gPROMS Product family

Hybrid Multizonal gPROMS–CFD

High-precision multizonal gPROMS models with automated CFD coupling

Multizonal (or multicompartment) models approximate the effects of non-ideal mixing in industrial-scale processes by representing them as networks of **well-mixed zones**.

However, in the past, the wide application of such models has been limited by the difficulty of establishing zone connectivity and calculating inter-zonal flowrates.

Hybrid Multizonal …

- combines multizonal (multi-compartment) models in gPROMS with CFD
- offers unprecedented modelling accuracy for optimisation of design and operations
- addresses traditionally "difficult" processes, including crystallisation, polymerisation, and fluidised-bed reactions
- allows solution of both steady-state and dynamic simulation problems within reasonable computational time
- delivers new value from both CFD and process modelling investment via model re-use.

PSE's Hybrid Multizonal gPROMS–CFD (Hybrid Multizonal) software is a unique and powerful tool that enables multizonal models in gPROMS to make use of computational fluid dynamics (CFD) models for the prediction of the network connectivity and the inter-zonal flowrates.

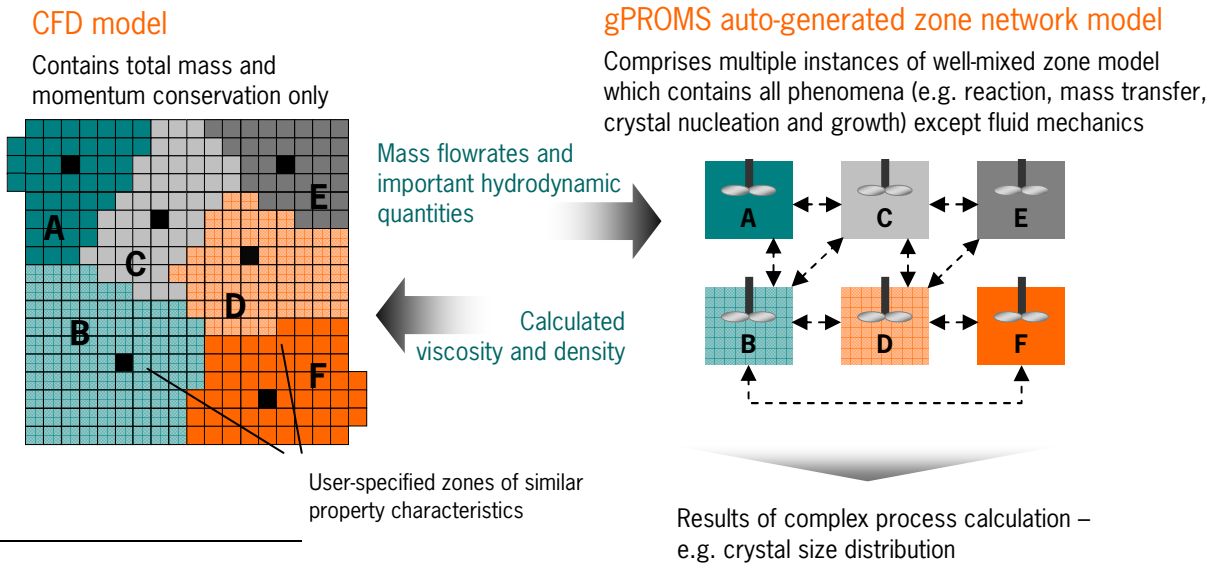
In the past, creating such links has been a time-consuming and error-prone process. With Hybrid Multizonal, all the user has to do is provide a single gPROMS model[1] (of any level of complexity) of a well-mixed zone, and specify the number of zones to be considered and the approximate (*x*,*y*,*z*) co-ordinates of their centres in the CFD model. Hybrid Multizonal does the rest automatically.

How the gPROMS Hybrid Multizonal CFD tool works

Hybrid Multizonal uses the specified (*x*,*y*,*z*) co-ordinates to group the cells in the CFD model into a number of zones of irregular geometry. This information is used to automatically create a multizonal model in gPROMS, by connecting multiple instances of a gPROMS model for a single well-mixed zone.

On execution, gPROMS reads initial inter-zone mass flowrates from the CFD model, performs the internal gPROMS calculations for each zone, and returns the zonal viscosities and densities to the CFD model, which then re-computes the mass flowrates. Iteration between the two models (typically only 1 -3 cycles) proceeds until the returned values are within tolerance.

If necessary, the CFD model can also return zone volume-averaged hydrodynamic quantities (e.g. turbulent energy dissipation rate), which may affect some of the physical phenomena represented within the gPROMS zone model (e.g. the rate of nucleation in crystallisation models).



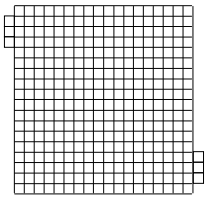
[1] PSE provides the Advanced Model Library for Solution Crystallisation (AML:SC) for sophisticated zone models of crystallisation processes. Similar reaction and polymerisation models can be supplied under PSE's ModelCare programme.

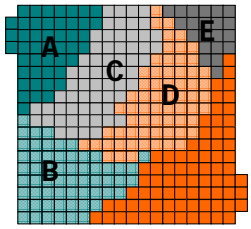
Using the Hybrid Multizonal gPROMS–CFD software – a simple step-by-step guide

The typical workflow for hybrid multizonal gPROMS–CFD modelling involves the following steps:

A. Prepare the CFD zone information

Step 1: Prepare a CFD model of the equipment of interest, incorporating total mass and momentum balances only

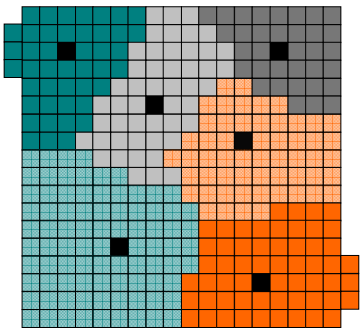




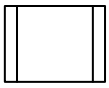
Step 2: Perform a preliminary CFD calculation using nominal values of viscosity and density

Step 3: Inspect the solution and identify approximately well-mixed zones

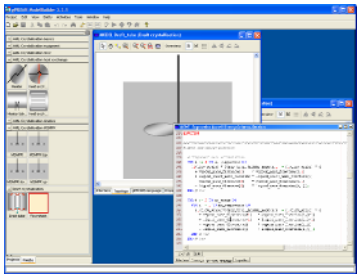
Step 4: Specify the number of zones and the (*x*,*y*,*z*) co-ordinates of the centre of each zone in a simple text file



Step 5: Run a utility that identifies the cells belonging to each zone, the volume of each zone, and the zone connectivity



B. Prepare the gPROMS models

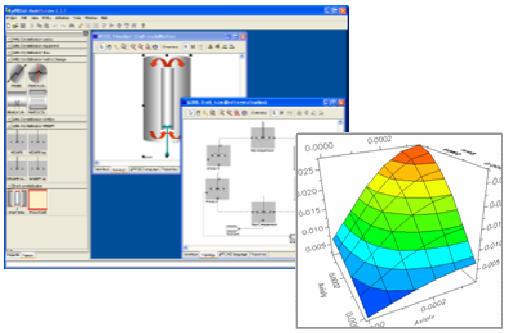


Step 6: Making use of the gPROMS ModelBuilder, prepare a gPROMS model of a single well-mixed zone

C. Execute the combined simulation

Step 7: Execute a gPROMS simulation of the Multizonal model. gPROMS automatically creates the zone flowsheet

Step 8: View the results of the calculation using gPROMS' standard facilities



Licensing, supported platforms and pre-requisites

The Hybrid Multizonal gPROMS–CFD software is licensed as an option under the gPROMS ModelBuilder. The licence includes the utility for the automatic construction of the zone network, a Foreign Object for gPROMS–CFD communication during execution, and a self-configuring gPROMS multizonal network model.

Pre-requisites are:

- gPROMS ModelBuilder for Linux
- Fluent® version 6.1.22 for Linux or later