Press release

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gO:CFD - CFD with complex chemical reactions

Powerful, easy-to-use link between CFD and gPROMS process modelling

PSE today released the **gPROMS Object for Reactive CFD** (gO:CFD), a unique and powerful new tool that for the first time allows users of Computational Fluid Dynamics (CFD) packages easily to **model complex reaction systems by combining CFD's** spatial modelling capabilities with the power of PSE's **gPROMS process modelling environment**.

gO:CFD's combination of the best of CFD and process modelling technologies into a single multi-scale model of reaction systems leads to an unprecedented level of accuracy, providing detailed quantitative information for reactor design, troubleshooting and operational decision support.

gO:CFD is supplied with built-in Reaction Objects for five different types of reaction – including implicit sets of reaction equations, such as those arising from chemical reaction equilibrium, and a variety of heterogeneous reaction systems – and provides capabilities far more sophisticated and complex than those available via the standard CFD reaction facilities. Using gO:CFD demands very little additional effort from the CFD practitioner over the effort required for building a non-reactive model.

PSE have worked closely with CFD industry leader Fluent Inc. to develop and prove gO:CFD. Fluent's Director of Strategic Partnerships, Barbara Hutchings, says "we have supported PSE from early on in the development of the gO:CFD capabilities and we believe many applications involving reaction can take advantage of this easy integration between FLUENT and gPROMS."

PSE Technology Director Costas Pantelides says "this is part of our drive to place gPROMS at the heart of process modelling, and to break down the traditional boundaries between complementary parts of the design and operational support activities within organisations. The chemists and engineers developing process models of the reaction systems can work closely with their CFD colleagues to combine their knowledge into quality designs."

gO:CFD links a gPROMS model of reaction kinetics and other physical and chemical phenomena, prepared and tested in the gPROMS ModelBuilder environment, to every CFD cell. This ensures that the gPROMS reaction calculation takes into account the spatial variations in flow, concentration of species and mixing conditions determined by the CFD solution. In turn, the CFD mass and enthalpy continuity equations incorporate the rates of generation or consumption of species and energy resulting from the reactions and other important phenomena, such as mass and heat transfer limitations, modelled in gPROMS. The state-of-the-art software architecture and advanced numerical solvers of the gPROMS Server ensures that all of this is done with remarkable computational efficiency.

The Reaction Objects for heterogeneous systems include detailed modelling of mass and heat transfer, allowing the concentrations of reactants, and temperatures within the system to be predicted with unprecedented

accuracy. Kinetic and other critical model parameters can be determined accurately from experimental or plant data using gPROMS' parameter estimation capabilities before the model is linked to the CFD package.

A key benefit is that reaction models are implemented in an easily-maintainable and easily-extendible form (the gPROMS modelling language) and can be used for further design and optimisation work across the modelling lifecycle.

The prerequisites for running gO:CFD are the gPROMS ModelBuilder for creating reaction models and Fluent 6.0 or greater. PSE will release versions of gO:CFD for other CFD packages in the near future.

Notes for Editors

The advantages of combining CFD and process modelling

CFD and process modelling are highly complementary technologies, each with well-developed features for dealing with the key phenomena of reaction systems. CFD packages' strengths are their ability to model in detail fluid mechanics and mixing, to solve equations in irregular geometries, and to handle very large number of equations. On the other hand, gPROMS process modeling can also deal with very large numbers of equations, but in addition can model multi-component phase equilibria, multi-component inter-phase mass transfer, and complex reaction schemes including equilibrium reactions and other complex phenomena to a highly-accurate level of detail.

About gPROMS

gPROMS is one of the world's leading software packages for advanced process modeling, simulation and optimisation. Conceived and initially developed at London's Imperial College, the package has been developed and marketed by PSE since 1997. gPROMS is widely used throughout the process industries but in particular by large chemical manufacturers in the area of reactor systems engineering. Here it delivers powerful capabilities for building and solution of complex models of reaction systems, for the estimation of reaction kinetics and related process parameters, and for its industry-first dynamic optimisation capability. gPROMS is both a steady-state and dynamic simulator, but is most frequently used for the optimisation of process equipment and control design under dynamic conditions, the optimisation of complex operating procedures and for troubleshooting of operation using detailed process models.

About Process Systems Enterprise Ltd

PSE (http://www.psenterprise.com) is one of the world's leading providers of model-based technology and services for design and decision support to the process manufacturing industries. The company was founded in 1997, originally to deliver and support in the commercial market innovative process modelling technology originating from London's Imperial College. Among its unique offerings are advanced software packages, services and expertise for modelling and simulation of manufacturing processes and optimal design, planning, scheduling and operation of flexible manufacturing facilities. PSE has established itself as a leading independent high-tech provider to a growing, global customer base that encompasses the largest process manufacturing and automation companies in the world. The company is a winner of the prestigious UK Queen's Award for Enterprise and Innovation for 2001, for its gPROMS mathematical modelling framework and dynamic optimisation technology. It employs around 35 graduates and PhDs at its headquarters in London, UK, and recently initiated a Japanese operation in Tokyo.

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The model company