Dynamic modelling and simulation to overcome the initialization problem in steady state simulations of distillation columns

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Solvers for steady-state distillation models are notoriously difficult to initialise. A procedure that builds on a dynamic model is suggested. This procedure starts with an appropriate set of single phase systems of which pairs are encased in constant volumes each of these volumes representing a stage in the column. First the phases are brought into contact. This results in a thermal equilibrium followed by a chemical equilibrium. Next the liquid levels are adjusted and then the cooling is started. Then communication between the gas phases is slowly enabled followed by slowly heating up the column to operating conditions.
The procedure is demonstrated on a C-4 splitter.

1. The Issue

Modelling of chemical processes is today the foundation to almost any operation including design, control, planning, retrofitting. As varied as the use of models is its structure: models are built for a particular purpose, to meet the requirement of the application.
Though there is obviously a need for dynamic models, the most common models are steady-state models mostly used in designing and retrofitting, but also in some control and planning applications. With distillation being the most common separation unit, its models have been subject of studies for decades. The computation of steady-state distillation models is a notorious problem as it consists of a large number of equations which proliferates mainly with the number of components and number of trays. Solving such a model implies to solve this large-scale algebraic problem for a single set of roots representing the equilibrium state of the distillation. The numerical methods being used for this purpose have usually a very small convergence radius, which gave rise to a lot of research, for example C. D. Holland developing his θ-method (Komatsu and C.D. Holland 1977, C. D. Holland 1981) or methods that passed through the complex domain (Taylor et al. 1996). The problem with initializing such algorithms was also mentioned by Rabeau et al. (1997) and more recently by Grossmann et al. (2005). Thus whilst computing has improved tremendously, little progress has been made in solving the initialization problem.
This paper demonstrates an approach based on a dynamic distillation model.

2. The Typical Model

Models of distillations build on a description of two distributed phases (liquid and gas). This description can assume different levels of detail, according to the time scale resolution that the user wants to study. The thereby chosen granularity of the system reflects itself into the geometry chosen to capture the modelled phenomenon: for certain time scales it is enough to lump together each phase, while for others this simplification is not sufficient. In these cases at least parts of the plant have to be modelled in more details (finer granularity) for example modelling a distillation tray then may result in describing the complex two-phase behaviour of bubbles and drops.

Assumptions are also made about the capacities: the typical distillation model neglects the capacity of the gas phase taking into consideration that the mass is low compared to the mass of the liquid phase. This brings about a model where the dynamic equations for the liquid phase, which may or may not include the mass of the gas phase, are combined with the phase equilibrium relations and possibly steady-state relations for the gas phase.

As mentioned, the resulting models are difficult to initialise.

3. Idea

The idea for approaching the initialisation problem is to use a dynamic description that mimics the behaviour of a distillation column close enough so as to simulate a dynamic path starting with a very simple generic initial state and integrating up to the desired operating condition. Thereafter one may switch to a steady state description of the plant and continue the computations, if so required.

Dynamic simulations are very robust. Choosing an appropriate dynamic description and choosing reasonable initial conditions should enable the user to compute a solution that is sufficiently close to the desired steady state solution if one chooses in parts simpler elements for the description of the material behaviours.

Earlier studies have shown that bringing two isolated phases into contact will converge monotonically to the steady-state under the condition that the heat transfer is significantly faster than the diffusional mass transfer through the phase boundary (Asbjørnsen 1973, Preisig 2004). This is taken as a starting point to suggest a sequence of physical operations which will guide the dynamic model to converge to the desired steady-state condition. Thus by switching from a steady-state simulation to a dynamic simulation one substitutes the complex initialisation problem by a simple one plus an integration over a feasible physical path. Mathematically this implies that one solves a set of Differential Algebraic Equations (DAE) instead of a large set of algebraic equations. With DAE solvers having advanced tremendously over the past decades, using a dynamic model may even be competitive to using a steady state model.

The strength and robustness of the dynamic approach have been tested by the authors on a model for a distillation column working in total reflux.

4. The Dynamic Model

This section explains the dynamic model for a distillation column the authors developed.

The model is simple: each tray, boiler and condenser are considered as dynamic flashes each contained in a fixed volume (Preisig, 2004). Staking up such two-phase containments, the column becomes a tower of dynamic flash “drums” as shown in Figure 1.

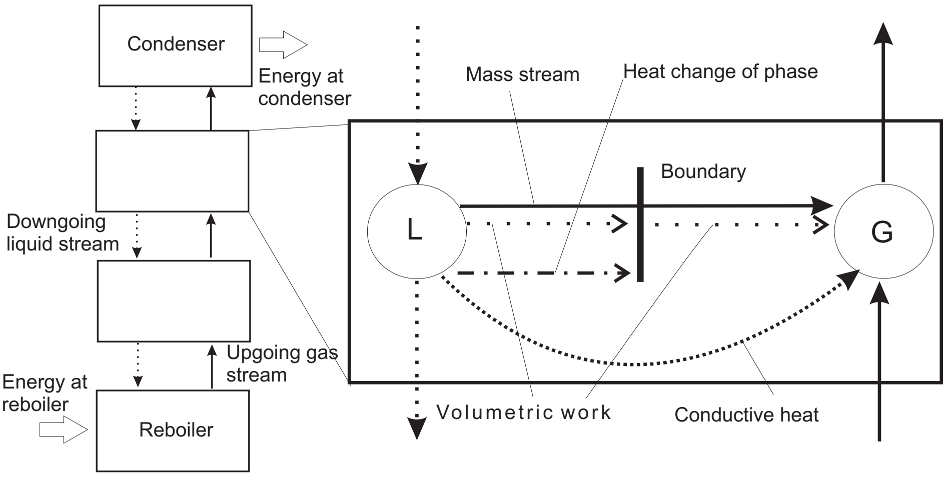

Figure 1 Model for a distillation column. L stays for liquid phase, G for gas.

For sake of simplicity, the material behaviour is simplified assuming ideal gas and liquid.

The procedure representing a feasible physical path leading to the desired steady state starts with a set of isolated containments forming pairs of gas and liquid both in isolation. Those are first brought in contact with each other, pair by pair thereby fixing the respective joint volume to represent the volume of the boiler, each stage and condenser, respectively. The individual phases are initialised within the domain of operation. Since a priori the two phases are not in equilibrium, they can exchange energy (in the form of heat and volumetric work) and mass both being diffusional processes through the common phase boundary. The conductive heat stream, driven by the different temperatures of liquid and gas phase, is significantly faster than the mass diffusion, which makes the temperatures in the two phases to converge quickly.

The mass exchange driven by the chemical potentials, accordingly to fundamental transfer laws, is slower. The mass stream induces also convective energy transfer as mass carries internal energy.

The heat transfer in the liquid phase is assumed to be very fast (event dynamics). This makes the temperature on the boundary identical to the liquid bulk temperature. The energy associated with the phase change is thus solely associated with the liquid phase.

This simplifies also the computations as otherwise one has to compute the conditions on each phase boundary, which involves solving for roots of a set of algebraic equations (dimension: number of components + 1 for each boundary). The first step is completed when the two phases in each part of the column have reached an equilibrium.

Then it is time for the second step: adjusting the liquid levels. If the liquid level is too little, meaning the fluid does not reach up to the weir height on each stage, liquid is added on the top with the overflows modelled with the weir equation (see for example Coulson and Richardson, 1977, p.117). In case there is too much fluid, one may have to drain some out of the boiler so as to adjust the overall hold-up.

With the next step energy is drawn in form of heat from the liquid phase of the condenser driven by the difference between the temperature of the liquid phase and the temperature of a cold reservoir. This procedure excludes anything like drop or film formation.

Up to this point the gas phases are not connected. Only at this point this communication of mass driven by the pressure difference is enabled. The transfer model consists of two parts, namely a resistance in the construction, the dry tray resistance, and the hydraulic pressure drop on the tray.

Finally heat is supplied to the liquid phase of the boiler driven by the difference in temperature between a warm reservoir and the liquid phase excluding any bubble formation.

The complete model consists for each stage of number of components mass balances for the gas phase and the liquid phase, and an energy balance for each liquid and gas phase.

5. Some Results

Studies implementing the above-described approach showed that the suggested procedure is indeed very robust with respect to the chosen initial conditions for a two component mixture, which was taken from an industrial problem, namely the C-4 splitter.

Below a representative example is shown. The graph in figure 2 shows the pressure history in a column consisting of a condenser, 15 trays and a boiler. The reader should note that the chosen initial conditions lead initially to an inverted pressure profile, that is, the pressure on the top is higher than the pressure in the boiler. The thick lines show the two ends, namely the condenser (dashed) and the boiler (solid). Adjusting the liquid levels on the trays does not have a large effect on the pressure distribution. Only once the cooling is enabled, the pressure changes drastically in the condenser, which starts to propagate into the column once the heating is started and gas connections are enabled. In the following period the pressure profile is inverted going through a largely increased overall pressure difference between the top and the bottom after which it converts monotonically to the final pressure profile. The temperature profile reflects the same qualitative transition behaviour. All the final results, that are the pressure, temperature and concentration profiles, assume physical meaningful steady-state values.

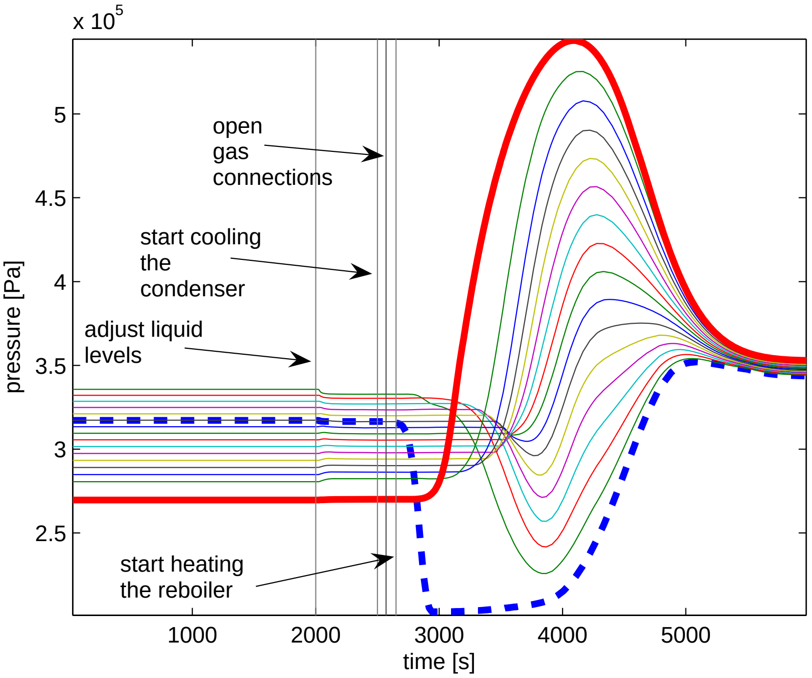

Figure 2 Pressure profile in the column. The highlighted lines represent condenser (dashed line) and reboiler (solid line).

Whilst the overall procedure looks very promising and will be exploited further to initialize generic columns with arbitrary mixtures, the approach has some weak points. One of these is the stiffness of the equations faced by the DAE solver. The stiffness of the problem is particularly evident once changes are introduced in the system. For example, opening the gas connections between the gas volumes is a "shock" for the solver. This makes it necessary to enable the gas connections slowly, which is done by adding a virtual controller that enables the flows slowly starting with a zero slope. The same approach has been applied to the external cooling in the condenser and heating in the reboiler.

6. Conclusions

A procedure solving the problem to initialise solvers of steady-state distillation models has been suggested. It is based on a dynamic model for the flashes representing the boiler, the trays and the condenser. The procedure suggests a feasible physical path along which the model can be integrated. It starts with each stage being represented as two isolated volumes that are first brought into contact. The approach uses the fact that dynamic models for two phase systems for which the diffusional heat transfer is faster than the diffusional mass transfer converge monotonically. This makes the initialisation problem trivial, but puts the burden on the dynamics the system. Anything that is associated with changing the conditions in the gas phase represents a computational problem, as the model is very stiff indeed.

The procedure has been tested on the industrial example of a C-4 splitter. The procedure is very robust with respect to the chosen initial conditions but sensitive to changes associated with the gas phase.

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