

Mass transfer modelling

As real as it gets

Most process modelling undertaken today makes the assumption that phase separation operations and reactions proceed to equilibrium. However in reality, systems are rarely at equilibrium. In many cases the rate of an operation is limited by how fast material and energy can be transferred across tiny spaces – the rate of mass transfer.

Typical operations where mass transfer is the dominant step are falling film evaporation and reaction, total and partial condensation, distillation and absorption in packed columns, liquid-liquid extraction and multiphase reactors. Many examples of these operations in industry have an unnecessarily high level of over-design to provide a safety margin for poorly-understood phenomena. Not only does this result in excessive capital and operating costs, it can also make such processes very difficult to control.

By modelling these processes accurately using detailed relationships for the mass transfer, you can eliminate or significantly reduce over-design and develop sound control structures, improving unit operating revenues.

Benefits

There are many benefits of detailed process modelling. With a detailed mass transfer model, you can size equipment more accurately, quantify risks with confidence and devise optimal operating policies. This results in capital and operational savings, increased throughput and quality of products leading to increased revenue, and better compliance with safety and environmental requirements.

The more detailed the modelling, the more pronounced the benefits. Using mass transfer (or 'rate-based' modelling) is the closest you can come to reality – providing you with the means to push your plant design or operation as close to its limits as safely possible and gain essential competitive edge.

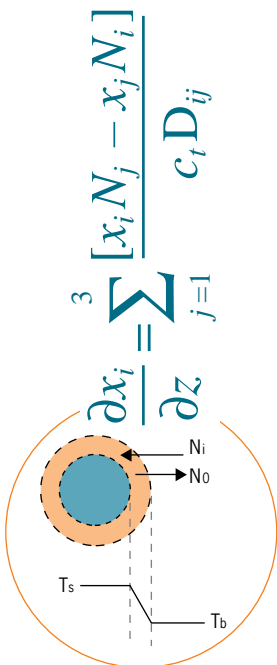
The rigorous mass transfer approach is especially recommended in situations where:

- accurate tracking of impurities in a separation operation is important
- molecules of components present in a mixture are of different size and nature
- a component is dragged against its driving force (reverse diffusion)
- a component is not transferred from one phase to another despite existence of a driving force (diffusion barrier)
- a high rate of mass and heat transfer drives the system far from equilibrium
- the mixture is highly non-ideal.

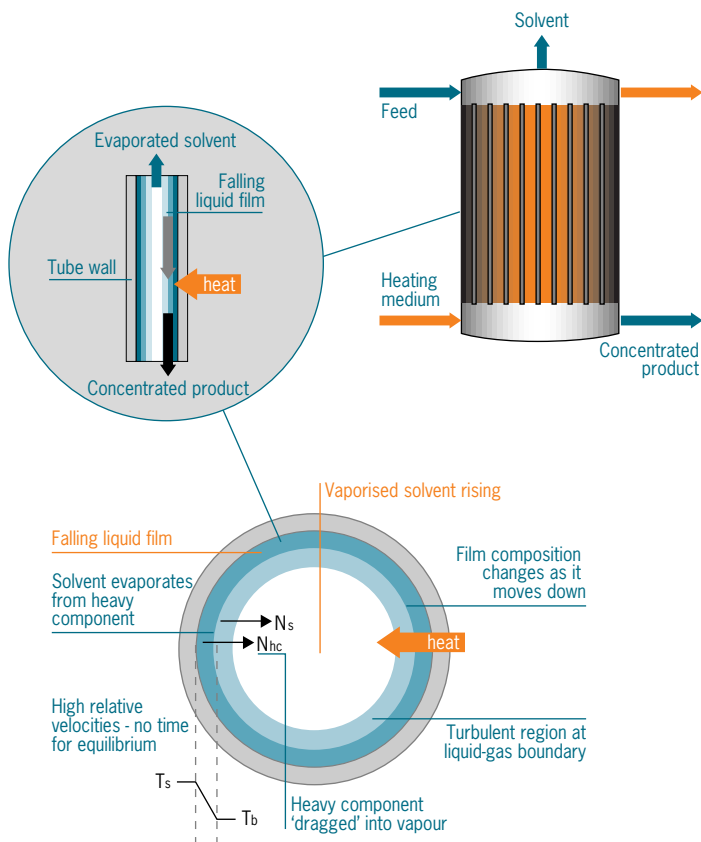
How does it work?

gPROMS provides all the facilities required for implementing process models to virtually any level of detail, and then simulating or optimising the model to achieve design or operational objectives. Mass transfer models are simply detailed models implemented using standard gPROMS modelling facilities.

The models use the Stefan-Maxwell formulation for diffusion kinetics to predict mass transfer accurately. The equation takes account of friction between components, so it can explain important phenomena that are simply impossible to predict under equilibrium assumptions.



$$\frac{\partial x_i}{\partial z} = \sum_{j=1}^3 \frac{[x_i N_j - x_j N_i]}{c_t D_{ij}}$$



Example application: falling-film evaporator

In this design application, a chemical compound is concentrated from a solvent by evaporating the solvent along the vertical tube walls of the evaporator unit.

Low-concentration fluid enters the tubes at the top and heating medium on the shell side. As heat enters the tubes from the shell side, it vaporises the solvent falling down the tube walls, concentrating the product. The relative velocities of vaporised solvent and film are high, causing turbulence at the interface. Consequently, the operation of the unit is driven far from equilibrium.

A key requirement in modelling of the falling film evaporator was avoidance of flooding or the formation of dry patches, which reduce efficiency or lead to local overheating of the products.

Detailed modelling in gPROMS established a novel technique for increasing throughput capacity and optimising the unit's operation. It also led to a new startup procedure, taking into account the thermal inertia in the tubes. The model was then used within a third-party steady-state simulator for flowsheeting studies.

Over and above the throughput enhancement, a major benefit of this application was that it gave design engineers the confidence to proceed with a low capital cost equipment option without the need to construct a pilot plant.

ModelCare

Mass transfer modelling is a specialist domain, and requires a very detailed knowledge of the underlying physics and chemistry governing the mass transfer process. Under our ModelCare consultancy service, PSE will provide highly skilled modelling personnel to work alongside your engineers and scientists for short periods, to deliver robust applications and to train your personnel in these advanced modelling techniques.