Chemical Process Modeling in Modelica

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Hierarchical modeling

Chemical processes are networks of equipments. It is natural to model these equipments hierarchically, as composites of smaller components. The smallest subcomponents are called **atomic units**. The atomic units are connected by **process streams**.

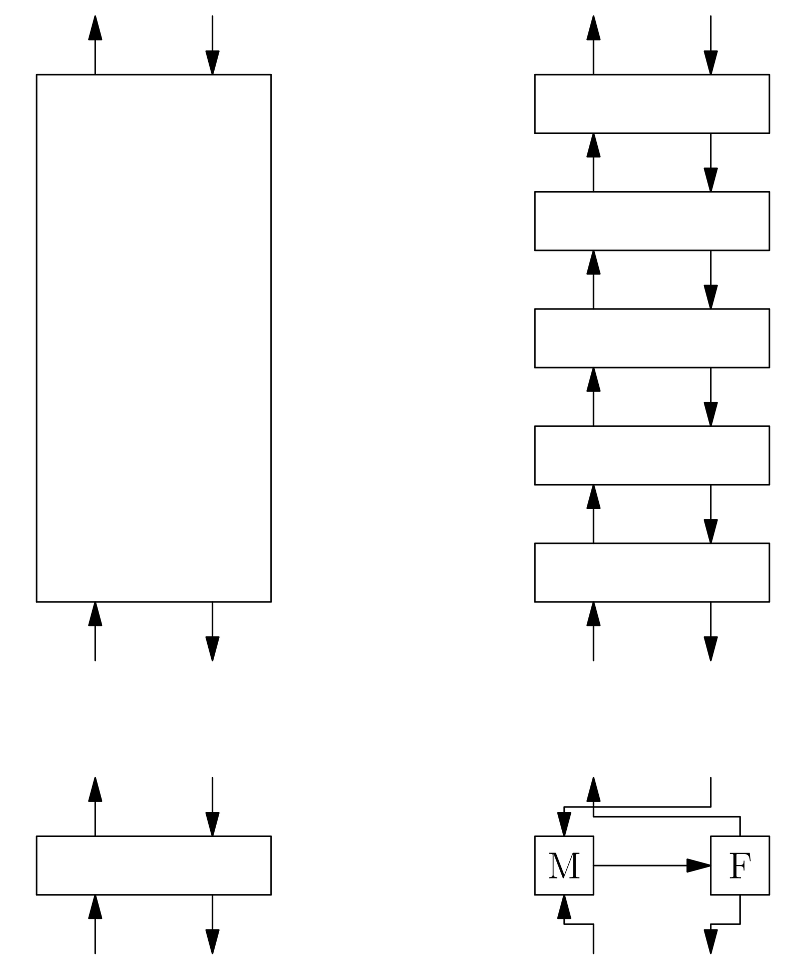


Figure 1: The vapor-liquid equilibrium cascade is decomposed into a cascade of stages, then a stage into a mixer M and a flash unit F.

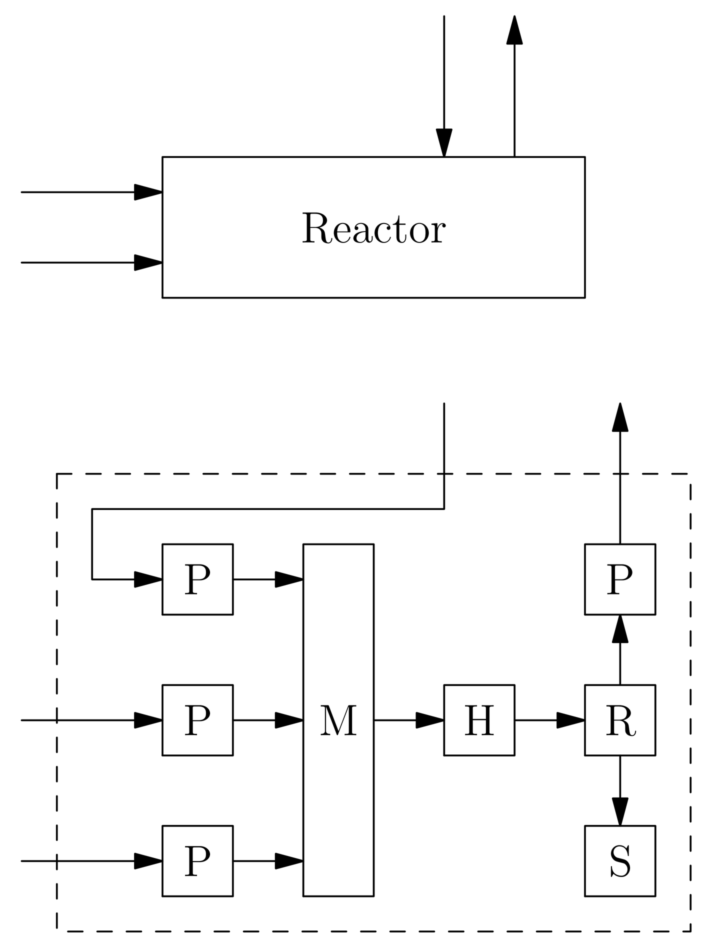


Figure 2: The reactor of Yi & Luyben [1] and its abstract decomposition into atomic units. P: pressure changer, M: mixer, H: heat exchanger, R: reactive flash, S: sink.

Connector class

Table 1: The $C+2$ independent variables characterizing a **process stream** of C chemical substances.

variable	physical meaning	SI unit
$f[i] \geq 0$	molar flow rate of substance $i = 1 : C$	mol/s
$p \geq 0$	pressure	Pa
H	enthalpy flowrate	J/s

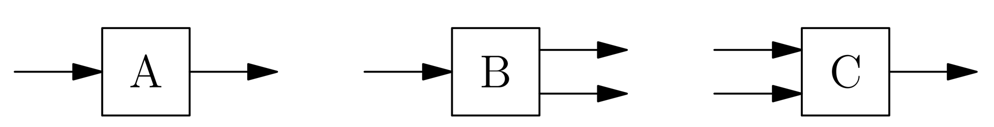
This choice of independent variables guarantees **linear material and heat balance equations.**

Why not Modelica.Fluid?

Modelica.Fluid is for modeling flows in networks of pipes and not for chemical process models.
We want to preserve the linearity of the material and heat balances. Our choice of the independent variables guarantee the linearity but Modelica.Fluid does not allow this choice.

Smallest subcomponents

The **atomic units** cannot be decomposed further to smaller, connected Modelica components. Their **structural types** are:



(A) heat exchanger, pressure changer, reactor, (B) divider, flash, (C) mixer.
The following **equations** apply to all atomic units:

- material and heat balances
- thermal and mechanical equilibrium conditions
- characterizing equations
- connections with other units
- specifications.

Note on the connector class

Table 2: The traditional choice of variables to characterize a **process stream**.

variable	physical meaning	SI unit
$F \geq 0$	total molar flow rate	mol/s
$x[i] \geq 0$	mole fraction of substance $i = 1 : C$	–
	$\Sigma x[i] = 1$	
$p \geq 0$	pressure	Pa
$T \geq 0$	temperature	K
h	specific enthalpy	J/mol

Issues. (1) The temperature is uniquely determined by the other variables and this relation is nonlinear (equation of state).
(2) The material and heat balance equations are nonlinear because mole fractions are used to describe the stream composition.
(3) The process stream definition involves the constraint $\Sigma x[i] = 1$.

Acknowledgement

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References

[1] Chang K. Yi and William L. Luyben. *Design and control of coupled reactor/column systems–Part 1. A binary coupled reactor/rectifier system.* Computers & Chemical Engineering, 21(1):25–46, 1996.

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

[3] Amy R. Ciric and Peizhi Miao. *Steady state multiplicities in an ethylene glycol reactive distillation column.* Ind. Eng. Chem. Res., 33: 2738–2748, 1994.

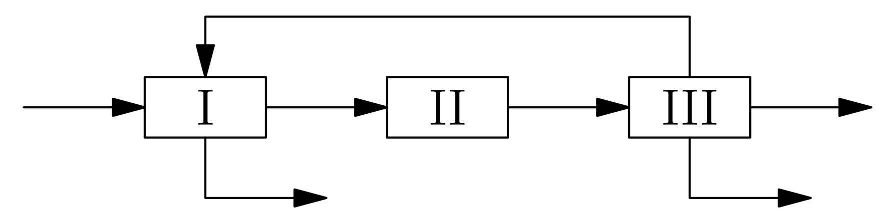
More on **structure-driven methods for large-scale optimization** on the project homepage `http://www.mat.univie.ac.at/~neum/structure.html`

Contributions

- Commonality and variability analysis (CVA) of chemical processes
- Connector class design preserves the linearity of the balance equations
- Smallest subcomponents and their equations based on CVA
- Application to separation operations of high industrial relevance

Application: separation operations

Three steps can be distinguished in a chemical plant: (I) preparation, (II) reaction and (III) purification. Input: raw materials, output: products and byproducts.



Both the first and the third step involves separation operations. In a typical chemical plant, **40–80% of the investment is spent on separation operation equipments.**
Many of the practically relevant equipments used in separation operations are internally a cascade, see Fig. 1. Their mathematical model can be solved in a sequential manner. **Identifying multiple steady states is critical** to proper design, simulation, control, and operation of these equipments. **The Modelica implementation was successfully tested on a distillation column** presented in [2], having 5 steady states.

Why is the structure so important?

Information on how the hierarchical components are connected can help to **make the solution procedure more robust, reliable and orders of magnitude faster.**

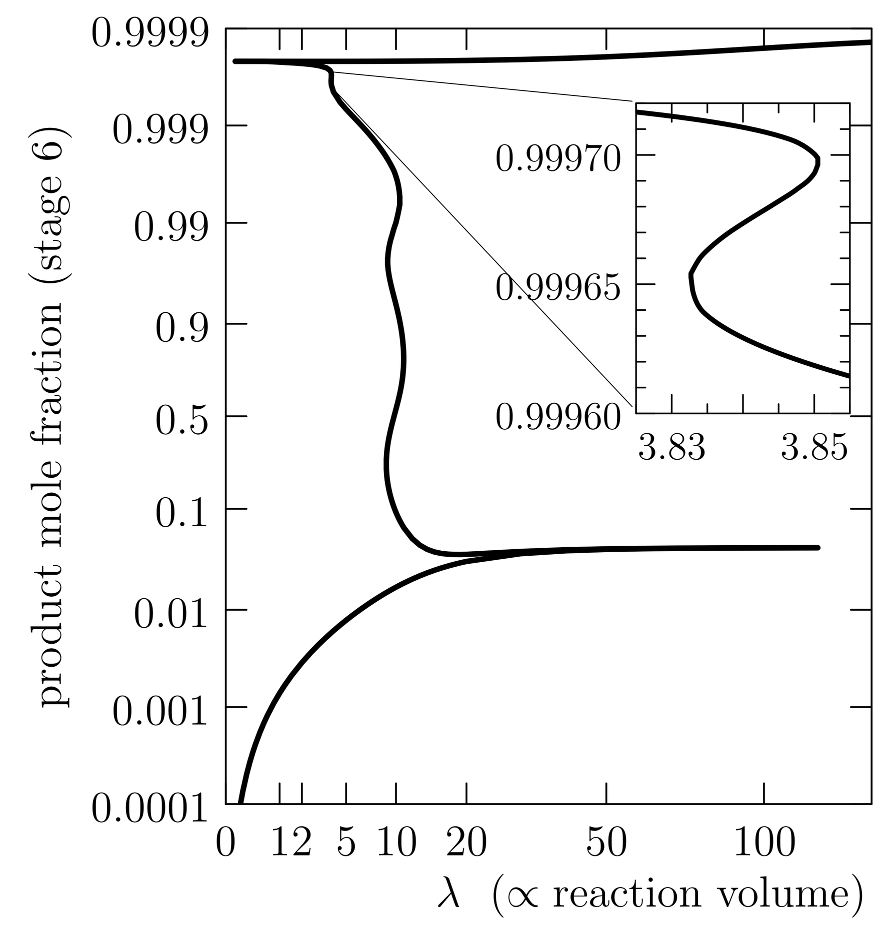


Figure 3: Bifurcation diagram with multiple steady-states in the reactive distillation column [3] for manufacturing glycol.

Fig. 3 was computed with our novel structure driven method. This problem is numerically challenging: State of the art general purpose methods failed on this problem.
Our ultimate goal is to develop structure-driven optimization methods for solving nonlinear programming problems (NLP).