

The gPROMS Object for Reactive CFD Heterogeneous catalytic reaction applications

In contrast with previous approaches for linking CFD and process modelling systems, the gO:CFD provides an “off-the-shelf” capability for achieving the benefits from combining the two technologies.

Prerequisites are

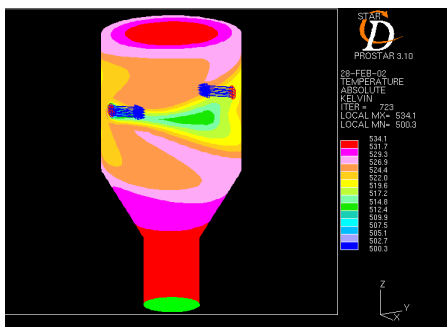
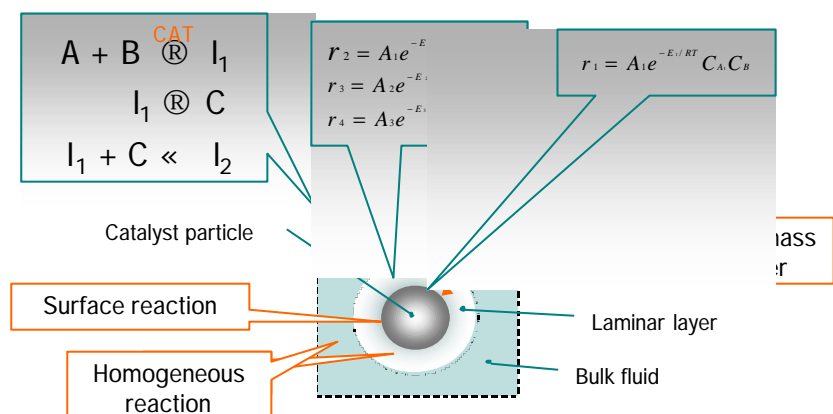
- a CFD model of the geometry
- a gPROMS model of the reaction system

The gPROMS Object for Reactive CFD (gO:CFD) is a unique and powerful tool that enables reaction engineers to combine the power of Computational Fluid Dynamics (CFD) packages for fluid flow and mixing modelling with gPROMS’ capabilities for modelling of complex reaction systems. See the brochure “gPROMS Object for Reactive CFD – An overview” for more information.

This application brief uses an example of a heterogeneous catalytic reaction taking place in a reactor to illustrate gO:CFD’s key advantages and benefits.

Reaction chemistry and physics

A heterogeneous catalytic reaction occurs on the surface of catalyst particles suspended in a liquid. Further non-catalytic reactions occur in the laminar layer surrounding the catalyst particles as well as in the bulk fluid, as shown in the diagram below.



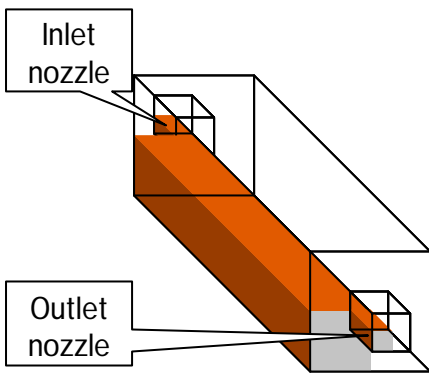
Combined gPROMS/STAR-CD computations in reactor with two tangential inlet nozzles

The laminar layer formed around each catalyst particle in a turbulent flow field provides a resistance for mass and heat transfer which limits the rate of reactions. As a result, the temperature and the reactant concentrations on the catalyst surface can differ significantly from those in the bulk liquid. As one of the non-catalytic reactions is irreversible, the reactant conversion and the product selectivity achieved in this heterogeneous reacting system will, in general, be different from those that would be observed in a homogeneous reaction environment.

Implementation in gO:CFD

The above heterogeneous reactive systems is one of those supported as standard by the gO:CFD. Using the gPROMS ModelBuilder, the user can define the chemistry and kinetics for both the catalytic and non-catalytic reactions, and specify the geometric and other characteristics of the catalyst particles – all with minimal effort.

The gO:CFD automatically includes in the model a complete description of multi-component mass and heat transfer based on the Maxwell-Stefan formulation.



CFD reactor modelling

The reactor employed for performing the above reaction has a simple rectangular box geometry, with centred inlet and outlet nozzles, as shown on the left. Because of the reactor's intrinsic symmetry, it is sufficient to model only a quarter of this system (shaded in red on the left), thereby reducing the number of CFD cells by a factor of 4.

The CFD model for this example is constructed in the STAR-CD CFD package. The model is one of a pseudo-homogeneous liquid-phase system involving the 5 chemical species A, B, C, I_1 and I_2 . Neither the existence of the solid catalyst particles nor the physics and chemistry of the reaction are included in the model. However, the model does include mass and heat source terms for the CFD equations for species mass and energy conservation respectively. These terms are calculated externally by the gO:CFD during the execution of the CFD model.

Results

Close coupling of a CFD simulation and a detailed, high-fidelity reacting system model allows accurate prediction of product quality at all points in the reactor. As can be seen in the concentration profiles shown on the left:

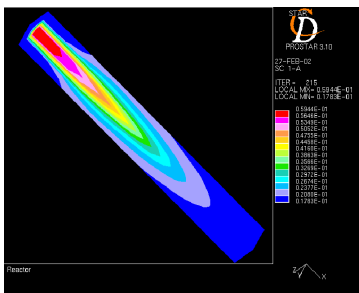
- The main reactant A starts being consumed as soon as it comes into contact with the catalyst. The effects of the geometry on the flow pattern are evident in the shape of the 'plume' of reaction downstream from the inlet nozzle.
- The concentration of the intermediate product I_1 peaks around the middle of the reactor. The calculation takes into account the microscale phenomena of diffusion kinetics of reactants and products along the diffusion path between the bulk liquid and the catalyst surface.
- The concentration of the main product C builds up toward the end of the reactor, as expected.

Conclusions

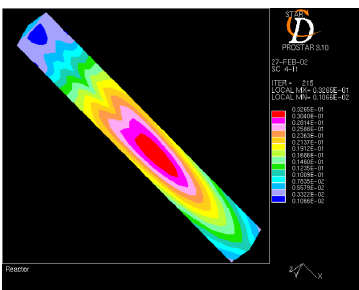
This detailed 3D modelling of the complex reacting system under consideration can be achieved only by gO:CFD's combination of gPROMS with CFD technology. The results contain information that is invaluable both to the designers of new reactor equipment and to operations personnel attempting to maximise product yield and quality from existing reactors. For example:

- The rigorous prediction of the mass and heat transfer limitations in the reacting system allows confident prediction of the required reactor volume. In fact, the results indicate that the volume is not sufficient, and also that it is possible to achieve higher conversion by improving distribution of the feed to make better use of the volume around the inlet nozzle.
- The concentration of reactant C is highest in the stagnant corners adjacent to the outlet. This indicates that a higher product purity could be obtained by re-designing the reactor geometry in order to eliminate dead areas (indicated by the highest product concentration)

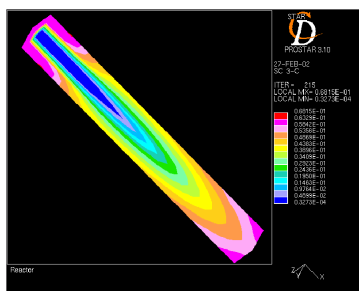
The predictive capability of the gO:CFD model is such that new reactor designs and/or improvements to operating conditions can be tested with confidence, quite simply by implementing the proposed changes in the model and repeating the calculations.



Concentration of reactant A



Concentration of intermediate I_1



Concentration of product C