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Modelling and Simulation of Reaction-Separation Processes using gPROMS ProcessBuilder

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Modelling and simulation play a vital role in modern chemical engineering by enabling safer, more efficient, and sustainable process development. As industries face increasing pressure to optimize energy consumption, reduce emissions, and minimize waste, digital tools such as process simulators become indispensable. In this context, the concept of a *digital process twin* — a virtual replica of a real process — is gaining traction due to its potential for predictive analysis, optimization, and decision-making support. This work focuses on the application of the gPROMS ProcessBuilder to develop such digital twins.

Our methodology involves the creation of fundamental dynamic models of unit upstream and downstream operations based on physical knowledge of the process. The models are used to assess the effectiveness of the plant configuration and to observe system responses to step changes in operational parameters. Building on this foundation, we simulate more complex systems, such as coupled reaction-separation processes.

We study esterification of acetic acid in a continuous stirred tank reactor followed by a distillation column. Reaction kinetics follows the data from the literature. Different designs and operations of a distillation column were investigated to enhance the separation efficiency.

Secondly, we study the kinetics of plastic pyrolysis. Our work involves the estimation of model parameters. We employ the parameter estimation module within gPROMS ProcessBuilder, which enables kinetic models to be fitted to the experimental data through nonlinear regression. This enables the development of predictive models that can simulate the behavior of thermal decomposition processes under various conditions.

The simulations studied contribute to a deeper understanding of chemical systems and support future activities such as process optimization, control design, and the transition from laboratory to industrial applications.

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