Film Flow Down On An Inclined Plate
Outcome of Simulations on NETL Supercomputer

Film flow down on an inclined plate was investigated using the commercial CFD code “Ansys Fluent 14.0” installed on the NETL Supercomputer. This simulation study develops fundamental insights on the hydrodynamics of film flow over an inclined surface. Specifically, the influence of solvent properties, such as viscosity, surface tension, and flow configurations were investigated. This information may be used in the design of structure packing elements, such as one would find in solvent absorption.

The computational flow domain was modeled and discretized in GAMBIT. Proper meshing is a critical step in simulation in order to achieve converged and accurate results. In this context, the number of meshes in the domain was varied with 1.26-1.50M, depending on the case. The simulations were initially run on 32 cores with a time step of $5 \times 10^{-4}$ sec. However, these simulations tended to diverge indicating smaller time steps were needed. Ultimately, a typical case took around 96 hrs wall time to complete.

The availability of 9 ANSYS HPC packs and 384 dedicated cores allowed for a wide ranging parametric investigation. Specifically, these resources permitted 3 cases to be run simultaneously with each parallel simulation using 128 cores. More than 250 simulations, involving different solvent properties and configurations, have been run. Several new insights in the field of film flow have been achieved using the results from this investigation.

Additional computing resources, in terms of cores and software licenses, are needed to complete the overall goal of this research project on time. In particular, the primary goal is to develop a more accurate closure model for interfacial interaction forces for solvent absorption which in turn may be used to develop a large-scale CFD. Accordingly, the next step in this study involves simulating countercurrent gas-liquid flow between smooth and then corrugated sheets. This setup should serve to be representative of the gas-liquid flow through real structured packing. The main challenge foreseen in this simulation is the flow in the inflexion region of the packing. This location will require a very fine mesh to adequately capture the flow behavior and achieve converged results. Thus, more computational resources will become necessary to simulate this setup.

Tecplot and Ensight, which are already installed on the Supercomputer, have been used for post processing of the results and data visualization. Tecplot has enriched user control capabilities for CFD post processing and plot presentation. Both software packages enable better post processing and analysis of the simulation results and excellent presentation of flow visualization.

Using these resources a manuscript addressing the fundamentals of film flow is in preparation for possible publication in peer reviewed journal. A detailed report will soon be submitted to the Carbon Capture Simulation Initiative (CCSI) under which this research is being conducted. Details and results of the project are briefly presented in the next section.
Hydrodynamics of film flow over an inclined plate: Effects of solvent properties

Solvent absorption is usually carried out in a countercurrent gas liquid flow in the tower, where the gas flows upward and liquid falls in downward direction. The purpose is to preferentially dissolve one or more of the constituents of the gas, such as carbon dioxide (CO₂), into the liquid. The tower is filled with a packing material that provides enhanced surface area for gas-liquid contact. Surface area is important because very little reaction will occur without adequate contact of the gas and liquid. Structured packing is popular because it provides a large surface area for mass transport between both phases while minimizing pressure drop. This packing is generally made of corrugated sheets arranged in crisscrossing fashion to form a single layer of packing material (see Fig. 1). Accurate design of the packed column requires knowing essential hydraulic characteristics of the packing element across the operating range. Computational fluid dynamics (CFD) model is a useful tool to capture local hydrodynamics and complex behaviors associated with chemical reaction, mass transfer, etc.

Absorption columns are characterized by length scales of several meters with diameters that may range from 5-10m and overall column heights of 20-30m. In contrast, the characteristic dimensions of the packing are much smaller with the length scale of a typical layer of corrugated structured packing on the order of 20 centimeters. Finally, the dimension of liquid film thickness is on the order of tenths of millimeters for structured packing. These scales cannot be resolved simultaneously within a single computational model. That is, it is computationally infeasible to run computations at large scales while taking into account the local gas-liquid interactions and the real geometry of the packing. This problem requires a multi-scale approach.

In this CFD investigation, Volume of Fluid (VOF) multiphase flow simulations are being used to develop closures models for two fluid model simulations and/or process models. Among the computational methods of multiphase flow, the VOF method is well suited for simulation of two immiscible fluids. This method has been successfully applied by others for stratified flow such as drop dynamics, film flow, etc.

Fig. 1: Schematic of the structure packing tower showing the countercurrent gas-liquid flow. Exploded view shows the orientation of the corrugated packing sheet inside the tower.
Recent work focused on investigating the micro-scale hydrodynamic of the falling film flow above an inclined plane using a commercial CFD code “Ansys FLUENT 14.0” running on the NETL Supercomputer. This particular problem was primarily selected because results from several experimental (Hoffmann et al., 2006 and Iso et al., 2013) works are available which allows for validation of the present simulations. Gaining a better understanding of the fundamentals of liquid flow over an inclined surface (e.g., flow transitions, film thickness, wetted area, etc) is another important aspect of this study. Note that the liquid behavior on the structured packing plays a critical role in the mass transfer between the liquid and gas phases and therefore on the overall efficiency of the absorption column.

The geometry and flow conditions of the present simulations are similar to the studies mentioned earlier. A schematic of the simulation setup is presented in Fig. 2. The domain consists of a stainless steel smooth plate of dimensions 60 mm long by 50 mm inclined at an angle of 60 degrees with respect to the horizontal. The depth was taken as 7 mm. Air (density ($\rho$) = 1.185 kg/m^3, viscosity ($\mu$) = 1.831 $\times$ 10^{-5} Pa-s) and water ($\rho$ = 997 kg/m^3, $\mu$ = 0.8899 $\times$ 10^{-3} Pa-s, surface tension ($\sigma$) = 0.0728 N/m) were used as working fluids. Water enters the domain at the top and exits the bottom in the presence of gravity. At this stage, air was considered a stationary phase. The plate and side walls were set as no-slip walls with the static contact angle of 70°. The outlet and top boundary were set to pressure outlets with zero gauge pressure. The liquid inlet was defined as a uniform flow given by a constant velocity perpendicular to the boundary. In this effort, the dimension of the liquid inlet was given by the width of the plate (50 mm) and the depth of the domain (7 mm).

Fig. 2: Schematic of the flow domain used for the study of liquid film development over an inclined plate.

The flow domain was modeled in GAMBIT, a preprocessor tool of FLUENT. Mesh generation is a critical step for the convergence, stability and accuracy of the numerical simulations. In this context, one needs a sufficiently resolved mesh to capture the micro-scale phenomenon of the film flow, such as droplet formation and breakup, rivulets, etc. Accordingly, the flow domain was discretized with a non-uniform hexahedral mesh with 1.37M cells (Fig. 3). To capture the steep gradients of flow (see Fig. 3) required a very fine grid density inside the liquid film near the plate and at the center of the domain in the flow direction. Transient flow simulations were conducted with a variable time step $\Delta t$ having a value between ($10^{-5} - 10^{-4}$) corresponding to a Courant number of 0.50. Note that small time steps are the result...
of the very fine mesh needed to capture the micro scale hydrodynamics of film flow. The simulations were run until pseudo-state steady conditions were reached, which was determined by an approximately constant liquid flow rate at the exit. The total time needed to reach a convergent solution was generally around 2.0 sec. This simulation required approximately 48 hours wall time using 128 cores. In the study, a number of such simulations (more than 250 runs) were conducted to investigate the hydrodynamics of film flow. For some cases, such as for highly viscous solvent, the simulation time had to be extended to 3-5 sec. Accordingly, these simulations were more expensive (wall time of 48-96 hrs).

The effect of varying liquid flow rate (inertia), with flow rates ranging from $1.05 \times 10^{-6}$ to $1.05 \times 10^{-5}$ kg/m$^3$, was examined first for validation purposes. The Weber number ($We$) was used to characterize the importance of inertial forces to surface tension and was evaluated based on Nusselt film theory (Nusselt, 1916): $We = \frac{\rho V_{in} \delta_N}{\sigma}$, where $V_{in}$ and $\delta_N$ are the velocity and thickness of the liquid film, respectively. The impact of inertia on the flow behavior is demonstrated in Fig. 4, which shows a snapshot of the flow pattern once pseudo-steady state has been reached for different Weber numbers. The results represent the iso-surface defined by a volume fraction of liquid phase equal 0.5, which corresponds to the interface between the gas and liquid phase. At low $We (=0.03)$, where surface tension dominates over inertial force, droplets eventually form. The surface tension force tends to reduce the surface area thereby reducing the surface energy. As the flow rate increases (higher inertial forces), rivulets develop due to breakup of the film. Finally, at high $We (=1.10)$ film flow develops as evident by the fully wetted plate. The normalized wetted area of the plate compare well with the experimental results of Hoffmann et al (2005). Note that the wetted area of the plate is normalized by its total area of the plate.
Apart from liquid inertia, physical properties of the liquid (e.g., viscosity, surface tension, etc.) also play a significant role in the liquid film behavior (i.e., interfacial area, liquid thickness and flow regime), and therefore on the mass transfer between liquid and gas. The impact of varying liquid viscosity, surface tension, inclination angle was systematically investigated. The effects of viscosity on wetted area and film thickness at moderate value of viscosity (~2.5 mPa-s) has been previously investigated using VOF simulation (Gu et al., 2004; Valluri et al., 2005; Sebastia-Saez et al., 2013) and experiment (Nicolaiewsky et al., 1999). However, some disagreement exists. In view of this, a systematical investigation of liquid film development over an inclined plate has been conducted for air and a range of viscous solvents. Since solvents have different physical properties, a dimensionless group, Kapitza number $Ka = \sigma/\rho(g \sin \alpha \nu^4)^{1/3}$ was selected, where $\sigma$, $\rho$, $\nu$, and $\alpha$ are surface tension, density, kinematic viscosity of solvent and inclination angle of the plate, respectively. The advantage of the Kapitza number is that it only depends on physical properties and it is fixed for each solvent. The numerical simulations have been conducted for a wide range of $Ka$ and $We$. For sake of brevity, only the results for high $We$ (~1.10 and 1.50) are shown. At both $We$ a fully wetted plate is observed for all $Ka$ values (see corresponding value of specific wetted area equal to one in Fig. 5).

![Fig. 4](image.png)

**Fig. 4:** Effect of the inertia on the flow pattern over the inclined plate. Flow develops from droplet to rivulet and finally to full film (a fully wetted plate).

![Fig. 5](image.png)

**Fig. 5:** Plot for showing the fully wetted plate for all $Ka$ at $We=1.10$ and 1.50.
The average film thickness is computed at a cross-section sufficient away from the inlet, where fully developed film is observed. The numerically predicted film thickness matches excellently with those computed from Nusselt theory (Nusselt 1917) for all $K_a$ examined (see Fig. 6 (a)). Further, the decrease in computed film thickness with increasing $K_a$ indicates that film thickness increases with solvent viscosity. Note that a higher value of $K_a$ corresponds to a less viscous solvent. A correlation is also being developed that shows that $\delta \propto 1/K_a^{1/4}$ (See Fig. 6(b)).

The results and discussions of the detailed investigations will be presented in the manuscript of the paper for possible publication in the peer reviewed journal.

References
Gu et al., Chemical Engineering and Technology, 2004, Vol. 27, No. 10, pp. 1099-1104
Hoffmann et al., Chemical Engineering Research and Design, 2006, Vol. 84, A2, pp. 147-154
Xu et al., Chemical Engineering and Technology, 2008, Vol. 31, No. 10, pp. 1445-1452.