Modeling Multi-Phase Systems Using Bond Graphs

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Abstract

This is the second in a series of three papers. The first paper [3] discussed the modeling of conductive as well as convective flows of a single homogeneous substance through a homogeneous medium. This second paper discusses the phenomena associated with phase change, i.e., it discusses, from a bondgraphic perspective, phenomena such as evaporation and condensation, solidification, melting, and sublimation. Assumptions of quasi-stationary or equilibrium conditions are minimized to ensure the largest possible degree of generality in the conclusions reached. Problems associated with modeling the dynamic behavior of multi-substance systems will be left for discussion in the third paper of the series [4]. A thermodynamic model of a pressure cooker shall serve as an example of a multi-phase system.

Keywords: Thermodynamics; Multiphase; Bond graphs; Condensation; Evaporation; Pressure cooker.

1 INTRODUCTION

This paper discusses primarily issues surrounding the thermodynamic modeling of evaporation and condensation. It does not consider effects such as undercooled steam or overheated liquid. Such effects are inherently unstable, and can only exist during a transitory period. They require a statistical approach for their treatment that is incompatible with the bondgraphic world view that has been embraced in this publication. On the other hand, phenomena involving other stable phase changes, such as solidification and melting, can be treated using approaches that are quite similar to the ones presented here. They were excluded only because of space limitations.

2 BACKGROUND

In the previous paper [3], C-fields were discussed that varied only in their position in space. In principle, multi-phase systems could be treated in the same fashion, as the bondgraphic topology of C-fields connected by R-fields remains the same in the presence of multiple state phases. Only the internal descriptions of the individual C-fields would have to be adapted to the new situation.

However, such an approach would lead to a further increase in complexity of the C-field models, and it would deprive the modeler of the possibility to analyse each phase separately. Also in multi-element systems (cf. [4]), it makes sense to separate the phases, as different elements of the same phase will be connected closer to one another than different phases of the same element. For this reason, the authors decided to introduce one CF-element for each phase and each substance.

Once the decision has been reached to model individual phases through separate C-fields, the question needs to be answered, how phase changes, such as evaporation and condensation, can be represented in the resulting bond graph. Since phase changes are of a dissipative nature, it makes sense to represent them as R-fields. However, it will be necessary to let go of the demand that R-fields should not contain any element data, as these phenomena will indeed depend on the substances that they are applied to. At this point, it is therefore necessary to leave the parallels of network theory [1].

As explained earlier, no quasi-stationary or equilibrium assumptions shall be made, i.e., different phases can be at different temperatures and different pressures (although they will not differ much). It turns out that this decision actually simplifies the modeling task. It means, of course, that the new modeling elements will have to be supplied with saturation data.

3 EVAPORATION AND CONDENSATION

Evaporation occurs when the state of a liquid is forced to pass through the saturation line into the area of wet vapor. Evaporation is by itself a statistical event, i.e., it occurs at all times – sometimes stronger, sometimes less strong. It represents the reaction of a fluid molecule to energy boosts obtained from other molecules in collisions.

Condensation is the counterpart of evaporation. It represents the chance of the gas to reach a more stable state. It occurs whenever the state of the gas reaches the wet vapor area after passing through the dew line (gas in the wet vapor area already contains liquid).

When modeling different phases by separate C-fields, a phase transition element is needed that takes boiling (i.e., evaporating) liquid from the C-field, representing the fluid state, over to the C-field, representing the gaseous state. This element can be designed in analogy to the generalized RF-element, as its flows will be driven also by differences in potentials.

Inside the wet vapor area, pressure and temperature are no longer linearly independent, i.e., either of them can be calculated from the other. Suppose, the saturation pressure is calculated for a given temperature ($p_{sat} = p(T)$). If the true pressure is compared with the saturation pressure, the following cases can be distinguished:

- fluid state
  - $p_{sat} \leq p_{fl}$: The state of the fluid is outside the wet vapor area. For modeling purposes, it can be postulated that no evaporation occurs, as the statistical molecular movements lead only to a small amount of evaporation. This evaporation can be ignored except if the simulation is to extend over a very long time period.
  - $p_{sat} > p_{fl}$: The liquid is saturated (respectively oversaturated), and evaporating can be observed.
- gaseous state
  - $p_{sat} \geq p_{gas}$: The gas is too hot to condensate. Statistical condensation can certainly be ignored, because its effects are always smaller than those of statistical evaporation. Consequently, a phase transition does not occur.
  - $p_{sat} < p_{gas}$: The dew line is crossed. In a sufficiently disturbed system (the presence of the disturbing butterfly will be assumed), fluid will fall out.

$$\dot{M}_{evap} = \begin{cases} 0 & \text{if } p \geq p_{sat}, \\ 0 & \text{if } M_{liq} = 0, \\ R_v \cdot (p_{sat} - p) & \text{otherwise} \end{cases} \tag{1}$$

$$\dot{M}_{cond} = \begin{cases} 0 & \text{if } p \leq p_{sat}, \\ 0 & \text{if } M_{gas} = 0, \\ R_c \cdot (p - p_{sat}) & \text{otherwise} \end{cases} \tag{2}$$

These equations could also have been written using the saturation temperature $T_{sat} = T(p)$ instead of the saturation pressure.

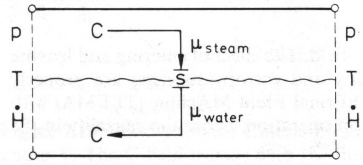

Figure 1: Cross-section through a fluid pipe with a supposed interface between 2 phases, steam and water. Here the exchange between the phases is driven by the chemical potential (Thoma [10])

A different approach had been suggested by Thoma [10]. He determined the resulting mass flow across the phase change directly as a function of the difference of the chemical potentials $\Delta\mu$ between the two phases (cf. Fig. 1). This approach would lead us around the need to supply the phase transition element with information about the saturation pressure (or the saturation temperature, respectively). Unfortunately, this seeming advantage is compensated by the fact that now, the chemical potentials of both phases need to be known, which is cumbersome, as the chemical potentials themselves change under evaporation and condensation. Furthermore, one needs to consider the situation that one of the two phases does not exist at all at some point in time. Computing the chemical potential of an emerging phase is essentially impossible, since the statistical effects at that instant are dominant.

Thoma's approach, although conceptually sound, has to the knowledge of these authors never been fully worked out. The description of Thoma's 'model' is sketchy at best. Furthermore, his model does not account for the fact that temperature and pressure will eventually equilibrate between the two phases independent of any phase transition flow. Also, Thoma let unresolved the question (he did not even ask it) of the corresponding volume flow. To answer that question, saturation data tables would have to be provided, even if Thoma's approach were being used.

Evaporation and condensation processes are - similar to the R-field - not allowed to change the mass of the surrounding system, i.e., the mass flow leaving the liquid phase must be identical to the one reaching the gaseous phase, and vice-versa. Furthermore, if the system in which the phase change occurs is closed, the same holds true for volume flows.

What happens to the entropy during evaporation? Like in all mass flows, the mass leaving the liquid phase carries its own entropy along. However, this does not account for everything that happens. From somewhere, the activation energy needs to be provided that allows the former liquid to turn itself into the more highly energetic gaseous phase. This requires a heat flow (latent heat) away from the liquid phase. The remaining liquid cools down in the process. In the literature, the corresponding enthalpy is usually referred to as r_0. It is larger than the enthalpy carried naturally with the mass by several orders of magnitude.

Let us provide an example of evaporating water at a temperature of T=353.15 K, and a pressure of p=1bar (reference [5]):

saturation pressure	0,4736 bar
specific volume	$1029{,}03\frac{cm^3}{kg}$
spec. saturation volume	$1029,30\frac{cm^3}{kg}$
spec. dewpoint volume	$43410000,00\frac{cm^3}{kg}$
$p_{fl} \cdot (v_{sat} - v_{fl})$	$0,000027\frac{kJ}{kg}$
change in specific entropy	$6,0437\frac{kJ}{kg \cdot K}$
enthalpy of evaporation $r_0 = T \cdot \Delta s$	$2134.33\frac{kJ}{kg}$

The entropy flow of the evaporation can be written as:

$$\xi_{evap} = \frac{\dot{M}_{evap}}{M_{fl}} \tag{3}$$

$$\dot{S}_{evap} = \xi_{evap} \cdot S_{fl} + \frac{\dot{M}_{evap}}{T_{fl}} \cdot r_0(T_{fl}) \tag{4}$$

where the first term denotes the transport of entropy with the converted mass, and the second term denotes the additional entropy needed to compensate for the activation energy.

Condensation is essentially the reverse process of evaporation. Condensation occurs, when the gas pressure is higher than the dew pressure (the latter one being identical to the saturation pressure on the fluid side). Yet, evaporation and condensation are not entirely reversible processes. The entropy needed to overcome the activation energy in the process of evaporation is taken from the liquid phase, whereas this energy stays as entropy in the gaseous phase during condensation, i.e. the processes of evaporation and condensation are indeed truly dissipative in nature.

Making use of the Heaviside function h,

$$h(x) = \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

the equations (1) and (2) for the mass flows of evaporation and condensation can be rewritten as:

$$\begin{aligned} \dot{M}_{evap} = R_v \cdot (p_{fl} - p_{sat}(T_{fl})) \cdot \\ \cdot h(p_{fl} - p_{sat}(T_{fl})) \cdot h(M_{fl}) \end{aligned} \tag{6}$$

$$\begin{aligned} \dot{M}_{cond} = R_c \cdot (p_{sat}(T_{gas}) - p_{gas}) \cdot \\ \cdot h(p_{sat}(T_{gas}) - p_{gas}) \cdot h(M_{gas}) \end{aligned} \tag{7}$$

Since both evaporation and condensation can occur simultaneously, the two flows can be merged by defining the evaporation as a positive and the condensation as a negative flow:

$$\dot{M} = \dot{M}_{evap} - \dot{M}_{cond} \tag{8}$$

The two volume flows can be written as:

$$q_{evap} = \dot{M}_{evap} \cdot v_{sat}(T_{liq}) \tag{9}$$

$$q_{cond} = \dot{M}_{cond} \cdot v_{sat}(T_{gas}) \tag{10}$$

where v_{sat} denotes the saturation volume, and merging the two volume flows, one obtains:

$$q = \dot{M}^{fl}_{evap} \cdot v^{fl}_{sat}(T_{liq}) - \dot{M}_{cond} \cdot v_{sat}(T_{gas}) \tag{11}$$

The equations for the entropy flow can be derived in the same way, as was done for the RF-element. In fact, the condensation-evaporation element looks structurally exactly like the RF-element. Only the internal equations describing it are different.

$$\xi = \frac{\dot{M}}{M} \tag{12}$$

$$\Delta\dot{S}_1 = (g_{fl} - g_{gas}) \cdot \dot{M} + (p_{fl} - p_{gas}) \cdot q \tag{13}$$

$$\dot{S_{fl}} = \begin{cases} \xi \cdot S_{fl} + \frac{r_0(T_{fl})}{T_{fl}} \cdot \dot{M} & \text{, if } \dot{M} > 0 \\ \dot{S}_{gas} + \Delta\dot{S}_1 + (T_{fl} - T_{gas}) \cdot \dot{S}_{gas} & \text{, otherwise} \end{cases} \tag{14}$$

$$\dot{S}_{gas} = \begin{cases} \xi \cdot S_{gas} - \frac{r_0(T_{gas})}{T_{gas}} \cdot \dot{M} & \text{, if } \dot{M} < 0 \\ \dot{S_{fl}} + \Delta\dot{S}_1 + (T_{fl} - T_{gas}) \cdot \dot{S_{fl}} & \text{, otherwise} \end{cases} \tag{15}$$

Obviously, this model is still somewhat simplified, as it only takes into account two separate phases. In reality, the model will have to deal with four separate C-fields:

- CF liquid, as discussed
- CF liquid, but distributed homogeneously in the gas phase
- CF gas, as discussed
- CF gas, as small bubbles in the fluid phase,

whereby the four CF-elements are connected by condensation-evaporation elements as shown in Fig. 2.

One question still needs to be answered: When does the fog leave the gas phase and join the fluid phase? When do the gas bubbles leave the fluid phase to merge with the gas phase? It can be assumed that fog that touches the surface of the liquid will join with it. Also, gas bubbles that rise to the surface of the liquid will merge with the gaseous phase above. Furthermore, gravitation will help gas bubbles to rise to the surface and will aid the heavier fog particles in sinking down to the liquid surface. These forces are opposed by cohesion forces. It turns out that this is a very difficult problem that can only be modeled in a statistical sense. It will not be discussed any further in this paper.

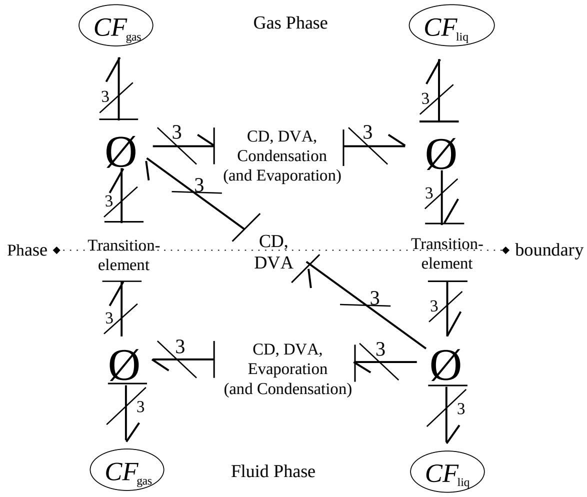

Figure 2: Modelling a two phase environment, using four C-fields.

Another problem that still needs to be discussed is the case that a phase may not exist at a given point in time. In that case, the (partial) pressure, volume, mass, and Gibbs enthalpy of that phase are zero, whereas its temperature and entropy are undefined. All model equations must be protected against division by zero and/or use of undefined variables. In the case of the CD- and DVA-elements introduced in the companion paper ([3]), this can be accomplished by a combination of a fudge factor ϵ, as proposed in the companion paper, and a boolean variable that distinguishes a non-existing phase from an existing one. Examinating the condensation-evaporation element for the case of a non-existing target phase, one discovers that it will be totally reversible, as the evaporating/condensating flow will not be mixed together with mass having another potential. During the first infinitesimal instant, the flow chart of this element can be redrawn as shown in Fig. (3).

Summarizing, the equations for the condensation-

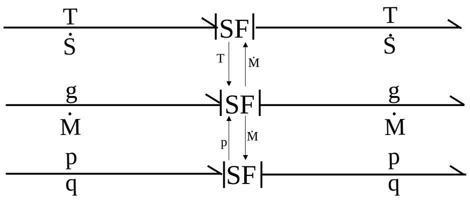

Figure 3: Condensation-evaporation element for the case of a not yet existing target C-field

evaporation element (KV) are given as follows:

$$\dot{M}_{evap} = R_v \cdot (p_{sat}(T_{liq}) - p_{liq}) \cdot \cdot h(p_{sat}(T_{liq}) - p_{liq}) \cdot h(M_{liq}) \tag{6}$$

$$\dot{M}_{cond} = R_c \cdot (p_{gas} - p_{sat}(T_{gas})) \cdot \cdot h(p_{gas} - p_{sat}(T_{gas})) \cdot h(M_{gas}) \tag{7}$$

$$\dot{M} = \dot{M}_{evap} - \dot{M}_{cond} \tag{8}$$

$$q = \dot{M}_{evap} \cdot v_{sat}(T_{liq}) - \dot{M}_{cond} \cdot v_{sat}(T_{gas}) \tag{11}$$

$$\Delta T\dot{S} = (g_{fl} - g_{gas}) \cdot \dot{M} + (p_{fl} - p_{gas}) \cdot q \tag{13}$$

$$\dot{S}_{liq} = \begin{cases} \xi \cdot S_{liq} + \frac{r_0(T_{liq})}{T_{liq}} \cdot \dot{M} & , \dot{M} > 0 \\ \frac{1}{T_{liq}} \left(\dot{S}_{gas} \cdot T_{gas} + \Delta T\dot{S} \right) & , \dot{M} < 0, M_{gas} > 0 \\ \dot{S}_{gas} & , \text{otherwise} \end{cases} \tag{16}$$

$$\dot{S}_{gas} = \begin{cases} \xi \cdot S_{gas} & , \dot{M} < 0 \\ \frac{1}{T_{gas}} \left(\dot{S}_{liq} \cdot T_{liq} + \Delta T\dot{S} \right) & , \dot{M} > 0,\ M_{liq} > 0 \\ \dot{S}_{liq} & , \text{otherwise} \end{cases} \tag{17}$$

4 CONDENSATION ON COLD SURFACES

Another phenomenon that needs to be discussed is the condensation on cold surfaces. If an adjacent surface has a lower temperature than the dew point temperature ($T_{tau} = T(p_{gas})$) of the element, there will be formation of dew on this surface. For the first time, an element is discussed, the behavior of which is primarily influenced by another element (the colder surface).

The problem here is that the dew point temperature can be computed, using tables, but the model has no direct way of knowing, when the dew point has been reached. To solve this problem, there are two meaningful ways:

- Taking the gas phase, one can calculate what pressure the gas would have if it were cooled down to the temperature of the adjacent surface. Using this fictitious pressure, one could then go on as usual and determine when the conditions for a condensation would be satisfied. However, the fictitious character of this methode would make it impossible to provide an explicit bond graph model — the modeler would have to be content with an iconic representation of the overall effects of the phenomenon.

- Closer to reality, but unfortunately associated with a higher computational cost, is the introduction of a boundary layer, as proposed by Luttmann [7]. The boundary layer can be represented by yet another C-field, the volume of which is a function of the gas volume. This C-field is connected on one side to the gas phase, and on the other side to the adjacent surface. Unfortunately, it is not trivial to model the proposed volume dependance. One possible solution is to connect the C-field of the gas and the one of the boundary layer by an RF-element with a volume flow that is proportional to the difference between the pressures of the two neighboring C-fields.

  The contact to the cold surface will be modeled using a (fast) CD-element. The other leg of the condensation element would either be placed directly in the fluid phase, or –as scetched in Fig. 4– in another boundary-layer element, representing the interface between the liquid face and the wall.

The former approach is computationally more efficient. The latter approach reflects somewhat better the physical reality, and thereby, is more in line with the bondgraphic spirit. Therefore, this is the approach that has been chosen in the research effort reported here.

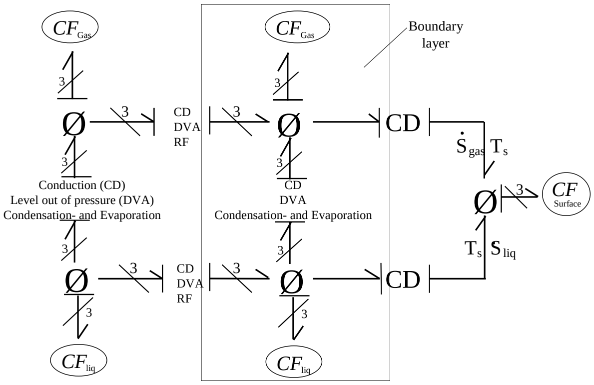

Figure 4: Bond graph model of an evaporation-condensation element including a cold surface and two boundary-layer elements. For readabilty, the cross-couplings were eliminated, although they exist in reality.

5 MODEL OF A PRESSURE COOKER

As an example for the discussed theory, a pressure cooker was simulated (cf. Fig. 5).

New in this model is the presence of a second element in the gas phase: air. Due to its presence, the equations had to be revised, and the pressure of the steam inside the condensation element had to be replaced by its partial pressure. The resulting model reflects the fact that humid air can exist even at room temperature, whereas, without the air, the steam would immediately condensate.

Modeling air and steam as ideal gases had the advantage, that the partial pressure of the steam could be computed fairly easily as $p_{steam} = \frac{p \cdot V}{V_{steam}}$. The disadvantage of this solution, in particular in the presence of liquid water, was that correctors had to be implemented.

For reasons of stability, a DVA-element was placed in parallel with the RF-element that controls the boundary layer.

At time=0, the pressure cooker, which at that time is at room temperature ($T \approx 293K$) and has just been closed ($p \approx 101Pa$, humidity ≈ 0.5) is placed on a hot surface ($T = 393K$). As expected, the pressure and the temperature rise. The pressure release valve was omitted that would prevent a real pressure cooker from exploding. It was assumed that the walls are strong enough to withstand arbitrarily high pressures.

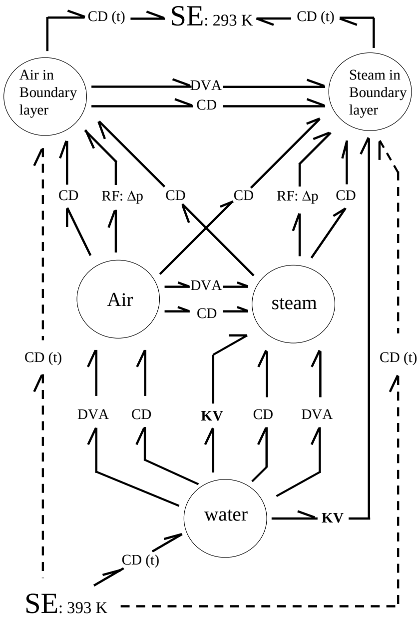

Figure 5: Bond graph model of the pressure cooker example. The circles represent C-fields together with their corresponding 0-junctions.

After half of the simulation period, the pressure cooker is removed from the stove and is placed under cold water (T=293K). Dew forms immediately in the boundary layer, whereas condensation across the phase boundary starts somewhat later.

For reasons of heat conduction, the stove is predominantly connected with the C-field of the water by a CD-element and the cold water source to the gas boundary layer. Figures 6 - 7 show the simulation results.

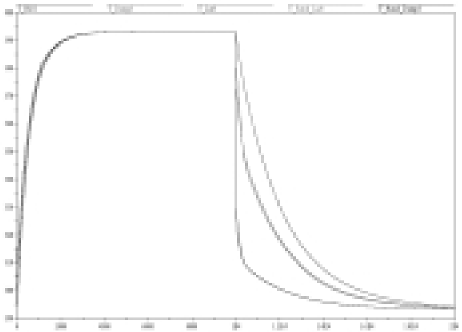

Figure 6: Temperature graphs of the simulated pressure cooker.

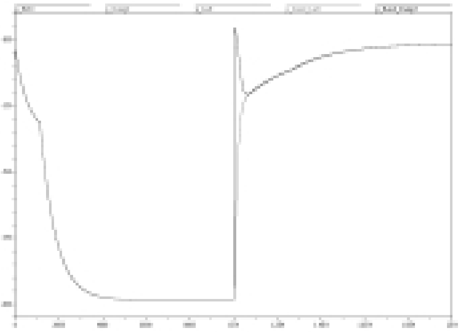

Figure 7: Pressure graphs of the simulated pressure cooker.

6 CONCLUSIONS

The paper discussed different aspects of the rather complicated processes of evaporation and condensation. It was found that describing phase transitions is not simple enough to model them without any assumptions. Yet, a convenient way was found to model simple phase transitions. The example of a pressure cooker was used to show the practicality of the advocated approach.

Earlier publications dealing with bond graph modeling of phase changes used two C-fields only, one for each phase. The new model is more detailed as it accounts for vapor within the gaseous phase and air bubbles within the fluid phase spearately, introducing separate C-fields for them. Also the treatment of condensation on cold surfaces by introducing a C-field representing the boundary layer is new.

The choice of state variables in modeling phase changes is non-trivial and has important consequences. This paper differs from earlier publications [8, 11] in its selection of state variables.

Due to space limitations, the paper is somewhat sketchy in its discussion of the details of the pressure cooker example. A full account of the pressure cooker model will soon be available [2]. An important problem that was not addressed in this publication is how the parameter values can be obtained. Some of them, such as R_v and R_c, are notoriously difficult to find [6, 9].

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