

Advanced modelling solutions Catalyst monolith reactors

PSE's microreactor modelling brings significant benefits to monolith reactor development, design and operation, including:

- optimised response to load changes
- economic manufacture
- reactor longevity

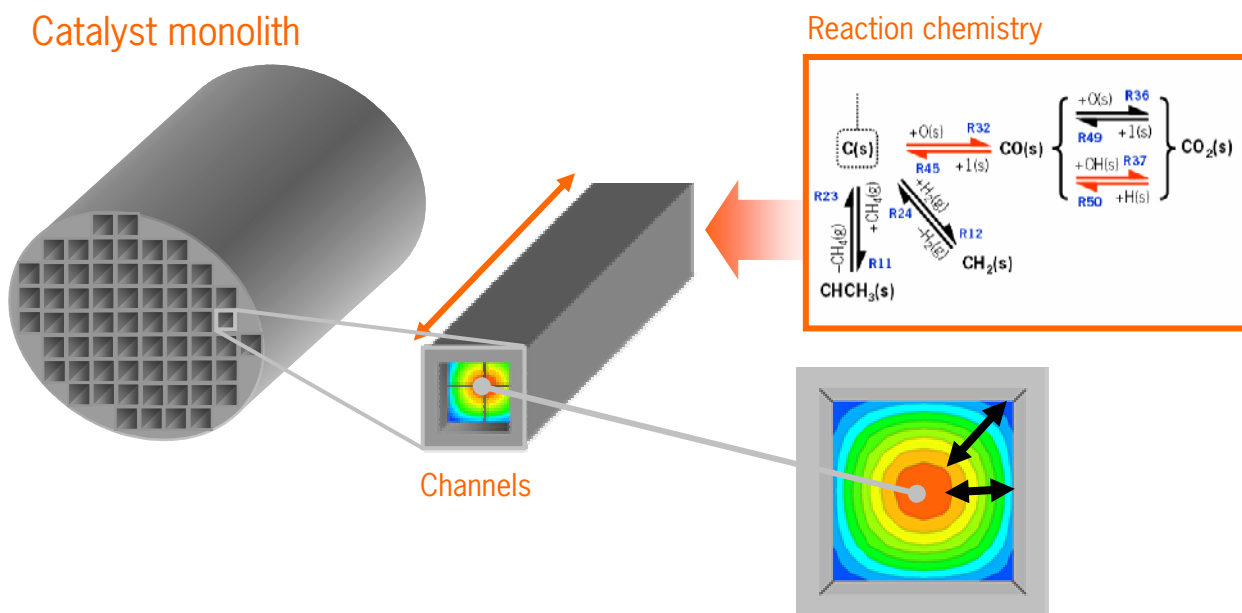
The benefits can be realised in a wide range of processes, such as:

- fuel cell reformers
- monolith ethylene production
- car catalytic reformers

Monolith reactors are particularly suitable for carrying out fast reactions in applications where space is at a premium – for example, in car exhausts, fuel cell reforming. They also provide a novel, highly scalable solution to large-scale industrial applications such as ethylene cracking.

Monolith reactors are divided into a number of channels. Reactions take place both in the fluid bulk and, primarily, on the catalyst-coated inner surfaces of the channels. Flow in the channels is laminar, and significant gradients in temperature and concentrations of reactants and products exist between the bulk fluid and the surface. Substantial heat transfer also takes place along the solid walls of the channels.

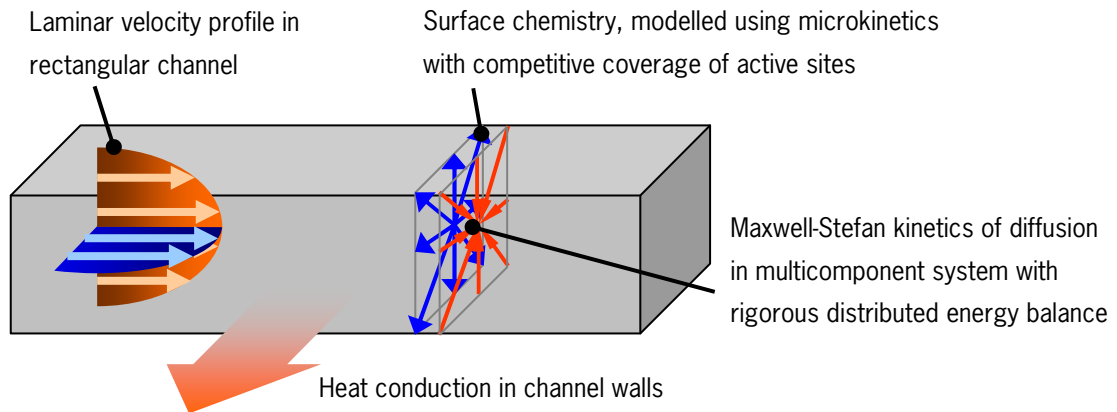
The detailed modelling of monolith reactors needs to be based on an understanding of the complex interactions between the reaction, mass and heat transfer and fluid flow phenomena. A first-principles approach is essential for truly predictive models that can quantify the effects of design and operating decisions on reactor performance. The effective utilisation of such predictive models can lead to significant commercial benefits such as reduced time-to-market, better utilisation of precious metal catalysts, higher efficiency of conversion, and better and more reliable reactor performance under a wide range of operating conditions.



PSE's monolith reactor model

Process Systems Enterprise has developed a comprehensive 3-dimensional microreactor model which incorporates the full range of fundamental physical phenomena occurring in monolith channels. Both steady-state and dynamic operations are supported.

The model employs detailed microkinetic descriptions of the surface and bulk chemistry, involving large numbers of elementary reactions and species including catalyst active sites. The use of microkinetics (instead of simple “global” reaction kinetics) ensures that the model retains its predictive capability over wide range of operating conditions.



Multicomponent mass and heat transfer between the bulk fluid and the catalytic surface are modelled using a rigorous Maxwell-Stefan formulation. This takes full account of the interactions between multiple species moving in different directions, which is particularly important under the high mass flux conditions prevailing in such systems.

PSE’s monolith reactor Advanced Modelling Solution

PSE’s monolith reactor model is implemented in gPROMS®, PSE’s state-of-the-art modelling software. This provides full access to advanced facilities including steady-state and dynamic simulation, rigorous mathematical optimisation of design and operation, and estimation of kinetic parameters from experimental data.

The model is provided as part of an **Advanced Modelling Solution** that includes a customisation service to tailor it to your particular system. Depending on requirements, the model can be supplied either as a box embedded in a MS Excel interface, or in **open source** form.

Example: Generation of hydrogen-rich fuel from gasoline

This study, undertaken by a major oil company, was concerned with the reforming of blended gasoline fuel into hydrogen-rich feed for fuel cells. PSE’s monolith model was used to optimise the utilisation of precious metal catalyst while ensuring satisfactory fuel conversion and maximising the lifespan of the reactor by controlling the temperature on the channel walls.

The microkinetic chemistry model used for this study involved 12 molecular species in the fluid bulk, ranging from octane and toluene down to hydrogen, as well as 23 surface species and 70 elementary reactions. gPROMS’ parameter estimation facilities were used to fit the kinetics to available experimental data.

The figures on the right show temperature and oxygen concentration profiles across the channel cross-section near the channel entrance. The substantial heat and mass transfer limitations that exist despite the small channel cross-section are clearly visible. These limitations have very significant effects not only on gasoline conversion but also on the achieved selectivity to hydrogen.

