# Computer-aided modelling of a distillation

## Background

The modelling software environment being developed in the PSE group is to generate code based on an ontology. The topology of the process model is handled by the ModelComposer, a hierarchical graph editor where the nodes and the arcs of the graph represent the capacities and the transport between the capacities.
Many processes, of which a distillation is a quite generic and important example, are modelled by making a good number of assumptions. This includes assumptions about relative capacities, like the gas phase has a negligible mass and thermal capacity. Other assumptions are based on the relative dynamics. In particular time scale assumptions with regard to pressure distribution. It happens several order of magnitude faster than the mass distribution as pressure waves propagate at the speed of sound and mass spreads through the liquid and gas streams through the various internal capacities.

## Description

The pressure distribution can be generated by splitting the time scales. This may mechanically be done in different ways.
At first we want to establish the mechanistic models that allow for the implementing the necessary time-scale assumptions. We then want to find the different ways of implementing the assumptions mathematically and at the same time we can make ourselves a picture on the order of magnitude on which the assumptions are commonly made. For example what is the change of internal energy from the inlet to the outlet of a pipe.
Once the mathematical framework is established, answers to the question where and when the established and agreed mechanism is being implemented.
It is expected that the implementation is simple, and that the main issue is to explore the feasible alternatives on how to achieve the goal without losing consistency of the model equations.
The distillation column has all the necessary components and at the same time, it is a very important process. Thus the objective shall be to establish a code that solves the distillation using the group's computational framework.

Once this goal is achieved we can extend towards other mechanistic-motivated reduction method that build on singular perturbation and nullspace methods.

## Supervision

Supervisor: Heinz Preisig
Daily contact: Tobias Elve and Heinz Preisig