

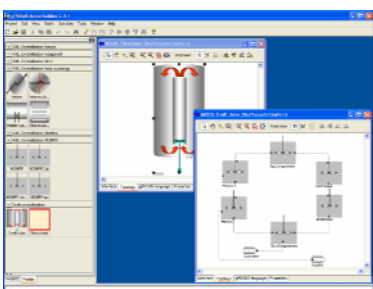
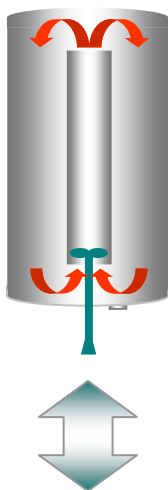
Linking gPROMS and CFD models

Harnessing the best of both solutions

gPROMS & CFD

The combination of gPROMS and CFD can bring considerable benefits:

- Operations can be scaled up with confidence
- Both non-ideal mixing and process complexity taken into account
- Highly accurate quantification of complex processes
- Easy multi-scale modelling
- Realistic run-times for complex calculations
- Powerful new technologies for accurate modelling of crystallisation and reaction processes.



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.

Computational fluid dynamic (CFD) software is designed to model mixing effects very well, but has limited capability for describing process phenomena. 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 as required to provide powerful predictive models for activities such as design scale-up.

However, in the past, creating such links has been a time-consuming and error-prone process. PSE has addressed this deficiency with a number of software products – validated through many years' work with industrial customers – that go as far as possible to automate the creation, linking and execution of combined CFD and gPROMS models.

Approaches for linking gPROMS process and CFD models

There are three different approaches, each applicable to a well-defined class of problems, and each covered by a PSE product:

1. Cell-linked models for strongly-coupled systems, used for – for example – volumetric reaction in a flowing fluid, surface reaction at a catalytically active surface, or reaction within a membrane separating two fluids [PSE product **gO:CFD**]
2. Surface-linked models for multitubular equipment [PSE product **Hybrid gPROMS-CFD Multitubular**]
3. Zone approach for weakly-coupled systems (PSE product **Hybrid Multizonal gPROMS-CFD**)

The common characteristic of all these technologies is that they combine CFD descriptions of fluid mechanics and mixing with gPROMS descriptions of all other phenomena (such as homogeneous or heterogeneous reaction, multicomponent mass transfer, heat transfer). This results in hybrid models of sufficient accuracy to support decisions on equipment design, retrofit, troubleshooting and scale-up with detailed, high-quality quantitative information.

In approaches 1 and 2, the CFD package is in control, calling the gPROMS model as a User-Defined Function. In approach 3, gPROMS calls the CFD package.

1. gO:CFD for cell-linked models

Cell-linked approach is used for strongly-coupled systems, i.e. those where the fluid dynamics have a strong effect on the process, and the process in turn has a strong effect on the fluid dynamics. The gPROMS model is called from every cell, on every iteration, using a well-designed technique that is extremely fast, even when dealing with complex phenomena. Typical effects modelled in the gPROMS model are multicomponent diffusion, complex reaction kinetics, electrochemistry, and heat transfer (for example through a catalyst pellet or catalytically-active surface).

PSE's **gO:CFD**, or “gPROMS Object for CFD” product caters for three types of cell-linked interaction:

1(a) gO:CFD for Volume Reaction

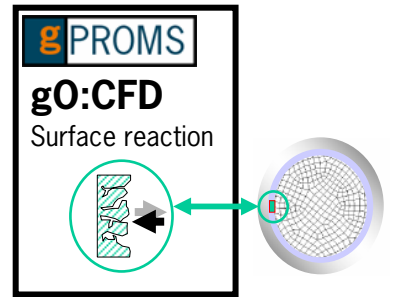
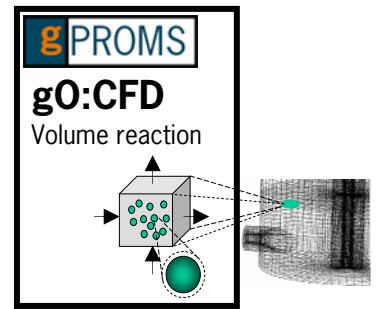
This is typically used for homogeneous and dispersed heterogeneous reaction. The gO:CFD object is called from every cell in the volume being modelled by the CFD model.

1(b) gO:CFD for Surface Reaction

This is typically used for catalytically-active surfaces, for example to model reaction on the surface of a catalyst monolith or catalyst wire.

1(c) gO:CFD for Membranes

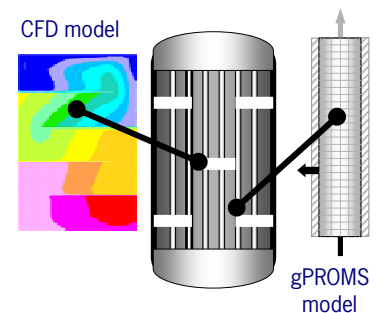
This is typically used to model configurations such as those found in fuel cells, where fluid effects on either side of a membrane and the membrane physics and chemistry are both important.



2. Hybrid gPROMS-CFD Multitubular for surface-linked models

In this case the gPROMS and CFD models are linked at a heat exchange surface, coupled via 1-D profiles along the tube length. A typical example is a multitubular reactor, where gPROMS is used to model the detailed catalytic reaction system, and the CFD package the fluid flows on the shell side. Other examples are multitubular equipment of all kinds, packed-bed reactors, and falling film equipment.

The Hybrid gPROMS-CFD Multitubular interface is supplied as an option with PSE's AML:FBCR advanced model library.



3. Hybrid Multizonal gPROMS-CFD for multizonal models

The zone approach is typically used for weakly-coupled systems such as crystallisation, where the fluid dynamics might have a strong effect on the process but the process has little effect on the fluid dynamics.

The PSE Hybrid Multizonal gPROMS-CFD software automates the creation of and linking of the CFD and gPROMS multizonal models and exchanges the required information between the two in a way that is transparent to the user.

