

Computer-aided modelling: A study on the dynamic flash

Heinz A Preisig*

Department of Chemical Engineering; NTNU; Trondheim, Norway

Abstract

The dynamic flash is a widely celebrated subject in the literature. It turns out to be also an excellent example for discussing issues around the representation and assumptions that are commonly made. Here we look into the representation and the conversion properties of a particular model using 2-film theory as a basis and suggest a more physical approach to solving the initialisation problem of partially-assumed steady state models.

Keywords : Distillation, modelling, dynamics

1 Introduction

The modelling approach our group has developed over the last years has proven itself as being very efficient. We see the students to get much further when following this approach and the computer implementation has now been used for over a year for building professional training simulators in an industrial environment. The models are not only constructed much faster, but they are also guaranteed to solve structurally and in most cases also numerically. They can also be modified very quickly and adapted to different use. Maintenance is significantly improved (Preisig (2004b), Westerweele (2003)). Here we shall continue the discussion cleaning out some important details and focusing on a very common, thus important subprocess, the flash. What first started with playing with alternatives turned out to be of a more wide interest, because the model has very good convergence properties.

2 Background

In last-years contributions (Preisig (2004a,b)) some of the basics were discussed and also the phase transition problem was touched on. This paper will expand on the basics with a focus on the phase transition problem.

The flash is a very widely celebrated subject of modelling obviously because the mechanisms playing in the flash are essential in many processes. A flash is a physical containment with a more or less constant volume containing at least two phases interacting with each other being a liquid and a gas phase. The flash is the main building block of distillation, which obviously plays an essential role as a separation process in the chemical industry. The discussion on the flash often focuses on the solution problems the model equations pose. The paper by Ponton and Gawthrop (Ponton and Gawthrop (1991)) uses

*e-mail: Heinz.Preisig@chemeng.ntnu.no

strong words when pointing out a certain rigor of their presented approach and the systematics they present circumventing the ever-appearing index problem. However, the index problem has certainly been known before 1982 as claimed by Ponton and so knew the chemical engineering community before 1988. The index problem is a characteristic that arises often when making assumptions, a fact, which indeed is pointed out in the same publication, though not, as claimed with the sufficient depth and rigor to uncover the problem more generally. A number of other groups worked on the problem including Gani and Michelsen (Gani et al. (1992), Michelsen (1993)) and most remarkably Asbjørnsen and Moe & Hertzberg (Asbjørnsen (1973), Moe (1996)). The Asbjørnsen publication is by far the most rigorous of them all. Its focus is the plate efficiency. This paper mainly places emphasis on a physical view, which should help understanding the source of the different mathematical problems and how they can be eliminated, though the limited space does not allow to go to the full extent.

3 A Physical View on the Flash

One of the most discussed problems is the initialisation problem (Moe (1996)). It arises from making assumptions of fast transfer and negligible capacity of the gas phase. Since the work reported here did not start with trying to solve the same problem, we took another view right from the beginning: we did not try to solve the flash as a stationary problem or did we aim at the stationary solution, but we thought about a description that represents the behaviour of a liquid-gas system over a wide range of dynamics. Thinking was going towards what happens if one brings together two phases to start with and what does the interface look like and how can one describe it. Whilst we have been initially experimenting with reduced models, as the ones discussed in the mentioned literature mostly are, we added more physical detail. The result is that we employed the celebrated two-film theory, going back to Lewis (Lewis (1924)). Its use added the feature to mechanically describe the adjusting of the two phases after the initial contact has been made. Thus we essentially expand the range of the time scale and consequently also allow for switching the time scale when appropriate, which from the physics point of view is quite a normal process, but which seems to have not found its way sufficiently into the chemical engineering community with the exception of Asbjørnsen's publication, which uses the same physical picture. Thus let us think of the process as having two phases ideally mixed at the beginning, that is, the intensive properties in the two phases are uniform.

Next we bring these two bodies in contact at which time the boundary is thought to adjust instantaneously to equilibrium at the surface, thus the surface is assumed to have no capacity, a fact we shall use later again. Two-film theory assumes at this point that on either side a diffusion process gets going driven by the chemical potential difference in the bulk of the phase and at the boundary. This process can be described as a distributed model, which we shall not do here. Rather we use the Nernst approximation where a film thickness is defined as the intersection of the tangent at the interface with the bulk both for the chemical potential or often the concentration is used instead. shows the approximation.

We now zoom into the boundary and look at it as a capacity. We abstract the flash into a topology shown in Figure 1, in which the boundary itself is now shown as a dynamic system and the diffusion processes are simplified to connections affecting the boundary

system.

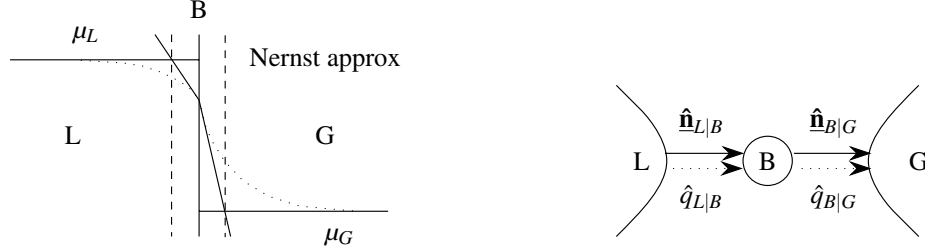


Figure 1. **On the left:** The celebrated 2-film model with Nernst's approximation of the films using the tangent at the interface, thus essentially the flux, as the measure for the film thickness. **On the right:** Zooming into the boundary and making the outer parts correspondingly large, the boundary may be seen as a dynamic system, a capacity in which the phase change takes place.

The model for the flash is then:

Component mass balances, the mass dynamics:

$$\dot{\mathbf{n}}_L := -\hat{\mathbf{n}}_{L|B}, \quad (1)$$

$$\dot{\mathbf{n}}_B := \hat{\mathbf{n}}_{L|B} - \hat{\mathbf{n}}_{B|G} + \begin{bmatrix} -\mathbf{I}_L & \mathbf{I}_G \end{bmatrix} \tilde{\mathbf{n}}_B, \quad (2)$$

$$\dot{\mathbf{n}}_G := \hat{\mathbf{n}}_{B|G}. \quad (3)$$

Component mass flows:

$$\hat{\mathbf{n}}_{L|B} := -\underline{\mathbf{L}}(\mu_B - \mu_L), \quad (4)$$

$$\hat{\mathbf{n}}_{B|G} := -\underline{\mathbf{G}}(\mu_G - \mu_B). \quad (5)$$

Production rates, $\tilde{\mathbf{n}}_B$ are not known. They describe the transition of the species between the phases.

The two matrices $\underline{\mathbf{L}}, \underline{\mathbf{G}}$ are measures of the diffusivities in the respective phases and here assumed to be diagonal and given. Note that this automatically includes the coupling condition of the distributed system, namely the equivalence of the chemical potentials.

The chemical potentials for $\alpha \in \{L, G\}$:

$$\mu_\alpha := \mu_\alpha(p_\alpha, T_\alpha) + RT_\alpha \ln(\mathbf{x}_\alpha), \quad (6)$$

$$\underline{\mu}_\alpha(p_\alpha, T_\alpha) := \underline{\mathbf{h}}(p_\alpha, T_\alpha) - \underline{\mathbf{s}}(p_\alpha, T_\alpha) T_\alpha, \quad (7)$$

$$\underline{\mathbf{s}}(p_\alpha, T_\alpha) := \underline{\mathbf{s}}^o(p_\alpha, T^o) + c_{p,\alpha} \ln\left(\frac{T_\alpha}{T^o}\right), \quad (8)$$

$$\underline{\mathbf{h}}(p_\alpha, T_\alpha) := \Delta \underline{\mathbf{h}}_f^o(p_\alpha, T^o) + \underline{\mathbf{c}}_{p,\alpha}(T_\alpha - T^o). \quad (9)$$

The concentration measures are state variable transformations:

$$\mathbf{x}_\alpha := (\mathbf{e}^T \underline{\mathbf{n}}_\alpha)^{-1} \underline{\mathbf{n}}_\alpha. \quad (10)$$

The energy is the second type of conserved quantity that describes the dynamics of the process.

Enthalpy balances: the energy dynamics :

$$\dot{H}_L := -\hat{H}_{L|B} - \hat{q}_{L|B}, \quad (11)$$

$$\dot{H}_B := \hat{H}_{L|B} - \hat{H}_{B|G} + \hat{q}_{L|B} - \hat{q}_{B|G} \quad (12)$$

$$\dot{H}_G := \hat{H}_{B|G} - \hat{q}_{B|G}. \quad (13)$$

The mass-flow-induced enthalpy flows are for $m \in \{L|B, B|G\}$:

$$\hat{H}_m := \mathbf{h}_m^T \mathbf{n}_m. \quad (14)$$

The heat flows are modelled with a gradient law, simplifying a heat diffusion process for $a|b \in \{L|B, B|G\}$:

$$\hat{q}_{a|b} := k_{a|b} (T_b - T_a). \quad (15)$$

Again, the equilibrium condition, namely the temperature on both sides of the boundary being the same is automatically included.

3.1 Singular Perturbation on the Boundary

In a first step we apply a singular perturbation for the boundary system, that is, we assume singular capacity effect in the boundary and set equation 2 and 12 to zero.

It is also quite easy to see that the unknown transition kinetics can be eliminated. We first split the liquid and the gaseous species:

$$\text{liquid : } 0 := \hat{\mathbf{n}}_{L|B} - \mathbf{I}_L \tilde{\mathbf{n}}_B, \quad (16)$$

$$\text{gaseous : } 0 := -\hat{\mathbf{n}}_{B|G} + \mathbf{I}_G \tilde{\mathbf{n}}_B. \quad (17)$$

Adding the two together eliminates the kinetics and makes inflow equal the out flow.

For the computation of the heat and mass flows, one needs the condition in the boundary, thus also the temperature, which is to be computed from the steady state energy balance:

$$0 := \hat{H}_{L|B} - \hat{H}_{B|G} + \hat{q}_{L|B} - \hat{q}_{B|G}. \quad (18)$$

The additional thing to observe is that the conditions in the convective heat streams, $\hat{H}_{L|B}$ and $\hat{H}_{B|G}$, switch when the direction switches, that is, the intensive quantities are always the ones of the source. For example, if the two mass flows are positive, then the temperature in the flow $\hat{H}_{L|B}$ is T_L and in the flow $\hat{H}_{B|G}$ it is T_B .

The problem is well posed given the quantities $\mathbf{L}, \mathbf{G}, R, \mathbf{s}_L^o, \mathbf{s}_G^o, \mathbf{c}_{p,L}, \mathbf{c}_{p,G}, \Delta \mathbf{h}_f^o, k_{L|B}, k_{B|G}$ and the initial conditions, the degree of freedom analysis gives equal numbers of equations and variables. Furthermore, one finds that the algebraic equations are lower mostly triangular with the exception of having to compute the temperature in the phase boundary using a root solver. Experience shows that most of these equation systems are indeed lower triangular. Only occasional they become block lower triangular in which case a numerical root search must be employed. Certainly the problem gets also more problematic to solve if one uses non-constant heat capacities; though it does not really add a principle problem. The only interesting part is, that the key variable, the temperature, appears then as the upper limit of an integral.

4 The Initialisation Problem

The above set of equations can be simulated and solve essentially the celebrated initialisation problem. The key to the claim of having solved the initialisation problem is in

proofing convergence. In view of the limited space, we show a reduced system for the proof. We make another order of magnitude assumption by setting the heat transfer parameters to large and applying a singular perturbation to heat flow topology. This then asks for the elimination of the heat streams which is achieved when adding the two remaining systems, namely the gas phase and the liquid phase together. This represents the null space for the heat flows (Preisig (2004a)). It eliminates the energy largely from the analysis and we are left with the mass communication system.

From the singularly perturbed mass balance of the boundary (16,) with the models for the mass flow (4, 5) and the state variable transformations (6, 10) one finds the chemical potential at the boundary:

$$\underline{\mu}_B := (\underline{\mathbf{L}} + \underline{\mathbf{G}})^{-1} (\underline{\mathbf{L}}\underline{\mu}_L + \underline{\mathbf{G}}\underline{\mu}_G). \quad (19)$$

which yields now a reduced model:

$$\dot{\underline{n}}_L := \underline{\mathbf{L}}((\underline{\mathbf{L}} + \underline{\mathbf{G}})^{-1} (\underline{\mathbf{L}}\underline{\mu}_L + \underline{\mathbf{G}}\underline{\mu}_G) - \underline{\mu}_L), \quad (20)$$

$$\dot{\underline{n}}_G := -\underline{\mathbf{G}}(\underline{\mu}_G - (\underline{\mathbf{L}} + \underline{\mathbf{G}})^{-1} (\underline{\mathbf{L}}\underline{\mu}_L + \underline{\mathbf{G}}\underline{\mu}_G)). \quad (21)$$

This together with the definitions of the chemical potential and the concentrations forms a DAE which can readily be substituted to an ODE in the component masses. The system converges uniformly, if the right-hand-side has a negative Jacobian. Since one of the Eigenvalues of the Jacobian will be zero, because the sum of the two systems is always zero, the second Eigenvalue needs to be computed. It is a rather cumbersome task to do so, and for the sake of limited space we just state the result for a binary system, which is

$$\lambda_1 := -\frac{RTGL(n_{L,2}n_{G,1}^2 + n_{L,2}n_{G,1}n_{G,2} + n_{L,1}^2n_{G,2} + n_{L,1}n_{L,2}n_{G,2})}{(n_{G,1} + n_{G,2})n_{G,1}(L + G)n_{L,1}(n_{L,1} + n_{L,2})}, \quad (22)$$

$$\lambda_2 := -\frac{RTGL(n_{L,1}n_{G,2}^2 + n_{L,2}n_{L,1}n_{G,1} + n_{L,1}n_{G,2}n_{G,1} + n_{L,2}^2n_{G,1})}{(n_{G,1} + n_{G,2})n_{G,2}(L + G)n_{L,2}(n_{L,1} + n_{L,2})}. \quad (23)$$

The fact that the differential equations, describing the inner solution of the singularly perturbed problem, are converging, can also be seen in another way: The chemical potential is a monotone function of the concentration and the mass in the system. The sum of the two sets of component mass balances is zero, whilst the difference is 2 times either of the two streams. Thus, if the left-hand side is monotone and moves towards the equilibrium state, the equations will converge. Let the star indicate equilibrium conditions. For example:

$$\dot{\underline{n}}_L - \dot{\underline{n}}_G := 2(\underline{\mu}_B - \underline{\mu}_L) - \underline{\mathbf{L}}(\underline{\mu}_B^* - \underline{\mu}_L^*), \quad (24)$$

$$:= 2\underline{\mathbf{L}}((\underline{\mathbf{L}} + \underline{\mathbf{G}})^{-1} (\underline{\mathbf{L}}\Delta\mu_L + \underline{\mathbf{G}}\Delta\mu_G) - \Delta\mu_L), \quad (25)$$

$$:= 2\underline{\mathbf{L}}((\underline{\mathbf{L}} + \underline{\mathbf{G}})^{-1} \underline{\mathbf{L}} - \underline{\mathbf{I}}) \Delta\mu_L + (\underline{\mathbf{L}} + \underline{\mathbf{G}})^{-1} \underline{\mathbf{G}} \Delta\mu_G. \quad (26)$$

Looking at the case, where $\mu_L > \mu_G$ the deviations are $\Delta\mu_L > 0$ $\Delta\mu_G < 0$, and $(\underline{\mathbf{L}} + \underline{\mathbf{G}})^{-1} \underline{\mathbf{L}} - \underline{\mathbf{I}} < 0$ thus the right-hand-side is indeed less than zero all the time and the equations converge uniformly towards the equilibrium. The same argumentation can be repeated for the opposite flow, when $\mu_L < \mu_G$. On the side: it is relatively straightforward to prove that $\mu_L \leq \mu_B \leq \mu_G$

5 Conclusions

A physical description of the flash problem has been given based on Lewis' two-film theory. The result is a set of equations in which only one undefined set of variables appears, namely the conversion rates describing the phase transition of the species in the form of a kinetic. These unknown transition rates are eliminated by singularly perturbing the boundary capacity and the condition of equality of the inflow with the outflow of the boundary results.

The agreeably unknown diffusion rates define the location of the interface potential (or concentration, if the gradient in the concentration was used in the transfer law (Asbjørnsen (1973))) and determine how quickly the two equations converge to the equilibrium. Thus if one is not interested in the inner solution, but only in the outer assuming fast transfer between the two phases, the choice of the two diffusivity matrices is not critical at all in contrary to Ponton's view. They must merely result in a sufficiently fast convergence, that is, about 10 times faster than the rest of the dynamics attached to the flash.

Convergence for the simplified case where the heat transfer is assumed to exhibit event dynamics on the time scale of the diffusional mass transfer between the phases. The inner solution solves the initialisation problem elegantly. The key is to think in time and length scales.

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