MODELING MULTI-ELEMENT SYSTEMS
USING BOND GRAPHS

Jürgen Greifeneder

Fakultät Verf.-technik und Techn. Kybernetik
Universität Stuttgart

70550 Stuttgart
Germany
J@Greifeneder.de
http://www.greifeneder.de/jg/

François E. Cellier

Dept. of Electr. & Comp. Engr.
The University of Arizona
P.O.Box 210104
Tucson, Arizona 85721-0104
U.S.A.
Cellier@ECE.Arizona.Edu
http://www.ece.arizona.edu/~cellier/

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ABSTRACT

This is the last in a series of three papers. The first paper (Greifeneder and Cellier 2001a) discussed the modeling of conductive as well as convective flows of a single homogeneous substance through a homogeneous medium. The second paper (Greifeneder and Cellier 2001b) discussed the phenomenona associated with phase change, i.e., it discussed, from a bond-graphic perspective, phenomenona such as evaporation and condensation, solidification, melting, and sublimation. This third paper deals in particular with the difficult problem of modeling multi-element systems. Together they offer a general methodology for modeling thermodynamical phenomenona using true, rather than pseudo-, bond graphs. No quasi-stationary or flow-equilibrium assumptions were made, such that the models generated using the proposed methodology would be kept as general as possible.

INTRODUCTION

Bond graphs enable the modeler to describe the dynamics of a physical system in a modular fashion using energy storage, dissipative power flow, energy source, and transformation elements. The basic bond-graphic icon library enables the user to model, in a systematic fashion, physical systems, the dynamic behavior of which is governed by power flows alone.

Systems with macroscopic mass flows add additional complexity to the modeling task, since the mass that flows through the system carries with it its stored internal free energy, which is thus transported from one location to another in a non-dissipative fashion.

In the most general sense, thermodynamics ought to be described by distributed parameter models. Since bond graphs are geared to be used for the description of lumped parameter models only, a simplifying assumption will be made, in that the system to be modeled is compartmentalized, whereby each compartment is considered to be homogeneous.

New bond-graphic macro-elements were introduced in the first two papers to describe the energy storage within a compartment as well as the mass (and energy) flows between neighboring compartments.

This paper discusses primarily issues surrounding the thermodynamic modeling of multi-element systems.

Contrary to earlier efforts related to the modeling of the thermodynamics of fluid flows, such as (Moksnes 1997; Thoma and Ould Bouamama 2000), which made use of pseudo bond graphs, the present discussion is based entirely on true bond graphs. True bond graphs, representing power flows across a system, offer a more realistic treatment of the interactions (energy exchange) between the three energy forms involved in fluid flows: the thermal, volume, and mass flows. Their use also simplifies drastically the interconnection of the fluid flow models with their environment.

BACKGROUND

In the previous papers (Greifeneder and Cellier 2001a, 2001b), systems were discussed that only included a single component. For dealing with multi-element systems, this paper needs the assumption of homogeneous, ideally mixed compartments. 'Ideally mixed' here means that the molecules are distributed at random, i.e., a prediction of what molecule becomes a neighbor of which other molecules is not possible.

A possible way of modeling an ideally mixed compartment would be, to define a single C-field (CF-element) representing the mixture, while changing its internal equations as a function of the composition of the mixture. However, such a decision would necessitate the definition of C-fields with $n + 2$ instead of 3 external cuts (n being the number of components in the mixture).
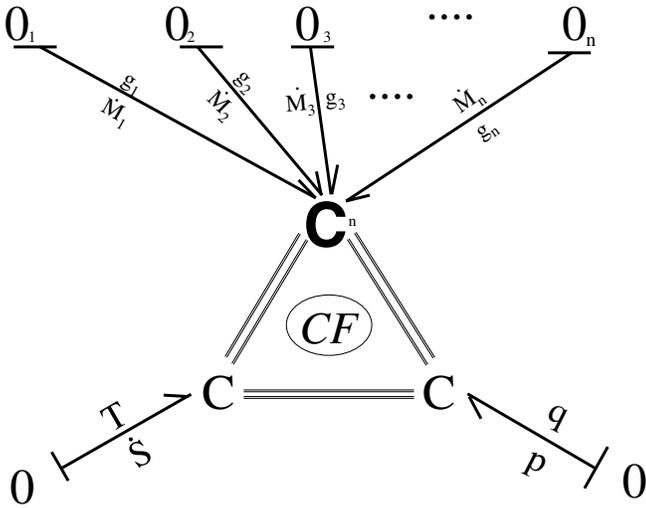
Figure 1: Modified CF-element, Using $n+2$ External Cuts

Such an approach would carry the advantage, that no constraint equations would need to be introduced and that the topological structure of the model of a complex system would be simpler and more easy to comprehend. However, the approach would also be characterized by serious disadvantages, namely that the previously introduced structure of the C-field would have to be extended, that the internal equations of the C-field would change in accordance with the composition of the mixture – an unnecessary complexity especially in the case of simple systems, and that processes would be hidden that the authors would like to make visible. However, as this would have been the classical thermodynamic approach to modeling multi-element systems, one could certainly have done so.

MONO PHASE SYSTEMS

The model discussed in this paper is based on the following idealizations. Let us assume the system to be considered contains n components that are mutually separated by moveable membranes. Let us further assume that the eigendynamics and the friction are neglected. We now make each compartment infinitely thin while preserving its volume. Thereby the surface of the boundary layers to the neighbors become infinitely large. We want to assume that each of these infinitely thin compartments is in contact with every other compartment, such that all compartments are direct neighbors of each other. Thence, if the initial temperature and pressure in the different compartments were distinct, the exchange between the compartments would guarantee that they would equilibrate infinitely fast. A system modeled in this fashion can be considered ideally mixed.

This conceptual system has been modeled by introducing one CF-element for each component of the mixture and by connecting them, using DVA- and CD-elements[1]. Sta-

bility analysis shows that the corresponding transfer rates cannot be chosen infinitely large. In fact, they must be limited such that the exchange between neighboring components is relatively slow for the simulation to work. Consequently, the temperature and pressure of different components of the ideal mixture can assume, in the simulation, somewhat different values, although if left alone, they will equilibrate eventually.

The primary advantage of this kind of modeling lies in the fact that the previously introduced structure of the CF-elements can be retained and that the disclosure of "imagined" flows among the components may improve our understanding of what is going on in mixtures.

IDEAL GASES

Let us start with the simplest case: a mixture of ideal gases. According to Dalton's law (Cellier 1991), ideal gases do not influence one another. When mixing such gases, their masses, volumes, and entropies simply add up. Therefore, the above model can be used for the most general case of such a mixture. However, the modeler must provide a consistent set of initial conditions, as the sum of all partial volumes must be identical to the volume itself.

Furthermore, some elements (e.g. phase transitions) are more conveniently expressed in terms of partial pressures than partial volumes. In multi-element systems, these elements have to be extended by an interface equation that determines the partial pressures as a function of the partial volumes and the overall pressure.

$$p_i^{partial} = \frac{V_i^{partial}}{\sum_{j=1}^{n} V_j^{partial}} \cdot p_i^{Gas} \qquad (1)$$

RF-ELEMENTS IN MULTI-ELEMENT SYSTEMS

The RF-element, describing macroscopic dissipative phenomena of mass and energy transfers between C-fields, can easily be generalized to multi-element systems[2]. If a mixture is being transported from one set of C-fields to another, each component of that mixture is transported as well. Consequently, an RF-element can be placed between each pair of CF-elements representing the same component of the two mixtures, and the flow rates across these RF-elements are computed in accordance with the volume fractions $(\frac{V_i^*}{\sum V_i^*})$ of the mixture of the emitting C-field.

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[1] The DVA- and the CD-element (Greifeneder and Cellier 2001a)

represent the exchange of volume and entropy, respectively, driven by the difference of the corresponding potentials (pressure and temperature, respectively).

[2] The CD-, DVA-, KA-, and KV-elements used in this paper describe dissipative phenomena, i.e., R-fields, as well. Yet, different mnemonics were used to isolate the different microscopic dissipative phenomena discussed in the paper, whereas the RF-element, as used in this paper, was restricted to describing macroscopic mass flow effects only.

Therefore, the multi-element transportation system can be identified as a parallel connection of single-element transportation systems, the throughput of which is determined by the composition of the emitting system (Figure 2).
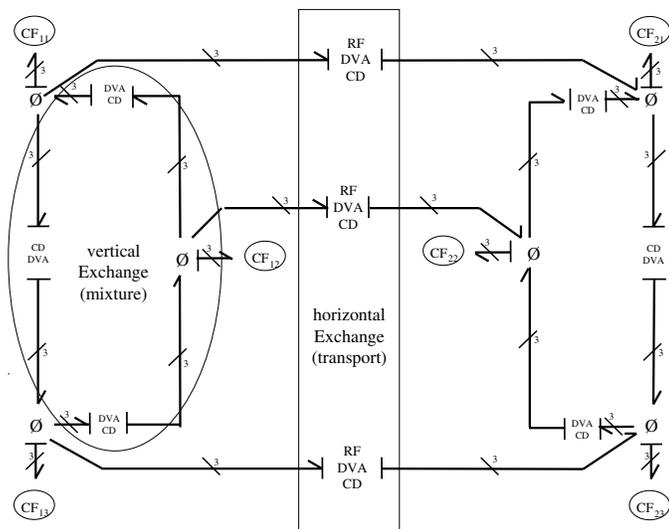

Figure 2: Multi-element Transportation System as a Sum of Coupled Single-element Systems. The Decomposition Illustrates the Difference Between Horizontal (Spatial Transport) and Vertical (Mixture) Exchange

EQUILIBRATION OF CONCENTRATIONS

There exists yet another phenomenon that needs to be discussed. Let us assume that each of the CF-Elements were connected to an outside source, a phase exchange element as discussed in the previous paper or anything equivalent. Consequently, the concentrations in the first compartment may become different from those in the second compartment. Thus, diffusion will take place to equilibrate the concentrations. This diffusion process is modeled using a new element, the KA-element. Its internal bond graph structure is identical to that of the RF-element described in the previous section. However, RF-elements were only provided with the state informations of the emitting CF-elements. Since in the diffusion, the resulting flow is no longer a function of potential differences, the corresponding KA-Elements will need to know the values of the variable to be equilibrated from both compartments. This variable – for example the molar or mass fraction – will be provided by the mixture information element discussed in the next section.

Diffusion is usually much slower than all of the other phenomena already discussed, yet the phenomenon cannot be neglected in the modeling effort, since otherwise, different concentrations of the same element in neighboring connected compartments may not be equilibrated at all, but may exist even in steady state, which is certainly incompatible with physical evidence. The KA-elements, contrary to the RF-elements described earlier, are not coupled, as they describe microscopic transport phenomena that occur for each element independently, except for the constraint imposed by the total mass balance.

IDEAL MIXTURES

Let us now proceed to the next more difficult case of a mixture. It is called "ideal mixture." An ideal mixture is defined in such a way that masses and volumes still add up, but additional entropy is produced in the process of mixing the components. Together with the entropy, also the free enthalpy changes.

At this point, the previously proposed way of modeling leads to a problem: CF-elements are not supposed to know about each other. Yet, the additionally generated entropy and free enthalpy need to be distributed among the participating components. To this end, we either need an additional bond graph element that distributes the newly generated entropy and free enthalpy among the participating CF-elements, or alternatively, each CF element needs to know its own molar fraction to compute the appropriate correction terms.

In our implementation, we chose the latter route. The required information is provided to the participating CF-elements by the Mixture Information (MI) element. Contrary to all previously introduced elements, the MI-element does not carry any energy (flows). It only provides information flows (Figure 3). Pure information flows are dubious from a physical perspective, but they are justified when they are used locally among bond graph elements that, in the physical reality, model different aspects of one and the same phenomenon, as is the case here.
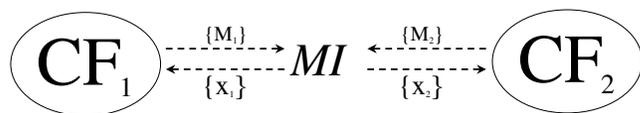

Figure 3: Mixture Information Element for Ideal Mixtures Shown Here for the Case of Only Two Components

When mixing two or more different components (chemical reactions are not being considered in this paper), their energy must be preserved. However in the case of an ideal mixture, irreversible processes are being considered, leading to an increase in entropy. Since the volume, pressure, temperature, and mass are conserved in an ideal mixture, the energy balance can be written as:

$$-\Delta S_{mixed}^{id} \cdot T = \Delta g_{mixed}^{id} \cdot M \qquad (2)$$

$$(\Longrightarrow \Delta H_{mixed}^{id} = \Delta g_{mixed}^{id} \cdot M + T \cdot \Delta S_{mixed}^{id} = 0) \qquad (3)$$

As requested, the enthalpy H is conserved. The change in specific entropy due to mixing can be written as (Stephan and Mayinger 1992)

$$\Delta s_{mixed}^{id} = -R \cdot \sum_k x_k \cdot ln(x_k) \qquad (4)$$

where x_k is the molar fraction, and consequently, the change of free (Gibbs) enthalpy can be evaluated as:

$$\Delta g_{mixed}^{id} = T \cdot R \cdot \sum_k x_k \cdot ln(x_k) \qquad (5)$$

How are these changes modeled using bond graphs? Evidently, as additional entropy is being generated irreversibly, thus using an RS-element, the corresponding heat flow must come from somewhere. The above equation shows, where the energy comes from. It is deducted from the mass flow, as the free enthalpy of the mass undergoing the mixture is reduced. This is shown in Figure 4.
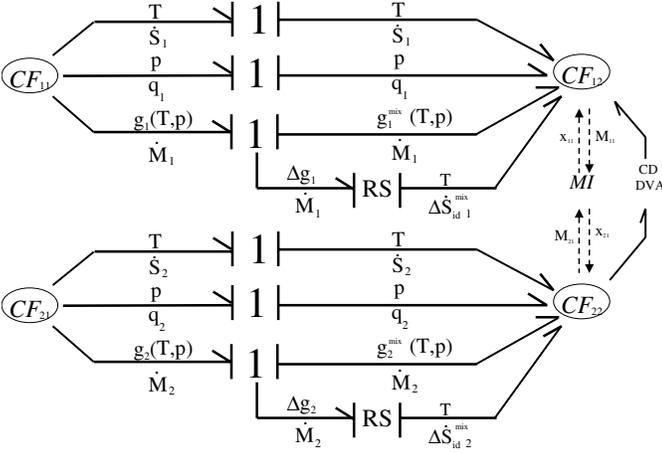

Figure 4: Entropy of Mixing (The 0-junctions Associated with Each of the C-fields Were Suppressed for Simplicity)

The left hand side of Figure 4 shows two components before mixing, represented by their corresponding CF-elements. The right hand side shows the same two components after mixing. The two RS-elements represent the generation of mixing entropy at the expense of free enthalpy.

What happens to temperature and pressure? It would be possible to compute the temperature T and the pressure p as functions of the specific enthalpy h and the specific volume v. Since neither h nor v are changed in the process, T and p cannot change either.

In our code, we compute T and p as functions of the specific entropy s and the specific volume v:

$$T = T(s, v) \qquad (6)$$
$$p = p(s, v) \qquad (7)$$

Since s changes its value, the formulae $T(s,v)$ and $p(s,v)$ must get modified in the process of mixing, such that T and p remain constant. Alternatively, it is possible to keep the formulae the same, but calculate a modified entropy value (a coordinate transformation) that corrects for the different formulae being used:

$$T = T(v, s^{intern}) \qquad (8)$$
$$p = p(v, s^{intern}). \qquad (9)$$

where:

$$s^{intern} := s - \Delta s_{mixed}^{id}. \qquad (10)$$

It may be of interest to briefly discuss causes and effects in Figure 4. Let us assume we start out with a pure substance M_1, and we now start to mix to it a substance M_2. Initially, the C-field CF_{22} inherits all of the properties of CF_{21}. However, as material flows in, CF_{22} computes the change in free enthalpy Δg_{mixed}^{id} in accordance with Equation 5, and thereby, the free enthalpy g_2^{mix} of CF_{22} changes. This change produces the required Δg_2, which in turn leads to an entropy flow $\Delta \dot{S}_{id_2}^{mix}$ into CF_{22}, which changes the specific entropy of the mixture.

What happens to CF_{12}? Since there is no mass flow of component M_1, no mixing entropy is produced. Yet, the entropy of the mixture changes, and consequently, T and p of CF_{12} will temporarily change. Now the equilibration elements between CF_{12} and CF_{22} become active, which equilibrate T and p, and in the process generate the additional mixing entropy required. In steady state, the temperature T and the pressure p of both CF_{12} and CF_{22} resume approximately their original values, and the total mixing entropy added to the mixture corresponds to that needed in accordance with Equation 4. The equilibration acts as a P-controller. There may remain a final bias, because, as soon as the total mass transfer into the mixture has taken place, there is no mechanism left to equilibrate the free enthalpy values, and a $\Delta g_2 \neq 0$ may remain that does not generate any entropy flow, since by now, the mass flow $\dot{M}_2$ is equal to zero.

In the worst case, the entire mass M_2 is added to the mixture in a single Dirac event. Consequently, the mass flow $\dot{M}_2$ is zero except during the event, when it is infinitely large. During the event, the entire mixing entropy should be generated, but numerically, our code has no way of accomplishing this. In the simulation, the mixing entropy will remain zero, and the temperature T of the mixture will assume a lower value accordingly.

NON-IDEAL MIXTURES

Non-ideal mixtures are defined in such a way that now, changes in volume due to the mixture are also considered. For example, if wine is mixed with water, the volume of the mixture is smaller than the sum of the volumes of the components. However, if the mixing takes place in a closed system, the volume of the mixture must be the sum of the individual volumes, and consequently, the pressure of the mixture will now be smaller than the pressure of its components.

Figure 5 shows the generation of mixing entropy in this case. Since T and p are no longer constant, additional energy flows $\Delta p \cdot q$ and $\Delta T \cdot \dot{S}$ are generated that result in two additional entropy flows into the CF-element of the mixture.

It can be seen that the process of mixing makes use of the general RF-element as introduced in (Greifeneder and Cellier 2001a). Evidently, entropy gets generated by means of the mRS-elements until the temperature of the mixture equals that of the components. If the components are at different temperatures (cold milk getting poured into hot coffee), the temperature of the mixture assumes a tem-
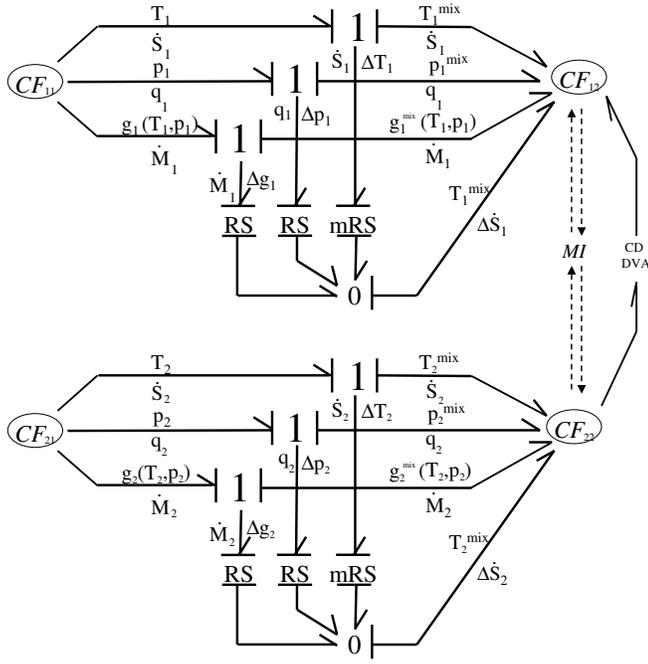
Figure 5: Entropy of Mixing in Non-ideal Closed Mixtures

perature in between those of the two components. Since the entropy flow is dictated by the mass flow, one of the mRS-elements "consumes" entropy (assumes a negative R-value), whereas the other generates it. Notice that the entropy "consumption" in one of the mRS-elements of the thermal domain is perfectly consistent with thermodynamics, since it is always overcompensated for by the generation of entropy in the other mRS-element. The reader is reminded that the separation of a mixture into component C-fields is only a mathematical construct, not physical reality.

In practice, the non-ideal mixture usually takes place in an open environment, i.e., the pressure remains constant, whereas the volume gets reduced. This process can be modeled as depicted in Figure 6.
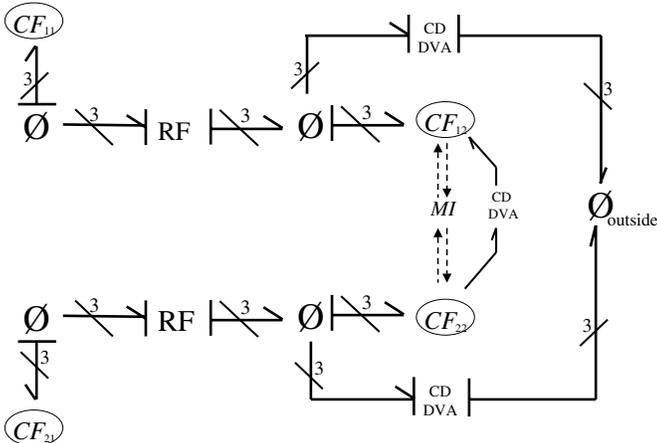

Figure 6: Entropy of Mixing in Non-ideal Open Mixtures

The CD-elements to the environment ensure that the temperature of the mixture approaches that of the environ-

ment, whereas the DVA-elements ensure that the pressure of the mixture, in steady state, equals that of the environment.

In the simulation code, these bond graphs are implemented as follows. The *specific excess volume* v^{Ex} and the *specific excess entropy* s^{Ex} of a non-ideal mixture are tabulated in the literature as functions of temperature and pressure. Given the current temperature T and the pressure p of the mixture, these quantities can be computed. Using these values, T and p can be corrected as follows:

$$T = T(v + v^{Ex}, s - s^{Ex}) \qquad (11)$$
$$p = p(v + v^{Ex}, s - s^{Ex}) \qquad (12)$$

A non-linear iteration takes place until T and p no longer change. These are the values that the mixture CF-elements put out initially. In general, both the temperature and the pressure will reduce their values during the initial iteration.

As a consequence, the RS-elements start to generate entropy, which flows into the mixture, and raises both the temperature and the pressure again. As long as the mass flow into the mixture continues, the temperature and pressure will rise, as additional entropy gets generated. In the steady state, the sum of the three entropy flows into the CF-element, $\Delta \dot{S}$, adds up to zero. At that time, the temperature is above that of the ideal mixture, whereas the pressure is still below that of the ideal mixture. The lower pressure is what is expected to happen in a closed system. The higher temperature is needed to compensate for the entropy generated by the difference in pressures of the unmixed and the mixed components. This phenomenon is often referred to as the *heat of mixing*. Temperature and pressure only get adjusted to the values of the environment if the CF-elements of the mixture exchange energy with the environment, as shown in Figure 6.

MULTI-ELEMENT MULTI-PHASE SYSTEMS

The authors propose to model each phase independent of the others (cf. the section on RF-elements in multi-element systems), and neglect influences of secondary importance as needed. This approach is meaningful, as the equilibration elements (the CD-elements and DVA-elements) have a tendency to stabilize the system and to reduce the importance of secondary effects.

By decoupling the phases, the fluid and gaseous phases may assume different flow velocities, which is commonly the case.

Figure 7 shows a system consisting of two components, each with a fluid and a gaseous phase traveling along a pipe that is compartmentalized. Only two compartments are shown.

The bottom half of the graph shows the fluid phase, whereas the top half depicts the gaseous phase. The left half shows one compartment, whereas the right half shows the other.
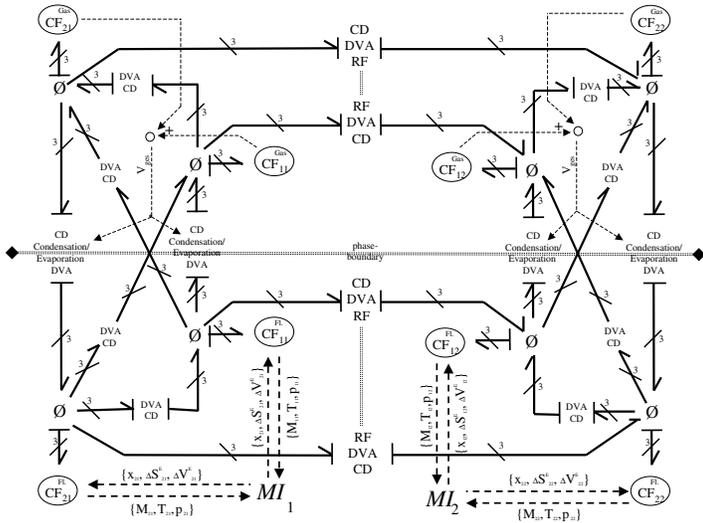
Figure 7: Model of a Two-element, Two-phase, Two-compartment Convective System

Figure 8: Simplified Pressure Cooker Model with Two Gaseous Phases and a Single Fluid Phase

The vertical bonds show the exchange of energy between the different phases of the same components. Beside the usual equilibration elements, thermal conduction and volume equilibration, also condensation and evaporation are being modeled (Greifeneder and Cellier 2001b). Activated bonds are used to indicate that the condensation and evaporation elements require knowledge of the overall volume to determine their own partial pressures.

The horizontal bonds show the convective flows from one comparment to the next. Beside from the equilibration elements, each phase uses coupled RF-elements to describe the convective flows. No KA-Elements were introduced, because diffusion effects are of second order small in the given context, and can therefore be neglected.

The diagonal bonds show secondary effects of temperature and volume interchange between two components, one in its fluid phase and the other in its gaseous phase.

Mixture information (MI) elements are shown for the fluid phase only, as the gases are assumed ideal.

MODEL OF A PRESSURE COOKER

As an example of the theory discussed in this paper, the model of a pressure cooker is being presented[3].

In a first approximation, the pressure cooker can be represented as shown in Figure 8. When the pressure cooker is heated, more and more of the water turns into steam by means of evaporation. The air component of the gas phase is needed to provide the pressure cooker at room temperature with the pressure of the environment. Without the air, some water would have to evaporate even at room tem-
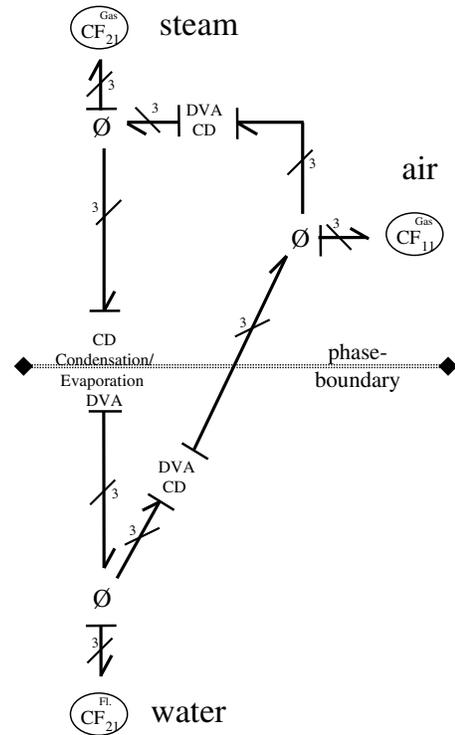
perature in order to produce equilibrium pressure, which would be considerably lower than 1 bar.

A more complete, yet more stylized, model is shown in Figure 9. Here, each bubble represents one component, i.e., one C-field together with its vector 0-junction. Beside from water, steam, and air, two more gaseous components were added, representing both air and steam in the boundary layer close to the wall of the pressure cooker. Thus, the gaseous phase has now two compartments, one representing the inside of the pressure cooker (the bulk), the other representing the boundary layer close to the wall. This compartmentalization was necessary, since the assumption of the entire gaseous phase being homogeneous is untenable, as it would lead to poor simulation results. At some point in time, the authors also considered the inclusion of air bubbles in the water and of water droplets in the air, but it was decided that the influences of these additional components were of second order small.

Air and steam were modeled as ideal gases. The inaccuracies associated with this assumption are of second order small. The assumption has the advantage, that the partial pressure of the steam can be computed easily as $p_{steam} = \frac{p \cdot V}{V_{steam}}$. The disadvantage of this solution is that the temperature and pressure tables for liquid water had to be slightly corrected in the vicinity of the boiling point in order to provide a clean transition to the gaseous phase.

The usual equilibration elements (the CD-elements and DVA-elements) were included between water and steam, between water and air, as well as between steam and air, both in the bulk and in the boundary layer. Only CD-elements were used between the two compartments (bulk and boundary layer), because the convective transport be-

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[3] The pressure cooker, a multi-phase, multi-element system, had already been used as example of a multi-phase system in (Greifeneder and Cellier 2001b), because multi-phase systems of a single element are hardly physical due to pressure/volume restrictions. However, lacking the multi-element-theory, the model could not be discussed in detail, which shall be done now.

tween these two layers (RF-elements) is driven by the pressure difference between these two layers. Hence the DVA-element and the RF-element would be competing for the equilibration of pressure, and a DVA-element is not needed since the RF-element will accomplish the desired equilibration of pressure. To model the necessary diffusion processes between the same elements of neighboring compartments, responsible for the equilibration of their concentrations, KA-elements were placed in parallel with the RF-elements for air and steam between the bulk and the boundary layer.
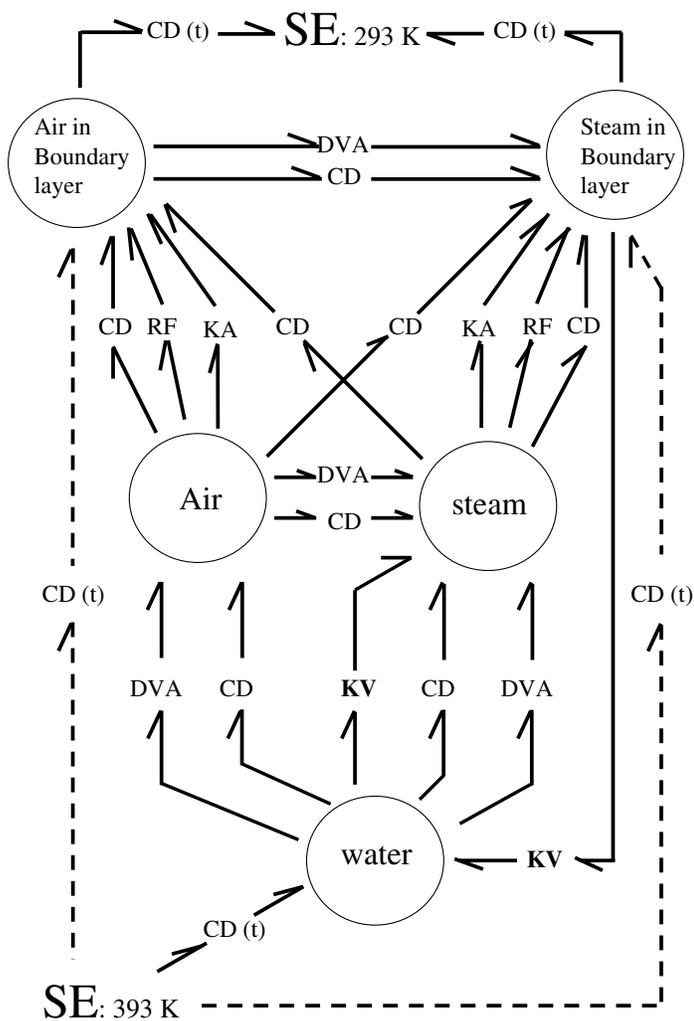

Figure 9: Stylized Bond Graph Model of the Pressure Cooker [4]

Additional CD-elements were included between steam in the bulk and air in the boundary layer and vice-versa. Evaporation and condensation (KV-element) take place between the water and the steam in the bulk. Condensation takes also place along the wall, i.e., between the steam in the boundary layer and the water. The SE-element at the bottom of Figure 9 represents the heating element, whereas

the SE-element at the top represents the cooling of the pressure cooker by letting cold water flow over it. Mixture information (MI) elements are not shown in Figure 9 for reasons of clearity. However, they are needed, first to provide the KV-elements with the total volume of the corresponding gaseous compartment and second to provide the RF-Elements with the information necessary for the diffusion process.

The following simulation experiment was conducted. At $time = 0$, the pressure cooker, which at that time is at room temperature, $(T \approx 293K)$, and has just been closed, $(p \approx 101kPa$, humidity $\approx 0.5)$, is placed on a hot surface $(T = 393K)$. As expected, both pressure and temperature rise. The pressure release valve, that would prevent a real pressure cooker from exploding, was omitted from the model. It was assumed that the walls are strong enough to withstand arbitrarily high pressure values. 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 in the bulk starts somewhat later.

Figure 10 shows the temperature trajectories of the five components as functions of time. During the heating phase, the five temperatures are almost identical. During the cooling phase, the boundary layer cools down most rapidly, the bulk follows somewhat more slowly, and the water cools down last.
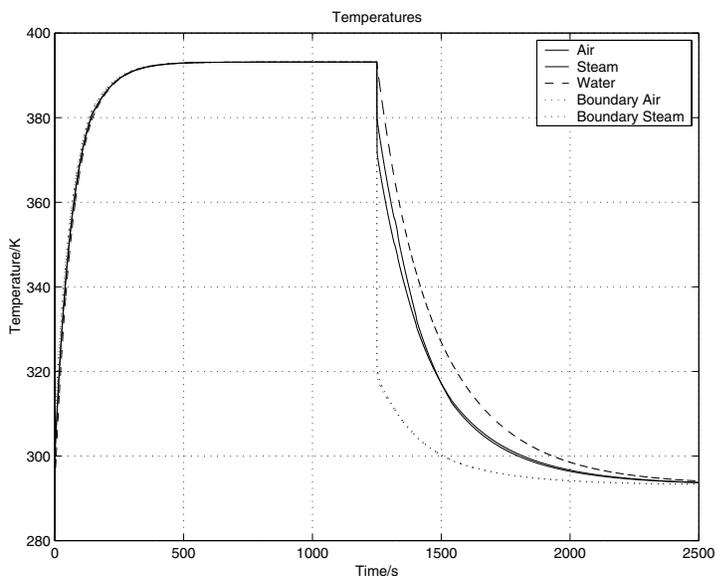

Figure 10: Temperature Graphs of the Simulated Pressure Cooker

Figure 11 shows the pressure trajectories. The pressure of the bulk is indistinguishable from that of the fluid phase. Only the boundary layer exhibits temporarily a pressure different from that of the other components. During the heating phase, all pressures are indistinguishable from each other. The knee in the curve (roughly at time 150 sec) represents the point where the water begins to boil. At that point in time, the temperature has reached a value of roughly 380 K, which, at a pressure of 130 kPa, indeed corresponds to the boiling point of water. During

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[4]The directions of the bonds are arbitrary. They were chosen from left to right and from the bottom up to coincide with positive power flows during the heating phase, except for those bonds describing condensation phenomena, where the direction of natural energy flow was chosen.

the cooling phase, the pressure in the boundary layer drops temporarily below that of the bulk, because the boundary layer cools down more rapidly than the bulk, and because water condensates more rapidly in the boundary layer, and the two RF-elements cannot resupply the boundary layer with air/steam mixture from the bulk arbitrarily fast.
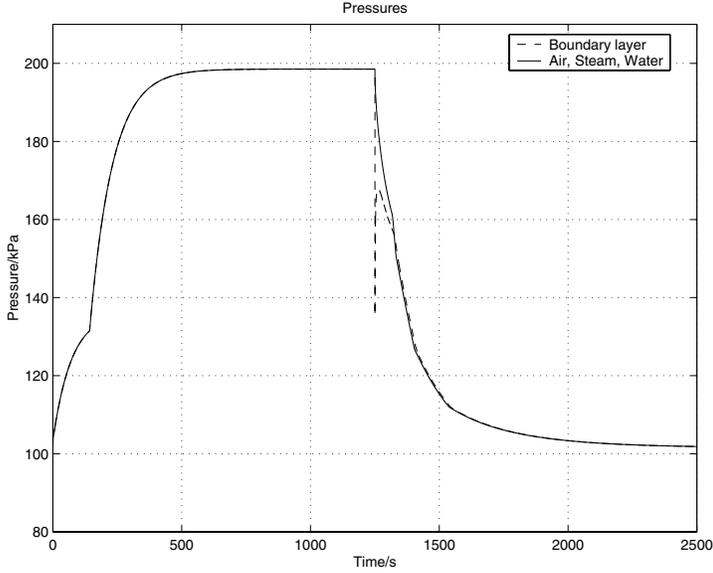

Figure 11: Pressure Graphs of the Simulated Pressure Cooker

Figure 12 shows the humidity trajectories of bulk and boundary layer. Humidity is defined as

$$\varphi = \frac{p_{steam}^{partial}}{p_{sat}^{H_2O}} \qquad (13)$$

whereby $p_{steam}^{partial}$ is the partial pressure of the steam, and $p_{sat}^{H_2O}$ is the saturation pressure of water at the given temperature.
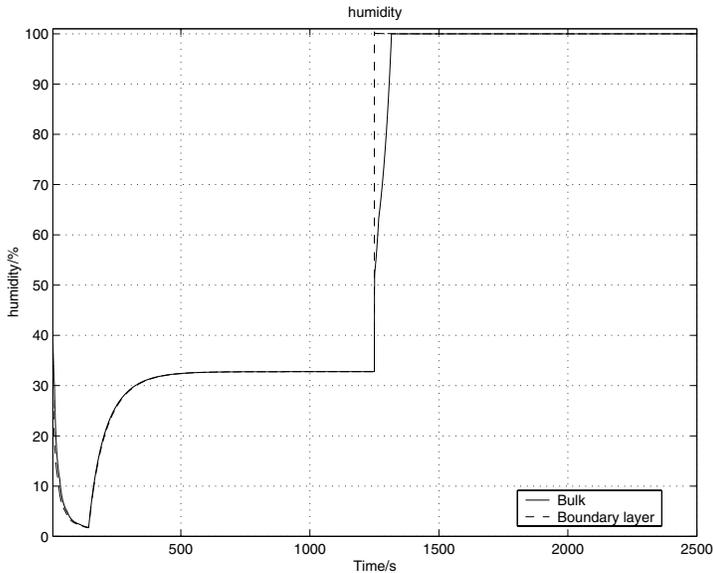

Figure 12: Humidity Graphs of the Simulated Pressure Cooker

The humidity is initially identically in both compartments. During the first part of the heating phase, the humidity decreases, as the saturation pressure – located in the denominator of the humidity – has the same gradient as the rising temperature. Small differences can be seen, as the boundary layer heats up a bit faster than the bulk, and therefore, its humidity decreases faster. The humidity starts climbing again after approximately 150 seconds. This is caused, just like the knee in the pressure trajectories, by the fact that the water begins to boil at this time. As the temperatures of the system no longer increase much and since additional steam will be present in the gaseous phase, the humidity in both compartments rises until it reaches an equilibrium state of approximately 32.75%.

As, with the beginning of the cooling phase, the temperatures in the boundary layer drop down rapidly, the corresponding humidity quickly reaches 100%, and dew starts to form on the cold surface of the pressure cooker. Now, the two gaseous compartments are no longer identical in their compositions, and therefore, diffusion occurs. The (slower) cooling down of the bulk together with the diffusion between the bulk and the boundary layer pull the humidity of the bulk up, until, roughly at time 1315 sec, the humidity of the bulk reaches 100%, and steam starts to condensate directly via the phase boundary.

The humidity inside the pressure cooker will remain at 100% until the end of the simulation, as the only way to lower the humidity would be to raise the temperature again, or open the pressure cooker.

Figure 13 shows the mass fractions of steam in the two gaseous compartments. The mass fraction of steam is defined as:

$$\varpi_{steam} = \frac{m_{steam}}{m_{steam} + m_{air}} \qquad (14)$$

i.e., it defines the percentage of steam contained in the gaseous phase.
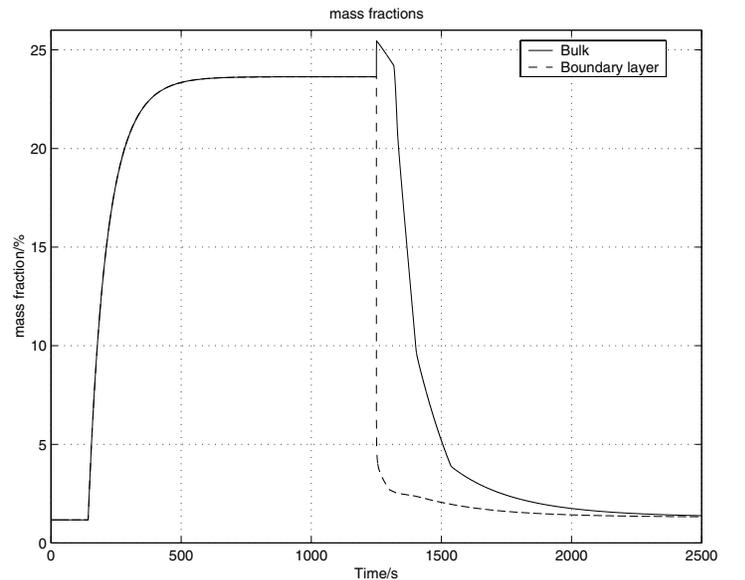

Figure 13: Mass Fractions of Steam in the Two Gaseous Compartments

The initial value of ϖ_{steam} is defined by the humidity of the air at the time when the pressure cooker is closed. It

stays constant, until, at time 150 sec, the water begins to boil. It then rises until the new flow equilibrium is reached. At that time, the percentage of steam in the gaseous phase has reached a value of 23.6%. When cooling starts, the boundary layer cools down more rapidly than the bulk. Also the pressure of the boundary layer drops more rapidly than that of the bulk. However, the pressure equilibrates much more rapidly than the temperature. Thus, the pressure in the bulk (and in the water) decreases more rapidly than the temperature, the boiling point of the water decreases, and consequently, additional water boils off. As a consequence, the mass fraction of steam in the bulk rises temporarily. However, the mass fraction starts dropping again due to pressure equilibration and diffusion. At time 1315 sec, steam starts to condensate from the bulk, and consequently, the mass fraction drops sharply. The final equilibration of the two mass fractions occurs primarily by means of diffusion.

CONCLUSIONS

The paper discusses different aspects of the rather complicated processes of modeling multi-element systems. It was found that modeling each element separately as a storage element (a C-field), and connecting them by means of dissipative elements (R-fields) simplifies the modeling task, offers insight into the physical functioning of multi-element systems, and leads to mathematical models that can be simulated in a numerically stable and highly accurate fashion.

The modeling methodology, as discussed in this paper, is still limited to multi-element systems without chemical reactions. The discussion of the latter may, in the future, form a paper on its own. The thermodynamics of chemical reaction systems were discussed already in (Greifeneder 2001).

The example of a pressure cooker was used to illustrate the functioning of the methodology, and to demonstrate the practicality of the advocated approach to modeling.

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AUTHOR BIOGRAPHIES

JÜRGEN A. GREIFENEDER is studying Technische Kybernetik (Engineering Cybernetics) at the University of Stuttgart, Germany. At the moment, he is working on his Diplomarbeit (final project), and expects to graduate withing the next six months. Mr. Greifeneder's main scientific interests concern modeling, simulation, and control methodologies. In 1999/2000, Mr. Greifeneder spent a year as an exchange student with the University of Arizona, where the foundations for the research effort presented in this paper as well as the previous two papers were laid.

FRANÇOIS E. CELLIER received his B.S. degree in Electrical Engineering from the Swiss Federal Institute of Technology (ETH) Zürich in 1972, his M.S. degree in Automatic Control in 1973, and his Ph.D. degree in Technical Sciences in 1979, all from the same university. Following his Ph.D., Dr. Cellier worked as a Lecturer at ETH Zürich. He joined the University of Arizona in 1984 as Associate Professor, where he is currently a Full Professor of Electrical and Computer Engineering. Dr. Cellier's main scientific interests concern modeling and simulation methodologies, and the design of advanced software systems for simulation, computer-aided modeling, and computer–aided design. Dr. Cellier has authored or co-authored more than 200 technical publications, among them a textbook entitled *Continuous System Modeling*, published by Springer-Verlag, New York in 1991. Dr. Cellier has organized numerous international conferences on Modeling and Simulation. Most notably, he was one of two co-founders of the *International Conference on Bond Graph Modeling and Simulation*, a series of conferences organized bi-annually by SCS, which has become the most important event related to bond graphs worldwide. Dr. Cellier currently serves as Vicepresident of Conferences of the Society for Modeling and Simulation, SCS.