

Rate-based separation modelling

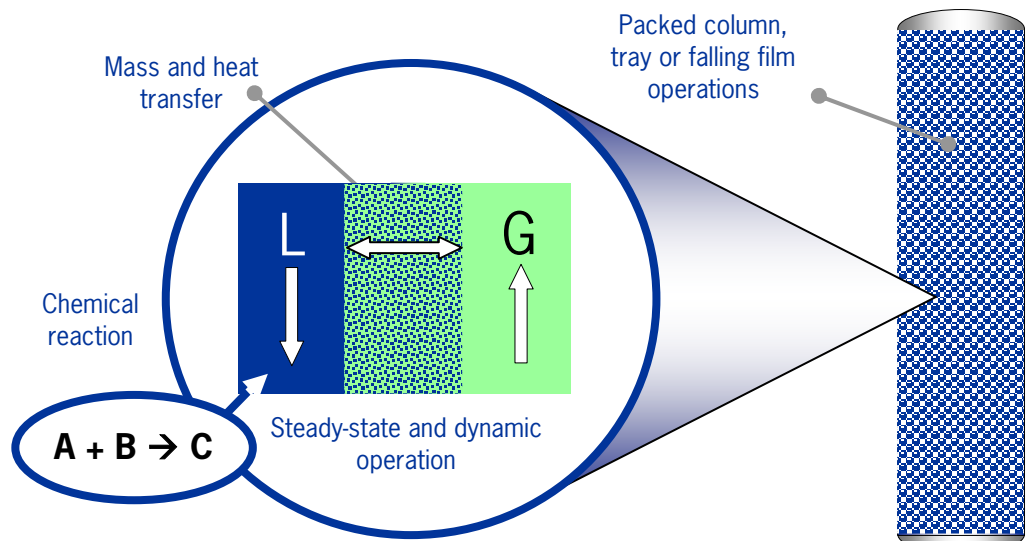
For reactive distillation, absorption and other complex separations

“With gPROMS we have already made remarkable progress compared to the tools that we used in the past”.

- Linde Engineering, following a three-month evaluation

Most of the modelling of separation processes currently performed assumes equilibrium between phases. However this is a poor assumption in many cases where mass and heat transfer considerations limit the rate of separation.

PSE's advanced rate-based separation models take into account mass and heat transfer limitation, liquid and vapour film diffusion effects, hydrodynamics and reaction mechanisms using detailed physical property calculations.



PSE's rate-based models can be applied to any process where mass or heat transfer dominate.

This includes many applications that have always been difficult to design and operate in the past, such as:

- **falling film evaporators** and **reactors**
- total and partial **condensers**
- **reactive distillation** and **absorption** in both tray and packed columns
- **liquid-liquid extraction**
- multiphase **reactors**

The models go well beyond the capabilities of current commercially-available software, allowing rigorous quantification of the operating envelope, and enabling you to optimise equipment and control designs rapidly based on realistic information. The result is capital and operational savings, increased yield and throughput, improved product characteristics and reduced risk of inadequate designs or off-spec operation.

The models, implemented within PSE's gPROMS environment, result from substantial R&D within PSE and validation on industrial problems. gPROMS' many proven capabilities for modelling of such systems include distributed modelling and advanced parameter estimation and optimisation capabilities, as well as the flowsheeting facilities necessary for optimising units within their operating context.

Why use rate-based modelling?

Rate-based modelling is necessary for:

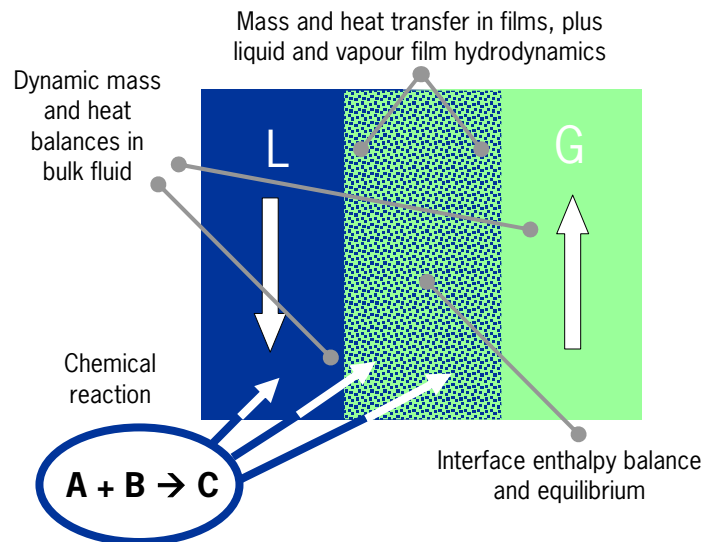
- prediction of departure from equilibrium caused by limited mass and heat transfer rates in high-throughput processes
- coupling of fast reaction with physical equilibrium in multi-phase processes
- prediction of reaction rates
- prediction of reverse diffusion and diffusion barriers

Modelling approach

Using the vapour-liquid case as an example, the model takes the phenomena shown in the diagram into account at each interface between phases.

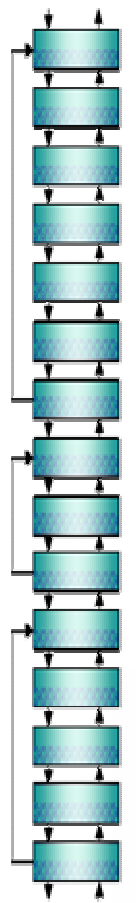
The Maxwell-Stefan equation is used to correctly relate fluxes across the interface to the composition (or chemical potential) gradients.

Physical property values are provided by gPROMS Multiflash properties, OLI Systems' electrolyte package or Aspen Properties Plus® as appropriate.



Example – caustic soda removal of CO₂

Caustic soda
Purified gas



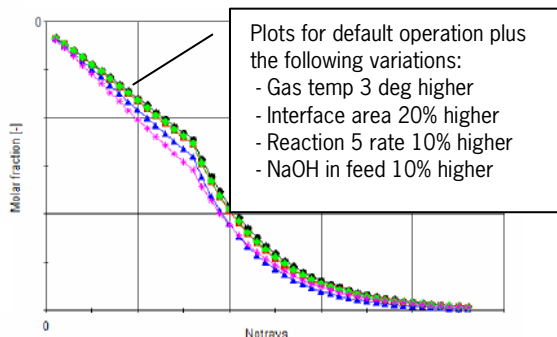
Linde Engineering used PSE's rate-based models to model caustic soda absorption of CO₂ from a gas feed stream to a catalytic reactor. It was important to remove as much CO₂ as possible (down to ppb levels) to prevent catalyst poisoning, thus extending the catalyst life as far as possible. Various configurations of tray columns with around 50 trays and recycles were studied.

The model used published kinetics for the CO₂ and OH reactions, as well as detailed Maxwell-Stefan heat and mass transfer relationships for ion diffusion within the liquid film.

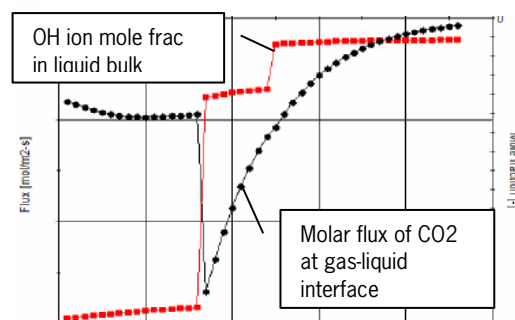
The preliminary case study for four selected operation parameters showed that the CO₂ concentration in the top product is most sensitive to the available interfacial area. The model also showed a well-developed profile of internal (intra-film) electric potential providing an extra driving force to keep the solution across the film electrically neutral. Selected results are shown below.

The preliminary results reflected the performance of the real unit with a high degree of accuracy, and this was validated by Linde against operating data.

CO₂ profile in gas phase



CO₂ removal profile



Reduce risks, ensure results

Process modelling brings major benefits to design and operation in:

- design optimisation
- scale-up
- quality and throughput enhancement
- controllability analysis
- optimisation of operating conditions
- optimisation of operating procedures and policy
- performance troubleshooting
- response to feedstock changes

PSE Advanced Modelling Solutions service

PSE supplies advanced separation models under the Advanced Modelling Solution programme, as a combination of models and configuration service. This means that PSE's existing knowledge base and wide experience in industrial application ensure rapid, low-risk implementation, a robust and accurate solution, and transfer of modelling know-how to your organisation. Models can be supplied in user-configurable or open source form, depending on your requirements.