Chemical Process Modeling in Modelica

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Structural information. Chemical process models are typically large-scale but highly structured. Information on how the hierarchical components are connected can help to make the solution procedure more robust, reliable and orders of magnitude faster. Our ultimate goal is to develop structure-driven optimization methods for solving nonlinear programming problems (NLP). The structural information is programmatically accessible in JModelica *before flattening*.

Connector class. Creating a component-based framework for chemical process modeling is the first step towards our final goal. The most challenging step was to design the connector class. Our choice of the independent variables in the connector class guarantees the linearity of the material and heat balances. The linearity of these equations is important for efficiency reasons. The Modelica.Fluid library superficially resembles our library, however Modelica.Fluid does not allow our choice of the independent variables.

Smallest subcomponents. The smallest Modelica subcomponents of our library are referred to as atomic units. The set of atomic units has been determined by recursively decomposing a variety of chemical processes. As a result, these atomic units are sufficient for general-purpose chemical process modeling.

High-level model building. Once the component library is finished, software with a graphical user interface can be used to build chemical process models. The process model creation involves only high-level operations on a GUI; low-level coding is not required. This is the desired way of input and this is also how it is implemented in commercial chemical process simulators.

Bridge towards the optimization community. Typical optimization problems in chemical engineering arise in process design, process control, model development, process identification and real-time optimization. AMPL is the de facto standard for model representation and exchange in the optimization community. We are aiming to create a 'Modelica to AMPL' converter. One could use the Modelica toolchain to create the models conveniently on a GUI. After exporting the Modelica model in AMPL format, the readily available AMPL-based environments can be used. Such a code generator to AMPL already existed in 2007 but it is no longer supported, and not publicly available.

Application. The Modelica library serves as a common language between mathematicians and chemical engineers. The library was tested on the model of JACOBSEN & SKOGESTAD [1], an industrial distillation column of high practical relevance. The distillation column has 5 steady-states in a certain region of the bifurcation parameter. The fact that the Modelica implementation gives the expected steady-states suggests that the implementation of the involved Modelica components is correct.

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References

[1] E.W. Jacobsen and S. Skogestad. Multiple steady states in ideal two-product distillation. *AIChE Journal*, 37:499–511, 1991.