Multiphase Modeling of Trickle-Bed Reactors

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Background

With respect to multiphase reactions involving solid-liquid-gas systems, trickle-bed reactors (TBR) have become the most widely used reactor in industry. TBR's are employed in the petroleum, petrochemical, and chemical industries in waste treatment, biochemical, and electrochemical applications (Al-Dahhan et al., 1997). TBR's are preferred to other fixed-bed reactors due to their large throughput of both gas and liquid phases (Ramachandran and Chaudhari, 1983). Furthermore, the flow pattern in a fixed bed reactor approaches plug flow and is preferred if conversion of a liquid reactant is desired or if the yield of an intermediate in a consecutive reaction scheme is to be maximized.

Trickle-beds are widely used despite the following drawbacks:

- Trickle-beds operated at low liquid flow rates exhibit inhomogeneous catalyst wetting
- Poor heat transfer in the reactor compared to other reactors (slurry, fluidized bed, etc.)
- TBRs can exhibit tremendous flow maldistributions with the potential for channeling, flow bypassing at the reactor wall, and clogging within the interstitial spaces of the catalysts.
- Because of differences in flow distribution between pilot and industrial scale reactors, scale-up is difficult in the design process

Due to the poor heat transfer, flow maldistribution, and clogging within TBRs, there is a great potential for non-isothermal regions within the packed bed. These non-isothermal regions contribute to inhomogeneous reaction rates, inhomogeneous conversion, and the possibility of hotspot formation.

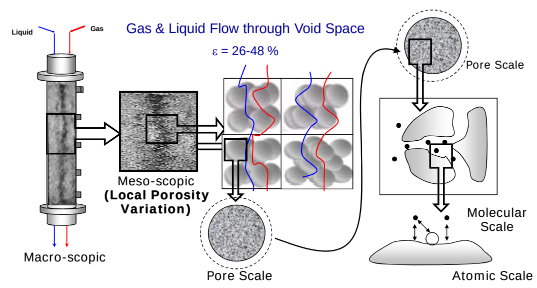
Previous Work

Previous work by Gunjal et Al. (2005) modelled single phase flow through interstitial spaces in a packed bed. This work utilized a unit cell approach to understand the heat and mass transfer characteristics as well as surface drag and form drag in the overall resistance to the flow through a packed bed. The model was validated against previously published experimental and computational results. In addition, a recent review by Dixon et al. (2006) mentioned research efforts in packed tubular modelling and catalyst design, noting that work must be done to improve the understanding of multiphase flow in trickle-bed reactor systems. Lastly, experimental work by Gladden et al. (2007) utilized MRI imaging techniques to track gas-liquid interfaces within gas-liquid-solid systems. Gladden's work proves to be a valuable tool in gaining insight into reaction dynamics and hydrodynamics of solid-liquid-gas systems captured from MRI image data. Furthermore, Gladden's work may help validate computed flow fields within multiphase systems.

Research Objectives

The objective of this work is to elucidate the role of flow inhomogeneity on the micro scale and it's affect on the overall performance and characteristics on the macroscale in trickle bed reactors. The work focuses on an interstitial flow model developed using computational fluid dynamics (CFD). Specifically, the model attempts to capture single and multiphase behavior in isothermal and non-isothermal systems. Finally, the overall objective of the work is to form a more detailed understanding of the role of maldistributions on reaction progress, hotspot formation, and the transport characteristics within a TBR based on models developed on multiple scales.

Scales Involved in the Trickle Bed Reactors

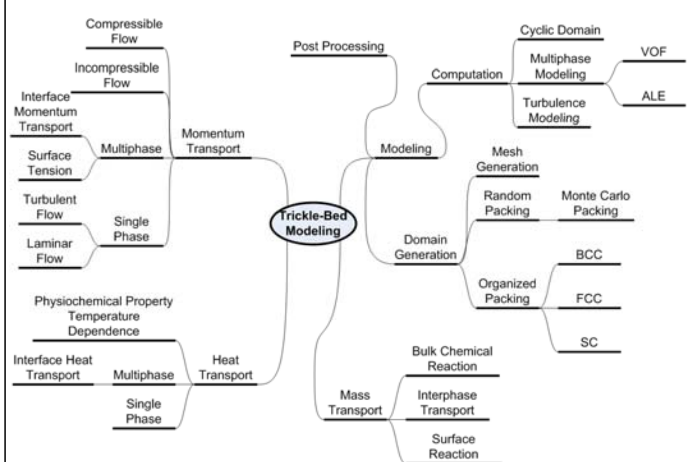


Gunjal Thesis

Hierarchy of Modeling for Trickle Bed Reactors

- Atomistic Modeling
  - Modeling at Atomic Level (Surface Chemistry)
  - Monte-Carlo Simulation/ Molecular Dynamic Simulation
- Microscopic and Mesoscopic Modeling
  - Multi-Component Heat and Mass Transfer in Catalyst Pores
  - Particle to Fluid Heat/Mass Transfer
  - Partial Wetting of Solid Particles
  - Multiplicity and Catalyst Effectiveness
- Reactor/Macroscopic Modeling
  - Flow Distribution
  - Distributor Design
  - Liquid Mal-distribution
  - Overall Heat and Mass Transfer

Research Complexity



Computational Tool (OpenFOAM)

Open Field Operation and Manipulation (OpenFOAM) is an open source CFD toolbox based on object oriented C++ (Weller et al., 1998). OpenFOAM focuses on a tensor calculus approach rather than a pure vector representation of partial differential equations in computational continuum mechanics.

The unique aspect of the OpenFOAM code is that high levels of the code resemble partial differential equation math notation. For example the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\phi) = 0$$

$$where \quad \phi = \rho U$$

Can be directly represented in OpenFOAM by:

```
fvMatrixScalar rhoEq
(
    fvm::ddt(rho) + fvc::div(phi)
) ;
```

Similarly, OF has also has the capability to model turbulence relatively easily. The momentum equation for a Reynolds-averaged simulation (RAS) is represented by:

```
fvMatrixVector Ueqn
(
      fvm::ddt(U)
    + fvm::div(phi,U)
    - fvm::lapalcian(tubulence.nuEff(),U)
    + turbulence.momentumSource()
);
```

OpenFOAM contains a large library of predefined solvers that are modified to meet the specific system. OpenFOAM also is able to import mesh data from numerous commercial software.

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