Modeling Convective Flows Using Bond Graphs

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Abstract

This article, together with two companion papers, offers a general methodology for modeling thermodynamical phenomena using true, rather than pseudo-, bond graphs. This paper deals in particular with the difficult problem of modeling mass flows in a thermodynamic sense, i.e. with the formulation of mathematical models of convective flows. 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.

Keywords: Thermodynamics; Convection; Bond graphs.

1 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 bondgraphic 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, convection 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 bondgraphic macro-elements are introduced to describe the energy storage within a compartment as well as the mass (and energy) flow between neighboring compartments.

2 THE C-FIELD (CF)

2.1 Choice of variables

Analysing the energy balance of a compartment, three different components can be distinguished: mass flow into and out of the compartment, heat exchange between neighboring compartments, and mechanical work. Three independent (state) variables are needed to describe a thermodynamical system – one more than for mechanical or electrical systems. Traditionally, temperature T, pressure p, and mass M are used as basic state variables, from which the specific terms of e.g. entropy s and enthalpy h are being calculated.

For each of the three state variables, T, p, and M, a corresponding adjugate variable can be found, such that the product of the two adjugate variables represents a facet of (co-)energy stored in the compartment. These are the entropy S for the temperature, the volume V for the pressure, and the free (or Gibbs') enthalpy $g = h - T \cdot s$ for the mass.

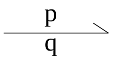

Figure 1: pneumatic-hydraulic power track

Since the pneumatic (hydraulic) bond is already defined in mechanics, as shown in Fig. 1, as temperature clearly defines a potential and not a field variable, whereas the mass intuitively has flow characteristics, it makes sense to use $\dot{S}$, $\dot{M}$, and q as flow variables, with T, g, and p being identified as the corresponding (adjugate) effort variables (it makes sense, to use g and not the enthalpy $h = g + T \cdot s$ as the effort variable, as a separate T,s-bond has already been defined [1]).

2.2 Computation of variables

Breedveld showed [2] that no inductance can exist in a thermal system, i.e. only flows can be accumulated. Therefore from a bondgraphic perspective, it makes sense to define the flow variables as the (independent) state variables, whereas the effort variables are indirect variables, i.e. they are dependent on the state variables.

$$\frac{dM}{dt} = \dot{M} \tag{2.1}$$

$$\frac{dS}{dt} = \dot{S} \tag{2.2}$$

$$\frac{dV}{dt} = \dot{V} = q \tag{2.3}$$

According to physics, none of the six variables T, S, p, V, g, and M can ever become negative. A compartment can only be emptied. Once empty, nothing further can be removed from the compartment. However, this can happen in a simulation due to numerical inaccuracies. It may therefore be better to define e.g. the mass of a system (analogous for volume and entropy) as

$$M = \max\{\epsilon, \int_{t_0}^{t} \dot{M}\, dt\}$$

where ϵ is a large enough number, such that divisions by M will still result in stable solutions.

The three different aspects of stored (co-)energy must not be treated as independent storage elements. If this were true, i.e., if the the three aspects could be modeled by three separate conventional capacitors, it would follow that: $T = T(S)$, $p = p(V)$, and $g = g(M)$. Evidently, at least the third of these equations is clearly in error, as a intensive variable (g) must not depend on the mass. Assuming incompressible fluids, the temperature equation would be correct, as $ds = c_p dT$. However, this would limit the generality of the envisaged approach to modeling. For the pressure, the situation is similar.

The reader may recall that any thermodynamical system can be completely described by two intensive and one extensive variables. That is exactly what the proposed three state variables are.

$$T = T(\frac{S}{M} = s, \frac{V}{M} = v) \tag{2.4}$$

This equation can be derived using the total differential:

$$dT = \left(\frac{\partial T}{\partial s}\right)_v ds + \left(\frac{\partial T}{\partial v}\right)_s dv \tag{2.5}$$

Using one of Maxwell's equations:

$$\left(\frac{\partial T}{\partial v}\right)_s = -\left(\frac{\partial p}{\partial s}\right)_v \tag{2.6}$$

and converting it as follows, whereby c_v is the 'constant volume heat capacity,'

$$\left(\frac{\partial T}{\partial v}\right)_s = -\left(\frac{\partial p}{\partial T}\right)_v \left(\frac{\partial T}{\partial s}\right)_v \tag{2.7}$$

$$\left(\frac{\partial T}{\partial s}\right)_v = \underbrace{\left(\frac{\partial T}{\partial u}\right)_v}_{=\frac{1}{c_v}} \cdot \underbrace{\left(\frac{\partial u}{\partial s}\right)_v}_{=T}, \tag{2.8}$$

the equation for the temperature can be determined as follows:

$$dT = \frac{T}{c_v} \cdot \left[ds - \left(\frac{\partial p}{\partial T}\right)_v dv\right] \tag{2.9}$$

For an ideal gas, the above equation can be converted to the well-known caloric state equation:

$$ds = \frac{c_v}{T} dT + R \cdot \frac{dv}{v} \tag{2.10}$$

Unfortunately, a (thermal) equation of state is also needed. If available, the pressure can be directly computed ($p = p(M, V, T)$). Lacking an equation of state, interpolation tables will have to be used instead. In this case, the total differential is not needed, as $\{T, p\} = \{T, p\}(v, s)$ can be directly obtained by interpolation[1].

Last not least, the equation for the free enthalpy must be determined. If a corresponding interpolation table is available, it may be easiest to use that table. Otherwise, another total differential may be used. Ultimately, an equation $g(v, s)$ is needed; however, since T and p have already been computed, it may be more convenient to determine $h(T, p)$, and then compute $g = h - T \cdot s$.

$$h(p_1, T_1) = \underbrace{h(p^0, T^0)}_{energy\ of\ formation} + \int_{T^0}^{T_1} \underbrace{\left(\frac{\partial h}{\partial T}\right)_{p^0}}_{=c_p} dT + \\ + \int_{p^0}^{p_1} \left(\frac{\partial h}{\partial p}\right)_{T_1} dp \tag{2.11}$$

Commonly a polynomial approach is used to determine the specific heat c_p. The variables $\alpha, \beta, \gamma, \delta$ are mostly constant and tabulated for $p = 1\ bar$.

$$c_p(T, p^\diamond) = \alpha(p^\diamond) + \beta(p^\diamond) \cdot T + \gamma(p^\diamond) \cdot T^2 + \delta(p^\diamond) \cdot T^3 \tag{2.12}$$

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[1] As most tables are provided in the form v,s(T,p), it may be necessary to first built $T(p, v)$ and $T(p, s)$ and find the value of p, for which $T(p, v) = T(p, s)$. This problem has an unique solution. To save time, this conversion should be done off-line once and for all, and not be implemented as part of the simulation algorithm.

For $p^\diamond \neq p$, Eq. 2.11 should be replaced by

$$h(p_1, T_1) = h(p^0, T^0) + \int_{T^0}^{T_1} \left(\frac{\partial h}{\partial T}\right) dT + \\ + \int_{p^0}^{p^\diamond} \left(\frac{\partial h}{\partial p}\right)_{T_0} dp + \int_{p^\diamond}^{p_1} \left(\frac{\partial h}{\partial p}\right)_{T_1} dp \tag{2.13}$$

2.3 Overall model

To represent the relationships between the storage (flow) and potential (effort) variables, a new bond graph element (Fig. 2) is introduced. It is called *capacitive field*, or *C-field*, and is introduced in the bond graph as the **CF**-element[2].

It is important to mention that specific material properties shall be modeled within the C-field only. All other elements will be totally generic.

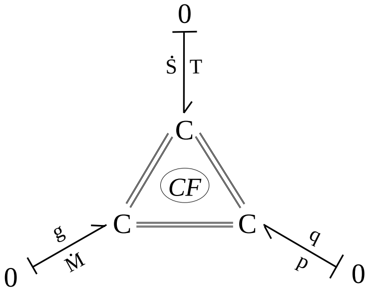

Figure 2: bond graph representation of the C-field

Analysing the $\{p/q\}$-bond properties, it may be noticed that a system loses energy for a positive volume flow and gains energy for a negative one. In order to avoid this asymmetry, the authors of this paper decided to define the pressure as *negative*. For example, the equation of state of the ideal gas is written as $R \cdot T = -p \cdot V$. In this way, the balance of the C-field becomes:

$$\frac{dU}{dt} = T \cdot \dot{S} + p \cdot \dot{V} + g \cdot \dot{M}, \tag{2.14}$$

This equation can be graphically interpreted as the sum over all bonds connecting to the C-field.

The kinetic energy of the CF-element has not been modeled, as the element is supposed to be stationary in space. The potential energy can easily be taken into account by adding E_{pot} to g; however in this case, the C-field must 'know' its own vertical position in space. Radiation can be included by modeling the entropy-cut of the C-field accordingly.

The equations of a C-field for air, using the assumption of an ideal gas, are as follows:

$$\frac{dM}{dt} = \dot{M} \qquad \frac{dS}{dt} = \dot{S} \qquad \frac{dV}{dt} = q \tag{2.1--2.3}$$

$$dT = \frac{T}{c_v} \cdot \left(ds - R \cdot \frac{dv}{v}\right) \tag{2.15}$$

$$p = -\frac{R \cdot T}{V} \tag{2.16}$$

$$dh = c_p dT \tag{2.17}$$

$$g = h - T \cdot s \tag{2.18}$$

$$c_v = c_p - R \tag{2.19}$$

$R = 0.2872 \frac{kJ}{kg \cdot K}$ and $c_p = 1.004 \frac{kJ}{kg \cdot K}$.

3 CONDUCTION (CD)

Conductive heat flow $\dot{Q}$ can be represented in a bond graph as a purely thermal phenomenon using bonds with T as effort and $\dot{S}$ as flow variables. If the C-field is exposed to such a heat flow only, then $\dot{M} = q = 0$ and $\frac{dS}{dt} = \dot{S} = \frac{\dot{Q}}{T}$. This is consistent with the second fundamental equation of thermodynamics (balance of entropy without mass flow).

Heat flow only occurs between two connected C-fields at different levels of temperature. The heat flow from the C-field located at the higher temperature to the C-field located at the lower temperature is proportional to the difference of temperatures and to the heat transfer coefficient λ:

$$\dot{Q} = \lambda \cdot (T_1 - T_2) \tag{3.1}$$

The entropy flows can be graphically depicted as shown in Fig. 3.

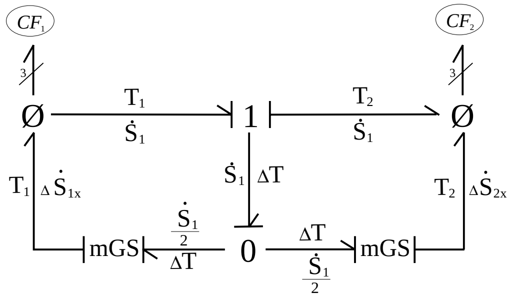

Figure 3: modelling heat flows

The **mGS**-element is a conductive source element [3] with a thermal primary side. The m denotes the

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[2] CF-fields have been previously used in the bondgraphic literature, but their purpose was simply to describe a network of conventional, i.e., independent, capacitors.

fact that the element is modulated, as the conduction G depends on the temperature:

$$G_{CD} = \frac{\lambda}{T_1 + T_2} = \frac{\lambda}{2 \cdot T_1 - \Delta T} = \frac{\lambda}{2 \cdot T_2 + \Delta T} \tag{3.2}$$

The notation is adopted from [1]. The authors prefer to use an mGS-element rather than an mRS-element because of the fixed causality of the autgoing bond. The secondary side of the mGS-element always represents an entropy (i.e., flow) source, and never a temperature (i.e., effort) source. The primary side of each mGS-element computes Ohm's law as follows:

$$\frac{\dot{S}_1}{2} = G_{CD} \cdot \Delta T \tag{3.3}$$

whereas the secondary sides compute the power flow continuity across the mGS-elements:

$$\Delta \dot{S}_{1x} = \frac{\dot{S}_1}{2} \cdot \frac{\Delta T}{T_1} \tag{3.4}$$

$$\Delta \dot{S}_{2x} = \frac{\dot{S}_1}{2} \cdot \frac{\Delta T}{T_2} \tag{3.5}$$

Heat flow is a dissipative phenomenon. In the process, additional entropy (but not heat) is being generated in the amount of $\Delta \dot{S}_{1x} + \Delta \dot{S}_{2x}$.

The reader may notice that the heat flow from the first to the second C-field is indeed:

$$\dot{Q} = T_1 \cdot (\dot{S}_1 - \Delta \dot{S}_{1x}) = T_2 \cdot (\dot{S}_1 + \Delta \dot{S}_{2x}) = \lambda \cdot \Delta T \tag{3.6}$$

as expected.

The conductive heat flow of Fig. 3 can be represented by a new macro bond element, the **CD**-element, as shown in Fig. 4.

Figure 4: Iconized conduction element

If one of the two C-fields is located outside the system, that C-field can be replaced by a one-port SE-element. Alternatively, the external C-field can be neglected, replacing the CD-element by a one-port SF-element.

4 VOLUME WORK AND EQUILIBRATION OF PRESSURE (DVA)

Ideal volume exchange does not pose any problem, as it is reversible and therefore does not generate entropy. In addition to this forced volume flow, there also exists a volume flow that is driven by differences between the pressure of two connected C-fields. An example for this phenomenon would be two systems, separated by a movable wall or membrane. It can be concluded that there will take place only a single volume flow, i.e., that the volume leaving the first system must be added to the second one.

Such a volume-exchange flow is proportional to the pressure difference and is of a dissipative nature (the power $\Delta p \cdot q \geq 0$ will be converted to heat).

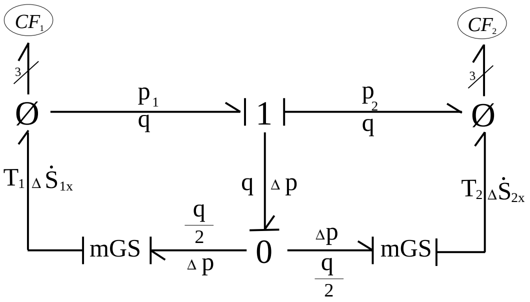

Figure 5: bond graph representation of the DVA-element

As in the case of conductive heat flow, the generated entropy will be distributed equally to both sides (Fig. 5).

The overall effects of pressure equilibration can be represented by a new bondgraphic macro element, the **DVA**-element.

Figure 6: Icon-representation of fig. 5

The attentive reader may have discovered that a triple bond, a so-called *bus-bond*[3], (Fig. 7) was used in the iconized representation (Fig. 6). As no mass flow takes place during pressure equilibration, the mass flow is set equal to zero.

The equations of the DVA-element can be summarized as follows:

$$\dot{M} = 0 \tag{4.1}$$

$$q = G_{DVA} \cdot (p_2 - p_1) \tag{4.2}$$

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[3] The literature mentions vector-bonds and multibonds as means to describe sets of bonds. However, these are used for the compact treatment of threedimensional mechanics, whereby each strand denotes one space dimension. In order not to confuse these different concepts, the authors of this paper decided on a different notation, borrowed from digital electronics, where multiple signal paths are connected into a signal bus. The bus-bond connects multiple power paths of different type into a single power bus.

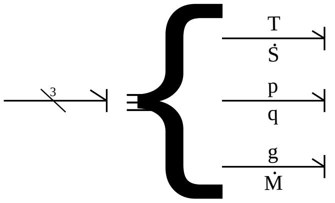

Figure 7: Bus bond

$$S_1 = \frac{q \cdot (p_2 - p_1)}{2 \cdot T_1} \tag{4.3}$$

$$S_2 = \frac{q \cdot (p_2 - p_1)}{2 \cdot T_2} \tag{4.4}$$

5 CONVECTION: THE R-FIELD

5.1 Introduction

So far, the paper only discussed entropy and volume flows, but did not use the third cut of the C-field: the mass flow. Unfortunately, mass flows are not independent (as entropy and volume flows could be), because mass has a volume and is carrying enthalpy. Obviously, it would have been possible, to model this by using a single bond (effort: (internal energy) $u = g+T \cdot s+\frac{p}{\rho}$; flow: $\dot{M}$), but in that case, a vector of *information* consisting of $\begin{pmatrix} T & p & \rho & s \end{pmatrix}$ would have to accompany the power flow, such that the internal energy bond could be decomposed into its components again further down the road.

Another possibility would have been to adopt the notation of Brown [4], who introduced a *convection bond*, whereby the power bond is given by $\{\mathrm{h},\dot{M}\}$ with

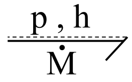

Figure 8: The convection bond introduced by von Brown [4]

the pressure superposed as information path. In our view, this approach carries three disadvantages:

- By superposing the pressure as an information path, the concept of pure power bonds is compromised.
- The decomposition of the enthalpy bond into a thermal bond and a mass flow bond at the entrance of the next compartment while recalculating the corresponding volume flow necessitates additional connection models. This complicates the modeling effort.
- Keeping track of mass flows from the entrance to the exit point of a compartment without an appropriate bondgraphic mass flow notation necessitates the introduction of additional information paths within the compartment models.

For these reasons, the authors decided to model mass flow phenomena as pure mass flows, i.e., with g as effort, and introduce the bus-bond as a convenient means to keep the accompanying volume and entropy flows together with the mass flow component in a compact power bus.

Will this make the use of activated bonds to describe information flows unnecessary? Unfortunately, this is not the case. Mass carries additional properties that may be needed in the computation of the mass flow characteristics, such as the density, ρ, and the total entropy contained in a C-field, S. These information paths will emanate from a C-field and end at the neighboring R-field downstream, i.e., they will stay fairly local. This is consistent with the fundamental principle of network theory [5], and could provide a hint for a future merger of these two ways of modeling physical systems.

Before the concept or the R-field is derived in detail, two additional notations need to be explained:

∅
describes a *bus-zero-junction.* Different busses can connect to a bus-zero-junction, whereby the normal rules of zero-junctions shall apply to each strang separately. If a regular bond (either thermic of hydraulic/pneumatic) is connected to a bus-zero-junction, it will be treated like a bus-bond with the other two bus-flow variables set to zero.

$\mathbf{0}_{T_i}$
This nomenclature is helpful for detail graphics. It represents the temperature-zero-junction of the CF-element named $'CF_i'$ (p, g will work analogously).

Using these abbreviations, an RF-schematic is provided in Fig. 9.

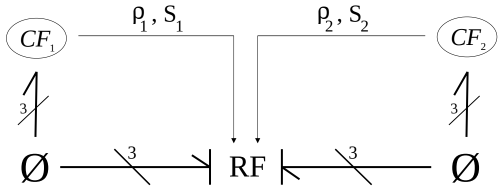

Figure 9: The resistive field

5.2 The basic RF model

For the time being, let us model the situation, where a fixed mass is being transported through a pipe at constant speed and without friction. The pipe is compartmentalized, such that each CF-element represents one section of the pipe. In this case, the following equations can be derived:

$$q = A \cdot v \qquad (5.1)$$

$$\dot{M} = q \cdot \rho \qquad (5.2)$$

Still missing is an equation for $\dot{S}$. Let us consider an amount Θ of a given homogeneous element with the mass M, the volume V, and the Entropy S (fig. 10). If a portion $\tilde{M}$ of this homogeneous mass is being cut off, that portion will obviously have the volume $\tilde{V} = \frac{\tilde{M}}{M} \cdot V$ and the entropy $\tilde{S} = \frac{\tilde{M}}{M} \cdot S$.

Generalizing to continuous infinitesimal flows, one can conclude:

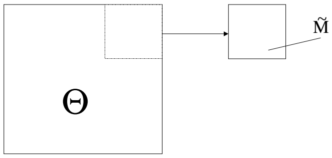

Figure 10: Cutting a portion $\tilde{M}$ off a given amount

$$\xi = \frac{\dot{M}}{M} \qquad (5.$$

$$\dot{S} = \xi \cdot S \qquad (5.$$

where ξ is the mass fraction.
To determine the flows leaving the R-field, it is knov that

$$\dot{M}_{out} \equiv \dot{M}_{in} \qquad (5.$$

because no mass is stored in the R-field. More ifficult is the case of the volume flow, as volume do not need to be preserved. Yet, it may make sen to assume volume preservation across the R-field, ar renegotiate the valume of an arriving flow at the ne: C-field downstream. Consequently, the volume flow is defined analogously to the mass flow:

$$\dot{V}_{out} = \dot{V}_{in} \qquad (5.6)$$

In this way:

- Mass, being transported from A to B, will arrive at B with the same volume that it had when leaving A, leaving it up to the C-field representing B to renegotiate its volume.
- The RF-element does not need to know, what volume flow $\dot{V}$ the mass flow $\dot{M}$ will have, after it got mixed with the mass at B.
- Modeling the case V_{CF} = const. (as it holds e.g. for pipes) inside the RF-element would not make much sense, as this would mean that there would be no volume flow at all. Furthermore, this would cause problems in section 5.3.
- Modeling volume changes within C-fields is more practical, as in this way, material properties can be mostly limited to individual C-fields, thereby minimizing the need for information flows (activated bonds) between neighboring bond-graph elements.

Last not least, the case of entropy flows across an R-field needs to be discussed. These flows constitute the most difficult case. Entropy certainly is not conserved. The R-field, in general, describes dissipation, and therefore, entropy is generated inside the R-field (fig. 11).

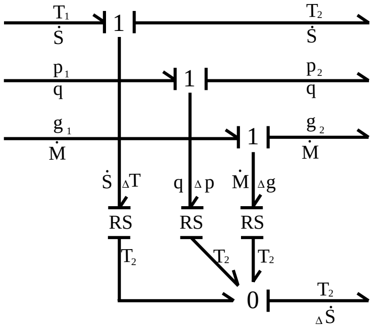

Figure 11: The R-field schematic

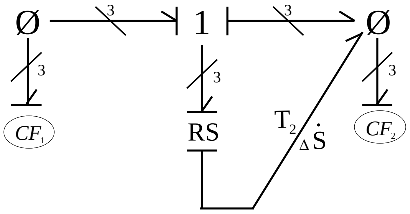

Figure 12: R-field schematic in bus-bond notation

If the two entropy flows $\dot{S}_{out}$ and $\Delta\dot{S}$ are combined, and if one takes into consideration that the R-field should be designed such that it can be used in both directions, a model as shown in figure 13 is obtained.

5.3 The general model

Up to this point, flows were supposed to have constant speed. As there is always friction, this was evidently a simplification. Based on the balance of impulses

$$\Delta p \cdot A = \Delta v \cdot \dot{M} \qquad (5.7)$$

a feedback loop of the pressure to the speed results, which is a function of the geometry of the pipe, the viscosity of the fluid, and the flow characteristics.
This leads to another simple generalization which accounts for varying cross-sections and the effects of

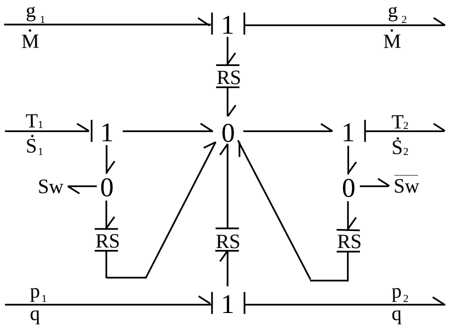

Figure 13: The R-field, considering both flow directions.

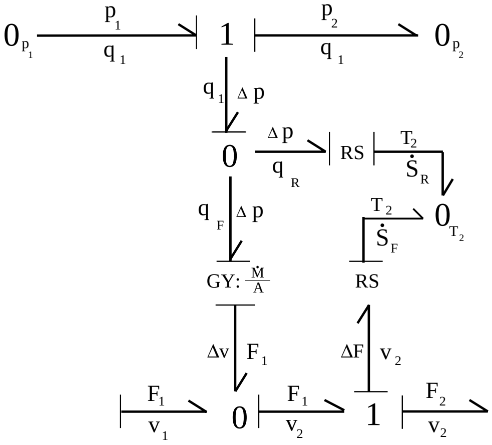

Figure 14: Hydraulic part of the RF-model

gravity.

$$p_1 \cdot A_1 - p_2 \cdot A_2 = \Delta v \cdot \dot{M} + cos\alpha \cdot G \tag{5.8}$$

where α is the vertical inclination of the flow.

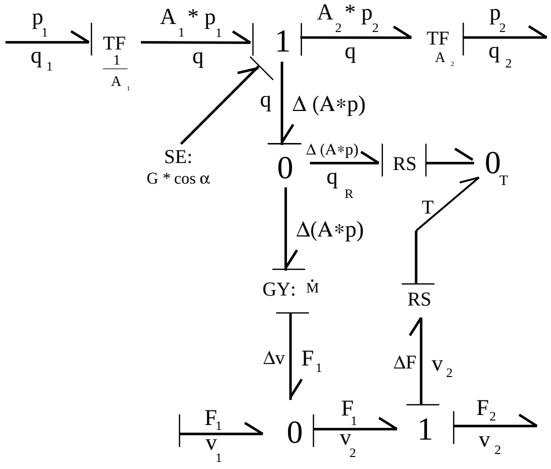

Figure 15: Part of the bond model of the generalized R-field.

5.4 Generalized Exchange Element

Merging the effects of the three previously introduced elements (CD – conduction, DVA – pressure and volume exchange, RF – convection), the following set of equations can be extracted from the combined bond graph:

$$q_{RF} = A \cdot v \tag{5.1}$$

$$q_{DVA} = R_{DVA} \cdot (p_2 - p_1) \tag{4.2}$$

$$q = q_{RF} + q_{DVA} \tag{5.9}$$

$$\dot{M} = q_{RF} \cdot \rho \tag{5.2}$$

$$\dot{S}_i^* = \frac{1}{T_i} \cdot \left(T_1 - T_2 + q \cdot \frac{p_1 - p_2}{2} \right) \tag{5.10}$$

$$\Delta \dot{ST} = q_R \cdot (p_1 - p_2) + \dot{M} \cdot (g_1 - g_2) + v \cdot (F_1 - F_2) \tag{5.11}$$

$$\dot{S}_1 = \begin{cases} \xi \cdot S_1 + \dot{S}_1^* & for \dot{M} > 0, \\ \frac{\Delta \dot{ST} + \dot{S}_2 \cdot T_2}{T_1} + \dot{S}_1^* & else \end{cases} \tag{5.12}$$

$$\dot{S}_2 = \begin{cases} \xi \cdot S_2 + \dot{S}_2^* & for \dot{M} < 0, \\ \frac{\Delta \dot{ST} + \dot{S}_1 \cdot T_1}{T_2} + \dot{S}_2^* & else \end{cases} \tag{5.13}$$

5.5 Special case: C-field with constant volume

Let us consider once more the example of the set Θ (fig. 10) where a part of the system $(\tilde{M}, \tilde{V}, \tilde{S})$ has been cut off. The remaining system will be characterized by $\{\mathrm{T}, \mathrm{p}, V^* = V - \tilde{V}, M^* = M - \tilde{M}, S^* = S - \tilde{S}\}$. Thinking of a leaking pipe or gas cylinder, the volume of which remains constant, a second setp is needed, in which the volume V^* of the remaining gas is expanded until it equals the volume V that the gas had occupied initially. The energy needed for this expansion must come from the inside of the C-field. This can be accomplished by making use of a controlled flow source that creates exactly the amount of volume that has left Θ. Considering the remaining energy balance (no mass flow)

$$0 = P + \dot{Q} \tag{5.14}$$

it is found that the flow source must be connected as a two port element to the temperature-entropy-cut of the C-field. The energy needed will thus be generated by a (reversible) entropy flow within the C-field, leading to a reduction of temperature in the pipe or gas cylinder, which is consistent with physical knowledge.

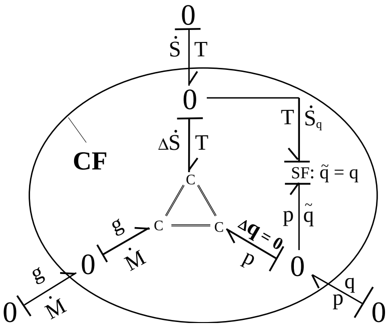

Figure 16: bond graph model for a constant CF-volume.

6 CONCLUSION

The elements introduced in this paper enable the modeler, to describe simple thermodynamical systems described by conduction and convection. The methodology introduced so far only deals with mono-elements and mono-phase systems. The description of multi-phase and/or multi-element systems is left to two companion papers [6] and [7].

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