Deriving fast distillation models: diploma thesis proposal

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Abstract

Distillation is the most important separation technology today. A trend in controlling distillation columns economically efficient is going toward using model predictive control (MPC) algorithms, which calculate an optimal input trajectory to the plant based on repeated simulations of a model of the process to predict the future behaviour of the plant with respect to disturbances and control inputs. Since the controllers operate in real-time, very fast process simulations are needed. In case of distillation, full models are usually too complex to be simulated sufficiently fast. Therefore, methods to derive reduced models are of high interest to both industry and research community. Our approach to derive a reduced model is based on tray aggregation, which means that the slow dynamics of a number of consecutive stages in the distillation column are approximated by a large "aggregation tray", and the fast dynamics are approximated by employing a quasi-steady-state assumption. These reduced models provide a good gain in computational performance while being sufficiently accurate to be used in an MPC. While the procedure to derive these models is straightforward, there are many structural and implementation degrees of freedom which can be used to further improve the performance of the method.

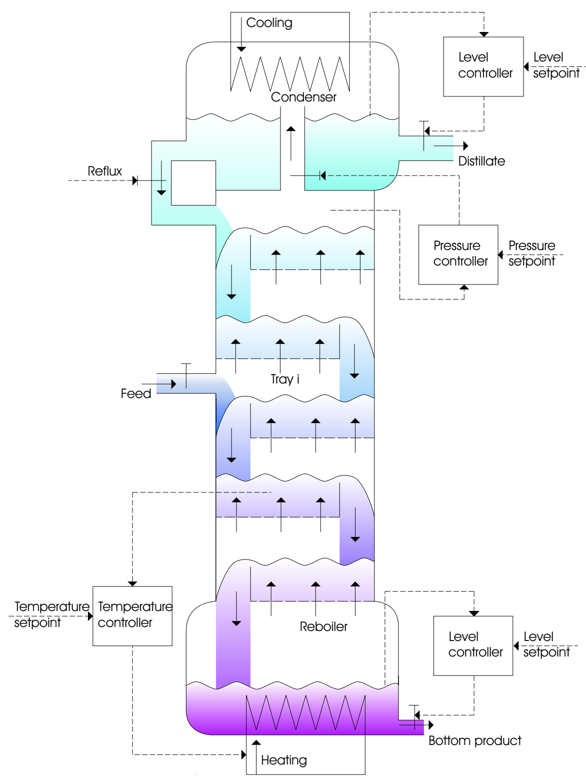

Figure 1: Schematic diagram of a distillation column.

Background

A distillation column is used to separate a mixture of different components, as for example crude oil or natural gas, by making use of the fact that the components have different volatilities. That means that if the mixture is boiling, the "lighter" components will have a higher concentration in the vapour than in the liquid, where the "heavier" components dominate. By stacking a number of trays with the boiling mixture on top of each other to a column, and allowing a certain amount of liquid and vapour to be exchanged between the trays, higher purities of the light and heavy components can be achieved towards the top and the bottom of the column. In the top of the column, the vapour is condensed into liquid and partially taken out of the column as distillate, and partially fed back into the column. In the top of the column, a part of the accumulating liquid is taken out as bottom product, and a part is being evaporated by reboiling the liquid. In the middle of the column, the mixture is fed into the column. This is illustrated schematically in figure 1.

In such a column, a stable operation has to be ensured by controlling certain physical quantities inside the column, typically the temperature and pressure, and the levels in the condenser and reboiler. Furthermore, for economical reasons, a high purity of the top and bottom products is desired. To achieve this, optimal values of certain degrees of freedom of the column, such as reflux rate and controller set points, have to be calculated. If no big changes in the operating conditions of the column are occurring, these optimal values can be determined by a steady-state optimisation. However, under conditions where for example the feed mixture composition and feed rate is fluctuating strongly, the optimal values have to be calculated in real-time by an MPC or similar algorithm.

Mathematical models of the process are used to design suitable controllers for the plant. In order to describe the process with a sufficiently high accuracy, rigorous models based on mass and energy balances are necessary. In the case of distillation, there is one mass balance equation for every component on every tray, in addition to one energy balance per tray. The thermodynamic properties of the mixture decomposed into vapour and liquid phases is described by some thermodynamic property correlations, for example the Soave-Redlich-Kwong equations. In the case of a two-component (binary) distillation, 3 dynamic variables M_1, M_2, U_{tot}, and 2 algebraic variables P, T per tray are needed. For a column with 70 trays, a model with around 360 equations with nonlinear terms for thermodynamic and flow relationships will result.

A model of this complexity is usually to slow to be used in real-time optimisation applications. A method to reduce the complexity of the model is tray aggregation. Certain trays in the column are assigned a time constant which is much larger than for a usual tray, whereas the chains of consecutive trays in between are modelled to be in "quasi-steady state". By this, the number of dynamic variables and equations is reduced to a much smaller number, typically around 40. If the choice of position and size of the dynamic trays is made carefully, such a reduced model will reproduce the dynamic behaviour of the full model quite accurately. However, the numerous quasi-steady-state trays contribute a large number of algebraic equations to the system. In order to reduce the computational burden caused by these equations, they can be solved off-line and the solutions can be stored and retrieved during simulation in a suitable way. Figure 2 shows schematically the structure of the reduced model.

If the reduced models are implemented efficiently, they are very well suited to enable MPC for complex distillation columns. This research is carried out as part of a European Union project on model reduction for large-scale system. As a case study, a C4-splitter column of the Statoil plant in Kårstø, Norway, is used.

Challenges

In the following, important issues concerning the derivation, implementation and utilisation in MPC of the reduced models are listed. Depending on the interests of the student, one or more topics can be selected for a diploma thesis. All topics are of high scientific interest and results will be part of scientific journal or conference publications.

- **Efficient handling of the algebraic equations:** One way to store and retrieve the solutions of the algebraic equations obtained by off-line computations is a look-up table with a suitable interpolation scheme to calculate values between the table grid points. These

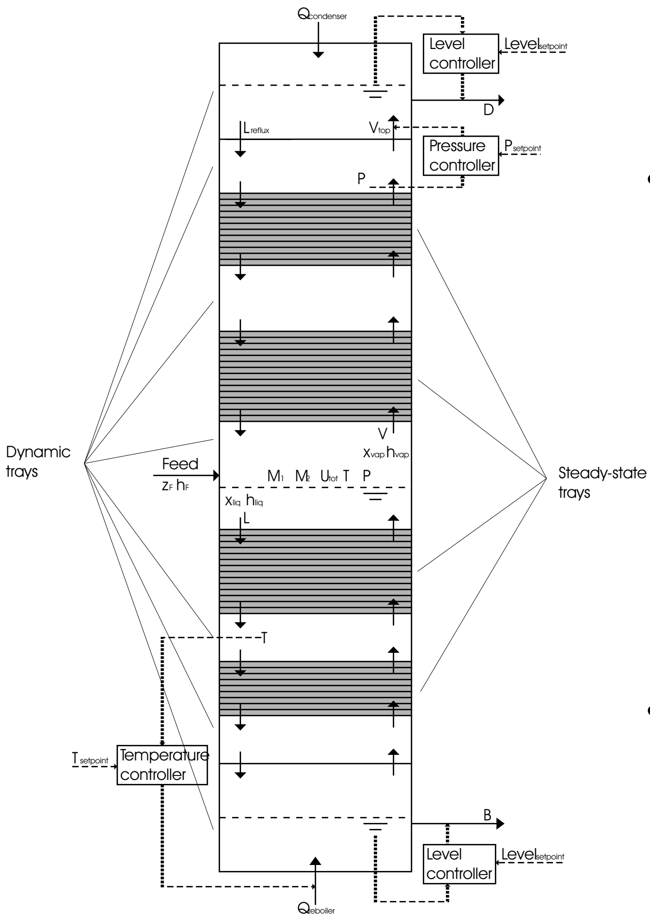

Figure 2: Schematic diagram of a reduced column model.

tables get very large, since for a binary distillation column, 5 dimensions corresponding to physical quantities on top and bottom of a chain of consecutive algebraic trays are needed. In order to achieve the best memory usage, the resolution in every table dimension can be adapted. The task here is to investigate further possibilities to store and retrieve offline solutions efficiently. Possibilities to do so are the proper choice of independent variables resulting in "well-behaved" functions, non-uniform table grids, sparse grids or functional approximations.

- **Extending the reduced model to more complex columns:** The currently developed reduced model is for a binary distillation column. In the case study column, around 20 components, of which at least 4 have a significant contribution to the dynamic behaviour of the column, are present. The task here is to investigate possibilities to extend the reduced models to a larger number of components. This is challenging because the dimensionality of the look-up tables cannot increased by more than one or two dimensions. A possibility could be linearisation or functional approximation of the component concentrations; another possibility is the creation of "pseudo-components" by component lumping.

- **Optimal choice of reduced model parameters:** The reduced model has certain degrees of freedom with respect to the position and choice of the dynamic trays. The task here is to investigate good choices of these parameters to achieve a high model accuracy. This can be done by using dynamic simulations for optimisation, and by obtaining a general understanding of the influence of the reduced model parameters

- **Base layer control interaction:** The base layer control, mainly the temperature and pressure controllers in the column, have a crucial influence on the dynamic behaviour of the whole column. Since their feedback loops are relatively short, their behaviour will be sensitive to changes inside the feedback loops when the trays of the full model are approximated by the reduced model. The task here is to investigate the optimal structure of the reduced model that allows for a authentic operation of the controllers, namely the choice of the positions and sizes of the dynamic trays inside the feedback loops. Another interesting question is how the controllers should be designed such that they can be easily integrated into a reduced model.

- **Deriving reduced models of simpler distillation models:** It is possible to simplify a distillation model by making certain assumptions, such as constant liquid flows from tray to tray or constant pressure difference between the trays. This will lead to simplified models which are of lower complexity than the original model. The performance of these models in combination with the tray aggregation model reduction method is to be investigated.

- **Application of reduced model in MPC:** An important question is the selection of the manipulated variables, which the MPC uses to control the model, and their update frequency. For example, the reflux and the temperature controller setpoint could be chosen as manipulated variables, while the pressure setpoint could be left constant. The reflux could be manipulated twice as often as the temperature setpoint. A clever choice will reduce the complexity of the overall optimisation problem. Since the model reduction method has a certain influence of the time-scales of the model, it seems advisable to investigate the interactions of these choices with the reduced model.