	4
Under-Relaxation Factor Ramp		Relaxation Scheme	Gauss-Seidel
Ramp Method	No Ramp	Acceleration method	Conjugate Gradient
AMG Linear Solver		Scaling	Auto
Verbosity	None	V Cycle	
Max Cycles	30	Pre-Sweeps	1
Convergence Tolerance	0.1	Post-Sweeps	1
Cycle Type	Flex Cycle	Max Levels	50
Parallel Migration Limit	25	Wale SGS Viscosity	
Enable direct-solver	☐	Temporary Storage Retained	☐
Maximum direct-solver equations	32	Solver Frozen	☐
Epsilon	0.0		
Group Size Control	Auto		
Group Size	4		
Relaxation Scheme	Gauss-Seidel		
Acceleration method	None		
Scaling	Disabled		
Flex Cycle			

Figure A-9: Solver settings for periodic LES simulations

Mesh 1		Reference Values	
Use Parallel Meshing	☐	Base Size	
Per-Region Meshing	☐	Value	0.4 mm
Interfaces	[mx_px_2, top_bot_2]	Automatic Surface Repair	
Regions	[Region 1]	Connected surface count limit	None
Verbose Output	☐	Connected surface size limits	None
OOB translation	☐	Minimum Proximity	
Interpolation Option	Nearest neighbor	Minimum Proximity	0.05
Models		Minimum Quality	
Polyhedral Mesher		Minimum Quality	0.05
Choose a Mesh Size Table	None	CAD Projection	
Enable Mesh Expansion Control	☐	Project to CAD	☒
Run Optimizer	☒	Number of Prism Layers	
Include Refinement	☐	Number of Prism Layers	6
Optimization Cycles	20	Prism Layer Stretching	
Quality Threshold	0.5	Prism Layer Stretching	1.05
Prism Layer Mesher		Prism Layer Thickness	
Stretching Function	Geometric Progression	Size type	Absolute
Stretching Mode	Stretch Factor	Absolute Size	
Gap Fill Percentage	25.0	Value	0.5 mm
Minimum Thickness Percentage	10.0	Surface Curvature	
Layer Reduction Percentage	50.0	Enable curvature deviation distance	☐
Boundary March Angle	75.0	Basic Curvature	
Concave Angle Limit	60.0	# Pts/circle	36.0
Convex Angle Limit	360.0	Surface Growth Rate	
Near Core Layer Aspect Ratio	0.0	Surface Growth Rate	1.1
Generate Standard Cells Only	☐	Surface Proximity	
Improve Subsurface Quality	☒	# Points in gap	2.0
Surface Remesher		Search Floor	0.0 m
Do curvature refinement	☒	Surface Size	
Do proximity refinement	☒	Relative/Absolute	Relative to base
Do compatibility refinement	☒	Size Method	Min and Target
Retain geometric features	☒	Relative Minimum Size	
Create aligned meshes	☒	Percentage of Base	20.0
Minimum Face Quality	0.05	Absolute Size	0.08 mm
Enable automatic surface repair	☒	Relative Target Size	
Choose a mesh size table	None	Percentage of Base	100.0
Surface Wrapper		Absolute Size	0.4 mm
Do proximity refinement	☐	Tet/Poly Density	
Do curvature refinement	☒	Density	1.0
Do gap closure	☐		
Do wrapper mesh alignment	☐		

Figure A-10: Mesh settings for single-phase periodic RANS simulations.

Physics 1			
Interfaces	{}	Multiphase Interaction	
Regions	[Region 1]	Phase Interactions	
Models		Phase Interaction 1	
Cell Quality Remediation		Index	1
Eulerian Multiphase		Interfaces	{}
Eulerian Phases		Regions	{}
Liquid		Models	
Index	1	Multiphase Material	
Interfaces	{}	Multiphase Material	
Regions	{}	Material Properties	
Models		Surface Tension	
Constant Density		Dimensions	Force/Length
Liquid		Method	Constant
H2O		Constant	
Database Material	H2O (Water) [Standard/Liquids]	Value	0.074 N/m
Material Properties		Surface Tension Force	
Density		Marangoni Convection	
Dimensions	Mass/Volume	VOF Phase Interaction	
Method	Constant	Primary Phase	Liquid
Constant		Secondary Phase	Gas
Value	997.561 kg/m^3	Multiphase Mixture	
Dynamic Viscosity		Mixture	
Dimensions	Pressure-Time	Mixture Properties	
Method	Constant	Dynamic Viscosity	
Constant		Dimensions	Pressure-Time
Value	0.00105 Pa-s	Method	Volume-Weighted Mixture
Turbulent		Volume-Weighted Mixture	
Gas		Turbulent Prandtl Number	
Index	2	Dimensions	Dimensionless
Interfaces	{}	Method	Constant
Regions	{}	Constant	
Models		Value	0.9
Constant Density		Realizable K-Epsilon Two-Layer	
Gas		Two-Layer Type	Shear Driven (Wolfstein)
N2		Convection	2nd-order
Database Material	N2 (Nitrogen) [Standard/Gases]	Normal Stress Term	
Material Properties		Two-Layer ReY*	60.0
Density		Two-Layer Delta ReY	10.0
Dimensions	Mass/Volume	Secondary Gradients	On
Method	Constant	Buoyancy Production of Dissipation	Boundary Layer Orientation
Constant		Cmu	0.09
Value	1.194 kg/m^3	C1e	1.44
Dynamic Viscosity		C2e	1.9
Dimensions	Pressure-Time	Ct	1.0
Method	Constant	Sigma_k	1.0
Constant		Sigma_e	1.2
Value	1.725E-5 Pa-s	Sarkar	2.0
Turbulent		Tke Minimum	1.0E-10
Gradients		Tdr Minimum	1.0E-10
Verbose		Reynolds-Averaged Navier-Stokes	
Gradient Method	Hybrid Gauss-LSQ	Segregated Flow	
Limiter Method	Venkatakrishnan	Convection	2nd-order
Least-Squares Quality Criterion	☒	Minimum Absolute Pressure	1000.0 Pa
Flat Cells Curvature Criterion	☒	Flow Boundary Diffusion	☒
Cell Skewness Criterion	☒	Secondary Gradients	On
Chevron-Cell Criterion	☒	Delta-V Dissipation	Off
Least-Squares Tensor Minimum Eigenvalue...	0.1	Three Dimensional	
Normalized Flat Cells Curvature Factor	1.0	Turbulent	
Maximum safe (positive) skewness angle (d...	75.0	Two-Layer All y+ Wall Treatment	
Minimum unsafe (positive) skewness angle (...)	88.0	Volume of Fluid (VOF)	
Gravity		Convection	2nd-order
Implicit Unsteady		Sharpening Factor	0.0
K-Epsilon Turbulence		Angle Factor	0.05
Multiphase Equation of State		CFL_l	0.5
		CFL_u	1.0

Figure A-11: Physics continuum settings for multiphase turbulent simulations.

Solvers			
Implicit Unsteady		Segregated VOF	
Time-Step	2.5E-4 s	Under-Relaxation Factor	0.6
Freeze Time	☐	Reconstruction Frozen	☐
Temporal Discretization	2nd-order	Reconstruction Zeroed	☐
Solver Frozen	☐	Temporary Storage Retained	☐
Wall Distance		Solver Frozen	☐
Verbosity	0	Under-Relaxation Factor Ramp	
Parallel memory optimization scaling factor	1.0	Ramp Method	Linear Ramp
Solver Frozen	☐	Linear Ramp	
Segregated Flow		Start Iteration	1
Reconstruction Frozen	☐	End Iteration	100
Reconstruction Zeroed	☐	Initial Value	0.04
Temporary Storage Retained	☐	AMG Linear Solver	
Solver Frozen	☐	Verbosity	None
Velocity		Max Cycles	30
Under-Relaxation Factor	0.45	Convergence Tolerance	0.1
Under-Relaxation Factor Ramp		Cycle Type	V Cycle
Ramp Method	Linear Ramp	Parallel Migration Limit	25
Linear Ramp		Enable direct-solver	☐
Start Iteration	1	Maximum direct-solver equations	32
End Iteration	100	Epsilon	0.0
Initial Value	0.04	Group Size Control	Auto
AMG Linear Solver		Group Size	4
Verbosity	None	Relaxation Scheme	Gauss-Seidel
Max Cycles	30	Acceleration method	None
Convergence Tolerance	0.1	Scaling	Disabled
Cycle Type	Flex Cycle	V Cycle	
Parallel Migration Limit	25	Pre-Sweeps	1
Enable direct-solver	☐	Post-Sweeps	1
Maximum direct-solver equations	32	Max Levels	50
Epsilon	0.0	K-Epsilon Turbulence	
Group Size Control	Auto	Under-Relaxation Factor	0.5
Group Size	4	Reconstruction Frozen	☐
Relaxation Scheme	Gauss-Seidel	Reconstruction Zeroed	☐
Acceleration method	None	Temporary Storage Retained	☐
Scaling	Disabled	Solver Frozen	☐
Flex Cycle		Under-Relaxation Factor Ramp	
Restriction Tolerance	0.9	Ramp Method	Linear Ramp
Prolongation Tolerance	0.5	Linear Ramp	
Sweeps	1	Start Iteration	1
Pressure		End Iteration	100
Under-Relaxation Factor	0.2	Initial Value	0.06
Pressure Reference Location	Automatic Selection	AMG Linear Solver	
Under-Relaxation Factor Ramp		Verbosity	None
Ramp Method	Linear Ramp	Max Cycles	30
Linear Ramp		Convergence Tolerance	0.1
Start Iteration	1	Cycle Type	Flex Cycle
End Iteration	100	Parallel Migration Limit	25
Initial Value	0.01	Enable direct-solver	☐
AMG Linear Solver		Maximum direct-solver equations	32
Verbosity	None	Epsilon	0.0
Max Cycles	100	Group Size Control	Auto
Convergence Tolerance	0.1	Group Size	4
Cycle Type	V Cycle	Relaxation Scheme	Gauss-Seidel
Parallel Migration Limit	25	Acceleration method	None
Enable direct-solver	☐	Scaling	Disabled
Maximum direct-solver equations	32	Flex Cycle	
Epsilon	0.0	Restriction Tolerance	0.9
Group Size Control	Auto	Prolongation Tolerance	0.5
Group Size	4	Sweeps	1
Relaxation Scheme	Gauss-Seidel	K-Epsilon Turbulent Viscosity	
Acceleration method	Conjugate Gradient	Under-Relaxation Factor	0.8
Scaling	Auto	Maximum Ratio	100000.0
V Cycle		Solver Frozen	☐
Pre-Sweeps	5		
Post-Sweeps	1		

Figure A-12: Solver settings for multiphase turbulent simulations.

Mesh 1		Reference Values	
Use Parallel Meshing	☐	Base Size	
Per-Region Meshing	☐	Value	0.85 mm
Interfaces	[]	Automatic Surface Repair	
Regions	[Region 1]	Connected surface count limit	None
Verbose Output	☐	Connected surface size limits	Minimum Face Count
OOB translation	☐	Minimum Proximity	
Interpolation Option	Nearest neighbor	Minimum Proximity	0.05
Models		Minimum Quality	
Polyhedral Mesher		Minimum Quality	0.1
Enable Mesh Expansion Control	☐	Minimum Connected Surface Face Co...	
Run Optimizer	☒	Minimum Connected Surface Face C...	400
Include Refinement	☐	CAD Projection	
Choose a Mesh Size Table	None	Project to CAD	☒
Optimization Cycles	6	Number of Prism Layers	
Quality Threshold	0.4	Number of Prism Layers	15
Prism Layer Mesher		Prism Layer Stretching	
Stretching Function	Geometric Progression	Prism Layer Stretching	1.07
Stretching Mode	Stretch Factor	Prism Layer Thickness	
Gap Fill Percentage	35.0	Size type	Absolute
Minimum Thickness Percentage	25.0	Absolute Size	
Layer Reduction Percentage	75.0	Value	1.0 mm
Boundary March Angle	50.0	Surface Curvature	
Concave Angle Limit	0.0	Enable curvature deviation distance	☐
Convex Angle Limit	360.0	Basic Curvature	
Near Core Layer Aspect Ratio	0.0	# Pts/circle	36.0
Generate Standard Cells Only	☐	Surface Growth Rate	
Improve Subsurface Quality	☒	Surface Growth Rate	1.3
Surface Remesher		Surface Proximity	
Do curvature refinement	☒	# Points in gap	2.0
Do proximity refinement	☒	Search Floor	0.0 m
Do compatibility refinement	☒	Surface Size	
Retain geometric features	☒	Relative/Absolute	Relative to base
Create aligned meshes	☒	Size Method	Min and Target
Minimum Face Quality	0.1	Relative Minimum Size	
Enable automatic surface repair	☒	Percentage of Base	8.0
Choose a mesh size table	None	Absolute Size	0.068 mm
Surface Wrapper		Relative Target Size	
Do curvature refinement	☒	Percentage of Base	100.0
Do proximity refinement	☒	Absolute Size	0.85 mm
Do gap closure	☐	Tet/Poly Density	
Do wrapper mesh alignment	☐	Density	1.0
		Growth Factor	1.02
		Tet/Poly Volume Blending	
		Blending Factor	1.0
		Wrapper Feature Angle	
		Angle	30.0
		Wrapper Scale Factor	
		Percentage	100.0

Figure A-13: Mesh continuum settings for multiphase CT geometry simulations.

Appendix B: SOP for Air-Water Column Operation

The following section is courteous of the Separations Research Program.

B-1. PROCESS DESCRIPTION

The 6" PVC Air-Water column is used to measure the hydraulic capacity and mass transfer efficiency of a variety of column internals. These data are collected by completing two different experimental. The experiments are designed to collect pressure drop and specific contact area.

The air-water system is composed of a 6" PVC column, a single centrifugal feed pump, a supply of compressed nitrogen, process instrumentation, and analytical equipment along with associated ancillary equipment. The operator utilizes the DeltaV DCS as well as manual valves to interface with, control, and direct flows properly. The main operator shall require an additional person to successfully complete the experiments.

A flow diagram of the air-water system is shown below:

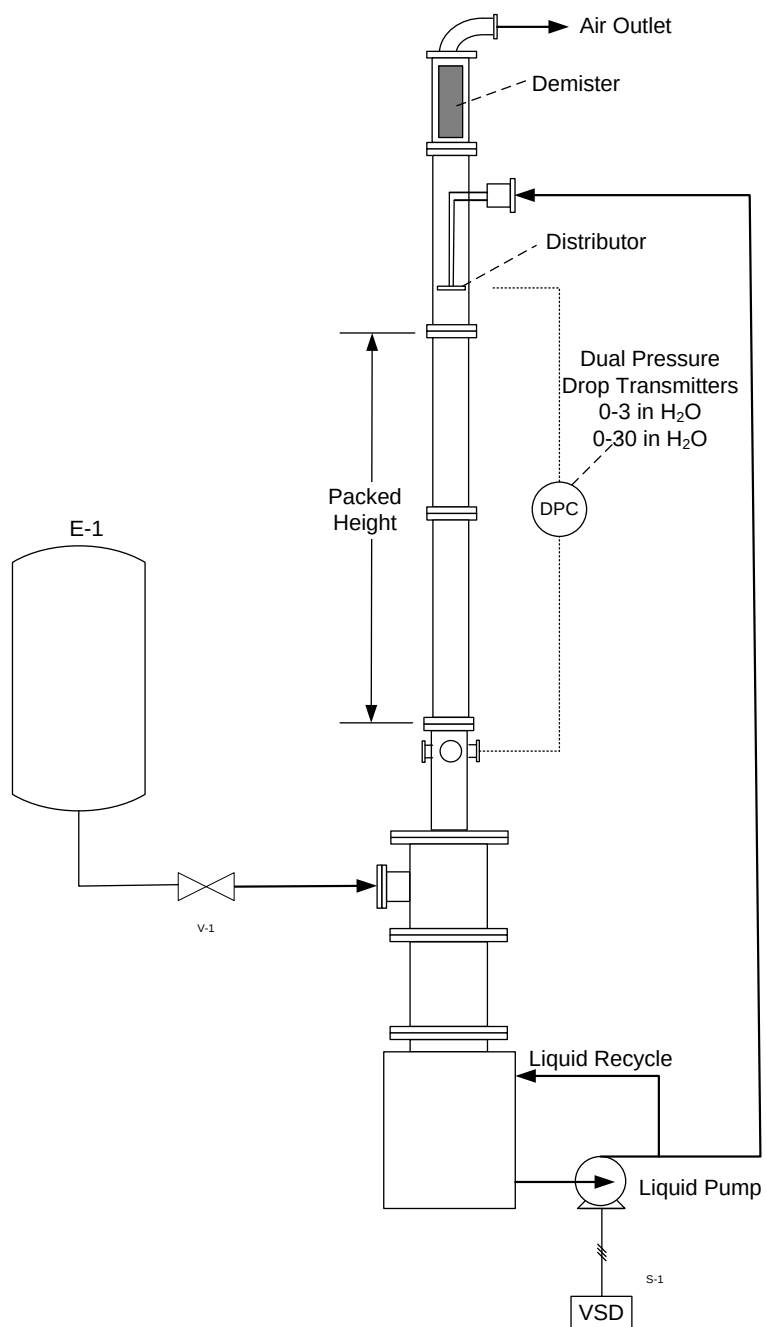


Figure B-1: Air-water system flow diagram

B-2. LIST OF EQUIPMENT, CHEMICALS, AND INSTRUMENTATION USED

Equipment:

250 Gallon Feed Tank

Feed Pump (P901)

Pneumatic Valve AV401 (to isolate liquid feed from column)

Inlet Sample Pump

Outlet Sample Pump

Horiba CO2 Analyzer

Chemicals:

Water (from tap)

Sodium hydroxide (pellet form)

Carbon dioxide (from pressurized cylinder)

Nitrogen (from pressurized cylinder)

Hydrochloric acid, fuming

Instrumentation:

MicroMotion flow meter (FT901)

Air Inlet Annubar

Pressure Drop Transmitter – High-Range (PDT901)

Pressure Drop Transmitter – Low-Range (PDT900)

Level Transmitter (LT900)

Assorted thermocouples

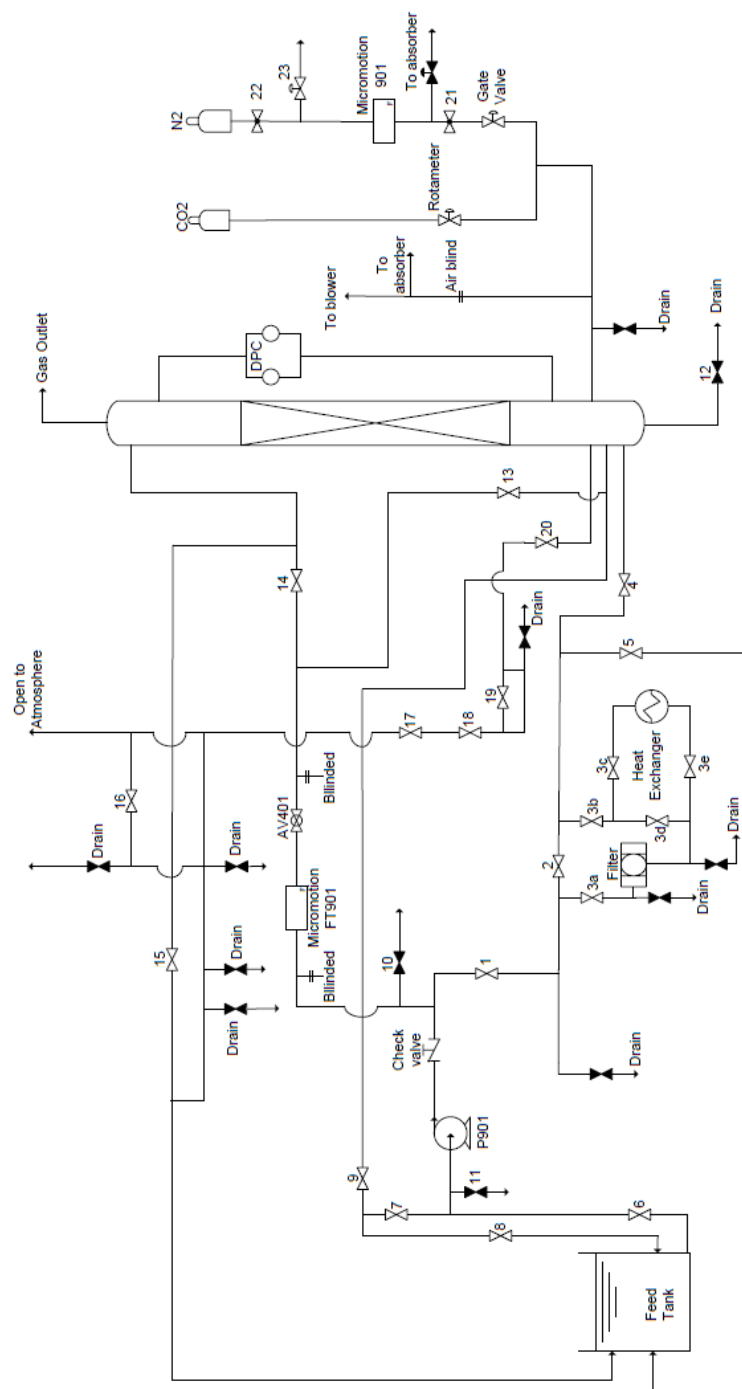
Wireless RTD (T902)

Nitrogen flow meter

Valve	Description	Liquid (L) / Vapor (V)	Comments
1	Pre-filter tank return	L	
2	Filter bypass	L	
3a/3b	Filter valves	L	
4	Sump return	L	
5	Post-filter tank return	L	
6	Pump suction (tank)	L	
7	Pump suction (sump)	L	
8	Tank return	L	
9	Sump outlet	L	
10	Pump discharge	L	Used for waste discharge into drums
11	Pump drainage	L	Only open during filling/drainage
12	Sump drainage	L	Only open during drainage
13	Dead-leg	L	Only open during drainage
15	Tank return valve	L	
14	Throttle valve	L	
16	Vent equilibration valve	L	Only open during leak check
17	Sight glass valves	L	
18			
19			
20	Sight glass valve		
21	Nitrogen sampling valve	G	
22	Nitrogen Spply Valve	G	
23	Bleed Valve	G	
AV401	Pneumatic valve	L	

Table B-1: Valves associated with air-water tower (shown in above figures).

B-3. AIR-WATER SYSTEM FLOWSHEET & PICTURES



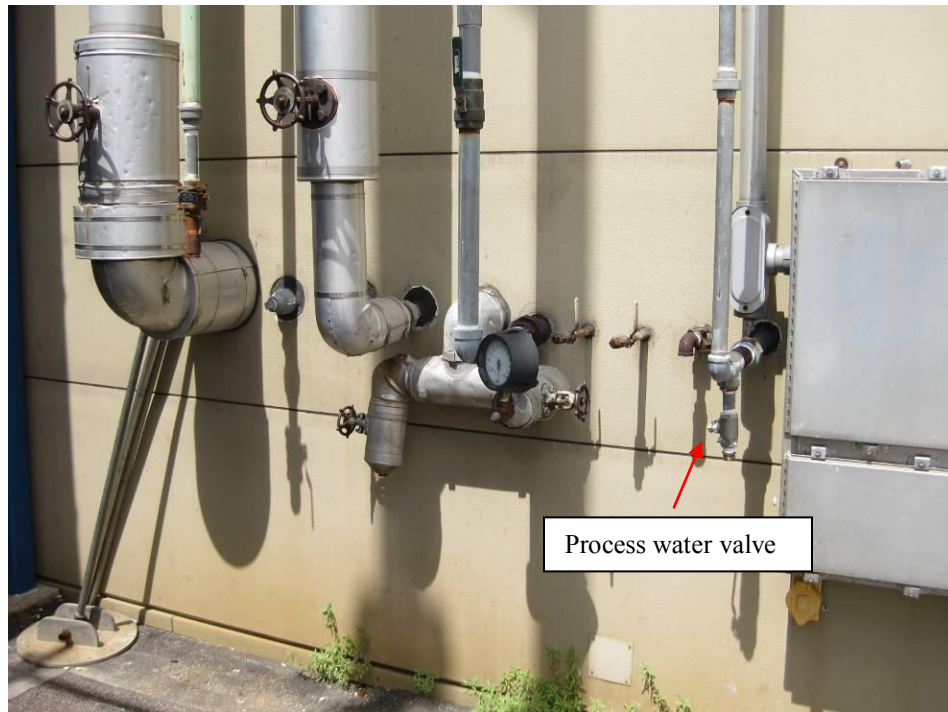


Figure B-2: Process water source

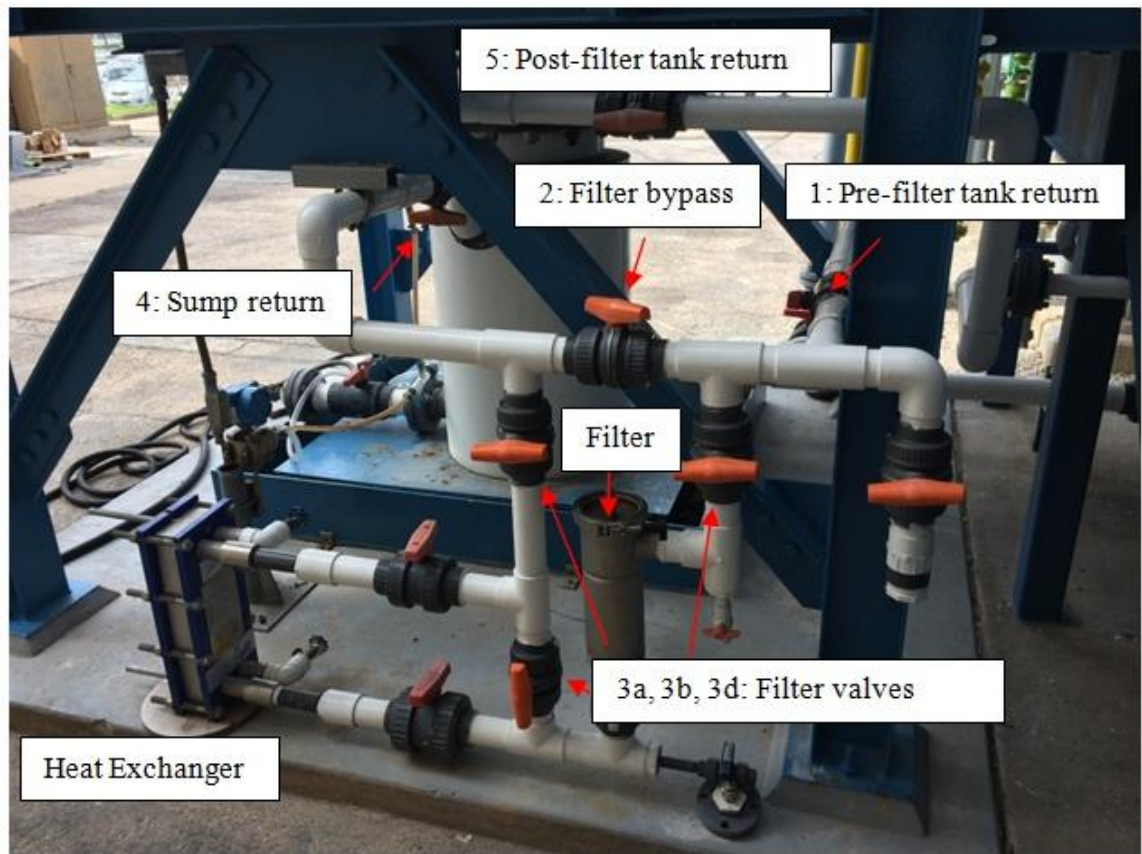


Figure B-3: Liquid line valves (north)

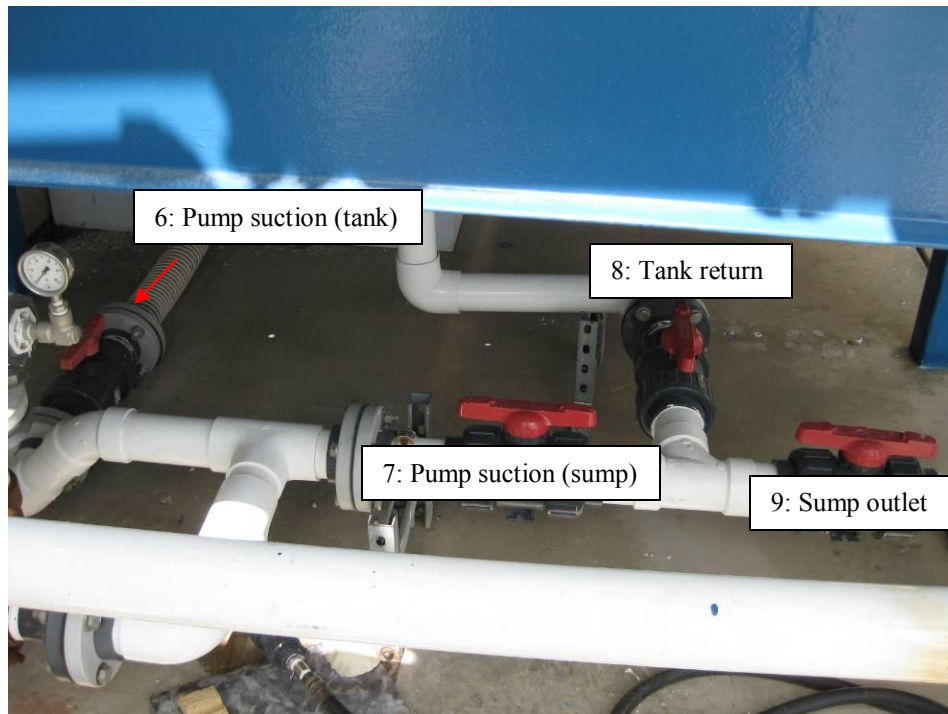


Figure B-4: Liquid line valves (south).

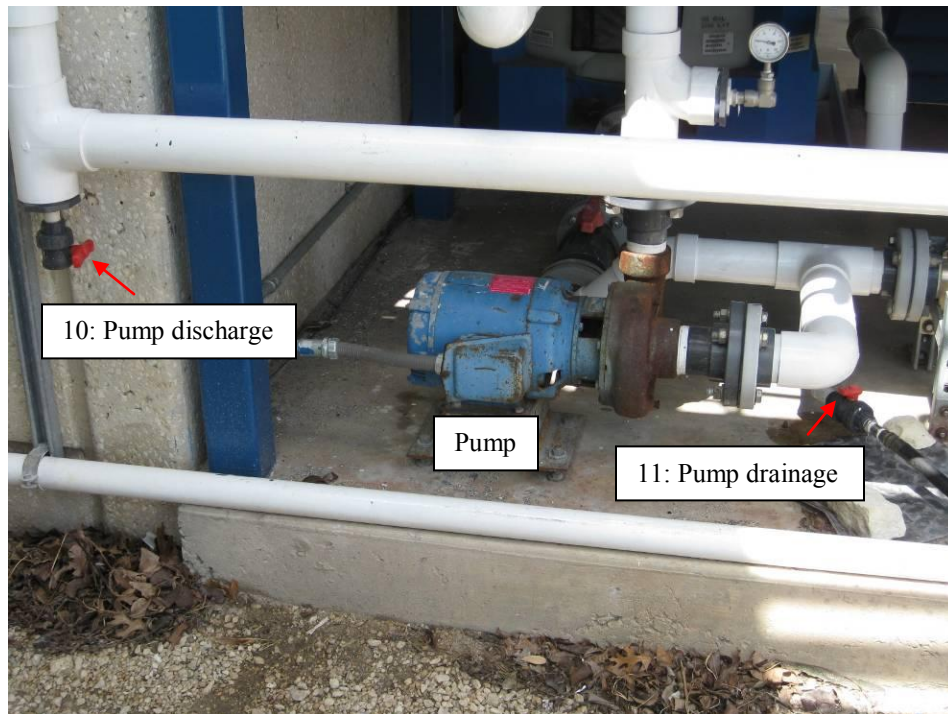


Figure B-5: Pump and associated valves.



Figure B-6: Column sump.

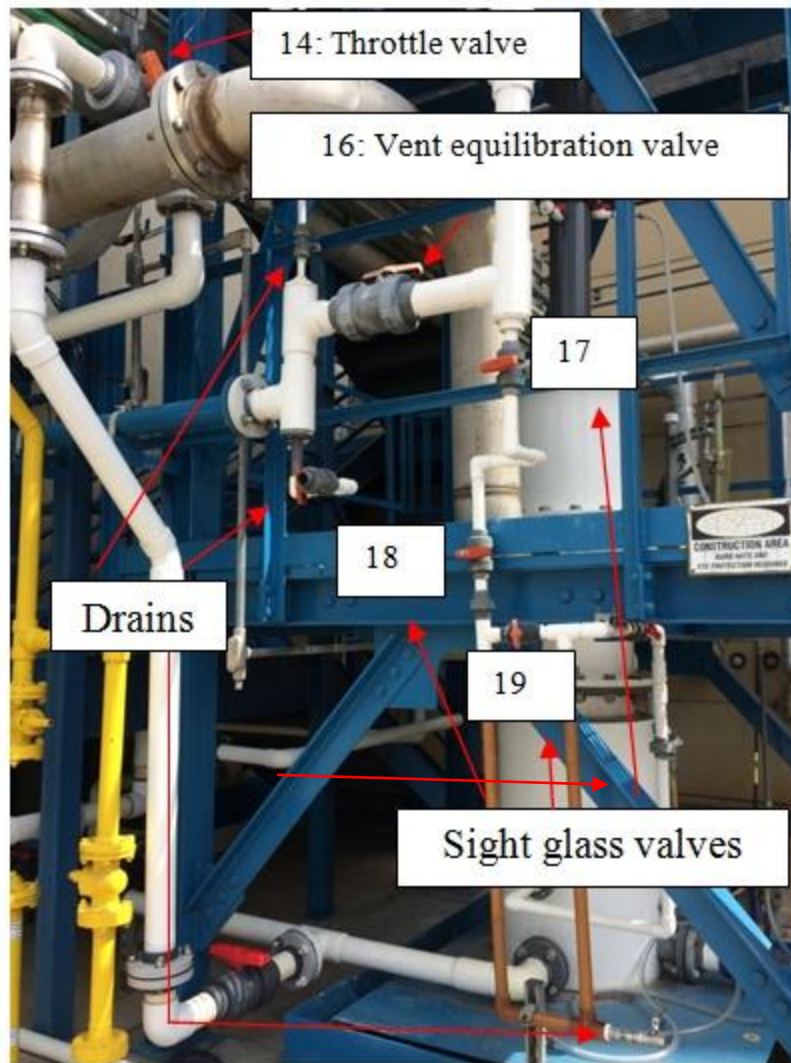


Figure B-7: MicroMotion outlet pipes and associated valves.

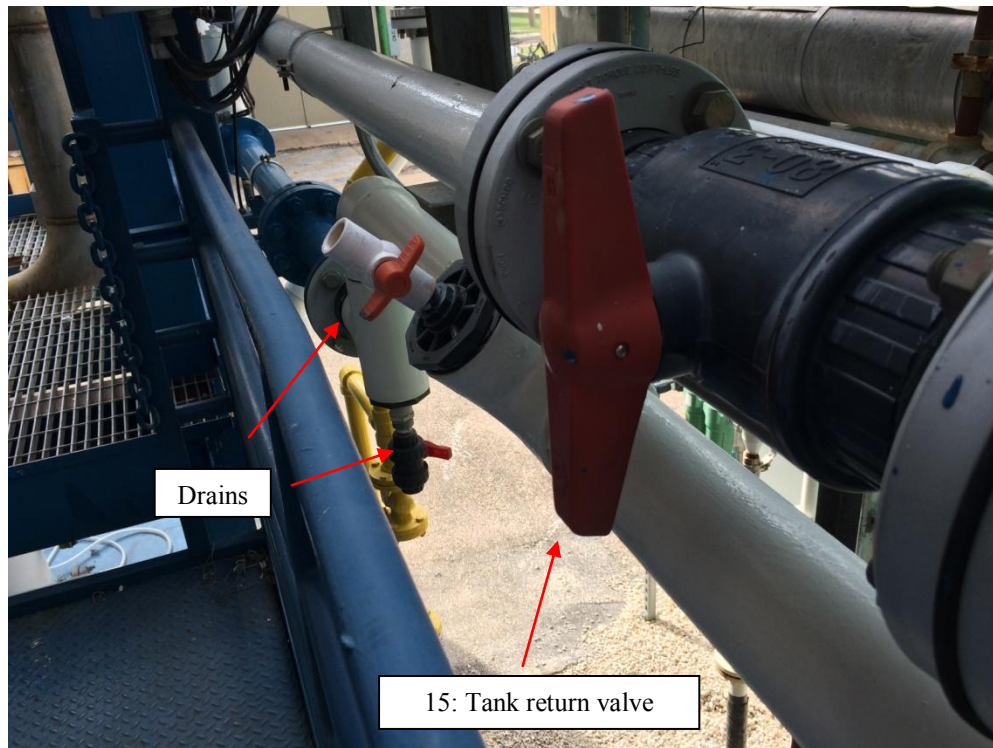


Figure B-8: Associated valves and drains.



Figure B-9: MicroMotion outlet flow associated valve.

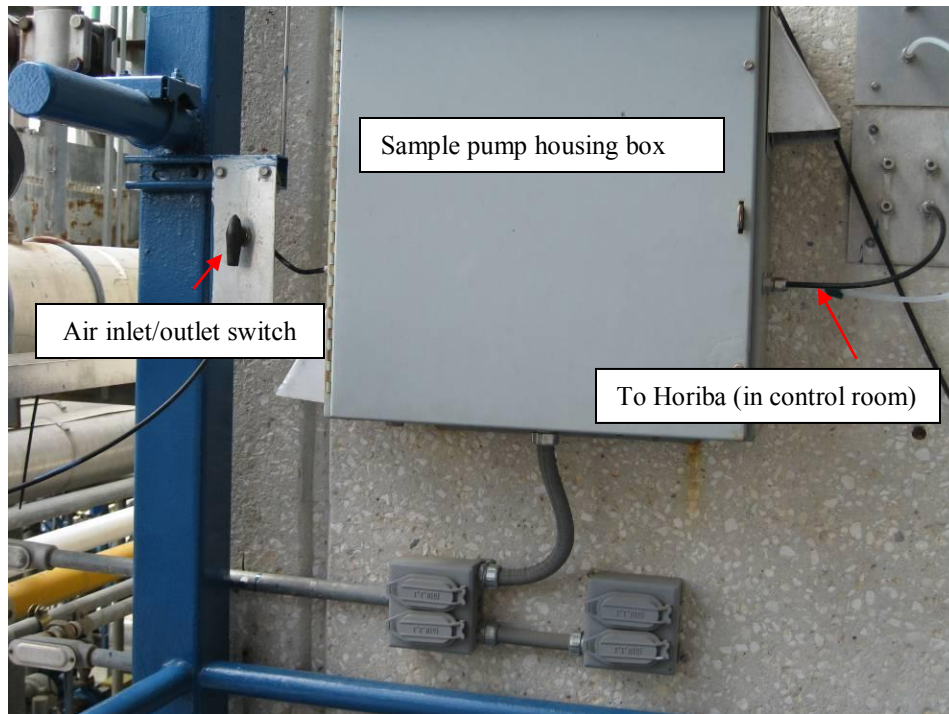


Figure B-10: Air sampling system.

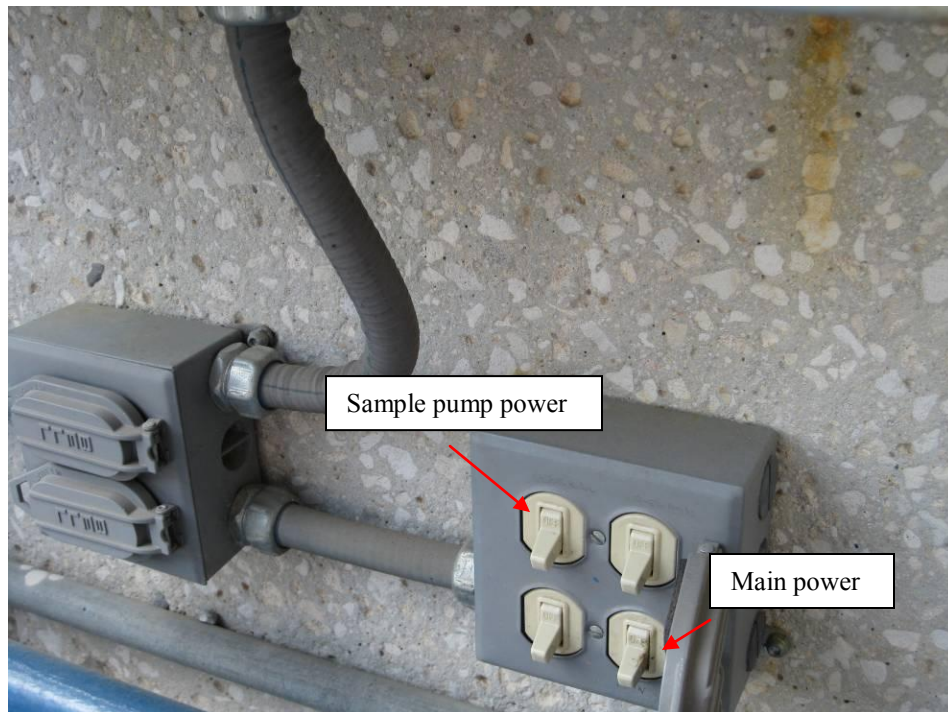


Figure B-11: Power for air sampling system.

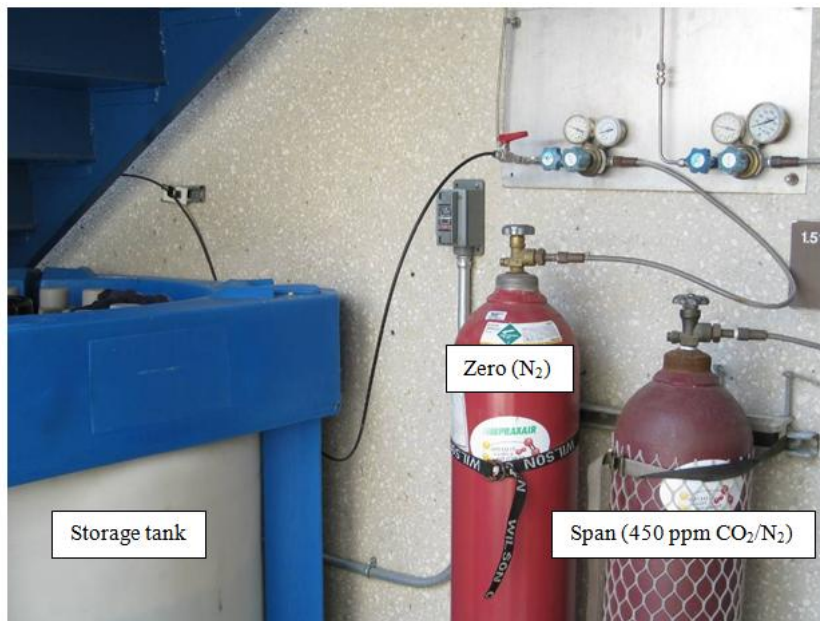


Figure B-12: Storage tank and gas cylinders.



Figure B-13: Column mid-section.

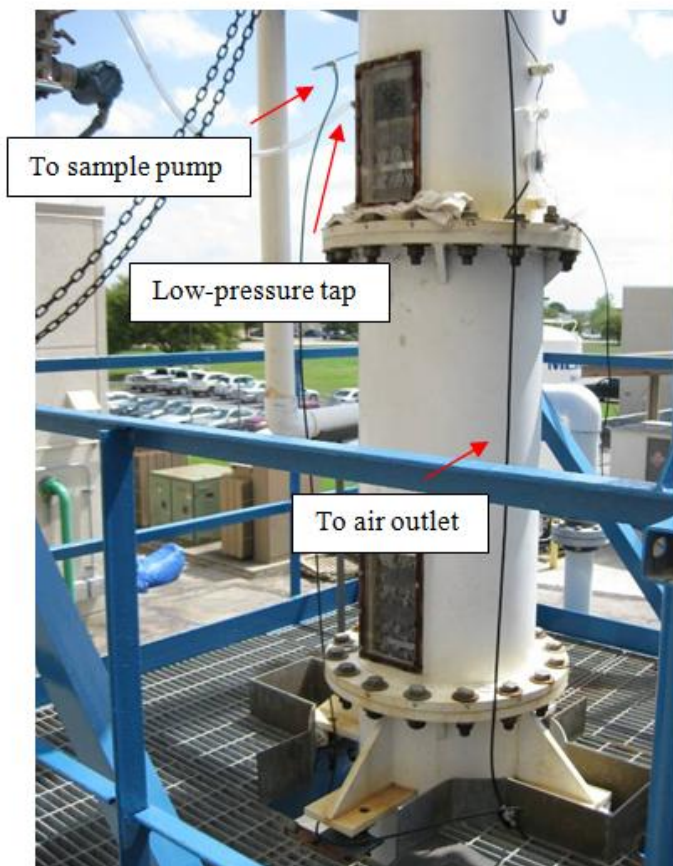


Figure B-14: Column top

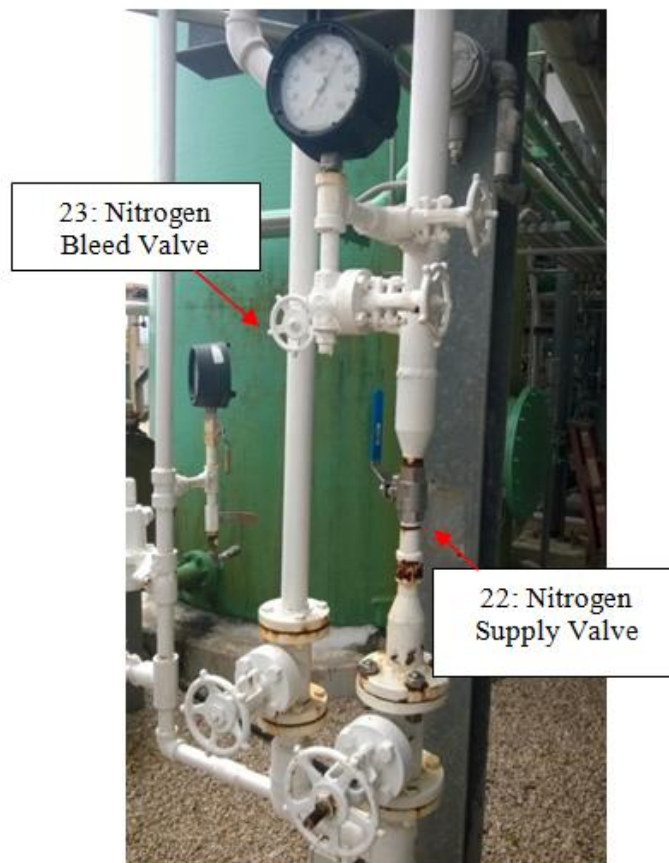


Figure B-15: Plant Nitrogen Supply Valve

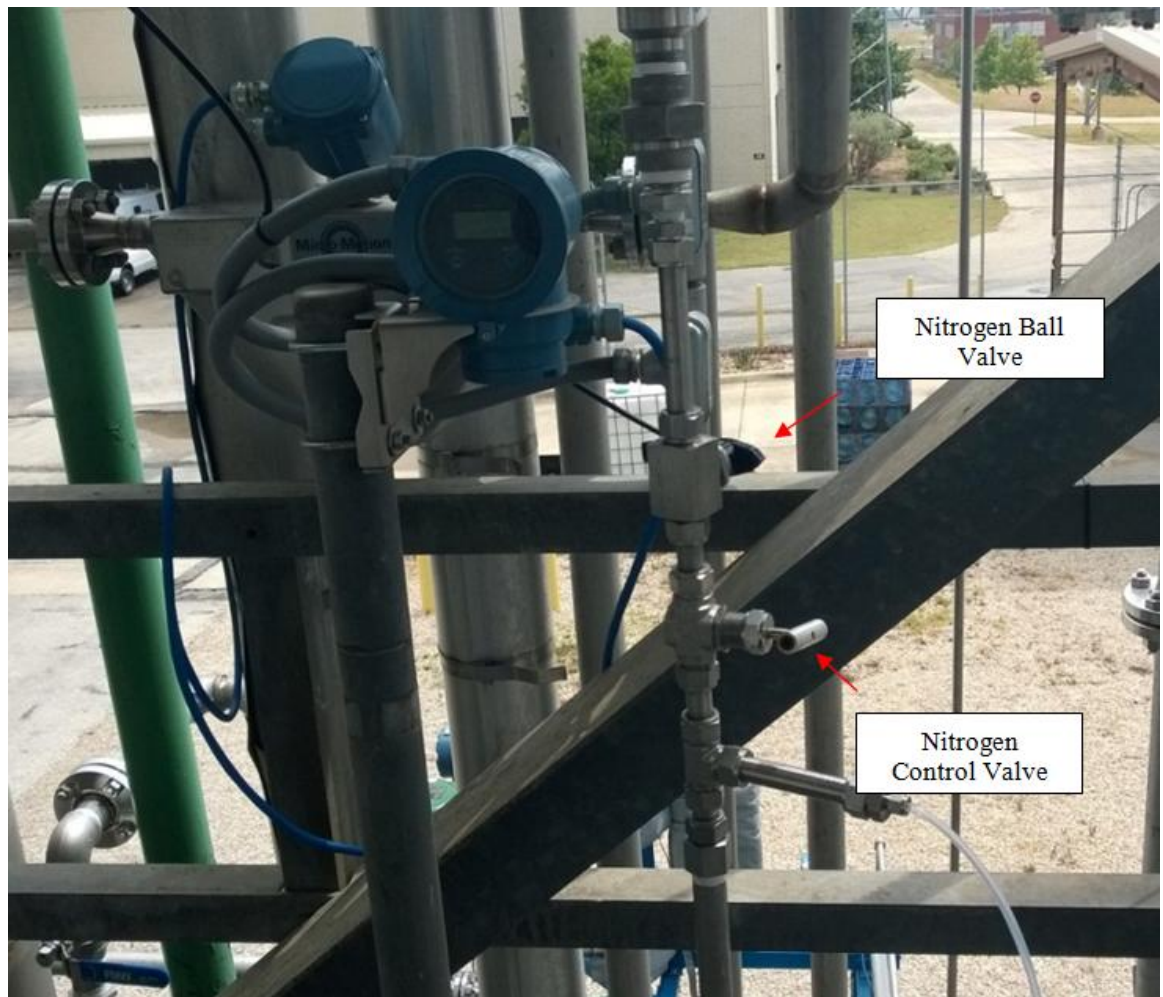


Figure B-16: Nitrogen Control Valve

B-4. START-UP PROCEDURE

I. Hydraulic Experiment

1. Open the Excel file going to:
Network - App - Logs - Air/Water - "AW Logs.Hydraulics_Roach"
Start a new file using following naming convention:
Network - App - Historical Data - Air-Water 6inch - "(File Name)".
2. Make sure the spreadsheets are ready to go.
3. Ensure air blind is in place, isolating the air column from the absorber and blower.
4. Fill storage tank with water (connection point: valve 11).
 - a. Open valves 1, 3a, 3b, 3d, 5, 6, 8, 9, 14 (manually) and use DeltaV to open AV401;
 - b. Close valves 2, 4, 7, 13, 15;
 - c. Add water from the wall to the column for 7.5 minutes;
 - d. Close valve 11 and disconnect the hose.
5. Ensure the liquid flow controller is in "MAN" mode with the output set at 40%.
6. Start nitrogen flow.
 - a. Ensure Nitrogen Supply Valve is open (valve22);
 - b. Open Nitrogen Ball Valve immediately upstream of Nitrogen Control Valve;
 - c. Use the radios to coordinate position of Nitrogen Control Valve to ensure proper gas rate. *This will require two people.*
7. Start experiment and record dry pressure drop using Excel log.
8. After completing dry pressure drop curve, start feed pump.
 - a. Enable pump on DeltaV Operator screen;
 - b. Depress the "ON" side of the knife-switch outside.

9. Wet packing by circulating liquid at 15 GPM/ft² (controlled by liquid VSD, %) with the gas rate at its lowest value for 15 minutes.
10. Start hydraulic experiment at lowest liquid and gas rates. Visually inspect the pipes for leaks.
11. Go to section 5.I. Hydraulic Experiment for steady-state operation instructions.

II. Liquid Holdup Experiment

The liquid holdup measurements are completed without gas flow. Without a need for nitrogen, the column can be assembled inside the high bay with a clear column sump to assist in measuring changes in volume.

1. Assemble column.
2. Hook up pump/flow meter cart.
3. Fill column from open column top.
4. Plug-in pump and cart.
5. Circulate liquid at 30 GPM/ft² for 10 minutes to wet the packing.
6. Establish baseline level by shutting-down pump and turning off pump simultaneously. Mark baseline height.
7. Start holdup experiment at lowest liquid rate.

III. Mass Transfer Efficiency, Gas Film Mass Transfer Coefficient Experiment

1. Fill system with 200 gallons of process water (connection point: valve 11).
 - a. Arrange valves so that all water flows once-through MicroMotion.
 - i. Open valves: 1, 5, 8, 9, 13 pneumatic valve (AV401);
 - ii. Closed valves: 2-4, 6, 7, 14.

- b. Track inventory in DeltaV Control Studio (EXTRACTION → EX_FLOW → FT420_FB).
 - c. Click the on-line button.
 - d. Double click PARAM1. Click TRUE - OK. Click FALSE - OK.
 - e. Open the valve in the wall to add water in the system.
 - f. Flow should be stopped when counter reaches 185-190 gallons, to account for dead space in system.
2. Start liquid circulation (recommended pump setting: 65% VSD).
 - a. Open valves 2, 4 and 6;
 - b. Close AV401 and valves 5 and 11. Start pump through DeltaV;
3. Add 8.00 lbs. of solid NaOH pellets to storage tank. Allow pellets to dissolve for 30 minutes.
4. Calibrate gas analyzer using zero and span gases from cylinders/zero air generator/flow controller.
5. Leak-check sample line tubing and sample pump.
 - a. Arrange valves so that analyzer draws from N₂ cylinder;
 - b. Turn sample pump on and adjust regulator so that gas is sampled under minimal pressure (< 1 psig). Analyzer reading should approach 7ppm;
 - c. Shut down sample pump afterward. Close valve and orient valve to draw from air outlet.
6. Allow liquid to circulate through packing. Ensure at least 5 or 6 liquid inventory turnovers for sufficient mixing.
 - a. Open valves 3a, 3b, 5, 14 and AV401;
 - b. Close valves 2 and 4;
 - c. Recommendation: 15 gpm/ft² for 1 hr.

7. Take sample (from spigot on column sump) and verify NaOH concentration.
 - a. Titrate 10 mL of solution with 0.1 N HCl and phenolphthalein indicator.

NaOH concentration should be within approximately 5% of 0.1 N.
8. Pre-wet packing at 25 gpm/ft² for 10 minutes.
9. Begin mass transfer experiment.

B-5. STEADY-STATE OPERATION

I. Hydraulic Experiment

If continuing operation from previous day and the column is left full of water, ensure the pressure drop is zero. Wait for conditions to remain steady for approximately 5 minutes before changing conditions. Very low liquid rates may require manipulation of the throttle ball valve (#14) located in the pump discharge line at the first platform. Closing down on the ball valve will allow the flow controller to better control lower flow rates.

In order to prevent pressure drop curves from overlapping, the data should be collected first by fixing the gas rate and increasing the liquid rate. Once all liquid rates have been completed, then the gas rate may be increased. This will prevent the constant liquid-rate curves from overlapping at the very low end. Remember to go back to the lower liquid rate when the gas rate is changed.

The experiment should start by fixing the gas rate in the following manner: adjust the nitrogen rate until it is at its lowest value. Only after all liquid rates have been tested (typically from 0 – 30 GPM/ft²) should the gas rate be increased. As the pressure drop curves become more spaced out, it becomes easier to keep the liquid rate constant and change the gas rate.

The gas rate should increase until the packing is flooded. Flood has been achieved when the column pressure drop surpasses 2 inches of H₂O per foot of packing. Once the packing has been flooded at the particular liquid rate, the gas rate should be lowered to recover the column. Take this time to check the impulse tubing of the differential pressure drop meters for entrained liquid. The lines should remain clear at all times. Also, monitor pressure drop trend during run to ensure steady state. If spikes, the column may be flooding.

II. Liquid holdup Experiment

There is only one data point collected per liquid rate. The difference in height is converted to a volume, and the fractional holdup is calculated for each liquid rate. The conditions should be repeated to accurately record the fractional holdup.

III. Mass Transfer Efficiency

An accurate initial sodium hydroxide concentration is very important. The hydroxide concentration calculator must be updated on the user interface screen after every data point in order to ensure a good prediction of sodium hydroxide concentration throughout the duration of the experiment.

Conditions can be changed after the carbon dioxide concentration has remained stable for five minutes. Each batch of caustic can only be used to complete one gas rate. Upon completion of the gas rate, data points at mid-range liquid rates should be done at different gas rates to demonstrate repeatability. The inlet CO₂ concentration should also be verified upon completion of a gas rate.

B-6. SHUTDOWN PROCEDURE

I. Hydraulic Experiment

1. Isolate nitrogen flow by closing Nitrogen Supply Valve (#22).
2. Turn off water pump in DeltaV.
3. Drain the system to the sanitary sewer by attaching hoses to valves 11 and 12 and stringing the hoses to the sewer. Open valves 2, 4, 5, 6, 7, 8, 9 13, and 15 allowing the system to drain.
4. After completely draining the system, put the hoses back into their places.

II. Liquid Holdup Experiment

1. Turn off pump.
2. Open all valves.
3. Close bottom ball valve in pump suction line.
4. Disconnect pump suction hose from pump and string to sewer port in floor.
5. Open column bottom/pump suction ball valve to drain system contents to sewer.

III. Mass Transfer Efficiency

1. Check inlet carbon dioxide concentration before stopping the blower.
2. Place gas and liquid flow controllers in “MAN” mode.
 - a. Place gas flow controller set point at 10%;
 - b. Place liquid flow controller set point at 40%.
3. Isolate nitrogen from system by closing nitrogen supply valve.
4. Shut pump discharge throttle valve at first platform to isolate liquid flow from the packing.
5. Align valves around filter so that liquid flows between the storage tank and the sump
 - a. Open valves: 1, 2, 4;
 - b. Close valves: 3, 5.
6. Raise the liquid flow controller set point to 60%.
7. Wearing long gloves, sleevelets, and a respirator, add hydrochloric acid to storage tank. Add slowly, wait 10 minutes, and check the pH of the solution by drawing a sample from the sample spigot in the column sump. Add hydrochloric acid until the pH of the solution is between 6 and 9.

8. Lower the set point of the liquid flow controller to 40%. Turn off the pump in DeltaV.
9. Drain the system to the sanitary sewer by attaching hoses to valves 11 and 12 and stringing the hoses to the sewer. Open all valves and allow system to drain.

B-7. METHOD OF DATA ACQUISITION

Before starting any experiment, prepare a new data sheet in Excel by opening one of the template files stored on the App station specific to that experiment. There are also different Log sheets for each experiment stored on the App station.

Log sheets are used to pull data from the DeltaV Continuous Historian. The data is copied from the Log sheets and pasted into the Excel files as the experiments are being conducted. All parameters for all experiments are pulled from the Continuous Historian.

B-8. DATA ANALYSIS EXAMPLE

Data analysis is accomplished using functions built-into the experiment-specific Excel files. Spreadsheets calculate important packing performance data from pressure drop per foot to effective contact area.

B-9. SAFETY AND RISKS

The proper personal protective equipment must be worn at all times. Operators must wear the following PPE:

- Hard hat
- Safety glasses
- Long Pants

When handling samples, nitrile gloves should be worn. The addition of chemical to the system also requires the use of nitrile gloves. When handling packing, cut-resistant gloves should be worn, and no more than one element of packing should be carried at one

time. A safety harness should also be worn at any point in which a ladder must be climbed.

Any physical injuries should be reported to Dr. Seibert and Micah Perry immediately. A binder that details SRP's emergency response protocols is kept beside the phone in the control room. Follow the procedures outlined in the binder when responding to a physical injury.

The response to any chemical exposures should follow the guidelines listed in the MSDS for the chemicals being used attached to this document. The closest shower and eye wash station is immediately out the control room door towards the high bay. If someone requires the safety shower, all clothing should be removed in order to prevent the chemical from sticking close to the skin. Anyone using the eye wash should keep their eyes in the water streams for at least 15 minutes to ensure a good flush. Chemical exposures should be reported immediately to Dr. Seibert and Micah Perry.

The test order usually allows leaks to be detected when only air and water are in the system. However, the risk of leaks in liquid lines is everpresent. The system is at relatively low pressure, so spray-like events would not be common. Portions of the liquid stream are under pressure. Frequent inspections of the system should be made to detect leaks as soon as possible.

The sodium hydroxide solution used in these experiments is relatively dilute, but exposure to the caustic scrubbing solution should still be treated quickly.

Appendix C: Wetted Area Calculations and Experimental Conditions

Water Flow FT901 (GPM/ft2)	Water In T901 (F)	Air Annubar TT403 (F)	N2-Flow (ACFM)	Pressure Drp (high) PDT901 (in H2O)	Press Drp (low) PDT900 (in H2O)	CO2 In (ppm)	CO2 Out (ppm)
25.37	61.73	50.68	40.79	3.24	3.34	396.00	223.46
19.33	61.17	50.83	40.63	1.80	1.90	396.00	235.67
15.10	60.71	50.24	40.43	1.42	1.53	396.00	238.74
10.00	59.85	48.85	40.14	1.15	1.28	396.00	245.83
5.36	59.13	48.46	40.06	0.95	1.09	396.00	258.42
29.98	58.11	48.19	19.97	2.19	2.33	370.00	125.67
25.39	57.75	48.70	19.99	0.98	1.15	370.00	131.25
19.97	57.45	50.07	19.99	0.47	0.60	370.00	136.98
15.15	57.22	52.23	20.01	0.28	0.42	370.00	144.84
10.22	56.98	53.99	20.08	0.20	0.34	370.00	154.74
5.36	56.57	53.93	20.08	0.16	0.30	370.00	167.59
25.69	56.56	51.84	39.99	3.11	3.23	406.00	237.72
19.88	56.24	51.28	39.96	1.81	1.96	406.00	247.07
15.70	56.01	51.47	39.88	1.40	1.54	406.00	252.03
10.28	55.80	51.87	39.89	1.13	1.28	406.00	259.99
5.26	55.48	52.05	39.91	0.95	1.11	406.00	274.21
15.11	55.00	55.63	60.55	3.21	3.37	408.00	294.58
10.31	54.85	57.83	60.76	2.65	2.78	408.00	301.52
6.09	54.69	59.72	60.79	2.35	2.46	408.00	308.19

Table C-1: Wetted area experimental conditions.

WETTED AREA CALCULATIONS

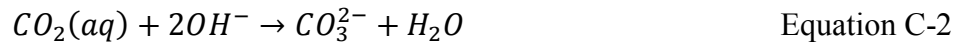
This section will summarize the development of Tsai, and interested readers are encouraged to read “Mass Transfer Area of Structured Packing” by Tsai.⁷¹ The first section details the chemical reactions that take place with absorption of CO₂ into a solution of sodium hydroxide. The second section details mass transfer enhanced by chemical reaction. The final section details the specific equations used.

Chemical Reactions and Kinetics

The chemical reactions occurring in the system are given by:



Reaction C-1b is significantly higher than the reaction rate of C-1a. Further, the concentration of bicarbonate can be considered negligible with sufficiently high free hydroxide. Thus, the overall reaction can be written as:



This reaction can be considered irreversible. The reaction rate can be written as:

$$r = k_{OH^-}[OH^-][CO_2] \quad \text{Equation C-3}$$

where k_{OH^-} is the second-order reaction rate constant. With a sufficiently low concentration of CO_2 and excess hydroxide ion, this can be rewritten a pseudo first-order reaction.

$$r \cong k_1[CO_2] \quad \text{Equation C-4}$$

where k_1 is the first-order rate constant given by:

$$k_1 = k_{OH^-}[OH^-] \quad \text{Equation C-5}$$

Mass Transfer Enhanced by Chemical Reaction

The flux of CO_2 across between the gas and liquid can be written as:

$$N_{CO_2} = K_G(P_{CO_2} - P_{CO_2}^*) \quad \text{Equation C-6a}$$

$$N_{CO_2} = k_G(P_{CO_2} - P_{CO_2}^i) \quad \text{Equation C-6b}$$

$$N_{CO_2} = k'_G(P_{CO_2} - P_{CO_2}^i) \quad \text{Equation C-6c}$$

where K_G is the overall mass transfer coefficient based on gas phase concentrations, P_{CO_2} is the partial pressure of CO_2 in the gas phase, $P_{CO_2}^*$ is the equilibrium concentration, $P_{CO_2}^i$ is the partial pressure of CO_2 at the interface, k_G is gas-film mass transfer coefficient, and k'_G is the liquid-film mass transfer coefficient given by:

$$k'_g = \frac{Ek_L^0}{H_{CO_2}} \quad \text{Equation C-7}$$

where E is enhancement factor to account for increased mass transfer due to chemical reaction defined below, k_L^0 is the physical liquid-film mass transfer coefficient, and H_{CO_2} is the Henry's law coefficient for CO_2 . The enhancement factor for a pseudo-first order reaction is given by:

$$E = \sqrt{1 + \frac{k_1 D_{CO_2,L}}{(k_L^0)^2}} \quad \text{Equation C-8}$$

where k_1 is the pseudo-first order reaction rate constant, and $D_{CO_2,L}$ is the diffusivity of CO_2 through the liquid phase. The Hatta number for a pseudo-first order reaction is given by:

$$Ha = \frac{\sqrt{k_1 D_{CO_2,L}}}{k_L^0} \quad \text{Equation C-9}$$

For a sufficiently large Hatta number (as was the case for these experiments), the Hatta number and enhancement factor are approximately equal, and k'_g can be written as:

$$k'_g \cong \frac{\sqrt{k_1 D_{CO_2,L}}}{H_{CO_2}} = \frac{\sqrt{k_{OH^-} [OH^-] D_{CO_2,L}}}{H_{CO_2}} \quad \text{Equation C-10}$$

where k_{OH^-} is the second-order reaction rate constant, and $[OH^-]$ is the molar concentration of OH^- . Using equations C6a-C6c, a resistance model relating mass transfer coefficients to each other can be written as:

$$\frac{1}{K_G} = \frac{1}{k_G} + \frac{1}{k'_g} \quad \text{Equation C-11}$$

The differential mass balance for carbon dioxide through a column filled with structured packing is given by:

$$U_{GS} \frac{dy_{CO_2}}{dz} = K_G a_e RT (y_{CO_2}^* - y_{CO_2}) \quad \text{Equation C-12}$$

where U_{GS} is the superficial gas velocity, y_{CO_2} is the molar gas fraction of CO_2 , z is the length variable, a_e is the effective wetted area, R is the molar gas constant, T is the

temperature, and $y_{CO_2}^*$ is the equilibrium concentration of CO_2 . As any CO_2 absorbed into the liquid is reacted, $y_{CO_2}^*$ can be considered 0. Integrating this equation and solving effective wetted area yields:

$$a_e = \frac{U_{GS} \ln\left(\frac{y_{CO_2,in}}{y_{CO_2,out}}\right)}{ZK_GRT} \quad \text{Equation C-13}$$

where Z is total packed bed height, $y_{CO_2,in}/y_{CO_2,out}$ is the inlet/outlet concentration of CO_2 in the gas phase. Using dilute caustic (~ 0.1 mol/L) and sufficiently high gas velocities [greater than ~ 0.6 m/s (~ 2 ft/s)], the absorption of CO_2 is dominated by the liquid-film mass transfer resistance, allowing Equation C-13 to be written as:

$$a_e \cong \frac{U_{GS} \ln\left(\frac{y_{CO_2,in}}{y_{CO_2,out}}\right)}{Zk'_gRT} \quad \text{Equation C-14}$$

U_{GS} and Z are controlled experimental conditions. Mole fractions and temperature are measured during the experiments. This leaves k'_g as the only unknown variable needed to calculate a_e . Equation C-10 shows that four parameters (k_{OH^-} , $[OH^-]$, $D_{CO_2,L}$ and H_{CO_2}) are necessary. The equations for determining these equations are detailed below.

Model Equations

The equations necessary for calculating the rate constant are given by:

$$\log_{10} \left(\frac{k_{OH^-}}{k_{OH^-}^\infty} \right) = 0.221I - 0.016I^2 \quad \text{Equation C-15}$$

$$\log_{10}(k_{OH^-}^\infty) = 11.895 - \frac{2382}{T} \quad \text{Equation C-16}$$

$$D_{CO_2,L} = \frac{D_{CO_2,w}\mu_w}{\mu_L} \quad \text{Equation C-17}$$

$$\log_{10} D_{CO_2,w} = -8.1764 + \frac{712.5}{T} - \frac{2.591 \cdot 10^5}{T^2} \quad \text{Equation C-18}$$

$$\mu_w = 0.02414 \cdot 10^{\left(\frac{247.8}{T-140}\right)} \quad \text{Equation C-19}$$

$$\log_{10} \mu_L = \frac{878.159}{T} - 3.0254 + 0.1103([OH^-] + 2[CO_3^{2-}]) + 0.08947 \left(\frac{[CO_3^{2-}]}{0.5[OH^-] + [CO_3^{2-}]} \right) \quad \text{Equation C-20}$$

where the subscript of w indicates the given property for water, the subscript of L indicates the property is evaluated for the liquid phase (i.e. a dilute caustic solution), and $k_{OH^-}^\infty$ is the second-order reaction rate constant at infinite dilution. The Henry's law coefficient is given by:

$$-\log_{10} H_{CO_2,w} = 9.1229 - 5.9044 \cdot 10^{-2}T + 7.8857 \cdot 10^{-5}T^2 \quad \text{Equation C-21}$$

$$\log_{10} \left(\frac{H_{CO_2}}{H_{CO_2,w}} \right) = \sum I_i h_i \quad \text{Equation C-22}$$

$$h_i = h_+ + h_- + h_g \quad \text{Equation C-23}$$

$$I = 0.5 \sum c_i z_i \quad \text{Equation C-24}$$

$$\sum I_i h_i = I_{NaOH} (h_{Na^+} + h_{OH^-} + h_{CO_2}) + I_{Na_2CO_3} (h_{Na^+} + h_{CO_3^{2-}} + h_{CO_2}) \quad \text{Equation C-25}$$

where I_i is the ionic strength, c_i is the concentration of the, z_i is the charge number of the ion, $H_{CO_2,w}$ is the Henry's coefficient for CO₂ in pure water, H_{CO_2} is the Henry's coefficient for CO₂ for the caustic solution, and h_i is the contribution to the Henry's law coefficient by the various species given by:

$$h_{Na^+} = 0.091$$

$$h_{OH^-} = 0.066$$

$$h_{CO_3^{2-}} = 0.021$$

$$h_{CO_2} = 4.364 \cdot 10^{-7} \cdot T_C^3 - 3.297 \cdot 10^{-5} \cdot T_C^2 + 1.204 \cdot 10^{-4} \cdot T_C - 6.847 \cdot 10^{-3}$$

No other unknowns are present, and thus the effective area can be determined.

Appendix D: Liquid Holdup at the Contact Points

Liquid droplets were observed in multiphase simulations at contact points between adjacent sheets of packing. A rudimentary analysis of this phenomenon was undertaken to characterize how much liquid was held up where packing sheets contacted and the relevant fluid properties.

METHOD

Within the periodic simulations, five threshold geometries were created at the coordinates shown in Table D-1. The thresholds consisted of mesh cells with centroids within 4.0 mm of the indicated coordinates. The created volumes are shown in Figure D-1, highlighted in pink. The liquid volume fraction was integrated over these threshold geometries to determine total liquid holdup present. As a note, this was only performed at one instant in time. Future studies should average the liquid volume over a period of time.

Contact Point	x-coordinate (mm)	y-coordinate (mm)	z-coordinate (mm)
Middle	17	-21	0.025
Top Left	0	-1.5	0.025
Top Right	34	-1.5	0.025
Bottom Left	0	-42.02	0.025
Bottom Right	34	-42.02	0.025

Table D-1: Location of the four contact point sphere centers for contact point studies.

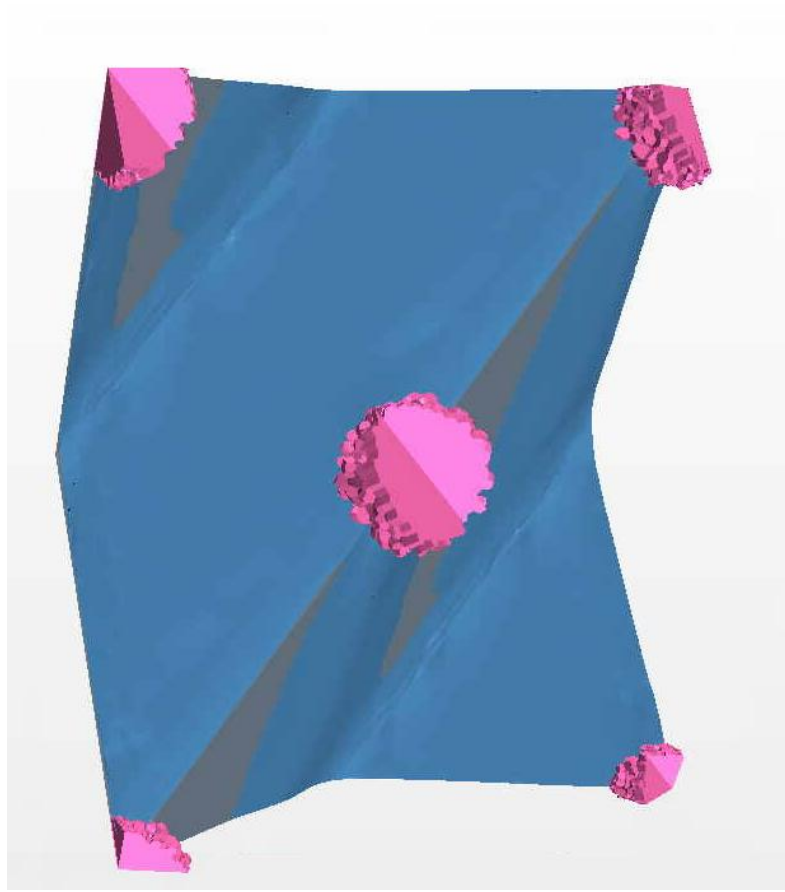


Figure D-1: Threshold geometries used to determine the contact point liquid holdup.

In total, the five thresholds had a total volume of 122.15 mm^3 . The total volume of the periodic geometry was 14570 mm^3 , making the threshold sections 0.84% the total volume present in the simulations. On average, the liquid at the contact points represented 4.5% of the total liquid in the system. Values ranged from 2.0-6.7%. In chapter 6 (Figure 6-22), it was found that liquid holdup could successfully be parameterized as:

$$h_L \left(\frac{\rho_L}{\rho_{ref}} \right) \left(\frac{\mu_{ref}}{\mu_L} \right) = A_1(\theta_c) f(Re_L) \quad \text{Equation 6-2}$$

$$Re_L = \frac{\rho_L Q}{\mu_L L_p} \quad \text{Equation 6-3}$$

This approach was adopted once again. However, rather than total liquid holdup, the local liquid holdup is used. It is defined as the volume of liquid present at the contact points divided by total contact point volume (i.e. 122.15 mm³). The results for a contact angle of 0° are summarized in Figure D-2. It is clear there is some weak dependence on surface tension. For equivalent Reynolds numbers, the diamond markers, which correspond to the highest surface tension examined ($\gamma=0.074$ N/m) tend to have higher local liquid volumes. This indicates surface tension acts to hold larger droplets together and, thus, result in increased droplet size.

To account for surface tension, the holdup is scaled by the surface tension as:

$$h_{L,droplet} \left(\frac{\rho_L}{\rho_{ref}} \right) \left(\frac{\mu_{ref}}{\mu_L} \right) \left(\frac{\gamma}{\gamma_{ref}} \right)^{-0.14} = A_1(\theta_c) f(Re_L) \quad \text{Equation D-1}$$

where γ_{ref} is a reference surface tension (chosen to be 0.074 N/m in this case). The results of this correlation are plotted in Figure D-3. No longer are low surface tension data points consistently lower than the high surface tension data. A power law prediction was generated as:

$$h_{L,droplet} \left(\frac{\rho_L}{\rho_{ref}} \right) \left(\frac{\mu_{ref}}{\mu_L} \right) \left(\frac{\gamma}{\gamma_{ref}} \right)^{-0.17} = 0.446 Re_L^{0.57} \quad \text{Equation D-2}$$

The power law model demonstrates an R^2 value of 0.99, and an average percent difference of 11.3% when compared to CFD data. Rearranging Equation D-2 yields:

$$h_{L,droplet} = 0.446 \left(\frac{\rho_{ref}}{\mu_{ref}} \right) \left(\frac{Q}{L_p} \right)^{0.57} \left(\frac{\mu_L}{\rho_L} \right)^{0.43} \left(\frac{\gamma}{\gamma_{ref}} \right)^{0.17} \quad \text{Equation D-3}$$

In this form, it is clear that a reduction in surface tension will result in a reduction in liquid holdup. To verify this model, X-ray CT scan data should be collected with an emphasis on determining how much holdup is in the region where adjacent packing sheets contact. This localized data can be compared to CFD predictions to provide ongoing data validation for the multiphase model selection.

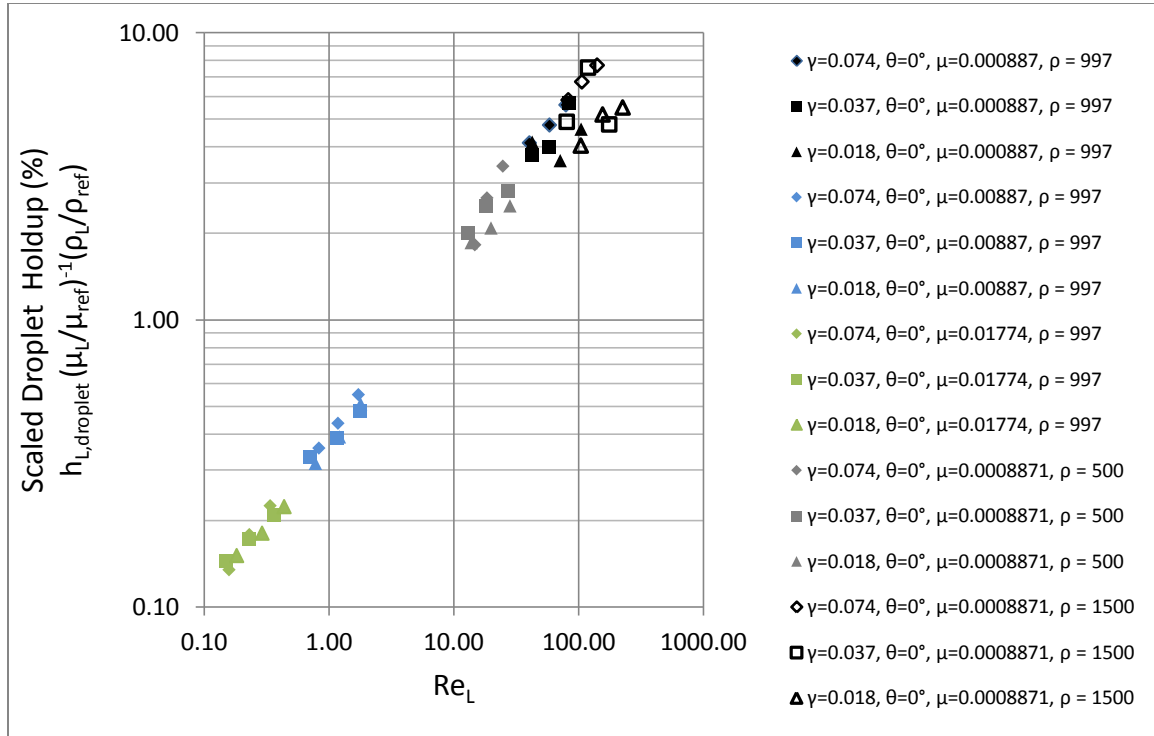


Figure D-2: Summary of local liquid holdup for simulations with a contact angle of 0° . Diamonds are high surface tension. Squares are middle surface tension. Triangles are low surface tension. Solid black markers are a base case with a liquid density of 997.561 kg/m^3 and viscosity of $0.0008871 \text{ Pa}\cdot\text{s}$. Hollow black markers have a density of 1500 kg/m^3 . Grey markers have a density of 500 kg/m^3 . Blue markers have a viscosity of $0.008871 \text{ Pa}\cdot\text{s}$. Green markers have a viscosity of $0.01774 \text{ Pa}\cdot\text{s}$.

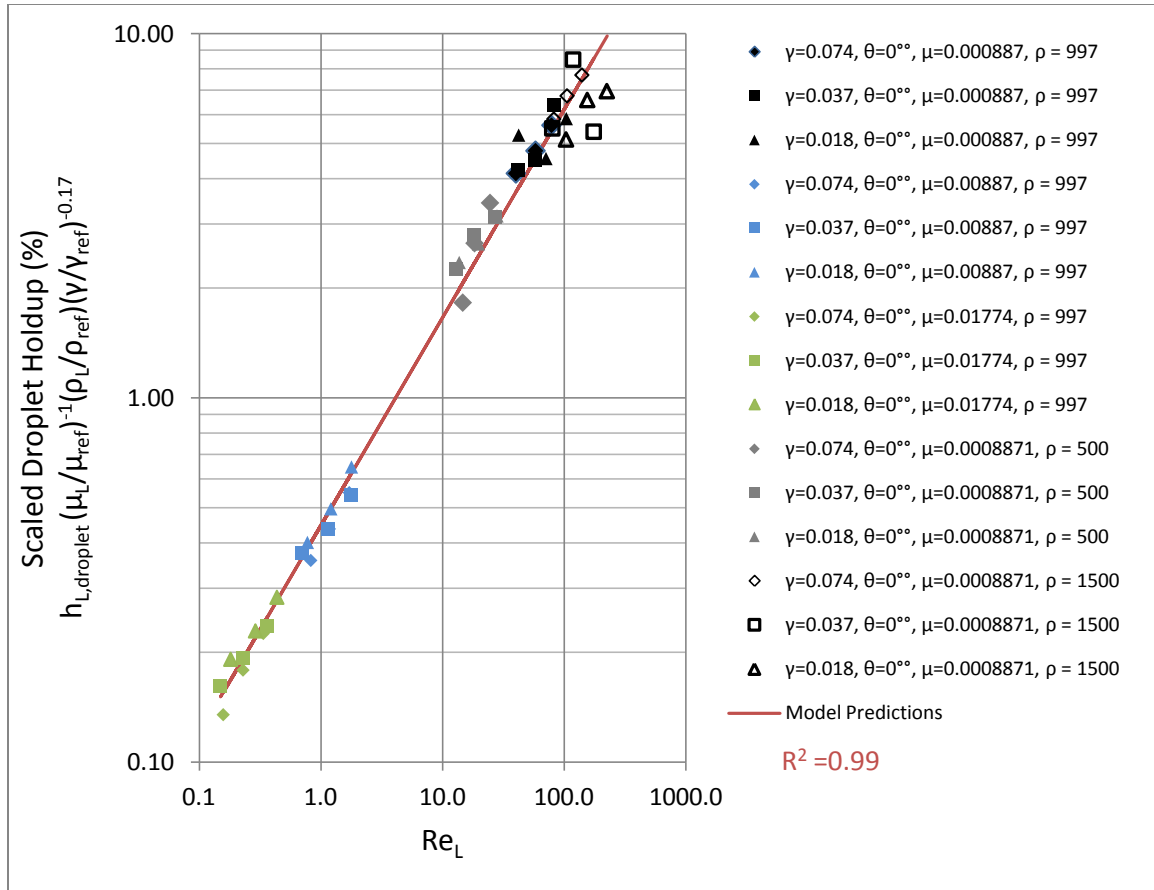


Figure D-3: Summary of local liquid holdup for simulations with a contact angle of 0° with a surface tension correction. Diamonds are high surface tension. Squares are middle surface tension. Triangles are low surface tension. Solid black markers are a base case with a liquid density of 997.561 kg/m^3 and viscosity of 0.0008871 Pa-s . Hollow black markers have a density of 1500 kg/m^3 . Grey markers have a density of 500 kg/m^3 . Blue markers have a viscosity of 0.008871 Pa-s . Green markers have a viscosity of 0.01774 Pa-s . A Power law model generated is shown as the red line (Equation D-2).

Glossary

A_c = cross-sectional area of column [m²]

a_p = packing specific surface area [m²/m³]

a_e = effective area of packing [m²/m³]

b = channel base length [m]

$C_\mu, C_{\varepsilon 1}, C_{\varepsilon 2}, C_{\omega 1}, C_{\omega 2}$ = constants related to two-equation turbulence models

CFD = Computational Fluid Dynamics

d_{hG} = hydraulic diameter of triangular channel used in Delft model $\left(\frac{2bh}{b+2s}\right)$

$d_{h,rhombus}$ = hydraulic diameter of rhombus channel $\left(\frac{bh}{s}\right)$ [m]

F-factor = gas capacity factor $(U_{GS}\sqrt{\rho_G})$ [Pa^{0.5}]

f_E = friction factor for pressure drop due to friction between packing and gas

f_H = friction factor for pressure drop due to horizontal gas velocity

f_i = volumetric body force in Navier-Stokes equations [m/s²]

F_i^γ = force of surface tension [N/m³]

GPM = gallons per minute

g_i = gravitational vector [m/s²]

GCI = Grid Convergence Index

h = channel height [m]

h_L = fractional liquid holdup [%]

h_{pb} = height of packed bed [m]

h_{ru} = height of a repeating unit in structured packing [m]

k = turbulent kinetic energy [m²/s²]

k'_g = liquid phase mass transfer coefficient [kmol/m²-Pa-s]

k_{OH^-} = second order rate constant [m³/kmol-s]

k_{SGS} = subgrid turbulent kinetic energy [m²/s²]

H_{CO_2} = Henry's Law constant for CO₂ [m³-Pa/kmol]

Liquid load = volumetric liquid flow through column divided the cross-sectional
area of the column (Q/A_c) [m³/m²-hr] or [GPM/ft²]

L_c = length of repeating flow channel through structured packing $\left(\frac{h_{ru}}{\sin \alpha}\right)$ [m]

L_p = wetted perimeter of packing $\left(\frac{4s}{bh}A_c\right)$ [m]

LES = Large Eddy Simulation

$\hat{n}$ = unit normal of interface pointing into the heavy phase

$\hat{n}_i^{wall}$ = unit normal of wall for VOF simulations

$[OH]^-$ = concentration of hydroxide ion [mol/L]

p = pressure [Pa]

P = modified pressure [Pa]

$\bar{P}$ = filtered pressure in LES equations [Pa]

$\langle P \rangle$ = Averaged modified pressure for RANS equations [Pa]

Q = volumetric flow rate of liquid through column [m³/s]

R = ideal gas constant (8314.5 m³-Pa/kmol-K)

r = the grid refinement ratio

RANS = Reynolds-averaged Navier-Stokes

Re_{Ge} = Reynolds number used in Delft model $\left(\frac{\rho_G U_{GE} d_{hG}}{\mu_G}\right)$

Re_{GH} = Reynolds number based on horizontal gas velocity $\left(\frac{\rho_G U_{GHS}}{\mu_G}\right)$

$Re_{G,rhombus}$ = Reynolds number using effective gas velocity $\left(\frac{\rho_G U_{GE} d_{h,rhombus}}{\mu_G}\right)$

Re_L = Reynolds number of liquid phase $\left(\frac{\rho_L Q}{\mu_L L_p}\right)$

s = channel side length [m]

S_{ij} = strain-rate tensor $\left(0.5 \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)\right)$ [1/s]

$\bar{S}_{ij}$ = filtered strain-rate tensor [1/s]
 $\langle S_{ij} \rangle$ = averaged strain-rate tensor [1/s]
 $\hat{t}_i^{wall}$ = unit tangent of the wall directed into liquid phase for VOF simulations
 u_* = friction velocity $\sqrt{\frac{\tau_w}{\rho}}$ [m/s]
 U = velocity [m/s]
 $\bar{U}$ = filtered velocity for LES [m/s]
 $\langle U \rangle$ = time-averaged velocity for RANS equations [m/s]
 U_{LS} = superficial liquid velocity [m/s]
 u' = velocity fluctuations in RANS equations [m/s]
 U_{GE} = effective gas velocity through structured packing [m/s]
 U_{GH} = horizontal gas velocity through structured packing channel [m/s]
 U_{GS} = superficial gas velocity [m/s]
VOF = Volume of Fluid
 y = distance from wall (i.e. a solid surface) in CFD simulations [m]
 y^+ = dimensionless wall distance ($\frac{u_* y}{\nu}$)
 $y_{CO_2,in}$ = mole fraction of CO₂ at the inlet in absorption experiments
 $y_{CO_2,out}$ = mole fraction of CO₂ at the outlet in absorption experiments
 Z = packed bed height [m]

GREEK LETTERS

α = channel corrugation angle measured from horizontal [°]
 α_L = liquid volume fraction
 $\Delta P_{friction}$ = pressure drop due to friction between gas and solid [Pa]
 ΔP_{shear} = pressure drop due to the horizontal velocity [Pa]
 ΔP_{total} = total pressure drop through periodic packing geometry [Pa]

δ = Dirac delta function

δ_{Delft} = film thickness used in Delft model for calculating liquid holdup [m]

δ_{ij} = Kronecker delta

ε = dissipation of turbulent kinetic energy [m²/s³]

ϵ = packing porosity

ζ_{GG} = overall coefficient for gas-gas friction losses in Delft model

ζ_{GL} = overall coefficient for gas-liquid friction losses in Delft model

θ_c = static contact angle [°]

γ = surface tension [N/m]

γ_{sl} = solid-liquid interfacial tension [N/m]

γ_{sv} = solid-vapor interfacial tension [N/m]

κ = curvature of free surface [1/m]

μ = dynamic viscosity of fluid [Pa-s]

μ_L = dynamic viscosity of liquid in VOF simulations [Pa-s]

μ_G = dynamic viscosity of gas in VOF simulations [Pa-s]

ν = kinematic viscosity [m²/s]

ν_r = eddy viscosity of the residual motions [m²/s]

ν_t = eddy viscosity [m²/s]

ξ_{GG} = gas-gas friction factor in Delft model

ξ_{GL} = gas-liquid friction factor in Delft model

ρ = density of fluid [kg/m³]

ρ_L = density of liquid in VOF simulations [kg/m³]

ρ_G = density of gas in VOF simulations [kg/m³]

$\sigma_k, \sigma_\varepsilon, \sigma_\omega$ = constants in two-equation turbulence models

τ_{ij}^R = residual-stress tensor for LES [m²/s²]

τ_{ij} = Reynolds stresses [Pa]

Ψ = fraction of channels covered in liquid film in Delft model $\left(\frac{2s}{b+2s}\right)$

ω = specific dissipation rate of turbulent kinetic energy [1/s]

References

- (1) Kister, H. *Distillation Design*; 1 edition.; McGraw-Hill Professional: New York, 1992.
- (2) Chapas, R. B.; Colwell, J. A. *Industrial Technologies Program Research Plan for Energy-Intensive Process Industries*; US Dept. of Energy, 2007.
- (3) Menon, A.; Dus, M. *Pushing the boundaries in process intensification*; Sulzer Technical Review; Sulzer Ltd., 2011; pp. 1–17.
- (4) Green, D.; Perry, R. *Perry's Chemical Engineers' Handbook, Eighth Edition*; 8 edition.; McGraw-Hill Professional: New York, 2007.
- (5) Kister, H. Z.; Scherffius, J.; Afshar, K.; Abkar, E. Realistically predict capacity and pressure drop for packed columns. *Chem. Eng. Prog.* **2007**, *103*, 28–38.
- (6) Wang, G. Q.; Yuan, X. G.; Yu, K. T. Review of Mass-Transfer Correlations for Packed Columns*. *Ind Eng Chem Res* **2005**, *44*, 8715–8729.
- (7) Green, C. W.; Farone, J.; Briley, J. K.; Eldridge, R. B.; Ketcham, R. A.; Nightingale, B. Novel Application of X-ray Computed Tomography: Determination of Gas/Liquid Contact Area and Liquid Holdup in Structured Packing. *Ind. Eng. Chem. Res.* **2007**, *46*, 5734–5753.
- (8) Basden, M.; Eldridge, R. B.; Farone, J.; Feng, E.; Hussey, D. S.; Jacobson, D. L. Liquid Holdup Profiles in Structured Packing Determined via Neutron Radiography. *Ind. Eng. Chem. Res.* **2013**, *52*, 17263–17269.
- (9) Owens, S. A.; Kossmann, A.; Farone, J.; Eldridge, R. B.; Ketcham, R. A. Flow Field Visualization in Structured Packing Using Real Time X-ray Radiography. *Ind. Eng. Chem. Res.* **2009**, *48*, 3606–3618.
- (10) Owens, S. A.; Perkins, M. R.; Eldridge, R. B.; Schulz, K. W.; Ketcham, R. A. Computational Fluid Dynamics Simulation of Structured Packing. *Ind. Eng. Chem. Res.* **2013**, *52*, 2032–2045.
- (11) Olujić, Ž. Effect of Column Diameter on Pressure Drop of a Corrugated Sheet Structured Packing. *Chem. Eng. Res. Des.* **1999**, *77*, 505–510.
- (12) Hirsch, C. *Numerical Computation of Internal and External Flows: The Fundamentals of Computational Fluid Dynamics, Second Edition*; 2 edition.; Butterworth-Heinemann: Oxford ; Burlington, MA, 2007.
- (13) WS Atkins Consultants. BEST PRACTICE GUIDELINES FOR MARINE APPLICATIONS OF COMPUTATIONAL FLUID DYNAMICS.
- (14) CD-adapco. *USER GUIDE STAR-CCM+ Version 7.06*; CD-adapco, 2012.
- (15) Pope, S. B. *Turbulent Flows*; 1 edition.; Cambridge University Press: Cambridge ; New York, 2000.
- (16) Durbin, P. A. *Statistical Theory and Modeling for Turbulent Flows*; 1 edition.; Wiley: Chichester ; New York, 2001.
- (17) Andersson, B.; Andersson, R.; Håkansson, L.; Mortensen, M.; Sudiyo, R.; Wachem, B. van. *Computational Fluid Dynamics for Engineers*; 1 edition.; Cambridge University Press: Cambridge ; New York, 2012.

- (18) Prosperetti, A.; Tryggvason, G. *Computational Methods for Multiphase Flow*; 1 edition.; Cambridge University Press: Cambridge; New York, 2009.
- (19) Brackbill, J. .; Kothe, D. .; Zemach, C. A continuum method for modeling surface tension. *J. Comput. Phys.* **1992**, *100*, 335–354.
- (20) Bellet, M. Implementation of surface tension with wall adhesion effects in a three-dimensional finite element model for fluid flow. *Commun. Numer. Methods Eng.* **2001**, *17*, 563–579.
- (21) Rocha, J. A.; Bravo, J. L.; Fair, J. R. Distillation columns containing structured packings: a comprehensive model for their performance. 1. Hydraulic models. *Ind. Eng. Chem. Res.* **1993**, *32*, 641–651.
- (22) Rocha, J. A.; Bravo, J. L.; Fair, J. R. Distillation Columns Containing Structured Packings: A Comprehensive Model for Their Performance. 2. Mass-Transfer Model. *Ind. Eng. Chem. Res.* **1996**, *35*, 1660–1667.
- (23) Fair, J. R.; Seibert, A. F.; Behrens, M.; Saraber, P. P.; Olujic, Z. Structured Packing Performance-Experimental Evaluation of Two Predictive Models. *Ind. Eng. Chem. Res.* **2000**, *39*, 1788–1796.
- (24) Olujic, Z. Development of a complete simulation model for predicting the hydraulic and separation performance of distillation columns equipped with structured packings. *Chem. Biochem. Eng. Q.* **1997**, *11*, 31–46.
- (25) Olujić, Ž.; Kamerbeek, A. B.; de Graauw, J. A corrugation geometry based model for efficiency of structured distillation packing. *Chem. Eng. Process. Process Intensif.* **1999**, *38*, 683–695.
- (26) Olujic, Z.; Jansen, H.; Kaibel, B.; Rietfort, T.; Zich, E. Stretching the Capacity of Structured Packings†. *Ind. Eng. Chem. Res.* **2001**, *40*, 6172–6180.
- (27) Olujic, Z.; Behrens, M.; Colli, L.; Paglianti, A. Predicting the efficiency of corrugated sheet structured packings with large specific surface area. *Chem. Biochem. Eng. Q.* **2004**, *18*, 89–96.
- (28) Tsai, R. E.; Schultheiss, P.; Kettner, A.; Lewis, J. C.; Seibert, A. F.; Eldridge, R. B.; Rochelle, G. T. Influence of Surface Tension on Effective Packing Area. *Ind. Eng. Chem. Res.* **2008**, *47*, 1253–1260.
- (29) Tsai, R. E.; Seibert, A. F.; Eldridge, R. B.; Rochelle, G. T. A dimensionless model for predicting the mass-transfer area of structured packing. *AIChE J.* **2011**, *57*, 1173–1184.
- (30) Van Gulijk, C. Using computational fluid dynamics to calculate transversal dispersion in a structured packed bed. *Comput. Chem. Eng.* **1998**, *22*, Supplement 1, S767–S770.
- (31) Van Baten, J. .; Ellenberger, J.; Krishna, R. Radial and axial dispersion of the liquid phase within a KATAPAK-S® structure: experiments vs. CFD simulations. *Chem. Eng. Sci.* **2001**, *56*, 813–821.
- (32) Van Baten, J. M.; Krishna, R. Liquid-phase mass transfer within KATAPAK-S® structures studied using computational fluid dynamics simulations. *Catal. Today* **2001**, *69*, 371–377.

- (33) Van Baten, J. M.; Krishna, R. Gas and liquid phase mass transfer within KATAPAK-S® structures studied using CFD simulations. *Chem. Eng. Sci.* **2002**, *57*, 1531–1536.
- (34) Petre, C. F.; Larachi, F.; Iliuta, I.; Grandjean, B. P. A. Pressure drop through structured packings: Breakdown into the contributing mechanisms by CFD modeling. *Chem. Eng. Sci.* **2003**, *58*, 163–177.
- (35) Larachi, F.; Petre, C. F.; Iliuta, I.; Grandjean, B. Tailoring the pressure drop of structured packings through CFD simulations. *Chem. Eng. Process. Process Intensif.* **2003**, *42*, 535–541.
- (36) Szulczewska, B.; Zbicinski, I.; Górak, A. Liquid Flow on Structured Packing: CFD Simulation and Experimental Study. *Chem. Eng. Technol.* **2003**, *26*, 580–584.
- (37) Raynal, L.; Boyer, C.; Ballaguet, J.-P. Liquid Holdup and Pressure Drop Determination in Structured Packing with CFD Simulations. *Can. J. Chem. Eng.* **2004**, *82*, 871–879.
- (38) Ataki, A.; Bart, H.-J. Experimental and CFD Simulation Study for the Wetting of a Structured Packing Element with Liquids. *Chem. Eng. Technol.* **2006**, *29*, 336–347.
- (39) Haghshenas Fard, M.; Zivdar, M.; Rahimi, R.; Nasr Esfahani, M.; Afacan, A.; Nandakumar, K.; Chuang, K. T. CFD Simulation of Mass Transfer Efficiency and Pressure Drop in a Structured Packed Distillation Column. *Chem. Eng. Technol.* **2007**, *30*, 854–861.
- (40) Wen, X.; Akhter, S.; Afacan, A.; Nandakumar, K.; Chuang, K. T. CFD modeling of columns equipped with structured packings: I. Approach based on detailed packing geometry. *Asia-Pac. J. Chem. Eng.* **2007**, *2*, 336–344.
- (41) Raynal, L.; Royon-Lebeaud, A. A multi-scale approach for CFD calculations of gas–liquid flow within large size column equipped with structured packing. *Chem. Eng. Sci.* **2007**, *62*, 7196–7204.
- (42) Mahr, B.; Mewes, D. CFD Modelling and Calculation of Dynamic Two-Phase Flow in Columns Equipped with Structured Packing. *Chem. Eng. Res. Des.* **2007**, *85*, 1112–1122.
- (43) Mahr, B.; Mewes, D. Two-phase flow in structured packings: Modeling and calculation on a macroscopic scale. *AIChE J.* **2008**, *54*, 614–626.
- (44) Fernandes, J.; Simões, P. C.; Mota, J. P. B.; Saadjan, E. Application of CFD in the study of supercritical fluid extraction with structured packing: Dry pressure drop calculations. *J. Supercrit. Fluids* **2008**, *47*, 17–24.
- (45) Fernandes, J.; Lisboa, P. F.; Simões, P. C.; Mota, J. P. B.; Saadjan, E. Application of CFD in the study of supercritical fluid extraction with structured packing: Wet pressure drop calculations. *J. Supercrit. Fluids* **2009**, *50*, 61–68.
- (46) Raynal, L.; Ben Rayana, F.; Royon-Lebeaud, A. Use of CFD for CO₂ absorbers optimum design : from local scale to large industrial scale. *Energy Procedia* **2009**, *1*, 917–924.

- (47) Haroun, Y.; Legendre, D.; Raynal, L. Direct numerical simulation of reactive absorption in gas–liquid flow on structured packing using interface capturing method. *Chem. Eng. Sci.* **2010**, *65*, 351–356.
- (48) Rafati Saleh, A.; Hosseini, S. H.; Shojaee, S.; Ahmadi, G. CFD Studies of Pressure Drop and Increasing Capacity in MellapakPlus 752.Y Structured Packing. *Chem. Eng. Technol.* **2011**, *34*, 1402–1412.
- (49) Said, W.; Nemer, M.; Clodic, D. Modeling of dry pressure drop for fully developed gas flow in structured packing using CFD simulations. *Chem. Eng. Sci.* **2011**, *66*, 2107–2117.
- (50) Shojaee, S.; Hosseini, S. H.; Rafati, A.; Ahmadi, G. Prediction of the Effective Area in Structured Packings by Computational Fluid Dynamics. *Ind. Eng. Chem. Res.* **2011**, *50*, 10833–10842.
- (51) Shojaee, S.; Hosseini, S. H.; Razavi, B. S. Computational Fluid Dynamics Simulation of Multiphase Flow in Structured Packings. *J. Appl. Math.* **2012**.
- (52) Brunazzi, E.; Nardini, G.; Paglianti, A.; Petarca, L. Interfacial area of mellapak packing: Absorption of 1,1,1-trichloroethane by Genosorb 300. *Chem. Eng. Technol.* **1995**, *18*, 248–255.
- (53) Haroun, Y.; Raynal, L.; Legendre, D. Mass transfer and liquid hold-up determination in structured packing by CFD. *Chem. Eng. Sci.* **2012**, *75*, 342–348.
- (54) Subramanian, K.; Wozny, G. Analysis of Hydrodynamics of Fluid Flow on Corrugated Sheets of Packing. *Int. J. Chem. Eng.* **2012**, *2012*, 1–13.
- (55) Armstrong, L. M.; Gu, S.; Luo, K. H. Dry Pressure Drop Prediction within Montzpak B1-250.45 Packing with Varied Inclination Angles and Geometries. *Ind. Eng. Chem. Res.* **2013**, *52*, 4372–4378.
- (56) Zhang, Y.-L.; Zhu, H.-M.; Yin, Q.-X. CFD Study on the Local Mass Transfer Efficiency in the Gas Phase of Structured Packing. *Chem. Eng. Technol.* **2013**, *36*, 1138–1146.
- (57) Brinkmann, U.; Janzen, A.; Kenig, E. Y. Hydrodynamic analogy approach for modelling reactive absorption. *Chem. Eng. J.* **2014**, *250*, 342–353.
- (58) Haroun, Y.; Raynal, L.; Alix, P. Prediction of effective area and liquid hold-up in structured packings by CFD. *Chem. Eng. Res. Des.* **2014**, *92*, 2247–2254.
- (59) Aferka, S.; Viva, A.; Brunazzi, E.; Marchot, P.; Crine, M.; Toye, D. Tomographic measurement of liquid hold up and effective interfacial area distributions in a column packed with high performance structured packings. *Chem. Eng. Sci.* **2011**, *66*, 3413–3422.
- (60) Tsai, R. E.; Schultheiss, P.; Kettner, A.; Lewis, J. C.; Seibert, A. F.; Eldridge, R. B.; Rochelle, G. T. Influence of surface tension on effective packing area. *Ind. Eng. Chem. Res.* **2008**, *47*, 1253–1260.
- (61) Long, J.; Chen, P. Surface Characterization of Hydrosilylated Polypropylene: Contact Angle Measurement and Atomic Force Microscopy. *Langmuir* **2001**, *17*, 2965–2972.
- (62) Owens, S. A. Advanced analysis of structured packing via computational fluid dynamics simulation, 2010.

- (63) Waas, C. Hydraulic Studies of the Structured Packing Mellapak N250.Y and Evaluation of CFD-data for the Non-dimensionalization of the Dry Pressure Drop in Structured Packing, Technical University of Munich, 2014.
- (64) Casey, M.; Wintergerste, T.; European Research Community on Flow, T. and C. *Best practice guidelines: ERCOFTAC Special Interest Group on quality and trust in industrial CFD.*; ERCOFTAC: [Switzerland], 2000.
- (65) Roache, P. J. *Verification and Validation in Computational Science and Engineering*; Hermosa Pub: Albuquerque, N.M, 1998.
- (66) Khosravi Nikou, M. R.; Ehsani, M. R. Turbulence models application on CFD simulation of hydrodynamics, heat and mass transfer in a structured packing. *Int. Commun. Heat Mass Transf.* **2008**, 35, 1211–1219.
- (67) Stichlmair, J.; Bravo, J. L.; Fair, J. R. General model for prediction of pressure drop and capacity of countercurrent gas/liquid packed columns. *Gas Sep. Purif.* **1989**, 3, 19–28.
- (68) Bird, R. B.; Stewart, W. E.; Lightfoot, E. N. *Transport Phenomena, Revised 2nd Edition*; 2nd edition.; John Wiley & Sons, Inc.: New York, 2006.
- (69) Starov, V. M.; Velarde, M. G.; Radke, C. J. *Wetting and Spreading Dynamics*; CRC Press: Boca Raton, 2007.
- (70) Nicolaiewsky, E. M. A.; Fair, J. R. Liquid Flow over Textured Surfaces. 1. Contact Angles. **1999**, 284–291.
- (71) Tsai, R. E. Mass transfer area of structured packing. **2010**.
- (72) Seader, J. D.; Henley, E. J.; Roper, D. K. *Separation Process Principles: Chemical and Biochemical Operations*; 3 edition.; Wiley: Hoboken, NJ, 2010.
- (73) Green, C. W. *Hydraulic Characterization of Structured Packing Via X-ray Computed Tomography*; ProQuest, 2006.
- (74) Hashmi, A. A.; Dullenkopf, K.; Koch, R.; Bauer, H.-J. CFD Methods for Shear Driven Liquid Wall Films. **2010**, 1283–1291.
- (75) Bozzano, G.; Dente, M.; Corna, P. A Phenomenological Model for Fluid-dynamics Evaluation of Structured Packing Systems. *Chem. Eng. Trans.* **2007**, 12, 189–194.
- (76) Wang, C.; Perry, M.; Rochelle, G. T.; Seibert, A. F. Packing Characterization: Mass Transfer Properties. *Energy Procedia* **2012**, 23, 23–32.
- (77) Wang, C.; Perry, M.; Seibert, F.; Rochelle, G. T. Characterization of Novel Structured Packings for CO₂ Capture. *Energy Procedia* **2013**, 37, 2145–2153.

Vita

Michael Allen Basden was born in Elko, NV to David Basden and Carla Cole. He grew up in the small town of Kemmerer, WY. Upon graduation from Kemmerer High School as co-Valedictorian, he enrolled at the University of Wyoming located in Laramie, WY. He graduated Summa Cum Laude with a B.S. in chemical engineering in December 2009, and he earned M.S. in chemical engineering in May 2010 through the university's combined degree program. He then moved to the University of Texas at Austin in August of 2010. During the summer of 2011, he worked at Total Petrochemicals' styrenics research group in La Porte, TX. He has accepted employment with Shell.

Permanent email: michael.basden@gmail.com

This dissertation was typed by Michael Allen Basden