gPROMS and CFD

Combining hydrodynamics and chemistry

There are many examples in the chemical process industries where non-ideal mixing is a major factor affecting the performance of industrial-scale equipment. Equally, there are many processes that can only be described accurately using very complex, detailed models of the underlying physical and chemical phenomena.

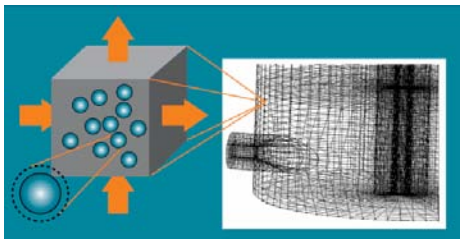
Why combine CFD and gPROMS?

Computational fluid dynamic (CFD) software is designed to model mixing effects very well, but has limited capability for describing complex process phenomena such as crystallisation and fermentation.

PSE's gPROMS modelling system, on the other hand, can model processes of arbitrary complexity, but has limited capabilities for describing and modelling 3-D geometries.

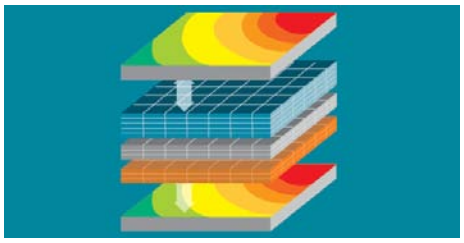
The combination of gPROMS and CFD models provides the perfect means to couple the microscale and macroscale effects in order to provide powerful predictive models for activities such as design scale-up.

PSE provides intefaces for a number of different situations:



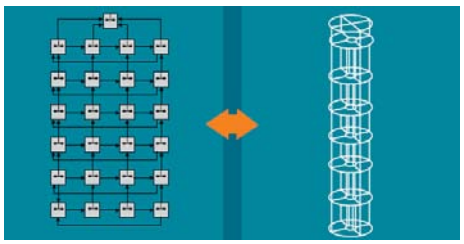
The gPROMS Object for CFD (gO:CFD)

This embeds a gPROMS model of homogeneous or heterogeneous reaction in each cell of a CFD model. A fast and efficient way of dealing with complex reactions (including species diffusion), gO:CFD adds relatively little overhead to a – for example – FLUENT® or STAR-CD® run.



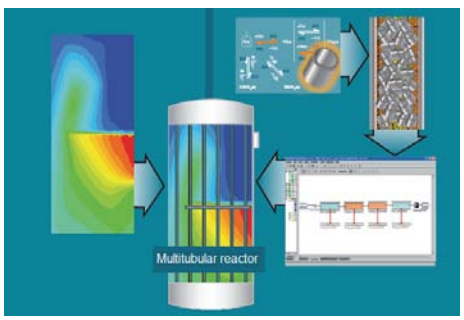
The gPROMS-CFD Fuel Cell Stack interface

An option to the Advanced Model Library for Fuel Cells, this links a gPROMS fuel cell membrane assembly model to a FLUENT model of the flow channels, enabling all relevant phenomena to be taken into account rigorously. Clever model reduction algorithms reduce the problem size by a factor of over 100 for full stack modelling.



The gPROMS-CFD Hybrid Multizonal interface

Hybrid Multizonal links gPROMS well-mixed zone models of complex 'population' processes such as crystallisation or fermentation to the corresponding zones (compartments) of cells in a FLUENT model of the equipment. This enables high-accuracy calculation in complex mixtures.



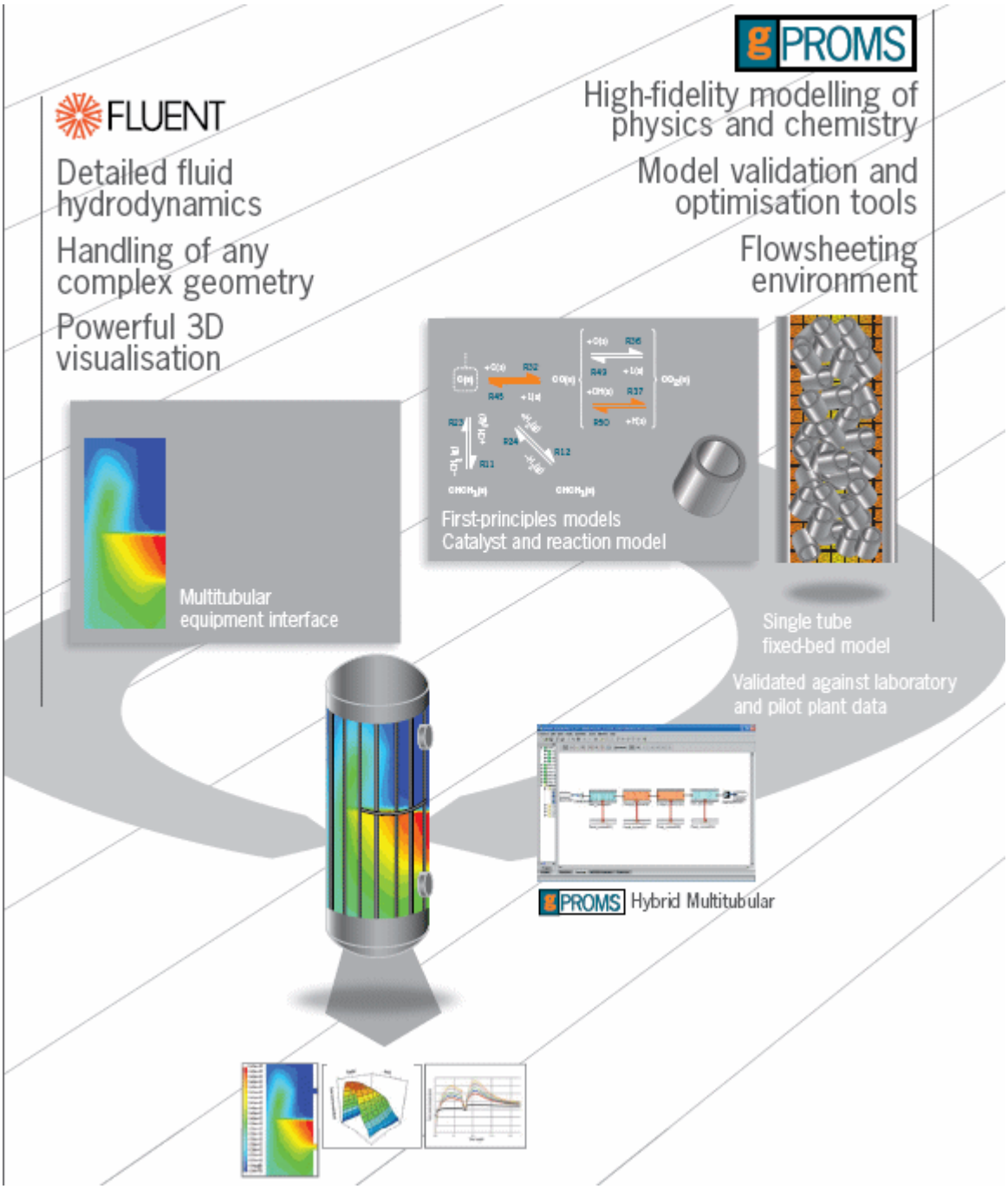
The gPROMS-CFD Hybrid Multitubular interface

An option to the Advanced Model Library for Fixed-Bed Catalytic Reaction, this links gPROMS tube models (2-D or 3-D catalytic reaction validated against laboratory and pilot plant data) to a FLUENT or STAR-CD model of the shell side fluid flow. The approach is the only known method for accurate detailed design of multitubular reactors (see overleaf for more information).

Note: selected interfaces are available with parallel computation options

Getting the best of both worlds: multitubular reactors

Multitubular reactors are complex items of equipment that need to be designed simultaneously taking into account the detailed hydrodynamics on the shell side with the complex catalytic reaction taking place inside the thousands of tubes – each of which experiences a different wall temperature profile. Hybrid modelling is the only effective way to do this.



The gPROMS-CFD Hybrid Multitubular interface

- Links gPROMS tube models (2-D or 3-D catalytic reaction validated against laboratory and pilot plant data) to a FLUENT or STAR-CD model of the shell side fluid flow
- Optional component of the Advanced Model Library for Fixed-Bed-Catalytic Reaction (AML:FBCR)

Accelerate innovation Manage risk

gPROMS