Final Project Report

Project Title: Advanced Hydraulic and Mass Transfer Models for Distillation Column Optimization and Design

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Executive Summary:

The project successfully developed a computational fluid dynamics (CFD) based simulation of the hydrodynamics of flow in a commercial structured packing element. This result fulfilled the prime objective of the research program. The simulation utilized commercial CFD code marketed by Fluent Inc. in combination with a novel graphical interface developed by Oak Ridge National Lab. The end product will allow the design of next generation column internals without the need for extensive experimental validation and will expand the fundamental understanding of the vapor-liquid contacting process.

In an effort to provide insight into the gas and liquid flow phenomena in an operating vapor-liquid contactor, a novel X-ray CT imaging technique was developed which allowed three dimensional visualization of the liquid and vapor flow paths. The information gained from X-ray studies provided useful information for the CFD effort and also assisted on-going efforts to develop accurate semi-empirical hydraulic and mass transfer models for contactors containing structured packing.

The CFD simulation and advanced semi-empirical models will facilitate the development of column internals which will reduce separations energy consumption and capital cost.

Task 1 - Imaging Technique Development

Introduction

Predictive models for packed column performance as they exist today incorporate macroscopic properties of the entire column, rather than focusing rigorously on underlying local variations of momentum-, heat-, and mass-transfer processes. It is necessary to gain further understanding of both hydraulic and mass transfer processes within packed columns in order to produce more accurate performance models and foster development of advanced column internals. Recently, various tomographic techniques have permitted non-invasive study of many types of process equipment, including packed columns. Specifically, it has been shown that X-ray computed tomography (CT) allows for quantification of packed column hydraulics and in addition provides qualitative evidence of phase distribution. This technique can be applied on a macro- or micro-scale and provides a pathway to the information necessary for development of more accurate predictive models.

This work will focus on potential improvements to predictive models for distillation column performance. Distillation is a highly energy-intensive unit operation that represents approximately 40% of the energy usage for the chemical processing industry. Distillation applications account for more than 2% of the nation's overall energy usage (U.S. DOE/Office of Industrial Technologies, 1998). Models which can achieve even a fractional improvement in prediction of the flooding point with relative certainty will allow columns to be operated much nearer their capacity, thus increasing the mass-transfer efficiency of the device. Greater efficiency will ultimately result in a reduction in energy consumption, magnified by the sheer volume of distillation equipment being operated in the United States today – in excess of 40,000 columns as of 1997 (Zanetti). More efficient packed columns utilizing advanced technologies will become the choice for future development and construction, adding to the potential energy savings.

Two of the most commonly used models for predicting column performance are the mass transfer model of Rocha, et al. (1996) and the hydraulic model of Rocha, et al. (1993). Both models rely on physical properties of the fluids as well as information about the column internals, specifically packing void fraction and the geometrical characteristics of the packing. One limitation of these models is the assumption of ideal, even liquid distribution throughout the column. Liquid maldistribution is common in both the axial and flow directions, which affects hydraulic and mass transfer performance. The ability to describe the conditions for and/or the effects of liquid maldistribution would greatly increase the accuracy of predictive models. Fundamental, first-principles knowledge of column operation on a micro-scale would be easily extendable to columns employing random packing, improving on models such as those of Stichlmair, et al. (1989) and Wagner, et al. (1997).

Models for column performance are typically developed using macroscopic data. Unfortunately such measurements do not provide the level of detail necessary to understand the underlying processes that occur during packed column operation. For example, dynamic liquid holdup is usually determined by measuring the amount of liquid that drains from a packed column after the liquid flow to the column is shut off. It is evident that, while providing a rough estimate of the amount of liquid in the column at a given time and under a given flow rate, the procedure does not provide any insight as to the distribution of the liquid, and represents an average over the entire height of the column. Two columns may exhibit identical holdup

measurements at a given flow rate but it is possible that the liquid distribution varies greatly between the two. If so, the efficiency of the two columns would likely be different due to a difference in interfacial area, a key component in mass transfer. Incorporation of information regarding local holdup or liquid distribution into predictive models would lead to a more accurate depiction of column operation.

Process tomography applications such as X-ray CT allow study of local level phenomena where a density gradient is present. The differences in density for liquid, gas, and packing material provide images where the locations of each phase may be identified. The scanning procedure involves acquisition of transmission data via a detector bank. X-rays are directed at the object of interest, and the beams are sampled after being attenuated by the object. The amount of attenuation is proportional to the density of the material that the beam passes through. The transmission data is collected at several different orientations by spinning either the source and detectors, or the object being imaged. Through a mathematical reconstruction algorithm, a cross-sectional image representing a slice of the object taken at the height of interest is produced. The resulting images can be processed using standard techniques, and in the case of a packed column, parameters including liquid holdup, liquid distribution, and interfacial area may be derived. Scanning the column at multiple heights provides insight to the flow behavior and hydraulic performance characteristics throughout the column. Three-dimensional models can be produced as an extension of X-ray CT by stacking slices taken at very close height intervals.

Literature Overview

The usage of process tomography to non-invasively image fluid flow has been well documented within the past 10 years. Applications of many different imaging technologies exist, including electrical capacitance tomography (ECT), electrical resistance tomography (ERT), nuclear magnetic resonance imaging (NMRI), gamma-ray tomography, and X-ray tomography. For the purpose of the current work, X-ray computed tomography was chosen for its ability to balance spatial resolution with temporal resolution. The high energy of X-ray sources permits the scanning of dense materials such as metal structured packing, which would be difficult with a lower energy source. Most studies involving gamma-ray and medical (<200 kV) X-ray sources have been limited to imaging plastic column internals. Spatial resolution for gamma-ray imaging systems is limited by gamma-ray detection technology. This prohibits the collection of data on the scale necessary for development of a more-rigorous, first-principles model of hydraulic behavior. Magnetic interference with metal objects inhibits the application of NMRI to the current study; X-ray CT scanning facilities are also more numerous and accessible than their NMRI counterparts.

While X-ray CT is limited in temporal resolution, the ability to analyze time-averaged flow images has been proven through previous work. Table 1 summarizes the key points from relevant publications over the last 10 years, including the most recent previous work performed as part of this project at The University of Texas.

The work of Xu and Kennedy (1999) used gamma-ray computed tomography to image an industrial scale Plexiglas column 3 feet in diameter, packed with 5 feet of random packing. The column operated under liquid-only flow conditions, with water serving as the fluid. Liquid holdup and distribution was determined from the transmission measurements. The image resolution was too low to gain any insight as to small-scale flow characteristics. However, this study showed the potential to validate any new models on industrial-sized equipment.

Table 1 - Applications of Process Tomography to Multiphase Flow in Packed Columns

Reference	Column Type (Diameter)	Internal Type	Phases Present	Measured Variables	Scanning Method
Xu & Kennedy (1999)	Packed column (0.9 m)	Random packing	Water, packing	Liquid holdup and distribution	□-ray
Yin et al. (2002)	Packed column (0.6 m)	Pall rings (metal)	Water, packing	Liquid holdup distribution	□-ray
Roy et al. (2004)	Packed column (30.48 cm)	Norton structured packing (metal)	Water, air, packing	Liquid distribution, void fraction	□-ray
Kantzas (1994)	Trickle bed (4.5 cm)	Glass beads	Water, packing	Liquid holdup	X-ray
Kantzas (1994)	Fluidized bed (10 cm)	Glass beads, polyethylene particles	Gas, packing	Gas holdup	X-ray
Toye et al. (1994)	Trickling filter (0.6 m)	Etapak 210	Water, packing	Liquid holdup	X-ray
Toye et al. (1996)	Trickling filter (0.6 m)	Etapak 210	Water, packing	Flow regime characteristics	X-ray
Toye et al. (1997)	Trickling filter (0.6 m)	CMR 1A	Water, packing	Liquid holdup and distribution	X-ray
Toye et al. (1998)	Packed column (0.6 m)	CMR 1A	Water, packing	Void fraction, liquid holdup and distribution	X-ray
Marchot et al. (1999)	Packed column (0.6 m)	CMR 1A	Water, packing	Liquid holdup and distribution	X-ray
Marchot et al. (2001a)	Packed column (0.6 m)	Mellapak 250Y (plastic)	Water, air, packing	Liquid distribution	X-ray
Marchot et al. (2001b)	Packed column (0.6 m)	Mellapak 250Y (plastic)	Water, air, packing	3-D Liquid distribution	X-ray
Schmitz et al. (1997a, 1997b)	Packed column (20 cm)	Ceramic spheres, Mellapak 250Y (metal)	Water, packing	Liquid holdup and distribution, water film thickness	X-ray
Schmitz et al. (1998)	Packed column (20 cm)	Optiflow structured packing	Water, air, packing	Liquid holdup and distribution	X-ray
Schmit & Eldridge (2004a)	Column (14.6 cm)	X-ray phantoms, film flow apparatus	Water, air, steel, acrylic	Liquid holdup, gas holdup, void fraction, liquid film thickness	X-ray
Schmit et al. (2004b)	Packed column (14.6 cm)	Mellapak 500Y (metal)	Water, air, packing	Liquid holdup and distribution, variance of X-ray attenuation	X-ray

More recent studies using gamma-ray tomography, such as those by Yin, et al. (2002) and Roy, et al. (2004) have focused on metal packing, both structured and random. Yin, et al. (2002) studied the effect of liquid distributor design on liquid distribution, verified by gamma-ray tomography and computational fluid dynamics (CFD) simulations, also under water-only flow conditions. Roy, et al. (2004) performed studies to establish the spatial resolution of a new gamma-ray scanner on a packed column exhibiting vapor-liquid countercurrent flow.

Kantzas (1994) used a modified medical X-ray scanner to measure holdup in trickle and fluidized beds. A complete slice could be acquired in 3 seconds using this equipment, as the source and detector rotated around the stationary object. Gas and liquid holdup values were calculated from the scans. While instantaneous flow dynamics were not realized, differences in time-averaged measurements could be obtained.

The experiments by Toye, et al. (1994, 1996, 1997, 1998) and Marchot et al. (1999, 2001a, 2001b) were all performed on the same 0.6 m-diameter packed column. Over the course of these studies, the column internals were changed, and the effect of liquid rate, vapor rate, and liquid distributor were studied. All internals used for these studies were plastic. Liquid holdup and distribution were successfully quantified; however, the area of liquid film formation has yet to be reported. Scan time was significantly longer than the work of Kantzas at 2.5 minutes per slice. The time-averaged values obtained still proved valuable in calculation of flow characteristics.

The work of Schmitz, et al. (1997a, 1997b) focused on X-ray CT imaging of random and structured packing in a 200 mm-diameter acrylic glass column. Analysis of the CT images provided liquid holdup and distribution information for countercurrent air-water flow. Holdup compared favorably to that of Suess and Spiegel (1992) for Mellapak 250Y. This work obtained water-only images by subtracting dry-bed reconstructed CT images from flow images; the previous work by Toye, Marchot, and coworkers subtracted transmission data before reconstructing a water-only image. Quantification of interfacial area became one step closer to reality with the successful calculation of liquid film thickness from X-ray CT images.

Schmit et al. (2004a, 2004b) developed a system for determining the optimal X-ray CT scanning parameters for an operating vapor-liquid contactor. The first portion of the experiment involved the imaging of phantoms to test the ability of a scanner to delineate the various interfaces observed in multiphase flow in a packed column. A second set of experiments showed the scanner's ability to resolve liquid film thickness on a simple geometry. Finally, a column containing Mellapak 500Y was imaged under air-water counterflow, and liquid holdup was calculated. Evidence of liquid accumulation at and above packing element joints was noted. Computer simulations of X-ray CT were completed to investigate the cause of ring-like artifacts in flow scans. These artifacts were attributed to a combination of liquid movement during transmission data acquisition and the use of subpositions in the data acquisition process.

Research Objective

The objectives of this research primarily consisted of local-scale quantification of hydraulic behavior in an operating vapor-liquid contacting device. Specifically, the use of X-ray CT to calculate liquid holdup, fluid distribution, as well as several types of area (effective, interfacial, and wetted) in a column utilizing stainless steel structured packing was studied. The effects of different packing types and vapor rates on hydraulic performance were evaluated. Methods of analysis were verified by calculating local void fraction within the packed bed under conditions of zero flow, with comparison to vendor-specified values for accuracy. Development of advanced computational techniques for image analysis were necessary to accurately describe the observed flow behavior. Values obtained for the previously mentioned hydraulic parameters were compared to those predicted by existing models as well as data obtained for various packings on both the distillation column and air-water column at the SRP pilot plant.

The first portion of the research focused on determining the optimal method for scanning the contactor. Air was used as the vapor phase, and water was chosen as the liquid phase. A wide range of vapor and liquid flowrates were studied, and Mellapak 250Y by Sulzer was chosen as the standard packing type. The column was scanned at several different heights within the packed section to give an adequate description of any potential flow deviation throughout the

column. Additionally, the area where two packing elements come together was of interest. Several slices were taken around the packing element joints to acquire the data necessary for studying flow transitioning from one element to the next. All of the parameters to be calculated from images can be extended to represent the column bulk by averaging the values obtained from multiple slices or three-dimensional models.

The difficulty in analyzing the resultant CT images lies in the ability to accurately define the three phases present in the column under flow conditions - packing, liquid, and vapor. Ideally, each phase would be represented by one gray level, but in reality, the continuous physical domain that is the column becomes discretized. The images consist of a matrix of pixels, with each discrete pixel being assigned a gray level. Blurring is a common effect associated with X-ray procedures, resulting in an approximate Gaussian distribution of gray levels associated with a given phase. These distributions can overlap, especially in the case of the liquid and the packing material, making it difficult to distinguish which phase a given pixel actually represents. Another drawback of domain discretization is the so-called edge response function; the boundary between two different materials is usually blurred. Edges look fuzzy and it is difficult to accurately define the boundary between the two materials without going to a very high spatial resolution. To obtain high spatial resolution with X-ray CT, scan times usually must be increased, meaning that resulting images represent an even longer time-average of the flow being observed. Accurately classifying pixels is critical to developing techniques that can adequately describe the phase distribution within the column. Techniques for doing so were developed using the base case of air and water on Mellapak 250Y. In addition, it was necessary to develop routines which can be applied in three-dimensions in order to quantify behavior within a volume of packing when X-ray CT slices are stacked to create a 3D model.

Experimental Methods

Acquisition of X-ray CT data for this work was performed on two separate scanning systems. The first system, located in Austin, Texas, is owned and operated by 3-D Imaging and Development. The "101 B+" scanner has been described in detail by Schmit (2001). It utilizes a Philips 450 kV X-ray source and possesses a linear array of 125 discrete scintillator detectors. The detectors have a variable aperture that permits adjustment for pixel size from 0.2 to 1 mm. The scanning platform can hold a maximum weight of 50 lbs. The maximum scan height is 30 inches, and the maximum object diameter is 10 inches. The overall maximum object height is approximately 6 feet. As with most X-ray systems, the room containing the equipment is shielded to prevent exposure to stray radiation. The equipment is controlled from a computer workstation located outside the scanning bay.

The second system used for this work is owned and operated by General Electric. It is located at GE's Quality Technology Center in Cincinnati, Ohio. The system is an Industrial Computed Tomography machine, which uses a Varian Linatron X-ray source capable of producing X-ray energies of 2 MeV or 6 MeV. The detector array is digital, close-packed (no gaps between detectors), and consists of 1024 elements. The object platform is controlled by a 9-axis manipulator. The room is shielded with concrete, and an external computer workstation is used to operate the scanner.

Several key differences exist between the two scanners, the most important of which relates to the detector array. The machine at 3DID has discrete detectors with gaps in between each element. Therefore, in order to obtain transmission data that samples the entire cross-sectional slice plane, multiple rotations are required, each with a small translational shift to the object. Thus, depending on the desired spatial resolution, anywhere between 4 and 13 subpositions are required. This dramatically increases the scanning time, and results in ring-like image artifacts that affect the analysis. The GE detector bank is close-packed, or relatively continuous, meaning that one rotation yields transmission data for the entire width of the object.

Scan time is thus reduced from approximately 5 minutes to 50 seconds for comparable spatial resolution and scanner settings. Ring artifacts were noticeably less apparent when using the continuous detector array. The object is rotated 360° with either scanner to obtain a full set of transmission data; however, the 3DID scanner raises and lowers the object to obtain CT slices at different heights. The GE scanner does not raise the object but rather the source and detector array via an I-beam with a precision movement system.

Figure 1 – Air-water column, mounted on GE ICT scanner.

The column used for the experiments, seen mounted for scanning by the GE machine in Figure 1, was developed by Cartmel (1999) and Schmit (2001). The vapor-liquid contactor is operated countercurrently, and is constructed from sections of 5.75" ID acrylic tubing with a wall thickness of 1/8". The uppermost section of the column is 18" tall and contains a liquid distributor and a mist eliminator. The middle section is 24" in height. This section is where the packed bed is located, which varies in height depending on the packing type and number of packing elements used. The bed is supported on a metal grid. The bottom section of the column is constructed from aluminum. Vapor inlet and liquid drain lines are fixed to the column base, and a cone-shaped vapor distributor is mounted in the center of the base, facing upward towards the packed section. The base attaches securely to the scanner turntable to maintain a rigid bond

throughout the scanning process, minimizing column flex that could adversely affect analysis of the CT images.

The column is a closed-loop system. Figure 2 depicts the experimental system. A liquid level is held in the bottom of the column once steady state operation is achieved. A variable drive pump, controllable from outside the scanning bay, uses the column bottom level as a suction reservoir. The liquid is pumped out of the column, through a MicroMotion mass flowmeter, and back into the distributor in the top of the column. The flowrate is adjustable by varying the frequency seen by the pump drive. The liquid flowmeter signal is sent to a National Instruments signal acquisition board that is configured to communicate with LabView software run on a notebook computer. The air to the column is provided through an in-house air supply line or an external diesel compressor, depending on the scanning location being used. The air passes through a drying filter, and is then measured with a second MicroMotion mass flow meter. This signal is also sent to the laptop running LabView. Tygon tubing of varying diameters is used for all process connections to and from the column.

Figure 2 – Air-water contactor skid.

Data Analysis

Analysis of X-ray CT images was performed using standard image processing techniques paired with custom code written in IDL software from Research Systems, Inc. of Boulder, Colorado. Dr. Richard Ketcham of the Department of Geological Sciences, The University of

Texas at Austin assisted with the development of custom analysis techniques for CT images as well as three-dimensional models. The Department of Geological Sciences has additional software that was used to facilitate study of the three-dimensional modeling work.

Accurate classification of the liquid phase within a given CT image is the driving force for obtaining quality measurement of hydraulic parameters. The basic process necessary to analyze the CT images is a simple image subtraction. Pixel by pixel, a CT image under zero flow condition is subtracted from a CT image at the same height in the column under flow conditions. Assuming that the column does not move between the two scans, the resulting subtraction image will represent only material that was present during the flow scan but not during the dry scan. Thus, a visual representation of the location of water during the scan is obtained. The "water only" image can be analyzed to obtain the amount of water within the slice plane during the flow scan, which is easily converted to liquid holdup. Calculation of void fraction for dry scans is similar, but requires no subtraction. An appropriate gray level threshold is selected to produce a binary image representing only metal packing and air. Similar to the holdup calculation, the number of pixels representing metal are summed and divided by the area of the column in pixels, yielding void fraction.

Transmission data is collected over a finite period of time, thus any deviation in the flow can result in image artifacts. However, Schmit (2001) showed that the transmission data signal observed at several different detectors, while high in frequency, did not possess high amplitude, signifying that the time-averaging that occurs over the course of a scan (5 minutes with the 3DID scanner) is acceptable and produces a fairly accurate image. Reduction in scan time with the GE scanner (50 seconds) will help smooth out this associated noise.

The procedure for obtaining data includes collection of dry scans, flow scans, and scans where the packed section is completely full of water (flooded). A secondary method for holdup calculation scales the water present in a flow scan with the minimum water case (dry scan) and maximum water case (flooded scan). This technique was applied by Schmit (2001) to X-ray transmission data, or sinograms, with success.

Three-dimensional modeling is possible using software that stacks X-ray CT slices obtained continuously and connects the adjacent images to form a surface. This process has been used for reverse engineering for a number of years. The challenge that this work poses is the reconstruction of a flow scan data set that is constantly changing. The number of slices necessary to create a realistically sized model requires a large amount of time to obtain, on the order of several hours. By holding the liquid rate constant, the most accurate picture possible can be obtained. The effect of high frequency flow variation must be well understood before any conclusions can be drawn on three-dimensional reconstruction of flow data. It is highly desirable to obtain an understanding of where the liquid within a packed bed is located, and also observe where there is no liquid, as well as the flow type.

Two different methods exist for potentially producing "water only" model reconstructions, and they both rely on image subtraction. The first and most promising method requires each slice in the model to undergo a subtraction from the dry slice of the corresponding height, resulting in a new batch of files representing only water. These images can then theoretically be stacked to produce a model of only water. The second technique would involve reconstruction of the flow model and reconstruction of a dry model. A volume subtraction would then be applied to obtain a model that represents the surface differences between the two. This second method is subject to more artifacts, as the model reconstruction between the slices themselves is a discrete approximation of a continuous domain; a method that requires only one reconstruction would therefore inherently contain less error. Potential problems may arise when image artifacts are stacked to form false surfaces in the model. Therefore, accurate processing of the CT image slices will be necessary to minimize these effects. Further techniques were developed to calculate the portion of the packing surface that is wetted as well as the interfacial area available for mass transfer once accurate three-dimensional models can be created. These

models may be presented in the form of images or actual physical models created by CAD machines or inkjet layer printers, providing striking physical evidence of internal flows.

Results

Studies analyzing the performance of Mellapak 500Y and 250Y structured packing in an operating air-water column were performed using the 3DID X-ray CT scanner. Figure 3 shows CT images of both packing types under flow conditions below the load point, taken just above a packing joint.

**Figure 3 – CT images of Mellapak 250Y (left) and 500Y (right).
 $L = 20 \text{ GPM/ft}^2$**

Note the presence of circular artifacts in both images. This results from the need to translate the object several times during transmission data acquisition to account for the space between detectors on the 3DID 101 B+ scanner. Further observation shows a distinct difference in flow type for the two packings. The liquid is not observed to accumulate between packing sheets for the 250Y packing as much as it does for the 500Y packing. The liquid appears to flow as a film on the surface of the 250Y packing, whereas on the 500Y packing the water tends toward rivulet flow. Comparison to images taken in other areas of the packed bed verifies that the pooling of liquid in the 500Y image is not attributed solely to joint holdup. Another possible cause of the two different flow types is the relatively high surface tension of water. At approximately 70 dynes/cm, it is much larger than the hydrocarbon-like materials typically used with structured packings, which tend to have surface tensions closer to 20 dynes/cm. The high surface tension and large contact angle associated with water combined with the relatively high density of the packing and small area available for liquid flow causes the fluid to accumulate and form rivulets rather than spread and wet the packing surface.

The liquid distribution in early studies of Mellapak 500Y packing was observed to be poor throughout the bed. It is believed that packing joints tend to help redistribute the liquid flow within a packed bed. New, half-elements of both 500Y and 250Y packing were imaged. These half-elements are exactly one-half the height of a standard element. The new packing allowed for 3 packing joints to exist in the same height of packed bed as previously used. This also allowed for further study of liquid behavior at packing joints.

It was determined that accurate analysis of CT images for water could not be achieved with image artifacts present. A relationship was developed with General Electric that allows

imaging of the air-water column with a high-energy industrial X-ray CT scanner. Trips to the Quality Technology Center in Cincinnati have resulted in a large amount of data collected for the air-water column. Images of Mellapak 250Y half-elements can be seen in Figure 4. The circular image artifacts are no longer present, due to the close-packed detector array that the GE scanner uses. The image on the right is magnified to emphasize the liquid films on the packing surface. Liquid accumulation is noticeable in the corrugation troughs and at contact points between adjacent sheets. This is attributed to the high surface tension of water.

Using image subtraction techniques, the liquid holdup has been calculated throughout the packed bed at several different liquid and gas flow rates. Figure 5 shows the holdup profile throughout the column. Holdup is plotted versus CT slice number.

Figure 4 – CT images of Mellapak 250Y.

$$L = 15 \text{ GPM/ft}^2$$

The slices are taken in 1" increments, starting near the top of the packed bed and moving down. Peaks in the holdup profile can be observed at elevations 6, 12, and 16. Elevations 6 and 12 were located at or slightly above packing element joints. The peak associated with the lowest elevation, 16, near the bottom of the packed bed, is presumed to be due to the effects of vapor drag near the air distributor. The qualitative behavior among the different liquid rates is similar. Holdup is seen to increase with increasing liquid rate, which is expected.

Figure 5 – Liquid holdup at various elevations within packed section.

Vapor F-factor = 0.48

The normal scanning procedure involves an in-depth study of packing joints. A joint is selected for study, and a series of closely packed CT slices are acquired, centered around the joint. Figure 6 shows the holdup profile calculated from CT images across a packing element joint. The scanning heights associated with the slice numbers in this plot do not correspond to the same slice numbers or heights in Figure 5. The actual interface of the two packing elements is located between slices 4 and 5.

Figure 6 – Liquid holdup observed around packing element joint.

Vapor F-factor = 0.48

Again, the qualitative behavior of the profile curves is very similar for the different liquid rates. The holdup appears to be highest above the joint, transitioning to a still-higher-than-average value at the packing interface, and then leveling off, falling to a value more representative of the column-average holdup after the liquid transitions into the next packing element.

The superior scanning time that the GE scanner provided allowed much more data to be collected over the same time period when compared to the 3DID scanner. As a result, it was decided to pursue the collection of data necessary to construct a three-dimensional model of a portion of the packed bed. By collecting a large number of CT slices spaced very close together, imaging software allows for the creation of a surface represented by the sequential cross-sectional images. The first-pass attempt at modeling resulted in a 3" section of irrigated packing being imaged, which is shown in Figure 7. This reconstruction was performed by image processing technicians employed by GE.

Figure 7 – 3-D reconstruction of irrigated packing, 3” section
 $L = 15 \text{ GPM/ft}^2$, $G = 0.48 \text{ F-factor}$

The packing and column wall are realized with impressive clarity. The perforations in the packing surface, as well as the surface texturing, are also reproduced. It is difficult to distinguish where the liquid films reside. However, there are no gross areas of accumulation within the packing channels, supporting the theory that the liquid must be flowing in thin films on the packing surface. One possible explanation that has arisen relates to the detail of the surface texturing that is visible. Near the middle of the packing, the texturing is apparent, but is subdued when compared to areas of the packing nearer to the column wall. The texture here appears to be more pronounced, indicating that perhaps there is no liquid film covering this portion of the packing.

A subsequent trip to GE provided more time for three-dimensional modeling, and models were captured for greater heights of packing under dry and irrigated conditions. A dry bed model is shown in Figure 8 below. The images were reconstructed using Amira, a 3-D imaging software found on computers in the Department of Geological Sciences' High Resolution X-ray CT facility. These pictures represent a first-pass attempt at reconstructing CT slices for dry and irrigated beds for further analysis of the film thickness and interfacial and wetted areas.

Figure 8 – 3-D reconstruction of dry packing using Amira.

Task 2 – Computer-aided Modeling

Research Objective

The initially proposed computational objective of the research program was to develop a lattice-free-Boltzmann simulation of structured packing flow field. After review of this task by the project team, it was decided the most efficient path-forward would be to utilize existing commercial code (Fluent) and supplement the code to accurately reflect the geometry of the structured packing.

This path produced two critical deliverables, namely the simulation of single-phase flow through a pair of corrugated sheets and single-phase flow through packing elements consisting of stacks of corrugated sheets. Computational results (Figure 9) have been compared with data obtained from a dual plate experimental system (Figure 10). The experimental apparatus permits high-fidelity representation of its geometry. Results of average linear pressure drop from the comparative simulation agree very well (within 5%) with the corresponding experimental data. The gas flow factor range in the simulation spans realistic limits as required by the industrial participants in the project (0 to 2.5 ft/s (lb/ft³)^{0.5}). The calculations employ an 8 CPU cluster and entail the solution of the equations of motion for a Newtonian fluid (Navier-Stokes equations) via GAMBIT/FLUENT software.

Figure 9 – CFD results versus experimental dry pressure drop.

Figure 10 – Dual plate apparatus

In extending the model development to realistic packing elements, an automated and systematic interface was built and named GraSPI (Graphical Structured Packing Interface – Figure 11). The interface is but one deliverable of the project that allows industrial users to quickly assemble realistic packing elements and perform a single-phase flow simulation. The interface was built as

a plug-in for the GAMBIT/FLUENT software (Fluent Inc.). Fluent Inc. is a participant in the project and GraSPI could turn into a commercial product. The current version of GraSPI has a built-in library of commercial packing elements, and automatic problem setup for users unfamiliar with computational fluid mechanics. The interface creates the packing structure, defines the mathematical domain, and outputs scripts to drive the underlying solution software with minimum intervention from the user. As a bonus, a blue print of the geometry may be delivered for fabrication purposes.

Figure 11 – GraSPI user interface

GraSPI has been tested and used for analysis of typical commercial packings used in distillation columns. Recently a joint effort with the participants in the project (Dow Chemical, Fluent Inc, Sulzer Chemtech, and SRP UT-Austin) led to preliminary results from simulations using realistic packing geometry. Three packings (Figure 12) were used, namely, Mellapak 205Y, Montz B1-250Y, and Montz B1-250X, for the calculation of linear pressure drop and associated flow quantities, such as flow trajectories, kinetic energy, and velocity magnitude. Packing blocks with 10 and 14 sheets were used with simulations performed on an 8 CPU cluster.

Mellapak 250Y

Montz B1-250Y

Montz B1-250X

Figure 12 – Packings used for implementation of GraSPI

One aspect of the simulation was to assess the hardware investment industries need to make in order to take advantage of current computational fluid dynamic codes. Our conclusion so far is that clusters equipped with at least 10 CPU's are necessary for resolution of flow scales in one single packing element (the above packing elements are 7.5-in tall). The simulations have been suggesting interesting insights into the flow field not accessible to experimental methods at this

point. For instance, paths of individual fluid particles can be followed and local pressure drop evaluated as they zig-zag between the corrugated sheets (Figure 13). It was found that local pressure drop could be as high as 3 times the average between the ends of the packing element.

Figure 13 – Localized pressure profile

Task 3 – Pilot Plant Validation

Research Objective

The objective of this task was to validate the computer code and imaging results with experimental data obtained from the SRP pilot plant.

Comparison with experimental data (Figure 14) for the Montz B1-250Y obtained from the SRP air-water contactor (Figure 15) proved very encouraging. This data demonstrated that the initial phase of the model development for gas-only flow accurately represented the column hydraulics. Pilot plant generated interfacial area data for Montz B1-250 also was obtained (Figure 16) and qualitatively supported the level of packing surface coverage obtained from the X-ray imaging studies (Figure 7).

Figure 14 – CFD predicted dry pressure drop versus SRP column results

Figure 15 – SRP Air –Water Contactor

Figure 16 – Interfacial Area Measurements

Task 4 – Commercialization

Research Objective

The objective of this task was to ensure that the project deliverables were translated into commercially relevant products or technology.

Toward this goal, an agreement was reached between UT-Battelle and Fluent which provided a framework for provided the CFD software package to interested end-users. The GraSPI software will be supplied as an add-in package for the existing Fluent CFD software. Technical support will be a collaborative effort between Fluent and ORNL.

Follow-on commercial activities also involve use of the code by Dow Chemical to investigate column performance variations currently attributed to variations in structured packing geometry. There is some antidotal evidence that the imaging effort has lead to changes in structured packing geometry and promoted the use of non-invasive scanning techniques for the evaluate column of hydraulic performance.

Project Extension Scope of Work

Funding was received from DOE for a fourth year of the project. A summary of on-going CFD efforts supported by these funds is given below.

GraSPI has been enhanced to include perforations on the corrugated sheets, and to generate cylindrical packing elements suitable for stacking and filling of cylindrical vessels such as distillation columns (Figure 17). In addition, the spacing between the packing elements and the column wall is under implementation. Gas-liquid flow simulations are also in development in a collaborative effort with project sponsor Dow Chemical. The first test case is gas-liquid counterflow through a pair of corrugated plates of the experimental setup described in the previous section; experimental data has been collected for validation. Other cases with packing elements will follow.

Figure 17– GraSPI representation of cylindrical packing elements

With results achieved so far there is a possibility of extending GraSPI to the larger scope of modeling flow through a pilot distillation column of the size of the air/water column at SRP-UT Austin. That column is equipped with 16 packing elements of 7.5-in height each and 16-in diameter, resulting in elements with 34 corrugated sheets (Figure 18).

Figure 18 – GraSPI representation of SRP pilot plant packing elements

Simulations of this magnitude will involve 100 to 1000 CPU's and would represent a major step toward first-principles modeling of flow through distillation towers. The significance of this development is that US chemical industries would have access to a modeling tool with an unprecedented level of detail. This tool could be used in a variety of ways. Notably, the tool could be used for designing improved packings which could then be shipped to the SRP for testing under design conditions. Alternatively, industrial users of the tool could have the SRP test packing elements used to calibrate the tool for a proprietary scale-up design. In any scenario, the tool would satisfy the purpose of reducing energy consumption in the distillation industry through state-of-the-art design. Furthermore the tool could become a design standard in the distillation allied industry, and also be used for educating the future generation of engineers.

The main tasks involved in project extension are:

1. Improve and test GraSPI to generate packing elements with up to 35 corrugated sheets (currently the maximum tried has been 14). However the images above (generated by GraSPI as a replica of packing elements used at SRP) show that the task is feasible.
2. Fit a cylindrical duct around the packing with and without spacing.
3. Stack a pair of cylindrical packing elements rotated at an angle (the image above shows 90° degrees rotation).
4. Stack multiple packing elements.
5. Perform single-phase flow simulations.
6. Perform gas-liquid flow simulations.

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