TRICKLE BEDS

I-12. Flow Distribution in a High Pressure Trickle Bed Reactor

A. Problem Definition

Trickle-bed reactors (TBRs), in which liquid and gas flow concurrently downward through a packed bed of catalyst, are one of the most widely used in petroleum industry. Poor flow distribution and catalyst contacting in such reactors can be detrimental to the process efficiency. Particularly, liquid maldistribution often occurs and may lead to formation of liquid channels, hot-spots and incomplete catalyst wetting.

Already three engineers from TOTAL worked in CREL on hydrodynamics in TBRs. The previous studies had been performed at atmospheric pressure with an air-water system over beds packed with non-porous glass beads. This time we will focus on operating conditions and come closer to industrial set up by packing real catalyst support (porous trilobe extrudates), operating at elevated pressure (10 bar) and using both air-water and air-oil systems.

B. Research Objectives

The objective is to evaluate the effects of parameters such as gas and liquid flow rates and bed height on the phase distribution along the bed and provide experimental data to verify correlations and validate future Computational Fluid Dynamics (CFD) simulations.

The work consists of:

- Designing, constructing and testing a high pressure (up to 10 bar) 6-inch trickle bed reactor setup that can accommodate different distributor designs and bed heights and can be operated at a range of liquid and gas flow rates that covers the trickle flow regime.
- Using sock and dense packing methods and determining beds porosities, catalyst internal holdup and Ergun's coefficients of the bed to be used in CFD simulations.
- Measuring the two-phase pressure drop as well as static and dynamic liquid holdup.
- Evaluating phase distribution via outlet collection of both liquid and gas phases and determining the liquid saturation at different elevation by gamma-ray Computed Tomography (CT).

C. Accomplishments and Current Work

The design of the lab-scale reactor has been finished and the main parts have been ordered or fabricated.

Also some primary experiments have been performed to study the catalyst support which will be used for the experiments. Particularly, it seems that, at atmospheric pressure and for superficial gas velocities between 1 and 40 cm/s, the standard reported Ergun's coefficients (E_1=180 and E_2=1.8) predict with a good accuracy the single phase pressure drop through sock packed as well as densely packed beds. This result must yet be verified at higher pressure for which the inertial effects due to the tortuosity of the packing are predominant.

The current work is to assess the newly designed uniform distributor. Experiments have been carried out to evaluate the induced pressure drop for the gas phase and the inlet distribution of the liquid with and without the presence of gas. The post-treatment of these results is in progress.

D. Future Work and Milestones

The erection and calibration of the setup should be accomplished in early summer 2006. The experiments with pressurized two-phase systems and the associated data post-treatment will be performed in summer and fall 2006.

E. Acknowledgements

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I-13. Multiphase Kinetic and Reactor Models

A. Problem Definition

Several industrially important chemical processes, such as hydrogenation, hydro-de sulphurization, oxidation etc, are carried out in the trickle bed reactors. Often due to the complexity of reaction schemes involved in these processes, a robust mathematical reactor model is required for understanding the process, for training and trouble shooting purposes (e.g. identification of hotspots and any flow maldistribution) and for the reactor scale-up. The reactor model requires a good kinetic model for the successful simulation of the processes. The kinetic models are developed based on the experiments conducted in laboratory scale equipment, very often these days in autoclave, for high pressure three phase reaction systems. CREL has expertise in developing the laboratory and reactor scale models. CREL can assist industrial partners in designing the experiments, data analysis, developing robust kinetic model, developing suitable reactor model in a user-friendly format and training the industry personnel to use the models for trouble shooting purposes.

B. Research Objectives

The development of kinetic model involves the development of lab-scale reactor (autoclave) model and an appropriate parameter estimation model. The autoclave model consists of a set of component mass balance equations resulting in differential equations (in the absence of mass transfer limitations) or differential-algebraic equations (in the presence of mass transfer model) which are solved by stiff solvers. The parameter estimation program is an optimization routine which minimizes the sum of squares of errors between the model predictions and the experimental data and hence determines the kinetic constants. CREL has developed its kinetic parameter estimation program in a modularized form and hence any reaction rate forms, reaction species or the suitable solvers can be handled easily.

The trickle bed reactor model incorporates multiple reactions, non-isothermal effects, partial vaporization of volatile liquid phase components and the effect of partial external wetting of the catalyst. The reactor has been numerically modeled as network of cells. By this approach, a number of diverse reactor models can be obtained by simply choosing a scheme for connecting the cells. In each cell, the governing equations are presented for the mass transfer among the gas-liquid-solid phases. Energy balance is considered for the whole cell to get the local cell temperature. Gas, liquid and solid phase in each cell are assumed to be at the same temperature which is a reasonable assumption in a trickle bed. The above model equations are solved by boundary value problem solver or by non-linear algebraic solver.

The above models are used to simulate successfully the commercially important processes.

C. Accomplishments

CREL has developed in-house kinetic and reactor model programs (1-D and 2-D) which can be easily used for any processes. The reactor model includes several calculation to account for heat of vaporization, gas-liquid, liquid-solid, gas-solid mass transfer coefficients. Correlations to calculate the wetting efficiency and the liquid holdup are also included in the model. The mixture rule to calculate the properties of gas and liquid mixtures along the reactor length has also been coded in the model.

Another important feature of this model is its ability to predict the pressure drop across the bed using several correlations. It is to be recognized that the pressure drop correlations developed using water-air system at lower pressure conditions can not be used for higher pressure conditions. Hence appropriate pressure drop correlations have to chosen for the operating conditions. In addition to that, the Ergun constants used in the pressure drop correlations have to be tuned to the system of interest. CREL has large experience in guiding the experimental effort in this direction to identify the Ergun constants for the reactor and to develop suitable pressure drop correlation.

Effort is being undertaken to couple the catalyst particle level model with that of the reactor level model. This becomes very important when dealing with highly exothermic reactions, where partial wetting of the catalyst is a major issue.

CREL delivers the developed reactor model in user friendly Excel format.

Several doctoral dissertations are available in CREL which address some of the above modeling effort (Khadilkar (1998), Jing Guo (2005), S. Roy (2006), etc).

For detailed information and for a copy of the theses contact Prof. M.P. Dudukovic at CREL at dudu@wustl.edu, (314) 935 6021.