Model-based optimisation of tubular reactors for the production of LDPE

Peter M.M. Van Erdeghem, Filip Logist and Jan Van Impe
BioTeC - Chemical and Biochemical Process Technology and Control
Department of Chemical Engineering

Abstract

This project involves the model-based optimisation and design of tubular reactors for the production of low-density polyethylene (LDPE). Information obtained from literature and industry results in detailed but complex mathematical models, which are not directly suited for optimisation purposes. Hence a two-step strategy is proposed. In a first step, a basic model which captures the most important phenomena is constructed based on advanced model reduction techniques. This basic model is used to identify the most promising optimisation possibilities. In a second step, the optimisation is performed for different industrially relevant objectives. Depending on the objective, the reduced model will be further adjusted to the required level of detail.

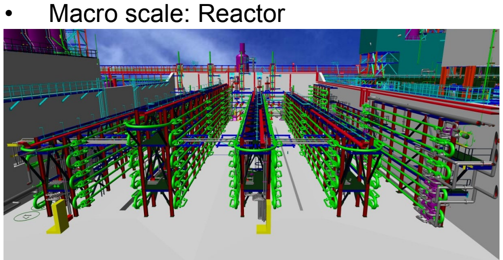
LDPE

Broad application area

Modeling

On a different level of detail

- Macro scale: Reactor



- Micro scale: Reactions

A **complex system** of (un)correlated differential (time and space) and algebraic equations.

Using model reduction techniques like **sensitivity analysis**

A **basic model** which still contains sufficient essential information and characteristics

$$\frac{d\mathbf{x}}{d\xi} = \mathbf{f}[\mathbf{x}(\xi), u(\xi), \xi]$$
$$0 = \mathbf{g}[\mathbf{x}(\xi), y(\xi), u(\xi), \xi]$$

Optimisation

Optimal control problem:

$$J = h[\mathbf{x}(\xi_f)] + \int_0^{\xi_f} g[\mathbf{x}(\xi), u(\xi)]dt$$

Subject to:

basic model

$$\frac{d\mathbf{x}}{d\xi} = \mathbf{f}[\mathbf{x}(\xi), u(\xi), \xi]$$
$$0 = \mathbf{g}[\mathbf{x}(\xi), y(\xi), u(\xi), \xi]$$

Heat transfer | Kinetics | Level of design detail

Re-increase in model complexity:

Detailed objective-specific model

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}_{\text{specific}}[\mathbf{x}(\xi), u(\xi), \xi]$$
$$0 = \mathbf{g}_{\text{specific}}[\mathbf{x}(\xi), y(\xi), u(\xi), \xi]$$

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For more information

jan.vanimpe@cit.kuleuven.be
www.cit.kuleuven.be/biotec
Tel.: +32 16 32 14 66
Fax: +32 16 32 29 91