# Chapter 3
Port-Based Modeling in Different Domains

C. Batlle, F. Couenne, A. Dòria-Cerezo, V. Duindam, E. Fossas, C. Jallut, L. Lefèvre, Y. Le Gorrec, B. M. Maschke, R. Ortega, K. Schlacher, S. Stramigioli, M. Tayakout

Abstract In this Chapter we present some detailed examples of modelling in several domains using port and port-Hamiltonian concepts, as have been presented in the previous chapters. We start with the electromechanical domain in Sect. 3.1, while in Sect. 3.2 it is shown how port-Hamiltonian systems can be fruitfully used for the structured modelling of robotics mechanisms. In Sect. 3.3, it is show how to model simple elastic systems either in the Lagrangian and Hamiltonian framework, while, in Sect. 3.4, an expressions of the models representing momentum, heat and mass transfer as well as chemical reactions within homogeneous fluids in the port-based formalism is proposed. To this end, the entropy balance and the associated source terms are systematically written in accordance with the principle of irreversible thermodynamics. Some insights are also given concerning the constitutive equations and models allowing to calculate transport and thermodynamic properties. As it will be shown, for each physical domain, these port-based models can be translated into bond-graph models, in the case of distributed as well as lumped parameters models.

3.1 Modeling of electrical systems

Electromechanical energy conversion has already been discussed in Sect. 1.9.3, and, in particular, the constraints imposed by energy conservation on the constitutive laws of the ports, Maxwell's relations, have been derived. As the name indicates, electromechanical systems (EMS) bridge the gap between the electrical and mechanical domains. In practice, on the electrical side one has an electric circuit of a very special class, what is called an *electronic power converter*, which, if the system is working as an electrical motor, takes the electrical energy from some source and provides a suitable voltage to the EMS so that the desired mechanical speed is reached; likewise, if the system acts as a generator, the power converter transforms the raw electrical energy into a form adapted for immediate use, storage or transportation. The main characteristic of electronic power converters is that they are *variable structure systems* (VSS). They contain a number of switches and diodes, of
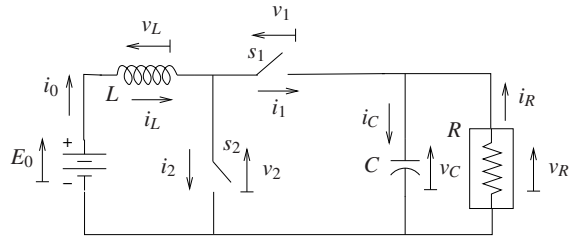
which the former can be opened or closed in a periodic manner by a suitable control algorithm, in order to effect the necessary electrical energy conversion.

Since electronic power converters are so important for EMS, and also for many other applications, such as portable equipment, energy supply systems in the aerospace industry, or uninterruptible power supply systems, we present first an explicit example of modelling of a power converter in the port-Hamiltonian framework. Next we discuss in detail the port-Hamiltonian description of a general EMS, and use it to describe an elementary electromagnet. Finally we couple both systems and display the complete port-Hamiltonian structure.

Although modelling of VSS in the port-Hamiltonian framework is straightforward, numerical simulation can be quite complex and time-intensive, due to the abrupt structure changes. Approximate, smooth models can be obtained from a VSS, using suitable averages of the state variables and the control signals. For completeness, we also present the simplest form of this averaging theory, which yields models which can be easily implemented in bond graph theory.

3.1.1 Electronic power converter circuits

Fig. 3.1 shows a functional model[1] of the boost (or elevator) converter (the detailed electronics of how the switches are implemented is not shown). The switches s_1 and s_2 are complementary: when s_1 is closed ($s_1 = 1$), s_2 is open ($s_2 = 0$), and vice-versa. Thus, the different circuit topologies can be described with a single boolean variable $S = s_2$.

The port Hamiltonian modeling of electric circuits can be done in a systematic way using tools from graph theory [145], but since we are dealing here with a circuit of very small size we will adopt a more pedestrian approach and concentrate on the problems presented by the switches, using the ideas of [74]. A more in-deep conceptual analysis of the switches can be found in [63, 73, 82]. The Hamiltonian dynamical variables of the boost converter are the magnetic flux at the coil, ϕ_L, and the charge of the capacitor, q_C. Hence we have two one-dimensional Hamiltonian

---

[1] In a real setup, one of the switches (s_1) is replaced by a diode. This may cause, under the appropriate conditions, the apparition of the so-called discontinuous conduction modes, which this simplified model cannot support.

subsystems, with a global Hamiltonian $H_B = H_C + H_L$,

$$\frac{dq_C}{dt} = i_C \qquad\qquad v_C = \frac{\partial H_B}{\partial q_C}, \qquad\qquad (3.1)$$

and

$$\frac{d\phi_L}{dt} = v_L \qquad\qquad i_L = \frac{\partial H_B}{\partial \phi_L} \qquad\qquad (3.2)$$

connected by Kirchhoff's laws

$$
\begin{aligned}
i_L &= i_1 + i_2 \\
i_1 &= i_C - i_R \\
v_2 + v_L &= E_0 \\
v_C + v_1 &= v_2 \\
v_C &= v_R \\
i_0 - i_L &= 0
\end{aligned}
\qquad\qquad (3.3)
$$

These 6 independent relations define a Dirac structure in $\mathbb{R}^{12}$, the space of the efforts and flows of the 6 interconnected electrical elements (the two switches, the capacitor, the inductor, the load and the voltage source).

Here we treat the switches as ports, with their correspondent effort and flow variables. For the time being we do not terminate the resistive port, i.e. we do not use $v_R = -Ri_R$ (the minus sign is necessary since we are adopting an input power convention for the rest of the system, hence an output power one for the resistor; we could get rid of this nuisance by introducing auxiliary variables at the resistive port). Using (3.1) and (3.2), the first four equations of (3.3) can be written as

$$
\begin{aligned}
\frac{\partial H_B}{\partial \phi_L} &= i_1 + i_2 \\
i_1 &= \frac{dq_C}{dt} - i_R \\
v_2 + \frac{d\phi_L}{dt} &= E_0 \\
\frac{\partial H_B}{\partial q_C} + v_1 &= v_2
\end{aligned}
\qquad\qquad (3.4)
$$

The second and third equations in (3.4) yield a Hamiltonian system with four inputs and $J = R = 0$:

$$\frac{d}{dt}\begin{bmatrix} q_C \\ \phi_L \end{bmatrix} = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} i_1 \\ v_2 \\ i_R \\ E_0 \end{bmatrix} \qquad\qquad (3.5)$$

Next we will use the constraints imposed by the switches to absorb the ports s_1 and s_2 into the Hamiltonian structure:

- $S = 0 \Rightarrow s_1 = 1,\ s_2 = 0 \Rightarrow v_1 = 0,\ i_2 = 0$;
- $S = 1 \Rightarrow s_1 = 0,\ s_2 = 1 \Rightarrow i_1 = 0,\ v_2 = 0$.

Hence, when $S = 1$ we already have the values of the port variables i_1, v_2 in (3.5), while if $S = 0$, using the first and fourth equations in (3.4),

$$i_1 = \frac{\partial H_B}{\partial \phi_L} \qquad\qquad v_2 = \frac{\partial H_B}{\partial q_C}$$

We can put together both results as

$$i_1 = (1-S)\frac{\partial H_B}{\partial \phi_L} \qquad\qquad v_2 = (1-S)\frac{\partial H_B}{\partial q_C}. \qquad (3.6)$$

Now

$$\frac{d}{dt}\begin{bmatrix} q_C \\ \phi_L \end{bmatrix} = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} (1-S)\frac{\partial H_B}{\partial \phi_L} \\ (1-S)\frac{\partial H_B}{\partial q_C} \\ i_R \\ E_0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 1-S \\ -(1-S) & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H_B}{\partial q_C} \\ \frac{\partial H_B}{\partial \phi_L} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} i_R \\ E_0 \end{bmatrix} \qquad (3.7)$$

which is a port Hamiltonian system with outputs

$$y = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} \frac{\partial H_B}{\partial q_C} \\ \frac{\partial H_B}{\partial \phi_L} \end{bmatrix} = \begin{bmatrix} v_C \\ i_L \end{bmatrix} = \begin{bmatrix} v_R \\ i_0 \end{bmatrix} \qquad (3.8)$$

Finally, we may terminate the resistive port using

$$i_R = -\frac{v_R}{R} = -\frac{v_C}{R} = -\frac{1}{R}\frac{\partial H_B}{\partial q_C}$$
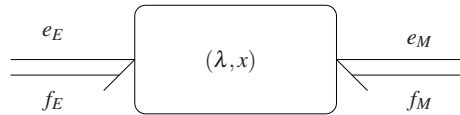
and get our final port Hamiltonian representation of the boost converter with resistive load

$$\frac{d}{dt}\begin{bmatrix} q_C \\ \phi_L \end{bmatrix} = \left\{ \begin{bmatrix} 0 & 1-S \\ -(1-S) & 0 \end{bmatrix} - \begin{bmatrix} 1/R & 0 \\ 0 & 0 \end{bmatrix} \right\} \begin{bmatrix} \frac{\partial H_B}{\partial q_C} \\ \frac{\partial H_B}{\partial \phi_L} \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} E_0 \qquad (3.9)$$

with natural output

$$y = \begin{bmatrix} 0 \\ 1 \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} \frac{\partial H_B}{\partial q_C} \\ \frac{\partial H_B}{\partial \phi_L} \end{bmatrix} = i_L = i_0. \qquad (3.10)$$

Fig. 3.2 A generalized elec-
tromechanical system.

Notice that the interconnection structure J is modulated by the boolean variable S. Designing a control for this system means choosing S as a function of the state variables.

3.1.2 Electromechanical energy conversion in the port-Hamiltonian framework

As explained Sect. 1.9.3, and in particular in Example 1.1, electrical domain systems with constitutive relations depending on geometric parameters develop additional mechanical ports through which power can flow and be exchanged with the electrical ports. Here we will cast the expressions for the constitutive laws of the ports into a Hamiltonian form. Consider the system displayed in Fig. 3.2. There are n_E generalized electrical ports (e_E, f_E) and n_M generalized mechanical ones (e_M, f_M), and the state variables are denoted by $\lambda \in \mathbb{R}^{n_E}$, $x \in \mathbb{R}^{n_M}$. Note that here we use a magnetic and translation mechanics notation, although the ports can be of any nature.

The equations of motion and the constitutive relations of the ports of this system, namely $\dot{\lambda} = e_E$, $\dot{x} = f_M$, $f_E = \frac{\partial H_E}{\partial \lambda}$, $e_M = \frac{\partial H_E}{\partial x}$, where $H_E = H_E(\lambda, x)$ is the energy function, can be expressed in explicit port-Hamiltonian form as:

$$\begin{bmatrix} \dot{\lambda} \\ \dot{x} \end{bmatrix} = \begin{bmatrix} e_E \\ f_M \end{bmatrix} \tag{3.11}$$

$$\begin{bmatrix} f_E \\ e_M \end{bmatrix} = \begin{bmatrix} \frac{\partial H_E}{\partial \lambda} \\ \frac{\partial H_E}{\partial x} \end{bmatrix} \tag{3.12}$$

This is just the purely electromagnetic part of an electromechanical system. In fact, the electromechanical system always contains some mechanical inertia, independently of whether the port is connected to other systems or not. To model this, consider a generalized mechanical element with n_I ports (e_I, f_I) and state variables $p \in \mathbb{R}^{n_I}$. The dynamical equations of the element, $\dot{p} = e_I$, $f_I = I^{-1}p$, are written in port-Hamiltonian form as

$$\dot{p} = e_I \tag{3.13}$$

$$f_I = \frac{\partial H_I}{\partial p} \tag{3.14}$$

with $H_I(p) = p^{\mathrm{T}} I^{-1} p$.

Fig. 3.3 Bond graph of a generalized electromechanical system with mechanical inertia included.
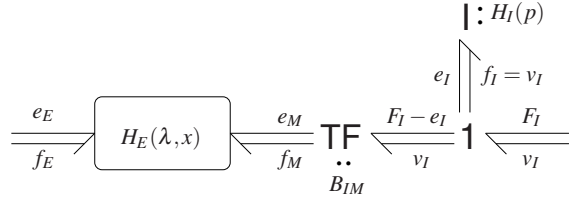
This purely mechanic part can be coupled to the electromagnetic part and to the rest of the system (if any), by means of

$$e_I = -B_{IM}e_M + F_I \tag{3.15}$$

$$f_M = B_{IM}^{\mathrm{T}} f_I \tag{3.16}$$

$$f_I = v_I \tag{3.17}$$

where the mechanical ports of the inertia element have been split into one contribution from the electromagnetic part, (e_M, f_M), and the connection to other subsystems, (F_I, v_I), with $F_I, v_I \in \mathbb{R}^{n_I}$. The matrix B_{IM} takes into account the fact that the mechanical ports may be connected to the electromagnetic part in a nontrivial way (or the fact that $n_I \neq n_M$), and the minus sign in (3.15) reflects Newton's third law (e_M is the force *on* the electromagnetic part, so a minus sign must be introduced to get the force on the mechanical element). Notice that the above relations define a Dirac structure in $\mathbb{R}^{n_M+2n_I} \times \mathbb{R}^{n_M+2n_I}$ with coordinates $(e_M, -f_M, -e_I, f_I, F_I, v_I)$, since the $n_M + 2n_I$ equations are clearly independent and can be written as

$$\underbrace{\begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix}}_{F} \begin{bmatrix} -f_M \\ -e_I \\ v_I \end{bmatrix} + \underbrace{\begin{bmatrix} 0 & B_{IM}^{\mathrm{T}} & 0 \\ -B_{IM} & 0 & I \\ 0 & -I & 0 \end{bmatrix}}_{E} \begin{bmatrix} e_M \\ f_I \\ F_I \end{bmatrix} = 0$$

with $EF^{\mathrm{T}} + FE^{\mathrm{T}} = E + E^{\mathrm{T}} = 0$. Notice that the two minus signs in $-f_M$ and $-e_I$ correspond to power flowing into the mechanical port of the electromagnetic subsystem and power flowing into the mechanical inertia, respectively, so that

$$F_I^{\mathrm{T}} v_I = e_I^{\mathrm{T}} f_I + e_M^{\mathrm{T}} f_M$$

The bond graph corresponding to the whole system is displayed in Fig. 3.3, where the power flow conventions can be clearly appreciated.

From (3.11), (3.12), (3.13), (3.14), (3.15), (3.16) and (3.17), one can express the equations of motion for the state variables in terms of the external inputs (e_E, F_I), and obtain also the corresponding outputs (f_E, v_I). Indeed, eliminating the internal port variables (e_M, f_M) and (e_I, f_I), one gets

$$\dot{\lambda} = e_E$$

$$\dot{x} = B_{IM}^{\mathrm{T}} \frac{\partial H_I}{\partial p}$$

$$\dot{p} = -B_{IM} \frac{\partial H_E}{\partial x} + F_I$$

$$f_E = \frac{\partial H_E}{\partial \lambda}$$

$$v_I = \frac{\partial H_I}{\partial p}$$

This can be given a port-Hamiltonian form, with total Hamiltonian

$$H_{EM}(\lambda, x, p) = H_E(\lambda, x) + H_I(p), \tag{3.18}$$

and

$$\begin{bmatrix} \dot{\lambda} \\ \dot{x} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & B_{IM}^{\mathrm{T}} \\ 0 & -B_{IM} & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H_{EM}}{\partial \lambda} \\ \frac{\partial H_{EM}}{\partial x} \\ \frac{\partial H_{EM}}{\partial p} \end{bmatrix} + \begin{bmatrix} I & 0 \\ 0 & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} e_E \\ F_I \end{bmatrix} \tag{3.19}$$

$$\begin{bmatrix} f_E \\ v_I \end{bmatrix} = \begin{bmatrix} I & 0 & 0 \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} \frac{\partial H_{EM}}{\partial \lambda} \\ \frac{\partial H_{EM}}{\partial x} \\ \frac{\partial H_{EM}}{\partial p} \end{bmatrix} \tag{3.20}$$

Many electromechanical systems of interest admit this explicit port-Hamiltonian form, including dc motors, levitating systems, elementary electromagnets (which will be presented in detail next) or microelectromechanical devices (MEMS). Alternating current machines can also be written in port-Hamiltonian form. However, several coordinate transformations are used in the electrical engineering literature to simplify the complex, geometry dependent constitutive relations involved in most of the cases. It turns out that, after carrying out those transformations, the system is still in port-Hamiltonian form, although with nontrivial, state dependent interconnection matrices. We will not pursue this here, but the interested reader is referred, for instance, to [16].

3.1.3 Elementary electromagnet

Fig. 3.4 shows an elementary electromagnet, a magnetic system with a moving part so that the flux linkage λ through the coil depends on a geometry variable, the "air gap" x. This can be written in the general form of electromechanical systems described above, with $n_E = 1$ and $n_M = n_I = 1$, $B_{IM} = 1$, $v_I = v$, $F_I = F$, $e_E = E$, $f_E = i$, and $H_I(p) = p^2/(2m)$. We just have to specify $H_E(\lambda, x)$, which we will deduce next from first principles, under suitable simplifications.

Fig. 3.4 An elementary electromagnet: a magnetic system with a moving part.
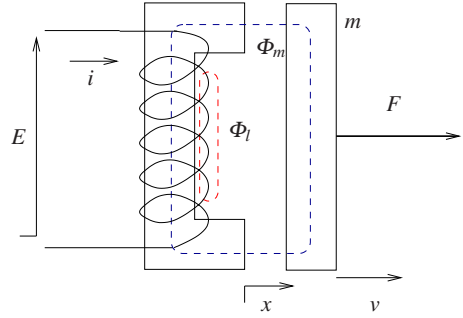
The flux linkage λ can be computed from the number of turns, N, and the magnetic induction flux, Φ, as

$$\lambda = N\Phi.$$

In turn, Φ has a leakage, Φ_l, and a magnetizing, Φ_m, parts, $\Phi = \Phi_l + \Phi_m$, which can be computed in terms of the reluctance of the respective paths:

$$\Phi_l = \frac{Ni}{\mathscr{R}_l} \qquad\qquad \Phi_m = \frac{Ni}{\mathscr{R}_m}.$$

The reluctance of the magnetizing path has a fixed contribution, the part of the iron path, and a variable one, the part of the air gap:

$$\mathscr{R}_m = \frac{l_i}{\mu_{ri}\mu_0 A_i} + \frac{2x}{\mu_0 A_g},$$

where μ_{ri}, the relative magnetic permeability of the iron core, is of the order of 10^3. Assuming that the sections of the iron and air gap paths are the same, $A_i = A_g = A$, one gets

$$\mathscr{R}_m = \frac{1}{\mu_0 A}\left(\frac{l_i}{\mu_{ri}} + 2x\right).$$

The relation between the current and the flux linkage can finally be written as

$$\lambda = \left(\frac{N^2}{\mathscr{R}_l} + \frac{N^2}{\mathscr{R}_m}\right)i = (L_l + L_m)i$$

with

$$L_m = \frac{N^2}{\mathscr{R}_m} = \frac{N^2 \mu_0 A}{\frac{l_i}{\mu_{ri}} + 2x} \equiv \frac{b}{c + 2x}.$$

Assembling these results, we can obtain the constitutive relation at the electrical port

$$i(\lambda, x) = \left(a + \frac{b}{c + 2x}\right)^{-1}\lambda, \tag{3.21}$$

where $a = L_l = N^2/\mathscr{R}_l$. As explained elsewhere in this book, the constitutive laws of a multi-port must obey Maxwell's reciprocity relations, which in this case read

$$\frac{\partial F}{\partial \lambda} = \frac{\partial i}{\partial x}. \tag{3.22}$$

One gets then from (3.21)

$$\frac{\partial F}{\partial \lambda} = \frac{2b}{(2ax + ac + b)^2}\lambda,$$

from which

$$F(\lambda, x) = \frac{b\lambda^2}{(2ax + ac + b)^2}. \tag{3.23}$$

Finally, $H_E(\lambda, x)$ can be computed from

$$H_E(\lambda, x) = \int_{(0,0)}^{(\lambda, x)} \left(i(\tilde{\lambda}, \tilde{x})\mathrm{d}\tilde{\lambda} + F(\tilde{\lambda}, \tilde{x})\mathrm{d}\tilde{x} \right),$$

or just using the result for linear magnetic materials. Either way, one gets

$$H_E(\lambda, x) = \frac{1}{2}\frac{c + 2x}{2ax + ac + b}\lambda^2. \tag{3.24}$$

The port-Hamiltonian structure is thus

$$\begin{bmatrix} \dot{\lambda} \\ \dot{x} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H_{EM}}{\partial \lambda} \\ \frac{\partial H_{EM}}{\partial x} \\ \frac{\partial H_{EM}}{\partial p} \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix}$$

$$\begin{bmatrix} i \\ v \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{\partial H_{EM}}{\partial \lambda} \\ \frac{\partial H_{EM}}{\partial x} \\ \frac{\partial H_{EM}}{\partial p} \end{bmatrix} \tag{3.25}$$

where

$$H_{EM}(\lambda, x, p) = \frac{1}{2}\frac{c + 2x}{2ax + ac + b}\lambda^2 + \frac{1}{2m}p^2.$$

Notice that, just replacing F with a constant gravitational force and expressing it as a gradient of the gravitational energy, which can then be added to H_{EM}, one obtains the model of the magnetically levitating ball of Example 2.2, albeit without the dissipation term.

Fig. 3.5 Coupling of the boost and the electromagnet.
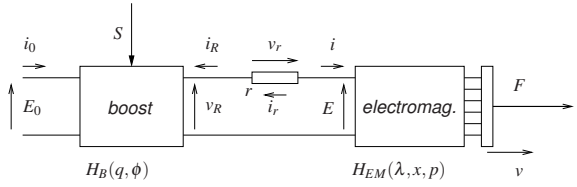
3.1.4 Coupling of the boost converter and the electromagnet

As a final example, we connect the boost converter, without the resistive termination, to the electromagnet, inserting a resistor r in series connection between them, as shown in Fig. 3.5, where we have renamed the boost variables to (q, ϕ). The series resistor obeys (we adopt an input power convention for this one)

$$v_r = r i_r \qquad (3.26)$$

and where the interconnecting Dirac structure is provided by Kirchhoff's laws

$$i_R = i_r \qquad\qquad i_r = -i \qquad\qquad E = v_R + v_r$$

From the first output relation of the boost subsystem, $v_R = \frac{\partial H_B}{\partial q}$, and the first one of the electromagnet, $i = \frac{\partial H_{EM}}{\partial \lambda}$, together with (3.26) and Kirchhoff's laws, one can express the internal port variables as

$$E = v_R + v_r = \frac{\partial H_B}{\partial q} + r i_r = \frac{\partial H_B}{\partial q} - r i = \frac{\partial H_B}{\partial q} - r \frac{\partial H_{EM}}{\partial \lambda}$$

$$i_R = -i = -\frac{\partial H_{EM}}{\partial \lambda}$$

Substituting these into (3.7) and (3.25), if $H(q, \phi, \lambda, x, p) = H_B(q, \phi) + H_{EM}(\lambda, x, p)$ one gets:

$$
\begin{bmatrix} \dot{q} \\ \dot{\phi} \\ \dot{\lambda} \\ \dot{x} \\ \dot{p} \end{bmatrix}
=
\begin{bmatrix}
0 & 1-S & 0 & 0 & 0 \\
-1+S & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & -1 & 0
\end{bmatrix}
\begin{bmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial \phi} \\ \frac{\partial H}{\partial \lambda} \\ \frac{\partial H}{\partial x} \\ \frac{\partial H}{\partial p} \end{bmatrix}
+
\begin{bmatrix} -\frac{\partial H}{\partial \lambda} \\ E_0 \\ \frac{\partial H}{\partial q} - r\frac{\partial H}{\partial \lambda} \\ 0 \\ F \end{bmatrix}
$$

This can be rewritten in explicit port-Hamiltonian form, with inputs E_0 and F and outputs i_0 and v, as

$$
\begin{bmatrix} \dot{q} \\ \dot{\phi} \\ \dot{\lambda} \\ \dot{x} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & 1-S & -1 & 0 & 0 \\ -1+S & 0 & 0 & 0 & 0 \\ 1 & 0 & -r & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial \phi} \\ \frac{\partial H}{\partial \lambda} \\ \frac{\partial H}{\partial x} \\ \frac{\partial H}{\partial p} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} E_0 \\ F \end{bmatrix} \tag{3.27}
$$

$$
y = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial \phi} \\ \frac{\partial H}{\partial \lambda} \\ \frac{\partial H}{\partial x} \\ \frac{\partial H}{\partial p} \end{bmatrix} \tag{3.28}
$$

3.1.5 Variable structure systems

Assume a VSS system such that the change in the state variables is small over the time length of an structure change, or such that one is not interested about the fine details of the variation. Then one may try to formulate a dynamical system for the time average of the state variables (*state space averaging*, or SSA)

$$
\langle x \rangle (t) = \frac{1}{T} \int_{t-T}^{t} x(\tau) \, d\tau, \tag{3.29}
$$

where T is the period, assumed constant, of a cycle of structure variations. Let our VSS system be described in explicit port Hamiltonian form

$$
\dot{x} = [J(S,x) - R(S,x)] \frac{\partial H}{\partial x}(x) + g(S,x)u, \tag{3.30}
$$

where S is a (multi)-index, with values on a finite, discrete set, enumerating the different structure topologies. For notational simplicity, we will assume from now on that we have a single index (corresponding to a single switch, or a set of switches with a single degree of freedom) and that $S \in \{0,1\}$. Hence, we have two possible dynamics, which we denote as

$$
\begin{aligned} S = 0 \Rightarrow \dot{x} = \left[J_0(x) - R_0(x) \right] \frac{\partial H}{\partial x}(x) + g_0(x)u, \\ S = 1 \Rightarrow \dot{x} = \left[J_1(x) - R_1(x) \right] \frac{\partial H}{\partial x}(x) + g_1(x)u. \end{aligned} \tag{3.31}
$$

Note that controlling the system means choosing the value of S as a function of the state variables, and that u is, in most cases, just a constant external input. Moreover, from (3.29) we have

$$
\frac{d}{dt} \langle x \rangle (t) = \frac{x(t) - x(t-T)}{T}. \tag{3.32}
$$

Now the central assumption of the SSA approximation method is that for a given structure we can substitute $x(t)$ by $\langle x \rangle(t)$ in the right-hand side of the dynamical equations, so that (3.31) become

$$
\begin{aligned}
S = 0 &\Rightarrow \dot{x} \approx \left[J_0(\langle x \rangle) - R_0(\langle x \rangle) \right] \frac{\partial H}{\partial x}(\langle x \rangle) + g_0(\langle x \rangle)u, \\
S = 1 &\Rightarrow \dot{x} \approx \left[J_1(\langle x \rangle) - R_1(\langle x \rangle)) \right] \frac{\partial H}{\partial x}(\langle x \rangle) + g_1(\langle x \rangle)u.
\end{aligned}
\tag{3.33}
$$

The rationale behind this approximation is that $\langle x \rangle$ does not have time to change too much during a cycle of structure changes. We assume also that the length of time in a given cycle when the system is in a given topology is determined by a function of the state variables or, in our approximation, a function of the averages, $t_0(\langle x \rangle)$, $t_1(\langle x \rangle)$, with $t_0 + t_1 = T$. Since we are considering the right-hand sides in (3.33) constant over the time scale of T, we can integrate the equations to get[2]:

$$
\begin{aligned}
x(t) = x(t - T) &+ t_0(\langle x \rangle) \left[\left[J_0(\langle x \rangle) - R_0(\langle x \rangle) \right] \frac{\partial H}{\partial x}(\langle x \rangle) + g_0(\langle x \rangle)u \right] \\
&+ t_1(\langle x \rangle) \left[\left[J_1(\langle x \rangle) - R_1(\langle x \rangle) \right] \frac{\partial H}{\partial x}(\langle x \rangle) + g_1(\langle x \rangle)u \right].
\end{aligned}
$$

Using (3.32) we get the SSA equations for the variable $\langle x \rangle$ (which we rewrite again as x to simplify the notation):

$$
\begin{aligned}
\dot{x} = d_0(x) &\left[\left[J_0(\langle x \rangle) - R_0(\langle x \rangle) \right] \frac{\partial H}{\partial x}(\langle x \rangle) + g_0(\langle x \rangle)u \right] + \\
&+ d_1(x) \left[\left[J_1(\langle x \rangle) - R_1(\langle x \rangle) \right] \frac{\partial H}{\partial x}(\langle x \rangle) + g_1(\langle x \rangle)u \right] \\
= &\left\{ \left[d_0(x)J_0(x) + d_1(x)J_1(x) \right] - \left[d_0(x)R_0(x) + d_1(x)R_1(x) \right] \right\} \frac{\partial H}{\partial x}(x) + \\
&+ \left[d_0(x)g_0(x) + d_1(x)g_1(x) \right]u,
\end{aligned}
\tag{3.34}
$$

where

$$
d_{0,1}(\langle x \rangle) = \frac{t_{0,1}(\langle x \rangle)}{T},
\tag{3.35}
$$

with $d_0 + d_1 = 1$. In the power converter literature d_1 (or d_0, depending on the switch configuration) is referred to as the *duty cycle*. Equation (3.34) is again a port-Hamiltonian system, with interconnection, dissipation and port matrices given by combinations of the individual topology matrices. Notice that this is a smooth system, whose numerical implementation is much easier than the original VSS. Discussion of these kind of averaged systems in the bond graph formalism can be found in [63]. In fact, this analysis can be extended to the case when higher order harmonics, and not just the zeroth order one considered here, are introduced; the result, as shown in [17], is again a system in port-Hamiltonian form.

---

[2] We also assume that u does not vary over this time scale; in fact u is constant in many applications.
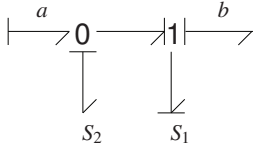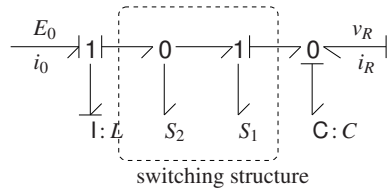
Fig. 3.6 The bond graph of the boost converter.

Fig. 3.7a Causality assignments of the switching structure of the boost converter: S_2 closed and S_1 open.
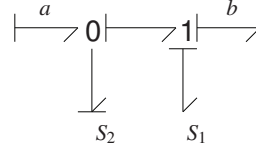
Fig. 3.7b Causality assignments of the switching structure of the boost converter: S_2 open and S_1 closed.

As an example, we can retake the boost converter discussed previously. In the above notation, for the case of an open load port, one has

$$J_0 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \qquad J_1 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \qquad g_0 = g_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

and no dissipation, i.e. $R_0 = R_1 = 0$. Putting this into (3.34) and denoting $\mu = t_0(x)/T$, one gets

$$\frac{d}{dt} \begin{bmatrix} q_C \\ \phi_L \end{bmatrix} = \begin{bmatrix} 0 & \mu \\ -\mu & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H_B}{\partial q_C} \\ \frac{\partial H_B}{\partial \phi_L} \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} ci_R \\ E_0 \end{bmatrix} \qquad (3.36)$$

This has exactly the same form that the exact, non-smooth model (3.7), with $\mu = 1 - S$, except for the fact that all the state variables are averages, and μ can take values in the continuum $[0,1]$. It is instructive to derive these results from a bond graph approach. Indeed, the bond graph of the boost converter, Fig. 3.1, considering the two switches as open ports, is displayed in Fig. 3.6. The interior bonds of the switching structure have no causality assignment, because it depends on the state of the switches. In fact, there are two possibilities, as shown in Figures 3.7a and 3.7b. Notice that the two possible interior assignments have the same output causality. In the first case represented in Fig. 3.7a, one has $v_2 = 0$ and $i_1 = 0$, since S_2 acts a zero voltage source while S_1 is a zero current source; the situation is reversed in the second case, illustrated in Fig. 3.7b. Writing down the bond graph equations for both cases, one arrives at the input/output relations

$$e_a = \mu e_b \qquad\qquad\qquad f_b = \mu f_a$$

with $\mu = 0$ in the first case, and $\mu = 1$ in the second one. This corresponds to the relations of an ideal transformer, and the associated bond graph is displayed in

Fig. 3.8 The bond graph of
the boost converter with a
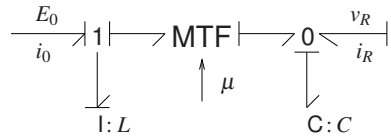transformer instead of the two
switches.

Fig. 3.9 Variable structure
and averaged 20-sim models
for the boost converter.
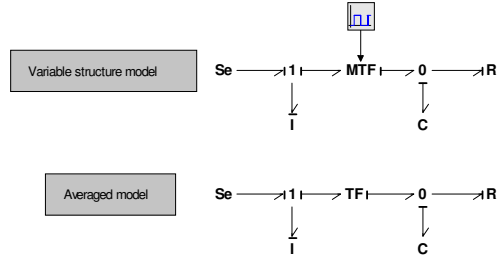
Fig. 3.10 Load voltage wave-
form for the VSS and aver-
aged models.
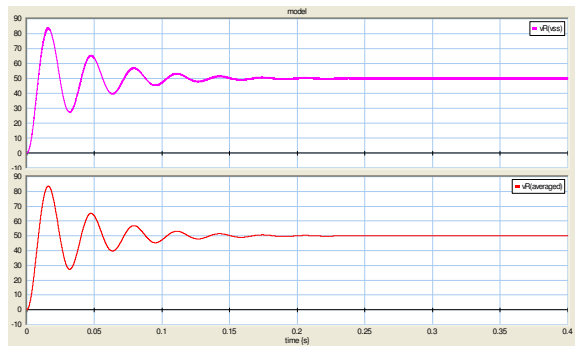
Fig. 3.8. If one writes the equations associated to this bond graph, the same form
as in (3.36) is obtained. From the point of view of the bond graph, μ could be a
boolean variable $\mu \in \{0, 1\}$ or a continuous one $\mu \in [0, 1]$. However, if the later op-
tion is taken the averaged model is recovered. Fig. 3.9 shows the 20-sim schemes for
both models, with the same system parameters, and Fig. 3.10 shows the load volt-
age for the corresponding simulations, for system parameters $C = 0.002$, $L = 0.002$,
$E_0 = 20$, and $R = 10$ (in SI units). For the variable structure model, a square pe-
riodic signal with $T = 0.0004$ s and duty-cycle $\mu = 0.6$ is injected into the MTF,
while for the averaged model the parameter transformer is $\mu = 0.6$. The averaged
model yields, indeed, the averages of the state variables of the VSS model; on closer
inspection it can be seen that the later has, however, a small ripple due to the commu-
tation, not present in the averaged model simulation. Notice that, in both cases, the
asymptotic output voltage is $E_0/(1 - \mu) = 50$ V, as expected for a boost converter.

3.2 Modeling of mechanical systems

3.2.1 Short introduction and motivations

In Chapter 1, we have introduced the basic notions of port-Hamiltonian systems. In this part we will show how it possible to use these techniques for the structured modeling of robotics mechanisms. If we would just start modeling the motion of a point mass, due to the geometry of the space it moves in, this could be done by just considering usual coordinates. The port variables would then be the usual vector forces and velocities and no extra structure would be necessary. To be more specific, a particle mass is easy to describe because its configuration can be associated to a point of the three-dimensional Euclidean space. After having chosen coordinates, each point can be associated to a triple of real numbers in $\mathbb{R}^3$; but the most important thing is that the algebraic and topological properties of $\mathbb{R}^3$ correspond to real physical properties of the motion of the particle: forces can be added; velocity vectors too; magnitudes of vectors correspond to magnitudes of forces and velocities; "orthogonality" of a force and velocity vectors gives zero power; the velocity and acceleration vectors are the time derivatives of the points position vector; Newton's Laws link a three-dimensional force vector to a three-dimensional acceleration vector, through the *apparently* scalar quantity "mass", for point masses, as well as spherically-symmetric rigid bodies such as planets and canon balls.

In contrast to the simplicity of the point mass motion properties, the motion and the dynamics of a rigid body are much more complex. A rigid body is composed of an infinite number of point masses, which are constrained not to move with respect to each other. It turns out that the dimension of the space necessary to describe the configuration of a rigid body is six: three dimensions for orientation, and three for translation. The force-acceleration relation is now a full six-by-six matrix, and not a scalar anymore. Moreover, the acceleration involved in this dynamic relation is *not* just the second-order time derivative of the position/orientation vector of the rigid body.

Even the short overview above should make clear that it is wrong to treat the six position/orientation coordinates of a rigid body in the same way as one treats the three position coordinates of a point: the *geometrical properties* of rigid bodies are fundamentally different from the geometrical properties of point masses. For example, if one continuously increases one of these six numbers (i.e., one that corresponds to orientation representation), the rigid body arrives at the *same* configuration after every rotation over 360 degrees. This "curvature" property does not occur when one indefinitely increases any of the three coordinates of a point configuration. Locally (i.e., in the neighborhood of a specific configuration) it *is* possible to describe a configuration using six real numbers, but this description is not an *intrinsic property* of the motion. (An intuitive definition of an "intrinsic property" is: any property that does not change if one changes the coordinate representation.)

A lot of powerful tools are available which allow to describe the motion of rigid bodies in a geometrical and global way. These methods are related to the geometry

of *lines* and *screws* and to the differential geometric concept of a *Lie group* (see Sect. B.1.4). Furthermore, the concept of a *Lie group* is the key structure which will allow to describe interconnection of rigid bodies by expressing common variables on which the interconnection is based. In a nutshell: it's not because one can use n numbers as coordinates on a given space, that the objects in that space have exactly the same properties as the n-tuples in $\mathbb{R}^n$!

3.2.2 Configuration and twist of a rigid body

We will now start introducing the concepts which are needed to handle multi-body systems.

3.2.2.1 Describing configurations

In case of a point mass moving in the Euclidean space $\mathbb{E}$, once an orthonormal reference frame Ψ has been chosen, we can associate with a bijective relation three numbers to it: $(x, y, z) \in \mathbb{R}^3$. Velocities with respect to an observer not moving with respect to Ψ and expressed in the same reference frame will be simply equal to $(\dot{x}, \dot{y}, \dot{z}) \in \mathbb{R}^3$.

   For rigid bodies this will be more complicated. In principle, a rigid body configuration is a six dimensional space (three translation and three rotations), but due to the topology of the space of rotations, there does not exist six global coordinates. In what follows, we will associate the configuration of a rigid body to a matrix which is called a homogeneous matrix once a reference has been chosen. First, for reasons based on projective geometry which can be further read in [196], it is convenient to describe the coordinate of a point using a four dimensional vector in which the first three components are the usual ones and the last is the scalar 1. For a point p expressed in an orthonormal frame Ψ_i, its coordinates will then be a vector of the following form:

$$P^i = \begin{bmatrix} x_i \ y_i \ z_i \ 1 \end{bmatrix}^{\mathrm{T}} \tag{3.37}$$

If we consider a second orthonormal reference frame Ψ_j, the same point will have a similar representation with different numbers if Ψ_i and Ψ_j do not coincide. It would be possible to see that the change of coordinates would be given by

$$P^j = H_i^j P^i \tag{3.38}$$

with

$$H_i^j = \begin{bmatrix} R_i^j & p_i^j \\ 0_3 & 1 \end{bmatrix} \tag{3.39}$$

where $R_i^j \in SO(3)$ is an orthonormal matrix, i.e. with determinant equal to 1 and such that $R^{\mathrm{T}} = R^{-1}$, and $p_i^j \in \mathbb{R}^3$.

If we now consider Ψ_i fixed to a body I and Ψ_j fixed to a body J, it is possible to describe their relative configuration by the relative configuration of the two frames which is represented by H_i^j using their change of coordinates. It could also easily be seen that H_i^j beside representing the change of coordinates of the same physical point from frame Ψ_i to frame Ψ_j, it also coincides with the physical motion which brings Ψ_j to Ψ_i for points expressed in either of the two frames; note that the inverse direction of the indices is not a typo. To be more precise, if we consider that a rigid body motion would bring frame Ψ_j to Ψ_i and this motion would also bring a point p to a point q, we would have that $q^i = H_i^j p^i$ and $q^j = H_i^j q^j$. For what it will follow later, it is important to notice that $(H_i^j)^{-1} = H_j^i$.

3.2.2.2 Relative instantaneous motions and twists

If a representation of a velocity of a point mass would be just the time derivative of its coordinate, we could consider as velocity of a rigid body the time derivative of the matrix H representing the relative configuration of the body with respect to another frame, the observer. This is in principle correct, but there are a number of problems related to this approach:

1. $\dot{H}$ has many more elements than necessary to express the six dimensional infinitesimal motion;
2. From the information of $\dot{H}$ would not be possible to have an idea of the relative motion without knowing H;
3. If we wanted to interconnect two bodies A and B using port variables, the velocity $\dot{H}$ could not be used since each of the bodies would have a different configuration H and a different $\dot{H}$. This would correspond to two vectors belonging to two different tangent spaces in a differential geometric context and therefore no natural operation can be performed among these vectors.

The solution to all the previous problems can be achieved by using the intrinsic structure of what is called a Lie group for the group of motions represented by the matrices $H \in SE(3)$. Properly speaking, the Lie Group $SE(3)$ is more general than a Lie group of matrices, but for what it will presented it is didactically sensible to describe what follows using matrix Lie groups. A Lie group is both a manifold, smooth nonlinear structure locally bijective to $\mathbb{R}^n$, and a group, it has a special point called the identity and an operation which allows to compose elements of the manifold, satisfying associativity and having for each element an inverse. This structure allows to associate to each element $(H, \dot{H}) \in T\,SE(3)$ belonging to the vector space $T_H SE(3)$ tangent to the manifold $SE(3)$ at the point $H \in SE(3)$ two unique vectors in the tangent space $se(3) := T_I SE(3)$ at the identity of the group, which in our case corresponds to the 4 identity matrix $I \in SE(3)$. These two vectors have a clear geometrical interpretation and they are called the *left* and *right translation* of $(H, \dot{H})$ to the Lie algebra $se(3)$.

Such a structure allows to naturally find unique representatives of velocities in a common space called a Lie algebra, allowing circumventing all previously de-

scribed problems. This is a generalization of what is done for rotations in which
the angular velocity vector can be easily and effectively used to describe rotational
motions in a coordinate free, body independent way; the role of angular velocity
for general rigid motions will be a twist. It could be shown that, following the no-
tation previously introduced we can indicate with $H_i^j(t) \in SE(3)$ the smoothly time
varying homogeneous matrix which can be used to change the homogeneous coor-
dinates of a point P from its representation in the two relatively moving frames Ψ_i
to Ψ_j. After we introduce a third frame Ψ_k, we could also consider the changes of
coordinate between any of these frames and it could be proven that ${}^k\tilde{T}_i^j := H_j^k \dot{H}_i^j H_k^i$
has always the following form:

$$ {}^k\tilde{T}_i^j := \begin{bmatrix} \tilde{\omega} & v \\ 0_3 & 0 \end{bmatrix} \tag{3.40} $$

where for any three dimensional vector ω, $\tilde{\omega}$ is the unique skew-symmetric matrix
such that for each x, $\omega \times x = \tilde{\omega}x$. In case $k = j$, the corresponding matrix is called
the *right translation* to the Lie algebra and in case $k = i$ the *left translation* to the
Lie algebra for reasons which can be found in any reference on Lie groups[3]. It can
be seen that in (3.40), only the six scalars of ω and v are independent, and therefore
we can also define the equivalent six dimensional vector representation

$$ {}^kT_i^j = \begin{bmatrix} \omega^{\mathrm{T}} & v^{\mathrm{T}} \end{bmatrix}^{\mathrm{T}} $$

This vector, which is called a twist, is a real geometrical object which describes the
relative instantaneous motion of the body rigidly connected to frame Ψ_i with respect
to the body rigidly connected to frame Ψ_j expressed numerically as a vector in the
frame Ψ_k.

It is possible to see that we can change coordinates of a twist using what is called
the Adjoint representation of the group which is represented by a 6×6 matrix:

$$ {}^kT_i^j = \mathrm{Ad}_{H_l^k} {}^lT_i^j \tag{3.41} $$

where

$$ \mathrm{Ad}_{H_l^k} = \begin{bmatrix} R_l^k & 0 \\ \tilde{p}_l^k R_l^k & R_l^k \end{bmatrix} \tag{3.42} $$

R_l^k is the rotation sub-matrix of H_l^k and $\tilde{p}_l^k$ is the skew-symmetric representation of
the position sub-vector of H_l^k.

For rotations, we can associate a vector called the angular velocity, which geo-
metrically completely expresses the instantaneous rotation of a body independently
of its pose at a certain instant of time. the direction of the angular rotation vector,
represents the instantaneous axis of rotation and direction (clockwise or anticlock-

---

[3] In Lie group theory, ${}^k\tilde{T}_i^j$ is introduced as the Adjoint transformation of the left or right translation,
for example ${}^k\tilde{T}_i^j = \mathrm{Ad}_{H_j^k}\left(R_{H_i^j}(H_i^j, \dot{H}_i^j)\right)$ where $R_{H^{-1}}$ indicated the right translation of the vector
$(H, \dot{H})$ to the Lie algebra $se(3)$.

wise around the axis) and its magnitude the angular velocity. In the same way, as shown by the Mozzi theorem [150], a twist is represented by a geometrical object which is called a screw since it is represented by an axis, a pitch, a direction and a magnitude. Mozzi's theorem says that we can always write a twist as:

$$\begin{bmatrix} \omega \\ v \end{bmatrix} = \|\omega\| \underbrace{\begin{bmatrix} \hat{\omega} \\ r \wedge \hat{\omega} \end{bmatrix}}_{rotation} + \alpha \underbrace{\begin{bmatrix} 0 \\ \hat{\omega} \end{bmatrix}}_{translation} \tag{3.43}$$

where ω and v are three dimensional vectors numerically expressed in k. The vector

$$\begin{bmatrix} \hat{\omega} \\ r \wedge \hat{\omega} \end{bmatrix}$$

represents a geometrical line passing through the point r and directed along ω. This line representation called Plücker coordinates has many advantages with respect to others like the fact that its representation has numerically a one to one relation to lines in the projective 3-space. The scalar coefficient α is called the pitch. The theorem basically says that each motion instantaneously can be seen as a screw motion: an instantaneous rotation around an axis, represented as just described, and an infinitesimal translation along this axis. The ratio of these two motions is given by the pitch coefficient α.

An essential feature of twists is that they are independent of the pose of a body and can therefore be used to describe relative motions of any body and are the key to define power ports in rigid multi-body mechanical systems. Twists play the role of flows and once we introduced the dual efforts, we will have the essential components to define a power port for rigid multi-body systems.

3.2.2.3 The dual of twists: wrenches

Since the space $se(3)$ of twists is a vector space, we can directly define the dual space $se^*(3)$ which will be a dual Lie algebra whose elements are called wrenches. Clearly, dimensionally, these elements are of the same size of twists (six dimensional) and the dual product of wrenches and twists will be a scalar representing the power exchanged by the wrench (generalization of the force) with the relative motion represented by the twist. A wrench in vector form can be indicated with

$$^kW_i^j = \begin{bmatrix} \tau^T & f^T \end{bmatrix}^T$$

and represents the wrench applied by i on j as a vector expressed in frame Ψ_k. Sometimes the presence of the index i may not be necessary. As a direct consequence of (3.41) and the dual nature of a wrench with respect to a twist, the change of coordinates of a wrench is expressed by:

$$\left({}^{k}W_i^j \right)^t = \mathrm{Ad}^t_{H_k^l} \left({}^{l}T_i^j \right)^t \tag{3.44}$$

To understand why such a quantity can be seen as the generalization of a force, the theorem of Pointsot can be used. This theorem states that any system of forces applied to a rigid body, can be simplified as the resultant of one force along a specific line in space and a torque oriented in the same direction. Similarly to (3.43), this dual theorem can be expressed as:

$$\begin{bmatrix} \tau \\ f \end{bmatrix} = \|f\| \underbrace{\begin{bmatrix} r \wedge f \\ f \end{bmatrix}}_{force} + \alpha \underbrace{\begin{bmatrix} f \\ 0 \end{bmatrix}}_{torque} \tag{3.45}$$

where the first vector indicates the linear force along the line oriented along f and passing through the point r and the second vector indicate the torque oriented in the same direction of f, but such that its application point does not matter being a torque. The ratio of these two magnitudes is expressed by the scalar pitch α.

3.2.2.4 Screw power ports

It is now possible to introduce the coordinate-free concept of a screw power-port. A screw power port is the pair of a twist and a wrench

$$\left({}^{k}T_i^j, \; {}^{k}W_\bullet^i \right) \in se(3) \times se^*(3)$$

and can be used as a mean to interconnect multi-body systems as we will see in more details later.

3.2.3 Rigid body dynamics

Using the concept of screws and Lie groups, we can introduce the inertia tensor which represents the complete inertial properties of a rigid body. The inertia tensor is a metric, positive definite quadratic form, which associates the kinetic co-energy to a certain twist of a rigid body:

$$H^*({}^{k}T_i^0) = \frac{1}{2} \left({}^{k}T_i^0 \right)^t {}^{k}I^i \; {}^{k}T_i^0 \tag{3.46}$$

where ${}^{k}I^i$ represents the inertia tensor of body i expressed in frame k and it is a 6×6 matrix corresponding to a quadratic form in $se(3)$. Using the inertia tensor we can also define what is called the screw-momenta which is a co-vector (belonging to $se^*(3)$) representing the 6-dimensional momenta of a rigid body:

$$\left(^{k}M^{i}\right)^{t} := ^{k}I^{i\ k}T_{i}^{0} \tag{3.47}$$

where $^{k}M^{i}$ indicates the screw-momenta of body i expressed in frame k. Using the expression of momenta we can now also write an expression for the kinetic energy as a quadratic form on $se^{*}(3)$:

$$H(^{k}M^{i}) = \frac{1}{2}{}^{k}M^{i}\left(^{k}I^{i}\right)^{-1}\left(^{k}M^{i}\right)^{t} \tag{3.48}$$

Newton's law for a point mass says that in an inertial frame the time change of momenta of a point mass is equal to the total force applied to it, i.e. $\dot{p}^{0} = F^{0}$. It could be shown that integrating this equation for a complete rigid body, it generalizes to:

$$^{0}\dot{M}^{i} = {}^{0}W_{\cdot}^{i} \tag{3.49}$$

where $^{0}M^{i}$ is the momenta of body i expressed numerically in the inertial frame Ψ_{0} and $^{0}W_{\cdot}^{i}$ the total wrench applied to body i expressed in frame Ψ_{0}.

Since the time derivative of the momenta is equal to a wrench, both terms of the equation transform identically with changes of coordinates and this is why the wrench is a co-vector. If we write the previous equation as an equality of column vectors, we have

$$\left(^{0}\dot{M}^{i}\right)^{t} = \left(^{0}W_{\cdot}^{i}\right)^{t},$$

It can be seen that by changing the coordinates to a frame Ψ_{k} rigid with the body, the previous expression becomes:

$$\left(^{k}\dot{M}^{i}\right)^{t} = \mathrm{ad}^{\mathrm{T}}_{{}^{k}T_{i}^{0}}(^{k}M^{i})^{t} + \left(^{k}W_{\cdot}^{i}\right)^{t}. \tag{3.50}$$

where

$$\mathrm{ad}^{\mathrm{T}}_{{}^{k}T_{i}^{0}} = \begin{bmatrix} -\tilde{\omega} & -\tilde{v} \\ 0 & -\tilde{\omega} \end{bmatrix}$$

and ω and v are the vectors composing $^{k}T_{i}^{0}$ and introduced in (3.40). After some calculations, it could be seen that

$$\mathrm{ad}^{\mathrm{T}}_{{}^{i}T_{i}^{0}}(^{i}M^{i})^{t} = (^{i}M^{i}\wedge)\ ^{i}T_{i}^{0} \tag{3.51}$$

where

$$(^{i}M^{i}\wedge) := \begin{bmatrix} {}^{i}\tilde{M}^{i}_{\omega} & {}^{i}\tilde{M}^{i}_{v} \\ {}^{i}\tilde{M}^{i}_{v} & 0 \end{bmatrix} \tag{3.52}$$

and $^{i}\tilde{M}^{i}_{\omega}$ and $^{i}\tilde{M}^{i}_{v}$ are the skew-symmetric form of three-vectors corresponding to respectively the first and last three components of $^{i}M^{i}$.

By looking closer at (3.50) it can be seen that the configuration of the rigid body does not appear in the equation at all. The equation is useful because in body fix coordinates the expression of the inertia tensor which we will need in order to calculate $^{k}M^{i}$ is a constant matrix which can be easily calculated. The equation (3.50)

is only dependent on the momenta and the effect of an applied wrench on it. This equation is all we need if we want to study a single rigid body independently. On the other hand, if we want to calculate dynamics of interconnected mechanisms, each of the quantities, like applied wrenches between bodies, will have to be described in the same coordinate systems. We need therefore a common reference frame in which we can take operations among tensors. Furthermore, if we want to consider gravity, its direction and effect will change in body coordinates and therefore it is necessary to keep track of the pose of a rigid body. We can tackle all these problems by considering in the open model of a rigid body a potential energy function of the configuration of the rigid body with respect to a common, inertial coordinate system.

3.2.3.1 Potential energy

The configuration of a rigid body is homeomorphic to $SE(3)$ and can be associated to a homogeneous matrix $H_i^0 \in SE(3)$ as seen previously. This means that any potential energy function of a rigid body will be expressed by a function of the form:

$$V : SE(3) \to \mathbb{R} \tag{3.53}$$

Normally, we would calculate the corresponding force field of a potential energy by taking the differential of the function, but in the case of a rigid body this is not direct since the argument of the function is a matrix of a specific form: the arguments are a set of variables on which constraints hold. A way to tackle this would be to find a minimal parametrization of $SE(3)$ which would then allow to take the differential in the usual way. This approach would be strictly local and not general. A much more elegant and effective approach is instead the usage of exponential coordinates of the group $SE(3)$ which, for matrix Lie groups, corresponds to the matrix exponential:

$$\phi_i^0 \mapsto H_i^0 = e^{\tilde{\phi}_i^0} \tag{3.54}$$

where the tilde operation in the argument of the exponential corresponds to the same tilde operation as for twists. The entity ϕ_i^0 is geometrically also belonging to $se(3)$ and it corresponds to what is called the *finite twist* (rather than infinitesimal). By means of the exponential map, we can express a potential function using a minimal set of coordinates. In this way we could write a corresponding potential function to (3.53) as $V_\phi : se(3) \to \mathbb{R}$, with

$$\phi_i^0 \mapsto V(\log(\phi_i^0)) \tag{3.55}$$

where log is a periodic function which can be calculated easily with the techniques presented in [213].

For what follows, it is necessary to know the map which relates the time derivatives of the exponential coordinates ϕ_i^0 to the instantaneous twist ${}^iT_i^0$ in the following way:

$$^iT_i^0 = K(\phi_i^0)\dot{\phi}_i^0 \tag{3.56}$$

where could be proven that

$$K(\phi_i^0) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(k+1)!}\,\mathrm{ad}_{\phi_i^0}^k \tag{3.57}$$

and can be calculated easily using the techniques introduced in [213]. From (3.56), the adjoint relation follows directly:

$$\gamma = K^t(\phi_i^0)\,^iW_. ^i \tag{3.58}$$

where γ is a dual of the time derivative of the exponential coordinates like is the case for

$$\frac{\partial V_\phi}{\partial \phi_i^0} \in se^*(3)$$

We can therefore calculate the wrench which the potential energy V_ϕ generates as:

$$W = K^{-t}(\phi_1^0)\frac{\partial V_\phi}{\partial \phi_i^0} \in se^*(3) \tag{3.59}$$

We can now finally give a port-Hamiltonian expression of the dynamics of a rigid body. The Hamiltonian will be a sum of the kinetic and potential energy and will be:

$$H(^kM^i,\phi_i^0) = \frac{1}{2}\,^kM^i\left(^kI^i\right)^{-1}\left(^kM^i\right)^t + V_\phi(\phi_i^0) \tag{3.60}$$

and the port Hamiltonian equation become:

$$\begin{bmatrix} \dot{\phi}_i^0 \\ (^k\dot{M}^i)^t \end{bmatrix} = \begin{bmatrix} 0 & K^{-1}(\phi_i^0) \\ -K^{-t}(\phi_i^0) & (^iM^i\wedge) \end{bmatrix}\begin{bmatrix} \frac{\partial H}{\partial \phi_i^0} \\ \frac{\partial H}{\partial ^kM^i} \end{bmatrix} + \begin{bmatrix} 0 \\ I \end{bmatrix}\,^iW_.^i \tag{3.61}$$

$$^iT_i^0 = \begin{bmatrix} 0 & I \end{bmatrix}\begin{bmatrix} \frac{\partial H}{\partial \phi_i^0} \\ \frac{\partial H}{\partial ^kM^i} \end{bmatrix} \tag{3.62}$$

or expliciting all ports, a single matrix representing the interconnection structure and changing the coordinates of the interconnection port we obtain:

$$\begin{bmatrix} \dot{\phi}_i^0 \\ (^k\dot{M}^i)^t \\ -\,^0T^0 \end{bmatrix} = \begin{bmatrix} 0 & K^{-1}(\phi_i^0) & 0 \\ -K^{-t}(\phi_i^0) & ^iM^i\wedge & \mathrm{Ad}^t_{e^{\phi_i^0}} \\ 0 & -\mathrm{Ad}_{e^{\phi_i^0}} & 0 \end{bmatrix}\begin{bmatrix} \frac{\partial H}{\partial \phi_i^0} \\ \frac{\partial H}{\partial ^kM^i} \\ ^0W_.^i \end{bmatrix} \tag{3.63}$$

In the previous equation, the matrix represents the Dirac structure composed of three ports:

$$\left(\dot{\phi}_i^0,\ \frac{\partial H}{\partial \phi_i^0}\right)$$

corresponding to the flow of potential energy,

$$\left({}^k\dot{M}^i, \frac{\partial H}{\partial {}^k M^i} \right)$$

corresponding to the flow of kinetic energy and

$$\left({}^0 T_i^0, {}^0 W_{\cdot}^i \right)$$

to the power port which can be used to interconnect and interact with the rigid body.

3.2.4 Rigid mechanisms: interconnections of rigid bodies

We will now discuss the topology of a mechanism and describe how to represent that in an elegant and effective way using the network structure represented by a Dirac structure. We will start looking at the constraints between pairs of rigid bodies.

3.2.4.1 Kinematic pairs

Consider now two rigid bodies whose relative motion is constraint. If we call these bodies i and j, we can describe the allowed motions by a subspace of $se(3)$ to which the twist ${}^0 T_i^j$ should belong. Let's call this subspace $\mathscr{T}_A$. This subspace will in general be function of the relative configuration H_i^j and possibly of time even if we will not specifically show that in the following equations for the sake of clarity. Suppose that this subspace is of dimension $n < 6$. In this case there will be n linear independent vectors whose span will coincide with $\mathscr{T}_A$. We will indicate these twists as $T_A^1, T_A^2, \ldots, T_A^n$. Due to these degrees of freedom, there will also be n linear independent wrenches which can be applied between the two bodies which can transfer energy to the relative motion. We will indicate these wrenches $W_A^1, W_A^2, \ldots, W_A^n$ and the subspace they span with $\mathscr{W}_A$. It is very important to realize that we cannot in general define $\mathscr{W}_A$ uniquely once $\mathscr{T}_A$ is known or the other way around due to the absence of a unique metric in $se(3)$. Nevertheless, we could use bi-invariant forms for this purpose like the hyperbolic form.

    What we can do in a unique way is to define the dual $6 - n$ dimensional spaces $\mathscr{W}_C := \mathscr{T}_A^{\perp}$ corresponding to the constraint wrenches (any of these wrenches will not transfer power $W_C^i T_A^j = 0 \ \forall i, j$) and $\mathscr{T}_F := \mathscr{W}_A^{\perp}$ corresponding to the forbidden motions (any applied wrench will not transfer energy to these directions $W_A^i T_F^j = 0 \ \forall i, j$). We can then define the non-singular 6×6 matrix

$$W^{\mathrm{T}} := \begin{bmatrix} W_A^1 \ \ldots \ W_A^n \ W_C^1 \ \ldots \ W_C^{6-n} \end{bmatrix} \tag{3.64}$$

It is now possible to consider for a kinematic pair k

$$W_k = W \begin{bmatrix} \tau \\ \lambda \end{bmatrix} \tag{3.65}$$

and dually

$$\begin{bmatrix} \dot{q} \\ v \end{bmatrix} = W^t T_k \tag{3.66}$$

where τ indicates the free torques which can be applied by external motors or actuators on the kinematic pair in order to generate or control motion in $\dot{q}$ and λ are indicating the Lagrangian multipliers which should be such to keep $v = 0$.

We can finally write (3.65) and (3.66) together to show the Dirac structure causally:

$$\begin{bmatrix} W_k \\ \dot{q} \\ v \end{bmatrix} \begin{bmatrix} 0 & W \\ -W^t & 0 \end{bmatrix} \begin{bmatrix} T_k \\ \tau \\ \lambda \end{bmatrix} \tag{3.67}$$

where the port (T_k, W_k) can be used to interconnect with the mechanism as it will be seen later, the port $(\dot{q}, \tau)$ can be used to drive and control the kinematic pair and therefore to supply or subtract energy to and from the mechanism and finally (v, λ) will be a port through which no power should be transferred since λ should be such that v would always be equal to 0.

3.2.4.2 Mechanism topology

Given a mechanism composed of rigid bodies, it is possible to find a network description of the mechanism similarly with what happens with electrical circuits, but now with complex six dimensional motions and time varying constraints. Suppose to have a mechanism composed of m rigid bodies indexed from 0 to $m - 1$ and such that the body 0 corresponds to a inertial base. Suppose that among those bodies we have n nodic elements that constraint relative motions of pair of bodies. We can describe this topology with a graph $G_P = (V_P, E_P)$ called *primary graph* in which V_P is the set of m rigid bodies and E_P the set of n edges corresponding to the pair constraints. We can define an *incidence matrix* $B \in \mathbb{R}^{m \times n}$ in which each column corresponding to an edge has a 1 in the row corresponding to the body to which the edge points and a -1 in the row corresponding to the body from which the edge stems from and zero everywhere else. We can then define a second graph $G_L = (V_L, E_L)$ called the *Lagrangian tree* which is composed of $m - 1$ edges stemming from each of the bodies which are not the inertial frames and all going toward the vertex 0. The graph which is obtained combining the primary and Lagrangian graph is called the *port connection graph*.

We can then define the fundamental $n \times (m + n)$ loop matrix

$$C := \begin{bmatrix} B^{\mathrm{T}} & I_{n \times n} \end{bmatrix} \tag{3.68}$$

Each of the rows of this matrix represents a loop of the port connection graph which can be obtained considering an edge of E_P and two edges of E_L which close the

edge of E_P via the body 0. To understand what this actually means we can see that
the following equation holds:

$$C \begin{bmatrix} {}^0T_1^0 \\ \vdots \\ {}^0T_m^0 \\ T_1 \\ \vdots \\ T_n \end{bmatrix} = 0 \tag{3.69}$$

where T_i indicates the relative twist corresponding to the i-th kinematic pair. This is
therefore a kind of Kirchhoff law which sums the relative twist around a loop to zero
as it is done in electrical circuits for the sum of relative potentials around a mesh.

Dually we can introduce the fundamental $m \times (n+m)$ *cut-set matrix*

$$Q := \begin{bmatrix} I_{m \times m} & -B \end{bmatrix} \tag{3.70}$$

Each row i of this matrix represents a cut-set corresponding to the sum of wrenches
on a body i. Such a cut-set has always one edge corresponding to the Lagrangian
tree which will represent the total wrench which will change the momenta of body
i and a number of other edges belonging to G_P corresponding to all wrenches the
kinematic pairs can apply to body i. This is similar to the Kirchhoff current law at
a node in an electrical circuit with the difference that in mechanics the non-nodicity
of inertial elements requires explicitly the presence of the Lagrangian tree. With the
usage of the fundamental cut-set tree, we obtain:

$$Q \begin{bmatrix} {}^0W_T^1 \\ \vdots \\ {}^0W_T^m \\ W_1 \\ \vdots \\ W_n \end{bmatrix} = 0 \tag{3.71}$$

where ${}^0W_T^i$ indicates the total wrench applied at body i and expressed in frame 0.

It can be easily seen that $CQ^t = 0$ and this actually corresponds to the Teleggen
theorem well known in electrical networks. In order to see that, a vector of twists
satisfying $C\bar{T} = 0$ can be also expressed using a image representation instead than a
kernel representation:

$$\bar{T} = C^T \alpha \qquad \forall \alpha$$

along a similar line of reasoning, any wrench set satisfying the network constrains
can be expressed using an image representation with

$$\bar{W} = Q^T \gamma \qquad \forall \gamma$$

If we now want to calculate the net power going into the network, we can just get the dual product of $\bar{W}$ and $\bar{T}$:

$$P = \bar{T}^t W = \alpha^t \underbrace{C Q^t}_{=0} \gamma = 0 \tag{3.72}$$

which indeed proves zero net power flow for any independent choices of $\bar{T}$ and $\bar{W}$ as known in Tellegen's theorem. We can also rearrange equations (3.71) and (3.69) to get to a general causal expression of the Dirac structure:

$$\begin{bmatrix} {}^0W_T^1 \\ \vdots \\ {}^0W_T^m \\ -T_1 \\ \vdots \\ -T_n \end{bmatrix} = \begin{bmatrix} 0 & B \\ -B^{\mathrm{T}} & 0 \end{bmatrix} \begin{bmatrix} {}^0T_1^0 \\ \vdots \\ {}^0T_m^0 \\ W_1 \\ \vdots \\ W_n \end{bmatrix} \tag{3.73}$$

It would then finally be possible to couple all ports ($\,^0T_1^0$, $\,^0W_T^i$) to the interconnection port of the rigid body model (3.63) and to connect the ports corresponding to each (T_k, W_k) to the corresponding port of a kinematic pair using the expression in (3.67).

In this way we obtain a model of the dynamics of the complete mechanism as the interconnection of various Dirac structures and port-Hamiltonian subsystem. This way of modeling is structured and very suitable for computer support. Furthermore, the usage of coordinate-free concepts ensures that the analysis is global and singularity free.

3.2.5 Flexible mechanisms

The modeling techniques presented in the previous sections can be generalized in order to define a systematic procedure, based on port concepts, for modeling and simulating mechanical systems with rigid *and* flexible links. The mathematical description of the whole mechanical system results from the interconnection of simpler components (e.g. rigid bodies, flexible links and kinematic pairs). Using the nonlinear model of a flexible link in distributed port-Hamiltonian form presented in [128] and, briefly, in Sect. 4.3.2, it is not necessary, in the definition of the dynamic model, to simplify the elastic and nonlinear effects present in the flexible parts, and therefore also mechanism with large deflections can be easily handled. This approach differs from what is illustrated in the next section, in which a more rigorous way for describing elastic systems is discussed. Moreover, the modularity of the approach can also be exploited for simplifying the simulation of such dynamical systems, even for control applications. In fact, if an object-oriented software package for model-

ing physical system is adopted, beside the mathematical derivation of the model also the numerical simulation of complex mechanisms can be carried out simply by port interconnection, thus leaving the solution of the causality of each sub-system to the simulation package. Among these software packages, one can mention the implementations of the Modelica language [78, 146] as Dymola [70] or Open Modelica [204], or the 20-sim package.

This is something completely different from what can be found in literature, where several methodological approaches for the definition of dynamic models of multi-body mechanical systems, taking possibly into account both rigid and flexible links, [9, 18, 26, 61, 62, 152, 190, 191, 199, 205] can be found. Moreover, a number of software packages, e.g. [4, 20, 50, 108, 194, 203] are also currently available for their numerical simulation. In case of flexible systems, these modeling approaches usually relay on finite dimensional approximations of the flexible link dynamics (e.g. modal expansion, finite elements or floating frame of reference) or on a simplification of the (nonlinear) elastic behavior of flexible links (Timoshenko or Euler-Bernoulli theory), and therefore they do not easily allow the description of mechanisms characterized by large deformations. Moreover, even if the simulation package is able to deal with large deformations and nonlinear effects (e.g. ABAQUS [194], ANSYS Multiphysics [4], or COMSOL Multiphysics [50]), in general it is not a trivial task to include the presence of state-feedback controllers. In fact, this requires the development of proper spatial discretization techniques for the elastic dynamics that are able to deal with time-varying boundary conditions, such as the torques applied at the extremities of each flexible link. These limitation are not present within the port Hamiltonian framework. Refer to [124, 128] for further information.

3.3 Modeling of simple elastic systems

3.3.1 Introduction

Simple elastic structures like strings, beams or membranes and plates are basic elements for many engineering fields. Roughly spoken, their mathematical models are approximations of certain equations of linearized elasticity. The mathematical models of elasticity, like other model in physics consist of two types of equations. The balance and/or conservation equations express that certain physical quantities or their sum are preserved. Typical representatives are the conservation of mass, charge, linear momentum, etc. The constitutive relations describe the behavior of the materials, typical representatives are Hook's law or friction relations. Within this setting one assumes that balance equations are never violated, whereas constitutive relations are often approximately known only.

Mathematical models of elastic structures are based on the conservation of mass and the balance of linear momentum and momentum of momentum, see

[133, 210, 221]. To simplify this complicated set of partial differential equations, one makes the strong constitutive assumption of the symmetry of the stress. This relation guarantees that balance of momentum of momentum is fulfilled, and we have to take conservation of mass and balance of linear momentum into account only. Additionally in simple elasticity, one assumes the existence of the stored energy function to express certain constitutive relations. If this function exists and the symmetry of stress is met, then the derived mathematical models have the structure of a Lagrangian or Hamiltonian system for a certain choice of the coordinates. The Lagrangian or Hamiltonian structure of these models is preserved by their linearization.

The models of structures, like beams or plates etc., with a small extension in one direction compared to the others, can be approximated by reduced models with less spatial variables. This way, the models of beams, plates, etc. are derived by the reduction of the linearized equations of simple elasticity. Of course, if the reduction process preserves the Hamiltonian or Lagrangian structure, then the resulting models will have this structure, too. Proceeding this way we show in an exemplary fashion how the Lagrangian or Hamiltonian formulation of the Euler Bernoulli beam can be derived in a straightforward manner. Furthermore, we use the simple example of the motion of a planar rigid body to illustrate the presented methods and ideas. But it is worth to mention that the presented methods can be applied to other mechanical structures like the Timoshenko beam (see [206] and Sect. 4.3.1), the Kirchhoff or Midline plate [123, 147], shell or membranes in an analogous manner.

3.3.2 Simple elasticity

The geometry of the general equations of elasticity are far beyond this contribution. Therefore, we confine ourselves to the case of simple elasticity, where the existence of the so called stored energy function is assumed. Furthermore, we describe the motion in an inertial frame with Euclidean coordinates and trivial metric. This choice is essential, since the following considerations are valid only in these coordinates. The Lagrangian and the Eulerian description are the most popular ones in continuum mechanics. Since we consider elastic bodies, we choose the Lagrangian description, which allows us to take into account the constitutive relations, which describe the behavior of material. Furthermore, we confine ourselves to the time invariant case, but we permit inputs like force or stress fields.

From now on, we use the standard tensor notation to keep formulas as short as possible and apply Einstein's convention for sums. Whenever the range of an index $i = 1, \dots, n$ is clear, we us the abbreviation

$$a^i b_i = \sum_{i=1}^{n} a^i b_i$$

Furhtermore, to avoid mathematical subleties we assume that all functions are sufficiently often continously differentiable, and that all regions for the integration are sufficiently nice.

We will consider functions, which depend on the time t and on the spatial coordinates X^I, $I = 1, \ldots, p$. Let x^i, $i = 1, \ldots, q$ denote the dependent coordinates, then $x^i = x^i(t, X)$ assigns the functions $x^i(t, X)$ to the coordinate x^i. Where no confusion occurs, we use the same symbol for the coordinate x^i and for the assigned function $x^i = x^i(t, X)$. Since we will deal with several higher order derivatives of these functions, we use the abbreviations

$$\partial_I = \frac{\partial}{\partial X^I} \qquad \partial_t = \frac{\partial}{\partial t} \qquad \partial_{IJ} = \partial_I \partial_J \qquad \partial_{tI} = \partial_t \partial_I$$

etc. We need also the derivative coordinates of first order x^i_t, x^i_I and higher order $x^i_{M\ldots}$ with the unordered multi index $M = m_1, \ldots, m_k, \ldots, m_r$, $m_k \in \{t\} \cup \{1, \ldots, p\}$, where $\#M = r$ is the order of the derivative. This notation is motivated by the assignment $x^i_M = \partial_M x^i(t, X)$, $\partial_M = \partial_{m_1} \cdots \partial_{m_r}$. We will also use the conventions $x^i_M = x^i$, $\partial_M x^i(t, X) = x^i(t, X)$ for $\#M = 0$.

Let us consider a function $f(t, X, x_M)$, $0 \leq \#M \leq m$. We say that the total derivative $(d_I f)(t, X, x_N)$, $0 \leq \#N \leq m + 1$ of f in the direction of I is the unique function $(d_I f)$, which meets

$$\partial_I f(t, X, \partial_M x(t, X)) = (d_I f)(t, X, \partial_N x(t, X)) \tag{3.74}$$

Obviously, the differential operator d_I or the total derivative into the direction of I is given by

$$d_I = \partial_I + x^i_{M,I} \partial^M_i = \partial_I + \sum_{\#M \geq 0} x^i_{M,I} \partial^M_i \qquad \partial^M_i = \frac{\partial}{\partial x^i_M}$$

with $I \in \{t\} \cup \{1, \ldots, p\}$.

3.3.2.1 Motion and coordinates

In general we need three coordinate systems for the modeling of an elastic body, the configuration space $\mathscr{C}$, where physics takes place, the reference space $\mathscr{R}$, where we do bookkeeping, and the more abstract space $\mathscr{G}$, which is used to parameterize maps from $\mathscr{R}$ to $\mathscr{C}$ by its generalized coordinates. Here, we choose $\mathscr{C} = \mathbb{R}^n$, $\mathscr{R} = \mathbb{R}^n$ and assume that $\mathscr{C}$, $\mathscr{R}$ are equipped with the Euclidean coordinates (x^i), (X^I), wit $i, I = 1, \ldots, n^4$. In addition $\mathscr{C}$ is an inertial space. The position of a mass point is given by $X \in \mathscr{B} \subset \mathscr{R}$, where $\mathscr{B}$ denotes the set of all mass points of the elastic body. A motion is a map

---

[4] Of course, values of $n \in \{1, 2, 3\}$ are of physical interest only. Since the following considerations are indpendent of choice of p, the value of p is unspecified.

Fig. 3.11 Motion of a planar
rigid body.
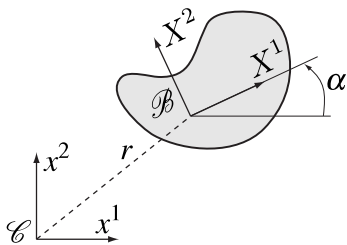
$$x^i = \phi^i(t,X) \qquad\qquad i = 1,\ldots,n \qquad\qquad (3.75)$$

which assigns the position x of a mass point X at time t. We assume that we can
invert ϕ such that $X = \phi^{-1}(t,x)$ is met. Fig. 3.11 illustrates the configuration and
reference space $\mathscr{C} = \mathbb{R}^2$, $\mathscr{R} = \mathbb{R}^2$ together with map (3.75) for the example of a
planar rigid body.

Throughout this contribution we equip the Euclidean space $\mathscr{C}$ with the trivial
metric. Let (v^i), (w^i) be two elements of the tangent space $T\mathscr{C}$ of $\mathscr{C}$, then their
product is given by

$$(v,w) = v^i g_{ij} w^j \qquad\qquad (3.76)$$

with

$$g_{ij} = \delta_{ij}$$

being δ_{ij} with the Kronecker symbol. The choice of the trivial metric is essential to
simplify the following. Before we can proceed with the balance laws, we introduce
the spatial velocity V and the velocity vector field v,

$$V^i = \partial_t \phi^i(t,X) \qquad\qquad v^i = V^i \circ \phi^{-1}(t,x) \qquad\qquad (3.77)$$

In addition we derive from (3.75) the so called deformation gradient

$$\left[J_I^i\right] = \left[\partial_I \phi^i\right] \qquad\qquad (3.78)$$

The inverse of $[J_I^i]$ is denoted by $[\bar{J}_i^I]$.

To parameterize the map (3.75) we choose further coordinates $\tilde{X}^{\tilde{I}}$ and $\bar{x}^{\bar{i}}$, with
$\tilde{I} = 1,\ldots,n$ and $\bar{i} = 1,\ldots,m$, and assume that the functions $\bar{x}^{\bar{i}}(t,\bar{X})$ depend on t and
$\bar{X}^{\bar{I}} = \tilde{X}^{\bar{I}}$ only, with $\bar{I} = 1,\ldots,\bar{n}$, or equivalently they are independent of $\hat{X}^{\hat{I}} = \tilde{X}^{\hat{I}}$,
with $\hat{I} = \bar{n}+1,\ldots,n$. A parameterization of (3.75) is given by the $2n$ functions ψ^i
and φ^I, i.e.:

$$x^i = \psi^i(X,\bar{x}_M) \qquad \#\bar{M} \geq 0$$
$$X^I = \varphi^I(\tilde{X}) \qquad\qquad\qquad\qquad (3.79)$$

such that the map φ is invertible and

$$\phi^i(t,X) = \psi^i(X,\partial_{\bar{M}}\bar{x}(t,\bar{X}))$$

is met for $\bar{x}^{\bar{i}} = \bar{x}^{\bar{i}}(t, \bar{X})$. Therefore, we choose the coordinates $(\bar{X}^{\bar{I}}, \bar{x}^{\bar{i}})$ for $\mathcal{G}$ and add the required derivative coordinates $\bar{x}^{\bar{i}}_{\bar{M}}$.

Let us take a look at the parametrization of the motion of the planar rigid body of Fig. 3.11. With $X^{\hat{I}} = \hat{X}^{\hat{I}}$, with $\hat{I} = 1, 2$, $\bar{x}^{\hat{i}} = r^{\hat{i}}$, with $\hat{i} = 1, 2$, and $\bar{x}^3 = \alpha$ one possibility is given by the well known relations

$$x^i = R^i_{\hat{I}}(\alpha)\hat{X}^{\hat{I}} + \delta^i_{\bar{i}} r^{\bar{i}} \qquad\qquad R = \begin{bmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{bmatrix} \qquad (3.80)$$

for $i = 1, 2$ with the rotary matrix R and the Kronecker symbol δ. Obviously, the coordinates (r, α) describe locally $\mathbb{R}^2 \times SO^2$ with the one dimensional rotary group SO^2.

3.3.2.2 Conservation of mass and balance of momentum

Let $\rho(t, x)$ denote the mass density in $\mathcal{C}$ and let $\mathcal{D}$ be an arbitrary subset $\mathcal{D} \subset \mathcal{B}$ such that we can integrate over $\mathcal{D}$. With the total time derivative d_t, and the volume forms $dx = dx^1 \cdots dx^n$, $dX = dX^1 \cdots dX^n$ on $\mathcal{C}$ and $\mathcal{R}$ we derive the identity

$$d_t \int_{\phi(t, \mathcal{D})} \rho(t, x)\, dx = d_t \int_{\mathcal{D}} \rho(t, \phi(t, X)) |J(t, X)|\, dX = \int_{\mathcal{D}} \partial_t \rho_{\mathcal{R}}(t, X)\, dX$$

with

$$\rho_{\mathcal{R}}(t, X) = \rho(t, \phi(t, X)) |J(t, X)|$$

where $|J(t, X)|$ denotes the determinant of J. Obviously, conservation of mass implies

$$\int_{\mathcal{D}} \partial_t \rho_{\mathcal{R}}(t, X)\, dX = 0 \qquad\qquad (3.81)$$

To proceed with the balance of linear momentum, we make the strong constitutive assumption of the symmetry of the Cauchy stress tensor $\sigma(t, x)$, see [133]. This assumption implies that the balance of momentum of momentum is met. Let $\partial \mathcal{D}$ denote the boundary of $\mathcal{D}$ and

$$\partial_i \rfloor dx = (-1)^{(i-1)}\, dx^1 \cdots \widehat{dx^i} \cdots dx^n$$

where the term $\widehat{dx^i}$ is omitted, be the ith surface element, then balance of linear momentum is given by

$$d_t \int_{\phi(t, \mathcal{D})} v^i(t, x) \rho(t, x)\, dx = \int_{\phi(t, \mathcal{D})} f^i(t, x)\, dx + \int_{\phi(t, \partial \mathcal{D})} \sigma^{ij}(t, x)\, \partial_j \rfloor dx$$

$$= \int_{\phi(t, \mathcal{D})} \left(f^i(t, x) + \partial_j \sigma^{ij}(t, x) \right) dx$$

with the body forces f. Using (3.81) we get

$$d_t \int_{\phi(t,\mathscr{D})} v^i(t,x)\rho(t,x)\,dx = \int_{\mathscr{D}} \rho_{\mathscr{R}}(X)\partial_t V^i(t,X)\,dX$$

and derive in a similar manner the force field F in Lagrangian description and the first Piola Kirchoff stress tensor P, see [133]:

$$F^i(t,X) = f^i(t,\phi(t,X))|J(t,X)|$$
$$P^{iJ}(t,X) = \sigma^{ij}(t,\phi(t,X))\bar{J}_j^J(t,X)|J(t,X)|$$

such that the relations

$$\int_{\phi(t,\mathscr{D})} f^i(t,x)\,dx = \int_{\mathscr{D}} F^i(t,X)\,dX$$

$$\int_{\phi(t,\partial\mathscr{D})} \sigma^{ij}(t,x)\,\partial_j \rfloor dx = \int_{\partial\mathscr{D}} P^{iJ}(t,X)\,\partial_J \rfloor dX \tag{3.82}$$

are met. Summarizing, we may write the balance of linear momentum in Lagrangian description in the form

$$\int_{\mathscr{D}} \rho_{\mathscr{R}}(X)\partial_t V^i(t,X)\,dX = \int_{\mathscr{D}}\left(F^i(t,X) + \partial_I P^{iI}(t,X)\right)dX \tag{3.83}$$

3.3.2.3 Equations of motion

The equations (3.81), (3.83) are incomplete, since the constitutive relations are missing. To overcome this problem, we have to parameterize the map (3.75) by generalized coordinates. The simplest choice is $\bar{X}^I = X^I$, with $I = 1,\dots,n$ for the independent, and $\bar{x}^i = x^i$, with $i = 1,\dots,n$ for the dependent spatial coordinates. Since the generalized coordinates $\bar{X}$ and $\bar{x}$ conincide with the coordinates X and x of $\mathscr{C}$ and $\mathscr{R}$ we suppress the accent here. If (3.83) holds for every "nice" subset $\mathscr{D} \subset \mathscr{B}$, then we may conclude that

$$\rho_{\mathscr{R}} x_{tt}^i = \left(F^i + d_I P^{iI}\right) \tag{3.84}$$

is met. For the present we allow that P^{iI} and F^i may depend on t, X and x_M, with $\#M \geq 0$. Therefore, we have to use the total derivative d_I, see (3.74), instead of the partial derivative ∂_I, like in (3.83). Multiplication of (3.84) with $(x_t^j g_{ij})$ and integration over $\mathscr{D}$ leads to

$$\int_{\mathscr{D}} \rho_{\mathscr{R}} x_t^j g_{ij} x_{tt}^i\,dX = \int_{\mathscr{D}}\left(x_t^j g_{ij} F^i + x_t^j g_{ij} d_I P^{iI}\right)dX$$

$$\int_{\mathscr{D}}\left(\rho_{\mathscr{R}} x_t^j g_{ij} x_{tt}^i + d_I\left(x_t^j g_{ij}\right)P^{iI}\right)dX = \int_{\mathscr{D}}\left(x_t^j g_{ij} F^i + d_I\left(x_t^j g_{ij} P^{iI}\right)\right)dX$$

or

$$\int_{\mathscr{D}} \left(d_t \left(\frac{\rho_{\mathscr{R}}}{2} x_t^i g_{ij} x_t^j \right) + \frac{1}{2} d_t \left(x_I^i g_{ij} x_J^j \right) S^{IJ} \right) dX =$$

$$= \int_{\mathscr{D}} \left(d_t \left(\frac{\rho_{\mathscr{R}}}{2} x_t^i g_{ij} x_t^j \right) + \frac{1}{2} d_t \left(C_{IJ} \right) S^{IJ} \right) dX =$$

$$= \int_{\mathscr{D}} x_t^i g_{ij} F^j dX + \int_{\partial \mathscr{D}} x_t^i g_{ij} P^{jI} \partial_I \rfloor dX$$

with

$$C_{IJ} = x_I^i g_{ij} x_J^j \qquad\qquad P^{iJ} = x_I^i S^{IJ} \qquad\qquad (3.85)$$

The Cauchy Green deformation tensor C, see [133], is symmetric by construction, whereas the symmetry of the second Piola Kirchhoff tensor S, see [133], is a consequence of the symmetry of the Cauchy stress tensor σ. In simple elasticity one assumes $S^{IJ} = S^{IJ}(X,C)$ and the existence of the stored energy function $e_E(X,C)$ such that

$$2 \frac{\partial}{\partial C_{IJ}} e_E(X,C) = S^{IJ}(X,C) \qquad\qquad (3.86)$$

is met. This is possible only, if S is symmetric. In this case the balance of energy is given by

$$\int_{\mathscr{D}} d_t (e_K + e_E) dX = \int_{\mathscr{D}} x_t^i g_{ij} F^j dX + \int_{\partial \mathscr{D}} x_t^i g_{ij} P^{jI} \partial_I \rfloor dX \qquad (3.87)$$

with the kinetic energy density

$$e_K(X,x_t) = \frac{\rho_{\mathscr{R}}}{2} x_t^i g_{ij} x_t^j \qquad\qquad (3.88)$$

Obviously, the coordinates (t, X^I, x_M^i), with $M = m_1, \ldots, m_r$, $m_k \in \{t\} \cup \{1, \ldots, n\}$ and $0 \le \#M \le 2$, are necessary to model a simple elastic system, and the equations of motion (3.84) are partial differential equations of second order. In addition, a simple elastic body allows two types of ports defined by the pairs $((x_t, F), (x_t, P))$ distributed over $\mathscr{B}$ and $\partial \mathscr{B}$. It is worth mentioning that $((x_t^i), (g_{ij} F^j))$ are elements of two linear spaces dual to each other. The analogous property is met by $((x_t^i), (g_{ij} P^{jI}))$. One can use these ports to connect the body to other systems in a power preserving manner. If sliding of the ports is permitted then the relations $x_t^i = \tilde{x}_t^i$, $F^i = -\tilde{F}^i$ and $x_t^i = \tilde{x}_t^i$, $P^{il} = -\tilde{P}^{il}$ must be met, where $\tilde{\cdot}$ refers to the second system.

3.3.3 The Hamiltonian and Lagrangian picture

To show that the equations (3.84) are of the Lagrangian type, it is sufficient to find a Lagrangian density $l(X, x_M^i)$, with $0 \le \#M \le 1$ such that the equations

$$\delta_i l + g_{ij} F^j = 0 \qquad\qquad (3.89)$$

with the variational derivative

$$\delta_i = \sum_{\#M \geq 0} (-1)^{\#M} d_M \partial_i^M \tag{3.90}$$

coincide with the equations (3.84), where $d_M = d_{m_1} \cdots d_{m_r}$. Obviously, the choice

$$l = e_K - e_E$$

with the kinetic energy of (3.88) and the stored energy function of (3.86) solves this problem because of

$$\delta_i l = -d_t \partial_i^t e_K + d_I \left(\frac{1}{2} S^{JK} \partial_i^I C_{JK} \right) = -\rho_{\mathscr{R}} x_{tt}^i + d_I \left(2 x_K^i \frac{1}{2} S^{IK} \right)$$

Furthermore, if the force field F meets the condition $\delta_{ij} F^j = -\partial_i e_F(X, x)$, then it can be included in the Lagrangian by $l = e_K - e_E - e_F$.

The Lagrangian equations (3.89) are implicit equations in general. Furthermore time and spatial variables are handled on the same footing, their different nature is expressed in the boundary conditions only. In the Hamiltonian picture the equations are explicit equations solved with respect to the time derivatives of the dependent variables. To derive them, we introduce the generalized momenta p_i by the Legendre transformation

$$p_i = \partial_i^t l = \rho_{\mathscr{R}} g_{ij} x_t^j \tag{3.91}$$

and proceed with the coordinates $(t, X^I, x^i, p_i, x_t^i, p_{i,t}, x_{\bar{M}}^i)$, where we have that $M = m_1, \dots, m_k, \dots, m_r$, $m_k \in \{1, \dots, n\}$ and $1 \leq \#M \leq 2$. The Hamiltonian density h is given by

$$h(X, x^i, p_i, x_M^i) = (p^i \partial_i^t l - l) = e_K(X, g^{ij} p_j / \rho_{\mathscr{R}}) + e_E \tag{3.92}$$

with $g^{ik} g_{kj} = \delta_j^i$, and the Hamiltonian equations take the form

$$x_t^i = \bar{\delta}^i h \qquad\qquad p_{i,t} = -\bar{\delta}_i h + g_{ij} F^j \tag{3.93}$$

with the variational derivatives

$$\bar{\delta}^i = \partial^i = \frac{\partial}{\partial p_i} \qquad\qquad \bar{\delta}_i = \sum_{\#M \geq 0} (-1)^{\#M} d_M \partial_i^M$$

in the new coordinates. Again, the Hamiltonian equations are partial differential equations of second order with respect to the spatial derivatives, but of first order only with respect to the time derivatives. The boundary conditions for both, the Lagrangian or Hamiltonian equations, follow from the same consideration like above.

3.3.4 The linearized scenario

To find the linearized equations of simple elasticity, we have to consider the relations (3.84), (3.86). Let us consider the equation (3.84) first. Now it is appropriate to introduce the Lagrangian strain tensor E:

$$2E_{IJ} = C_{IJ} + \delta_{IJ}$$

and displacement coordinates, see [133, 210, 221], by

$$x^i = \delta_I^i X^I + u^i$$

In the case of small strain one replaces E by the linearized small strain tensor ε:

$$2\varepsilon_{IJ} = u_I^i g_{ij} \delta_J^j + \delta_I^i g_{ij} u_J^j \tag{3.94}$$

Furthermore, we set $P^{iJ} \approx \delta_I^i S^{IJ}(X, \varepsilon)$. In this case the equations (3.84) simplify to

$$\rho_{\mathcal{R}} u_{tt}^i = \left(F^i + d_I \delta_j^i S^{JI} \right) \tag{3.95}$$

It is worth mentioning that nonlinear constitutive equations are still possible provided the strain remains small. Often one assumes that the stored energy function e_E takes the quadratic form

$$e_E(X, \varepsilon) = \frac{1}{2} \varepsilon_{IJ} E^{IJKL}(X) \varepsilon_{KL} \tag{3.96}$$

with $E = E^{JIKL} = E^{IJLK} = E^{KLIJ}$ then (3.86) simplifies to

$$S^{IJ} = \partial_{\varepsilon_{IJ}} e_E = E^{IJKL}(X) \varepsilon_{KL} \tag{3.97}$$

which is nothing else than Hook's law. Following these considerations and the previous section, it is straightforward to derive the Lagrangian or Hamiltonian equations for the linearized scenario.

3.3.5 Reduction

Often the equations (3.84) can be approximated by simpler ones. Examples are beams or plates, where the extension of the structure in a certain direction differs significantly from the ones in the others. The reduction under consideration here is based on the Lagrangian (3.89) or the Hamiltonian (3.91) description of (3.84). The main idea is quite simple. With the parameterization (3.79) one determines the Lagrangian $\bar{l}$ or Hamiltonian density $\bar{h}$ in the generalized coordinates and gets the equations of motion from this functions.

Let us discuss the reduction based on the Lagrangian equations first. Given (3.79) we extend these relations to the derivative coordinates by

$$x_t^i = d_{\bar{t}}\psi^i \qquad\qquad\qquad x_I^i = d_{\bar{I}}\psi^i D_I^{\bar{I}} \qquad\qquad (3.98)$$

where $\bar{D} = [\bar{D}_I^{\bar{I}}]$ denotes the inverse of the Jacobian $D = [\partial_{\bar{I}}\varphi^I]$. The total derivatives $d_{\bar{I}}$ in the new coordinates $(t, \bar{X}^{\bar{I}}, \bar{x}_{\bar{M}}^i)$ are given by

$$d_{\bar{t}} = \partial_t + \bar{x}_{\bar{M},t}^i \partial_i^{\bar{M}}$$

$$d_{\bar{I}} = d_{\bar{I}} = \partial_{\bar{I}} + \bar{x}_{\bar{M},\bar{I}}^i \partial_i^{\bar{M}} \qquad\qquad \bar{I} = 1,\ldots,\bar{n}$$

$$d_{\bar{I}} = \partial_{\hat{I}} \qquad\qquad\qquad \hat{I} = \bar{n}+1,\ldots n$$

Proceeding with (3.98) in an analogous manner we derive the relations for higher order relatives. Now the simplified Lagrangian density $\bar{l}$ follows as

$$\bar{l}(t, \bar{X}, \bar{x}_{\bar{M}}) = \int_{\widehat{\mathcal{X}}(\bar{X})} l(t, X, x_M) |D| \, d\hat{X}^{\hat{n}+1} \cdots d\hat{X}^n \qquad\qquad (3.99)$$

where we have to plug in the functions for X and x_M according to (3.79) and (3.98), and the relations for the higher order derivatives. The domain $\widehat{\mathcal{X}}(\bar{X})$ of integration meets $\mathcal{B} = \widehat{\mathcal{X}}(\mathcal{X})$ as well as $\bar{X}_a \neq \bar{X}_b$ implies $\widehat{\mathcal{X}}(\bar{X}_a) \cap \widehat{\mathcal{X}}(\bar{X}_b) = \emptyset$. To derive the force field $\bar{F}_{\bar{I}}$ from (3.89) we need the tangent map of (3.79) given by

$$\dot{x}^i = \partial_i^{\bar{M}} \psi^i \dot{\bar{x}}_{\bar{M}}^{\bar{i}} = \partial_i^{\bar{M}} \psi^i d_{\bar{M}} \dot{\bar{x}}^{\bar{i}} \qquad\qquad (3.100)$$

The functions $\bar{F}_{\bar{I}}$, also called generalized forces, follow from the relation

$$\int_{\mathcal{X}} \left(\int_{\widehat{\mathcal{X}}(\bar{X})} \partial_i^{\bar{M}} \psi^i \left(d_{\bar{M}} \dot{\bar{x}}^{\bar{i}} \right) g_{ij} F^j |D| \, d\widehat{X} - \dot{\bar{x}}^{\bar{i}} \bar{F}_{\bar{i}} \right) d\bar{X} = 0 \qquad\qquad (3.101)$$

which is supposed to hold for arbitrary $\dot{\bar{x}}^{\bar{i}} = \dot{\bar{x}}^{\bar{i}}(t, \bar{X})$, which vanishes on the boundary $\partial \mathcal{X}$. It is worth mentioning that (3.100) contains the differential operators $d_{\bar{M}}$. This is just the point, where the boundary conditions come into the play. Because of the complexity of this problem, we will consider special cases in the examples only. Finally, the Lagrangian equations follow as

$$\delta_{\bar{i}}\bar{l} + \bar{F}_{\bar{i}} = 0 \qquad\qquad (3.102)$$

To derive the reduced equations in the Hamiltonian picture, one can apply the Legendre transformation to (3.99). Provided this transformation exists and is a point transformation. Then one derives the Hamiltonian equations in a straightforward manner. Another way is to look for relations for the generalized momenta $\bar{p}_{\bar{i}}$. We require that

$$\int_{\mathcal{X}} \left(\int_{\widehat{\mathcal{X}}(\bar{X})} p_i \dot{x}^i |D\varphi| \, d\widehat{X} - \bar{p}_{\bar{i}} \dot{\bar{x}}^{\bar{i}} \right) d\bar{X} = 0 \qquad\qquad (3.103)$$

is met for p_i from (3.91), $\dot{x}^i$ from (3.100) and arbitrary functions for $\dot{\tilde{x}}^{\bar{i}}$, which vanish on the boundary $\partial \mathcal{X}$. If it is possible to determine the generalized momenta, then one can apply reduction procedure to the Hamiltonian density (3.92) analogously to the one for the Lagrangian density described above. To complete this section, we have to show, how the boundary conditions for the reduced model are derived. Because of the complexity of this problem we will discuss this in the example of Sect. 3.3.6 only.

3.3.5.1 The rigid body

Let us consider again the planar rigid body of Fig. 3.11, which is influenced by a force field F now. From (3.80), (3.98) we derive the relations

$$x_t^i = R_{\hat{I}}^i \Omega_{\hat{J}}^{\hat{I}} \alpha_t \hat{X}^{\hat{J}} + \delta_{\bar{i}}^i r_t^{\bar{i}} \qquad\qquad \Omega = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

Now it is well known, that the Lagrangian L takes the simple form

$$
\begin{aligned}
L(r, \alpha, r_t, \alpha_t) &= \frac{1}{2} \int_{\mathcal{B}} \left(R_{\hat{I}}^i \Omega_{\hat{J}}^{\hat{I}} \alpha_t \hat{X}^{\hat{J}} + \delta_{\bar{i}}^i r_t^{\bar{i}} \right) g_{ij} \left(R_{\hat{K}}^j \Omega_{\hat{L}}^{\hat{K}} \alpha_t \hat{X}^{\hat{L}} + \delta_{\bar{j}}^j r_t^{\bar{j}} \right) \rho_{\mathcal{R}} d\hat{X} \\
&= \frac{1}{2} \left(\theta (\alpha_t)^2 + M r_t^{\bar{i}} \delta_{\bar{i}\bar{j}} r_t^{\bar{j}} \right)
\end{aligned}
$$

with the rotational inertia θ, and mass M,

$$\theta = \int_{\mathcal{B}} X^I \delta_{IJ} X^J \rho_{\mathcal{R}} d\hat{X} \qquad\qquad M = \int_{\mathcal{B}} \rho_{\mathcal{R}} d\hat{X} \qquad (3.104)$$

provided the point $\hat{X}^I = 0$ is the center of gravity such that

$$\int_{\mathcal{B}} \hat{X}^{\hat{I}} \rho_{\mathcal{R}} d\hat{X} = 0$$

is met. With the tangent map, see (3.100)

$$\dot{x}^i = R_{\hat{I}}^i \Omega_{\hat{J}}^{\hat{I}} \dot{\alpha} \hat{X}^{\hat{J}} + \delta_{\bar{i}}^i \dot{r}^{\bar{i}}$$

and from, see (3.101):

$$\int_{\mathcal{B}} \left(\left(R_{\hat{I}}^i \Omega_{\hat{J}}^{\hat{I}} \dot{\alpha} \hat{X}^{\hat{J}} + \delta_{\bar{i}}^i \dot{r}^{\bar{i}} \right) g_{ij} F^j - \dot{\alpha} \bar{T} - \bar{F}_{\bar{i}} \dot{r}^{\bar{i}} \right) d\hat{X} = 0$$

we derive the generalized forces $\bar{F}_{\bar{i}}, \bar{T}$ as

$$\bar{F}_{\bar{i}} = \int_{\mathcal{B}} \delta_{\bar{i}}^i g_{ij} F^j d\hat{X} \qquad\qquad \bar{T} = \int_{\mathcal{B}} R_{\hat{I}}^i \Omega_{\hat{J}}^{\hat{I}} \hat{X}^{\hat{J}} g_{ij} F^j d\hat{X}$$

and finally the equations of motion

Fig. 3.12 Euler Bernoulli beam.
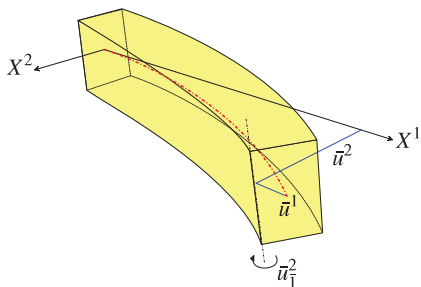
$$\theta \, \alpha_{tt} = \bar{T} \qquad\qquad M \delta_{\bar{i}\bar{j}} r^{\bar{j}}_{tt} = \bar{F}_{\bar{i}}$$

Since the derivation of the Hamiltonian counterpart to these equations is straightforward, it will be omitted here.

3.3.6 The Euler-Bernoulli beam

Beams are examples of two dimensional structures with different extensions in X^1 and X^2 directions. We choose a simple elastic material with the stored energy function, see (3.94) and (3.96):

$$e_E = \frac{1}{2} \left(a \left((\varepsilon_{11})^2 + (\varepsilon_{22})^2 \right) + 2b \varepsilon_{11} \varepsilon_{22} + c \, (\varepsilon_{12})^2 \right)$$

with $a, c \in \mathbb{R}^+$, $b \in \mathbb{R}$, $a > b$. Now, we apply the reduction, see (3.79) and [221]:

$$X^1 = \bar{X} \qquad X^2 = \hat{X} \qquad u^1 = \bar{u}^1 - \hat{X} \bar{u}^2_{\bar{1}} \qquad u^2 = \bar{u}^2 \qquad (3.105)$$

according to the assumptions for the Euler-Bernoulli beam, see also Fig. 3.12. Following the consideration from above we derive the additional relations

$$u^1_t = \bar{u}^1_t - \hat{X} \bar{u}^2_{t\bar{1}} \qquad\qquad u^2_t = \bar{u}^2_t$$
$$\varepsilon_{11} = u^1_1 = \bar{u}^1_{\bar{1}} - \hat{X} \bar{u}^2_{\bar{1}\bar{1}} \qquad 2\varepsilon_{12} = u^1_2 + u^2_1 = 0 \qquad \varepsilon_{22} = u^2_2 = 0$$

The Lagragian density $\bar{l} = \bar{l}(\bar{X}, \bar{u}^1_t, \bar{u}^2_t, \bar{u}^1_{\bar{1}}, \bar{u}^2_{\bar{1}\bar{1}}, \bar{u}^2_{t\bar{1}})$ follows according to (3.99) as

$$\bar{l} = \frac{1}{2} \int_{h/2}^{h/2} \left(\rho_{\mathscr{R}} \left((\bar{u}^1_t - \bar{u}^2_{t\bar{1}} \hat{X})^2 + (\bar{u}^2_t)^2 \right) - a \left(\bar{u}^1_{\bar{1}} - \hat{X} \bar{u}^2_{\bar{1}\bar{1}} \right)^2 \right) d\hat{X}$$

$$= \frac{h}{2} \left(\rho_{\mathscr{R}} \left((\bar{u}^1_t)^2 + \underbrace{\frac{h^2}{12} (\bar{u}^2_{t\bar{1}})^2}_{\approx 0} + (\bar{u}^2_t)^2 \right) - a \left((\bar{u}^1_{\bar{1}})^1 + \frac{h^2}{12} (\bar{u}^2_{\bar{1}\bar{1}})^2 \right) \right) \qquad (3.106)$$

Now we use (3.101) to derive the reduced field $\bar{F}$. From the relations

$$\int_0^L \left(\int_{-h/2}^{h/2} \left(F^1 \left(\dot{\bar{u}}^1 - \hat{X} \dot{\bar{u}}^2_{\bar{1}} \right) + F^2 \dot{\bar{u}}^2 \right) d\hat{X} - \bar{F}_{\bar{i}} \dot{\bar{u}}^{\bar{i}} \right) d\bar{X} = 0$$

$$\int_0^L \left(\dot{\bar{u}}^1 \int_{-h/2}^{h/2} F^1 d\hat{X} + \dot{\bar{u}}^2 \int_{-h/2}^{h/2} \left(d_{\bar{1}} F^1 \hat{X} + F^2 \right) d\hat{X} - \bar{F}_{\bar{i}} \dot{\bar{u}}^{\bar{i}} \right) d\bar{X} = \underbrace{\dot{\bar{u}}^2 \int_{-h/2}^{h/2} F^1 \hat{X} d\hat{X} \Big|_0^L}_{=0}$$

and the Lagrangian (3.106) one gets the inhomogenous wave equation

$$h \left(\rho_{\mathscr{R}} \bar{u}^1_{tt} - a \bar{u}^1_{\bar{1}\bar{1}} \right) = \bar{F}_1 = \int_{-h/2}^{h/2} F^1 d\hat{X} \tag{3.107}$$

for $\bar{u}^1$ and the well known beam equation

$$h \left(\rho_{\mathscr{R}} \left(\bar{u}^2_{tt} - \underbrace{\frac{h^2}{12} \bar{u}^2_{tt\bar{1}\bar{1}}}_{\approx 0} \right) + a \frac{h^2}{12} \bar{u}^2_{\bar{1}\bar{1}\bar{1}\bar{1}} \right) = \bar{F}_2 = \int_{-h/2}^{h/2} \left(d_{\bar{1}} F^1 \hat{X} + F^2 \right) d\hat{X} \tag{3.108}$$

for $\bar{u}^2$, provided the underbraced term is neglected in (3.106) and (3.108).

Finally, the evaluation of the boundary term of the energy relation (3.87) for $\bar{X} \in \{0, L\}$ with the lenght L of the beam to

$$\int_{-h/2}^{h/2} \left(\bar{u}^1_t S^{11} + \bar{u}^2_t S^{21} \right) d\hat{X} = \bar{u}^1_t \bar{u}^1_{\bar{1}} \int_{-h/2}^{h/2} a d\hat{X} - \bar{u}^2_t \bar{u}^2_{\bar{1}\bar{1}} \int_{-h/2}^{h/2} a \hat{X} d\hat{X}$$

$$= \left(\bar{u}^1_t \left(a h \bar{u}^1_{\bar{1}} \right) - \bar{u}^2_t \left(\bar{u}^2_{\bar{1}\bar{1}} \frac{a h^2}{2} \right) \right)$$

Therefore, we may introduce two ports at eauch boundary build up by the pairs $(\bar{u}^1_t, a h \bar{u}^1_{\bar{1}})$ and $(\bar{u}^2_t, \bar{u}^2_{\bar{1}\bar{1}} a h^2 / 2)$, wich can be used to connect the Euler Bernoulli beam to other structures.

Let us now take the Hamiltonian point of view. We determine the generalized momenta $\bar{p}_1$ and $\bar{p}_2$. According to (3.103), from

$$\int_0^L \left(\int_{-h/2}^{h/2} \left(\left(\bar{u}^1_t - \hat{X} \bar{u}^2_{t\bar{1}} \right) \left(\dot{\bar{u}}^1 - \hat{X} \dot{\bar{u}}^2_{\bar{1}} \right) + \bar{u}^2_t \dot{\bar{u}}^2 \right) \rho_{\mathscr{R}} d\hat{X} - \bar{p}_{\bar{i}} \dot{\bar{u}}^{\bar{i}} \right) d\bar{X} = 0$$

$$\int_0^L \left(\left(\bar{u}^1_t \dot{\bar{u}}^1 + \frac{h^2}{12} \bar{u}^2_{t\bar{1}} \dot{\bar{u}}^2_{\bar{1}} + \bar{u}^2_t \dot{\bar{u}}^2 \right) \rho_{\mathscr{R}} d\hat{X} - \bar{p}_{\bar{i}} \dot{\bar{u}}^{\bar{i}} \right) d\bar{X} = 0$$

$$\int_0^L \left(\left(\bar{u}^1_t \dot{\bar{u}}^1 + \left(\bar{u}^2_t - \frac{h^2}{12} \bar{u}^2_{t\bar{1}\bar{1}} \right) \dot{\bar{u}}^2 \right) \rho_{\mathscr{R}} d\hat{X} - \bar{p}_{\bar{i}} \dot{\bar{u}}^{\bar{i}} \right) d\bar{X} = \underbrace{- \frac{h^2}{12} \bar{u}^2_{t\bar{1}} \dot{\bar{u}}^2 \Big|_0^L}_{=0}$$

the relations

$$\bar{p}_1 = \rho_{\mathscr{R}} h \bar{u}_t^1 \qquad\qquad \bar{p}_2 = \rho_{\mathscr{R}} h \left(\bar{u}_t^2 - \frac{h^2}{12} \bar{u}_{t\bar{1}\bar{1}}^2 \right)$$

Obviously, it is straightforward to derive $\bar{p}_2$ as a function of $\bar{u}_t^2$ and its derivatives. But the determination of the inverse map requires the solution of a differential equation. Therefore the Legendre trasformation fails to be a point transformation. Therefore, we stop here and consider the simplified Lagrangian (3.106). Now, the determination of the generalized momenta $\bar{p}_1, \bar{p}_2$ is straightforward and the Hamiltonian density is given by

$$\bar{h} = \bar{p}_1 \bar{u}_t^1 + \bar{p}_2 \bar{u}_t^2 - \bar{l} = \frac{1}{2h\rho_{\mathscr{R}}} \left((\bar{p}_1)^2 + (\bar{p}_2)^2 \right) + \frac{h}{2} a \left((\bar{u}_{\bar{1}}^1)^2 + \frac{h^2}{12} (\bar{u}_{\bar{1}\bar{1}}^2)^2 \right)$$

With the variational derivatives, see also (3.93), one derives the Hamiltonian equations as

$$\bar{u}_t^1 = \delta^{\bar{1}} \bar{h} = \frac{1}{h\rho_{\mathscr{R}}} \bar{p}_1 \qquad\qquad \bar{p}_{1,t} = -\delta_{\bar{1}} \bar{h} = ah\bar{u}_{\bar{1}}^{\bar{1}}$$

$$\bar{u}_t^2 = \delta^{\bar{2}} \bar{h} = \frac{1}{h\rho_{\mathscr{R}}} \bar{p}_2 \qquad\qquad \bar{p}_{2,t} = -\delta_{\bar{2}} \bar{h} = -ah\bar{u}_{\bar{1}\bar{1}\bar{1}\bar{1}}^2$$

Of course, one can start with the Hamiltonian (3.92) and apply the reduction procedure. If one neglects the terms $\approx h^2$ in kinetic energy, then one derives the same set of equations.

3.3.7 Summary

The mathematical modeling of elastic structures can be significantly simplified by the use of differential geometric methods. Starting with the fundamental conservation and balance principles, one has to parameterize certain maps to bring the constitutive equations into the play. If one assumes the existence of the stored energy function in the presented manner, then one deals with simple elasticity. A further consequence of this assumption is, that one can rewrite the equations of motion in a Hamiltonian or Lagrangian manner. This fact is often used to derive simpler models, where the simplification is archived by adding holonomic constraints. Of course, one can also linearize the equations of motion. Exemplarily, these approaches has been presented for the rigid body and for the Euler Bernoulli beam such that the simplified equations of motion are derived by a systematic reduction procedure from the general ones. Since one can apply the presented methods to other mechanical structures like the Timoshenko beam (see [206] and Sect. 4.3.1), the Kirchhoff or Mindlin plate [123, 147], shell or membranes in an analogous manner, it is obvious, how their Lagrangian or Hamiltonian description can be achieved.

3.4 Port-based modelling and irreversible thermodynamics

Aim of this section is to express models of physico-chemical systems involving momentum, heat and mass transfer as well as chemical reactions in the port-based formalism. To this end, the entropy balance and the associated source terms will be systematically written in accordance with the principle of irreversible thermodynamics. Some insights will been given concerning the constitutive equations and models allowing to calculate transport and thermodynamic properties. These port-based models can be translated into bond-graph models, in the case of distributed as well as lumped parameter systems. Examples of this are reported in the concluding part of the section. The meaning of all the symbols appearing in this section has been reported in Appendix C.

3.4.1 Basic concepts

A thermodynamic system is a piece of matter containing a sufficiently high number of elementary particles (atoms, molecules, ions etc) so that macroscopic variables like pressure P, temperature T, mass density ρ, mass concentrations ρ_i can make sense. The energy of such a thermodynamic system is defined as the internal energy U. The other thermodynamic functions like enthalpy H, Gibbs free energy G are defined with respect to U as Legendre transforms (see Appendix B, Sect. B.2.6).

Some of the thermodynamic variables correspond to quantities subject to balance equations. These variables are extensive variables in the sense that they are dependent on the size of the system under consideration. For such variables, one defines specific mass or molar variables as well as fluxes, these concepts being necessary to derive balance equations. Some of them will lead to the definition of flow variables as they are defined in the port-based approach. As far as specific mass or molar variables are concerned, they can be considered as intensive variables in the sense that they are independent of the size of the system under consideration. Other intensive variables are not defined as specific variables. They will prove to be effort variables allowing the description of equilibrium situations (see Appendix B, Sect. B.2.2).

As far as only chemical reactions are considered, the total mass is conservative. This means that mass is neither destroyed nor created during the processes under consideration. In the case of distributed parameter systems, the total mass balance is as follows:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \rho \mathbf{v} \qquad (3.109)$$

where ρ is the mass density and $\mathbf{v}$ the fluid velocity.

When balances are established for distributed parameter systems, the conservation equations can be written under two forms [21]. If Y is a scalar quantity and y the corresponding quantity per unit mass, the partial derivative

$$\frac{\partial y}{\partial t}$$

is the time variation of y at a given point. In a frame moving according to the fluid velocity $\mathbf{v}$,

$$\frac{Dy}{Dt}$$

is the time derivative of y "following the motion" [21]. The relation between the two is obtained by applying the chain rule of derivation:

$$\frac{Dy}{Dt} = \frac{\partial y}{\partial t} + \mathbf{v} \cdot \nabla y \tag{3.110}$$

From that point, two forms of balance equations can be derived.

In a fixed frame, the balance of Y takes the general form:

$$\frac{\partial \rho y}{\partial t} = -\nabla \cdot \mathbf{f}_y + \sigma_y \tag{3.111}$$

where $\mathbf{f}_y$ is the flux of Y per unit of surface area and σ_y a possible volumetric source term. This source term can be either the result of a true destruction or creation of Y or the expression of a transfer with the surrounding that is expressed as a quantity by time and volume unit. In a frame moving according to $\mathbf{v}$, the total mass balance (3.109) being given, the Y balance becomes:

$$\rho \frac{Dy}{Dt} = -\nabla \cdot (\mathbf{f}_y - \rho \mathbf{v} y) + \sigma_y = -\nabla \cdot \mathbf{f}_y^R + \sigma_y \tag{3.112}$$

The source term is supposed to remain unchanged but the flux of Y is now a relative flux with respect to the convected one $\mathbf{f}_y^R = \mathbf{f}_y - \rho \mathbf{v} y$. The total mass balance can also be given in a frame following the fluid motion:

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v} \tag{3.113}$$

or by using the specific volume $v = \frac{1}{\rho}$:

$$\rho \frac{Dv}{Dt} = \nabla \cdot \mathbf{v} \tag{3.114}$$

If y is one of the components of a vector, equations (3.111) and (3.112) have their counterparts for the vector $\mathbf{y}$. In a fixed frame, the balance equation is:

$$\frac{\partial \rho \mathbf{y}}{\partial t} = -\nabla \cdot \Phi_y + \sigma_y \tag{3.115}$$

while in a frame moving according to $\mathbf{v}$:

$$\rho \frac{D\mathbf{y}}{Dt} = -\nabla \cdot (\Phi_y - \rho \mathbf{v} \mathbf{y}) + \sigma_y = -\nabla \cdot \Phi_y^R + \sigma_y \tag{3.116}$$

where Φ_y and Φ_y^R are tensors of order 2 representing respectively the absolute and relative flux of the **y** quantity and σ_y a vectorial source term per unit of volume.

3.4.2 Distributed parameter systems

In order to calculate output variables that can be measured like pressure, temperature and composition, the classical approach consists in deriving a balance equation for the internal energy. The internal energy balance equation has to be coupled to other balance equations (material and momentum). As far the port-based approach is concerned, the internal energy balance is replaced by the entropy balance.

3.4.2.1 Balance equations

The following material can be found in many textbooks (see for example, [21]). We restrict ourselves to an homogeneous fluid (in the sense that it is under the form of only one phase) subject to simultaneous mass, momentum and heat transfer. Chemical reactions are also supposed to occur in the system. The derivation of the equations is performed on a mass basis.

Two forms of energy have to be considered. The energy of the matter as a whole and the energy of the matter as a collection of elementary particles (atoms, molecules, ions ...). The total energy per mass unit is then given by:

$$\hbar = \frac{v^2}{2} + u \qquad (3.117)$$

that one can differentiate:

$$d\hbar = \mathbf{v} \cdot d\mathbf{p} + du \qquad (3.118)$$

where **p** is the momentum per mass unit. If one assumes that $\hbar$ is a conserved quantity, in the sense that it is never destroyed nor produced but only transformed from one form to another, it is possible to derive a balance equation for the internal energy. To this end, equation (3.118) is assumed to be valid for the substantial time derivatives:

$$\frac{D\hbar}{Dt} = \mathbf{v} \cdot \frac{D\mathbf{p}}{Dt} + \frac{Du}{Dt} \qquad (3.119)$$

so that

$$\rho \frac{D\hbar}{Dt} = \rho \mathbf{v} \cdot \frac{D\mathbf{p}}{Dt} + \rho \frac{Du}{Dt} = \rho \frac{D}{Dt}\left(\frac{v^2}{2}\right) + \rho \frac{Du}{Dt} \qquad (3.120)$$

is also valid.

Let us denote ρ_i as the mass concentration of component i in a mixture containing N species and $\omega_i = \frac{\rho_i}{\rho}$ its mass fraction. If one or more chemical reactions occur in the system, they will produce or consume component i: σ_i is the corresponding net source term expressed in mass of component i per unit of volume and time.

According to equation (3.111), the mass balance of component i is as follows:

$$\frac{\partial \rho \omega_i}{\partial t} = -\nabla \cdot \mathbf{f}_i + \sigma_i \qquad i = 1, \ldots, N \tag{3.121}$$

where $\mathbf{f}_i = \rho_i \mathbf{v}_i$ is the mass flux of component i per unit of surface area defined with respect to a fixed frame. If R chemical reactions occur in the system, σ_i is given by:

$$\sigma_i = \sum_{k=1}^{R} \bar{M}_i v_i^k r_k \tag{3.122}$$

where v_i^k is the stoechiometric coefficient of component i when it is involved in the kth reaction. It is more convenient to express r_k, the rate of the kth reaction per unit of volume, on a molar basis so that $\bar{M}_i$, the molar mass of component i, has been included in equation (3.122) to express σ_i. As far as the total mass is conservative, by summing equation (3.121) over all components, one recovers the total mass balance (3.109). $\mathbf{v}$, which turns to be the mass average velocity in the fixed frame, is defined by:

$$\left(\sum_{i=1}^{N} \rho_i \right) \mathbf{v} = \rho \mathbf{v} = \sum_{i=1}^{N} \rho_i \mathbf{v}_i \tag{3.123}$$

In a moving frame defined with respect to $\mathbf{v}$, according to (3.112), the component i mass balance becomes:

$$\rho \frac{D\omega_i}{Dt} = -\nabla \cdot (\mathbf{f}_i - \rho \mathbf{v} \omega_i) + \sigma_i = -\nabla \cdot \mathbf{f}_i^R + \sigma_i \tag{3.124}$$

The relative flux $\mathbf{f}_i^R$ per unit of surface area is the mass diffusion flux defined with respect to the mass average velocity $\mathbf{v}$.

Since $\mathbf{p}$ is the momentum per mass unit, it is clear that $\mathbf{p} \equiv \mathbf{v}$ but, contrary to the classical presentation, we distinguish here the velocity as an effort variable from the momentum as a flow variable. In a fixed frame, the momentum balance equation is as follows:

$$\frac{\partial \rho \mathbf{p}}{\partial t} = -\nabla \cdot \Phi_p + \sigma_p \tag{3.125}$$

The source term $\sigma_p = \sum_{i=1}^{N} \rho_i \mathbf{g}_i$ is due to the action of the external body force $\mathbf{g}_i$ exerted per mass unit on component i. σ_p is then an exchange of momentum with the surrounding. Φ_p is a second order tensor allowing to represent the momentum flux per unit of surface area. The same momentum balance can be considered in the moving frame according to (3.116):

$$\rho \frac{D\mathbf{p}}{Dt} = -\nabla \cdot (\Phi_p - \rho \mathbf{v} \mathbf{p}) + \sigma_p = -\nabla \cdot \Phi_p^R + \sigma_p \tag{3.126}$$

where $\rho \mathbf{v} \mathbf{p}$ is the convected momentum, while $\Phi_p^R = \Phi_p - \rho \mathbf{v} \mathbf{p}$ is the momentum flux defined with respect to the moving frame. This tensor can be split into two terms:

$$\Phi_p^R = P\mathbf{I} + \tau \tag{3.127}$$

where P is the pressure and τ the viscous part of the momentum flux (or shear stress tensor). In (3.127), we have assumed that the fluid under consideration is a non-elastic one [60].

3.4.2.2 The classical approach based on the internal energy balance

According to the first principle of thermodynamic, the total energy of the system being considered as a conserved quantity, the source term that will appear in its balance will necessary be only due to the action of external body forces – i.e. an exchange of energy with the surrounding:

$$\frac{\partial \rho \hbar}{\partial t} = -\nabla \cdot \mathbf{f}_\hbar + \sigma_\hbar = -\nabla \cdot \mathbf{f}_\hbar + \sum_{i=1}^{N} \mathbf{f}_i \cdot \mathbf{g}_i \tag{3.128}$$

and in the moving frame according to $\mathbf{v}$:

$$\rho \frac{D\hbar}{Dt} = -\nabla \cdot (\mathbf{f}_\hbar - \rho \mathbf{v}\hbar) + \sigma_\hbar = -\nabla \cdot \mathbf{f}_\hbar^R + \sum_{i=1}^{N} \mathbf{f}_i \cdot \mathbf{g}_i \tag{3.129}$$

By combining (3.119), (3.126) and (3.129), one obtain:

$$-\nabla \cdot \mathbf{f}_\hbar^R + \sum_{i=1}^{N} \mathbf{f}_i \cdot \mathbf{g}_i = -\mathbf{v} \cdot \left[\nabla \cdot \Phi_p^R\right] + \sum_{i=1}^{N} \mathbf{v} \cdot \rho_i \mathbf{g}_i + \rho \frac{Du}{Dt} \tag{3.130}$$

According to the following relations:

$$\sum_{i=1}^{N} (\mathbf{f}_i - \mathbf{v} \cdot \rho_i) \cdot \mathbf{g}_i = \sum_{i=1}^{N} (\mathbf{f}_i - \rho \mathbf{v} \cdot \omega_i) \cdot \mathbf{g}_i = \sum_{i=1}^{N} \mathbf{f}_i^R \cdot \mathbf{g}_i \tag{3.131}$$

$$\mathbf{v} \cdot \left[\nabla \cdot \Phi_p^R\right] = \nabla \cdot \left[\Phi_p^R \cdot \mathbf{v}\right] - \Phi_p^R : \nabla \mathbf{v} \tag{3.132}$$

(3.130) can be regarded as follows:

$$\rho \frac{Du}{Dt} = -\nabla \cdot \left(\mathbf{f}_\hbar^R - \left[\Phi_p^R \cdot \mathbf{v}\right]\right) - \Phi_p^R : \nabla \mathbf{v} + \sum_{i=1}^{N} \mathbf{f}_i^R \cdot \mathbf{g}_i \tag{3.133}$$

according to the general form (3.112):

$$\rho \frac{Du}{Dt} = -\nabla \cdot \mathbf{f}_u^R + \sigma_u \tag{3.134}$$

with

$$\begin{cases} \mathbf{f}_h^R = \mathbf{f}_u^R + \left[\Phi_p^R \cdot \mathbf{v}\right] \\ \sigma_u = -\Phi_p^R : \nabla \mathbf{v} + \sum_{i=1}^N \mathbf{f}_i^R \cdot \mathbf{g}_i = -P\nabla \cdot \mathbf{v} - \tau : \nabla \mathbf{v} + \sum_{i=1}^N \mathbf{f}_i^R \cdot \mathbf{g}_i \end{cases} \quad (3.135)$$

The internal energy is not a conserved quantity since the source term σ_u contains the positive term $-\tau : \nabla \mathbf{v}$ due to viscous dissipation. It is the expression of the transformation of mechanical energy into internal energy.

3.4.2.3 The port-based approach for modelling

The port-based approach formulates the entropy balance instead of the energy balance: it is based on the thermodynamic of irreversible processes concepts [60]. The main goal of this derivation is to obtain the expression of a source term since, according to the second principle of thermodynamic, the entropy is non-conservative.

The initial form of the Gibbs equation is concerned with macroscopic systems assumed to be at equilibrium [173]. As far as the internal energy of a macroscopic system U is considered as a function of its entropy S, its volume V and of the mass of each component M_i, the Gibbs equation gives the differential of U:

$$\begin{cases} dU = T dS - P dV + \sum_{i=1}^N \mu_i dM_i \\ \mu_i = \left(\dfrac{\partial U}{\partial M_i}\right)_{S,V,M_{k\neq i}} = \left(\dfrac{\partial G}{\partial M_i}\right)_{P,T,M_{k\neq i}} \\ \quad = \left(\dfrac{\partial H}{\partial M_i}\right)_{P,T,M_{k\neq i}} - T\left(\dfrac{\partial S}{\partial M_i}\right)_{P,T,M_{k\neq i}} = h_i - T s_i \end{cases} \quad (3.136)$$

where μ_i is the chemical potential of component i and $G = U + PV - TS = H - TS$ the Gibbs free energy (cf. Appendix B, Sect. B.2.6); s_i and h_i are respectively the partial entropy and enthalpy per mass unit. It can be seen that a fundamental assumption has been made in (3.136). Energy-conjugated variables associated to heat, space and mass transfer have been postulated for systems at equilibrium, respectively (T,S), $(-P,V)$ and (μ_i, M_i). As far as distributed parameter systems are concerned, a local version of (3.136) has to be derived.

According to the definitions of the quantities per mass unit $u = \frac{U}{M}$, $\mathbf{v} = \frac{V}{M}$, $s = \frac{S}{M}$ and the mass fraction $\omega_i = \frac{M_i}{M}$, with $M = \sum_{i=1}^N M_i$, (3.136) can be written as follows:

$$d(Mu) = T d(Ms) - P d(M\mathbf{v}) + \sum_{i=1}^N \mu_i d(M\omega_i) \quad (3.137)$$

After differentiation of each term, (3.137) becomes:

$$M du = M\left(T ds - P d\mathbf{v} + \sum_{i=1}^N \mu_i d\omega_i\right) + dM\left(\sum_{i=1}^N \mu_i \omega_i - (u + P\mathbf{v} - Ts)\right) \quad (3.138)$$

According to the definition of G and to (3.136), one can easily derive the differential of G:

$$dG = V dP - S dT + \sum_{i=1}^{N} \mu_i dM_i \tag{3.139}$$

where G is a function P, T and it is a first order homogenous function with respect to M_i (cf. Appendix B, Sect. B.2.1) so that Euler theorem can be applied [173]:

$$G = \sum_{i=1}^{N} M_i \left(\frac{\partial G}{\partial M_i} \right)_{P,T,M_{k \neq i}} = \sum_{i=1}^{N} M_i \mu_i = U + PV - TS \tag{3.140}$$

A similar equation can be written with the specific quantities by dividing (3.140) by M:

$$g = \frac{G}{M} = \sum_{i=1}^{N} \omega_i \mu_i = u + Pv - Ts \tag{3.141}$$

By combining (3.138) and (3.141), the local form of the Gibbs equation is as follows:

$$du = T ds - P dv + \sum_{i=1}^{N} \mu_i d\omega_i \tag{3.142}$$

If now one considers (3.118) and (3.142), a set of specific energy-conjugated variables $(\mathbf{v}, \mathbf{p})$, (T, s), $(-P, v)$ and (μ_i, ω_i) can be defined for a thermodynamic system at equilibrium and subject to heat, mass, momentum transfer and chemical reactions:

$$d\hbar = \mathbf{v} \cdot d\mathbf{p} + T ds - P dv + \sum_{i=1}^{N} \mu_i d\omega_i \tag{3.143}$$

This set of energy-conjugated variables is associated to the total energy of the system. As far as one is now interested in deriving a balance equation for the entropy, the balance equation for the internal energy as it has been derived above can be used.

When a system in not at equilibrium, its state variables vary with space and time. Irreversible phenomena and entropy production are partly due to these spatial variations. However, one can consider that at a sufficiently small scale, equilibrium is reached at each time. Balances are then considered in the frame following the fluid motion and the substantial times derivatives $\frac{Du}{Dt}$, $\frac{Dv}{Dt}$, $\frac{D\omega_i}{Dt}$ and $\frac{Ds}{Dt}$ are assumed to satisfy the local form of the Gibbs equation (3.142):

$$\rho \frac{Ds}{Dt} = \rho \left(\frac{Du}{Dt} + P \frac{Dv}{Dt} - \sum_{i=1}^{N} \mu_i \frac{D\omega_i}{Dt} \right) \frac{1}{T} \tag{3.144}$$

Once the expression of $\rho \frac{Ds}{Dt}$ is derived by using (3.144), the volumetric entropy production as well as the relative entropy flux $\mathbf{f}_s^R = \mathbf{f}_s - \rho \mathbf{v} s$ are obtained by identification to the general form of a balance equation (3.112).

Let us recall the internal energy balance, the mass balance of component i as well as the total mass balance as they have been already derived in the moving frame:

$$\begin{cases} \rho \dfrac{Du}{Dt} = -\nabla \cdot (\mathbf{f}_u - \rho \mathbf{v} u) + \sigma_u = -\nabla \cdot \mathbf{f}_u^R + \sigma_u \\[2mm] \rho \dfrac{D\omega_i}{Dt} = -\nabla \cdot (\mathbf{f}_i - \rho \mathbf{v} \omega_i) + \sigma_i = -\nabla \cdot \mathbf{f}_i^R + \sigma_i \\[2mm] \rho \dfrac{Dv}{Dt} = -\nabla \cdot \mathbf{v} \end{cases} \qquad (3.145)$$

By combining (3.144) and (3.145), the entropy balance expression with respect to the moving frame is as follows:

$$\rho \frac{Ds}{Dt} = -\frac{1}{T} \nabla \cdot \mathbf{f}_u^R + \frac{1}{T} \sigma_u + \frac{P}{T} \nabla \cdot \mathbf{v} + \sum_{i=1}^{N} \frac{\mu_i}{T} \nabla \cdot \mathbf{f}_i^R - \sum_{i=1}^{N} \frac{\mu_i \sigma_i}{T} \qquad (3.146)$$

To transform (3.146) into an equation having the general form of a balance equation, we use the following relations:

$$\begin{cases} \nabla \cdot \left(\dfrac{\mathbf{f}_u^R}{T} \right) = \dfrac{1}{T} \nabla \cdot \mathbf{f}_u^R + \mathbf{f}_u^R \cdot \nabla \left(\dfrac{1}{T} \right) \\[3mm] \nabla \cdot \left(\dfrac{\mu_i \mathbf{f}_i^R}{T} \right) = \dfrac{\mu_i}{T} \nabla \cdot \mathbf{f}_i^R + \mathbf{f}_i^R \cdot \nabla \left(\dfrac{\mu_i}{T} \right) \end{cases} \qquad (3.147)$$

According to the expression of σ_u (see (3.135):

$$\sigma_u = -P\nabla \cdot \mathbf{v} - \tau : \nabla \mathbf{v} + \sum_{i=1}^{N} \mathbf{f}_i^R \cdot \mathbf{g}_i \qquad (3.148)$$

the entropy balance becomes:

$$\rho \frac{Ds}{Dt} = -\nabla \cdot \left(\frac{\mathbf{f}_u^R - \sum\limits_{i=1}^{N} \mu_i \mathbf{f}_i^R}{T} \right) - \sum_{i=1}^{N} \mathbf{f}_i^R \cdot \nabla \left(\frac{\mu_i}{T} \right) - \sum_{i=1}^{N} \frac{\mu_i \sigma_i}{T}$$

$$+ \mathbf{f}_u^R \cdot \nabla \left(\frac{1}{T} \right) - \frac{\tau : \nabla \mathbf{v}}{T} + \frac{\sum\limits_{i=1}^{N} \mathbf{f}_i^R \cdot \mathbf{g}_i}{T} \qquad (3.149)$$

The relative entropy flux per unit of surface area and the volumetric entropy production are then as follows:

$$\begin{cases} \mathbf{f}_s^R = \dfrac{\mathbf{f}_u^R - \sum\limits_{i=1}^{N} \mu_i \mathbf{f}_i^R}{T} \\[2mm] \sigma_s = \mathbf{f}_u^R \cdot \nabla\left(\dfrac{1}{T}\right) - \dfrac{1}{T}\sum\limits_{i=1}^{N} \mathbf{f}_i^R \cdot \left[T\nabla\left(\dfrac{\mu_i}{T}\right) - \mathbf{g}_i\right] - \\[2mm] \hspace{3cm} - \sum\limits_{i=1}^{N} \dfrac{\mu_i \sigma_i}{T} - \dfrac{\tau : \nabla \mathbf{v}}{T} \geq 0 \end{cases} \qquad (3.150)$$

The relative flux of entropy is given by

$$\mathbf{f}_s^R = \frac{\mathbf{f}_q}{T} + \sum_{i=1}^{N} \mathbf{f}_i^R s_i$$

where $\mathbf{f}_q$ is the heat flux per unit of surface area by conduction. Then, according to the definition of the chemical potential (see (3.136)), the relative internal energy flux per unit of surface area can be expressed as follows:

$$\mathbf{f}_u^R = \mathbf{f}_q + \sum_{i=1}^{N} \mathbf{f}_i^R h_i \qquad (3.151)$$

According to the relation $\frac{\partial}{\partial T}\left(\frac{\mu_i}{T}\right) = -\frac{h_i}{T^2}$ [173],

$$\nabla\left(\frac{\mu_i}{T}\right) = \frac{(\nabla \mu_i)_T}{T} - \frac{h_i}{T^2}\nabla T$$

so that the volumetric entropy production can also be expressed as follows:

$$\sigma_s = -\frac{\mathbf{f}_q}{T^2} \cdot \nabla T - \frac{1}{T}\sum_{i=1}^{N} \mathbf{f}_i^R \cdot [(\nabla \mu_i)_T - \mathbf{g}_i] - \sum_{i=1}^{N} \frac{\mu_i \sigma_i}{T} - \frac{\tau : \nabla \mathbf{v}}{T} \geq 0 \qquad (3.152)$$

According to the second principle of thermodynamic, the source term σ_s correspond to a true creation of entropy. The first term is the entropy production due to heat conduction, the second one the entropy production due to diffusion and external body forces, the third one the entropy production due to chemical reactions and the fourth one the entropy production due to viscous effects.

The absolute temperature T is the power conjugated variable associated to σ_s since $T\sigma_s$ is a volumetric power. It represents the power that is locally dissipated due to irreversible processes. Another expression of this quantity can be derived from (3.150) by using the equality $\nabla\left(\frac{\mu_i}{T}\right) = \frac{1}{T}\nabla\mu_i + \mu_i\nabla\left(\frac{1}{T}\right)$. The dissipated power is then as follows:

$$T\sigma_s = -\mathbf{f}_s^R \cdot \nabla T - \sum_{i=1}^{N} \mathbf{f}_i^R \cdot (\nabla\mu_i - \mathbf{g}_i) - \sum_{i=1}^{N} \mu_i \sigma_i - \tau : \nabla \mathbf{v} \geq 0 \qquad (3.153)$$

Fig. 3.13 Micro Carnot engine.

$$\mathrm{d}\mathbf{f}_s^R = \frac{\mathbf{f}_q}{T}\mathrm{d}A$$

$T + \mathrm{d}T$

T

δW^{Rev}

$\mathrm{d}l$
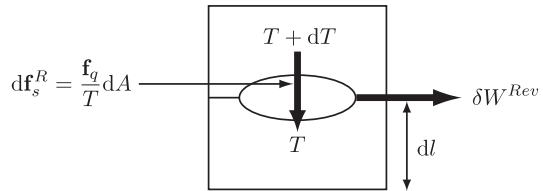
The significance of this dissipated power is more general then the ordinary dissipation due to friction or viscous effects. To understand this significance, we only consider the first term of the dissipated power $\mathbf{f}_s^R \cdot \nabla T$, and we assume that the entropy flux is only due to heat transfer by conduction, i.e. $\mathbf{f}_s^R = \frac{\mathbf{f}_q}{T}$.

Let us consider a piece of matter of volume $\mathrm{d}V$ at temperature T surrounded by a piece of matter at $T + \mathrm{d}T$ (see Fig. 3.13) and denote with $\mathrm{d}A$ the area of the contact surface between the two pieces. Let us imagine that a "micro Carnot engine" can be placed between the two pieces of matter. The power δW^{Rev} that this engine can produce reversibly is given by

$$\delta W^{Rev} = \mathrm{d}\mathbf{f}_s^R(T + \mathrm{d}T - T) = \mathrm{d}\mathbf{f}_s^R\mathrm{d}T = \mathbf{f}_s^R\mathrm{d}A\mathrm{d}T$$

and by unit of volume

$$\delta w^{Rev} = \mathbf{f}_s^R\mathrm{d}T\frac{\mathrm{d}A}{\mathrm{d}V} \propto \mathbf{f}_s^R\frac{\mathrm{d}T}{\mathrm{d}l}$$

If now the "micro Carnot engine" is removed, $\delta w^{Rev} \propto \mathbf{f}_s^R\frac{\mathrm{d}T}{\mathrm{d}l}$ is lost and one can see that $\delta w^{Rev} \propto \mathbf{f}_s^R\frac{\mathrm{d}T}{\mathrm{d}l}$ and $T\sigma_s = -\mathbf{f}_s^R \cdot \nabla T$ are similar. The minus sign of the expression of $T\sigma_s$ is due to the fact that $\mathbf{f}_s^R$ and ∇T are in the opposite direction. Finally, the dissipated power is a power that should have been produced reversibly by using appropriate systems.

Once the entropy production has been derived, one can reformulate the general equations according to the port-based approach. The flow variables balances are as follows in a fixed frame:

$$\begin{cases} \dfrac{\partial \rho\mathbf{p}}{\partial t} = -\nabla \cdot \Phi_p + \sigma_p \\[2mm] \dfrac{\partial \rho\omega_i}{\partial t} = -\nabla \cdot \mathbf{f}_i + \sigma_i \\[2mm] \dfrac{\partial \rho s}{\partial t} = -\nabla \cdot \left(\dfrac{\mathbf{f}_q}{T} + \sum_{i=1}^{N} \mathbf{f}_i s_i \right) + \sigma_s \end{cases} \qquad (3.154)$$

According to the fact that $\sum_{i=1}^N \sigma_i = 0$, the total mass balance is implicitly satisfied:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \rho\mathbf{v} \qquad (3.155)$$

Similarly, according to the expressions of σ_i, σ_s and σ_p, the total energy balance is also satisfied by using (3.143):

$$\frac{\partial \rho \hbar}{\partial t} = -\nabla \cdot \mathbf{f}_\hbar + \sum_{i=1}^N \mathbf{f}_i \cdot \mathbf{g}_i \tag{3.156}$$

The flux of $\hbar$ per unit of surface area is then as follows:

$$\mathbf{f}_\hbar = \rho \mathbf{v}\left(\frac{v^2}{2}+u\right)+\mathbf{f}_q+P\mathbf{v}+\tau\cdot\mathbf{v}+\sum_{i=1}^N \mathbf{f}_i^R h_i \tag{3.157}$$

This expression can be rearranged in order to exhibit the enthalpy per mass unit $h = u + Pv = u + \frac{P}{\rho}$:

$$\mathbf{f}_\hbar = \rho \mathbf{v}\left(\frac{v^2}{2}+h\right)+\mathbf{f}_q+\tau\cdot\mathbf{v}+\sum_{i=1}^N \mathbf{f}_i^R h_i = \rho\mathbf{v}\frac{v^2}{2}+\sum_{i=1}^N \mathbf{f}_i h_i+\mathbf{f}_q+\tau\cdot\mathbf{v} \tag{3.158}$$

The two first terms of (3.158)) represent the energy transported by the matter while the two last ones the energy flux due to heat conduction and to the work exerted by the shear stress tensor.

If the forces per mass unit $\mathbf{g}_i$ can be derived from a time independent potential Ψ_i so that:

$$\begin{cases} \mathbf{g}_i = -\nabla\Psi_i \\ \dfrac{\partial\Psi_i}{\partial t} = 0 \end{cases} \tag{3.159}$$

the total energy $\hbar'$ of the system (see (3.143)) is modified according to the following equation:

$$\begin{cases} \hbar' = \dfrac{v^2}{2}+u+\sum_{i=1}^N \omega_i\Psi_i = \dfrac{v^2}{2}+u+\Psi \\ d\hbar = \mathbf{v}\cdot d\mathbf{p}+Tds-Pdv+\sum_{i=1}^N \mu_i d\omega_i+\sum_{i=1}^N \Psi_i d\omega_i+\sum_{i=1}^N \omega_i d\Psi_i \end{cases} \tag{3.160}$$

A new set of energy-conjugated variables $(\mathbf{v},\mathbf{p})$, (T,s), $(-P,v)$, (μ_i,ω_i), (Ψ_i,ω_i) and (ω_i,Ψ_i) is defined while the total energy balance is given by:

$$\rho\frac{D\hbar'}{Dt} = -\nabla\cdot\mathbf{f}_{\hbar'}^R \tag{3.161}$$

The source term has disappeared since the exchange energy is now expressed as the variation of a potential energy. As far as a balance equation for the quantity

$$\rho\frac{D}{Dt}\left(\frac{v^2}{2}+\Psi\right) = \rho\left(\mathbf{v}\cdot\frac{D\mathbf{p}}{Dt}+\sum_{i=1}^N \Psi_i\frac{D\omega_i}{Dt}+\sum_{i=1}^N \omega_i\frac{D\Psi_i}{Dt}\right)$$

can be derived by using the component i balance (see (3.124)), an internal energy balance equation similar to (3.134) and (3.135) can be obtained:

$$\rho \frac{\mathrm{D}u}{\mathrm{D}t} = -\nabla \cdot \mathbf{f}_u^R + \sigma_u \tag{3.162}$$

with

$$\begin{cases} \mathbf{f}_{h'}^R = \mathbf{f}_u^R + \left[\Phi_p^R \cdot \mathbf{v} \right] + \sum_{i=1}^{N} \mathbf{f}_i^R \Psi_i \\ \sigma_u = -\Phi_p^R : \nabla \mathbf{v} + \sum_{i=1}^{N} \mathbf{f}_i^R \cdot \mathbf{g}_i = -P\nabla \cdot \mathbf{v} - \tau : \nabla \mathbf{v} + \sum_{i=1}^{N} \mathbf{f}_i^R \cdot \mathbf{g}_i \end{cases} \tag{3.163}$$

In this derivation, it has been assumed that:

- according to (3.159), the substantial time derivative of Ψ_i is reduced to

$$\frac{\mathrm{D}\Psi_i}{\mathrm{D}t} = \mathbf{v} \cdot \nabla \Psi_i = -\mathbf{v} \cdot \mathbf{g}_i$$

- the chemical reactions do not modify the potential energy, i.e. $\sum_{i=1}^{N} \Psi_i \sigma_i = 0$.

Neither σ_u nor the entropy balance are modified and the system represented by (3.160) can be seen as a port-based one in the same manner then previously.

3.4.3 Lumped parameter systems

In many circumstances, the derivation of models is based on the definition of a network of lumped parameter sub-systems (cf. Chapter 1). The state variables are supposed to be spatially uniform in each element of the network. In chemical engineering, a very famous element of such a network is the so-called CSTR (Continuous Stirred Tank Reactor) that is highly used for the modelling of chemical reactors [115]. Once the network is spatially defined, the balance equations are established for each element of the network. The total energy that is generally considered is reduced to the internal energy as far as the effects due to viscous dissipation are generally negligible with respect to those due to heat transfer or chemical reactions. A noticeable exception is the case of highly viscous fluids like polymers for example where the viscous dissipation has to be taken into account (see for example [48]). As in the case of distributed parameter systems, the objective of a model is to calculate the output variables P, T and the composition and the two approaches can be used to define state variables. The classical one consists in manipulating material and energy balances while the port-based one is based on material and entropy balances.

3.4.3.1 The classical approach

We will establish the balances on a molar basis so that $\bar{h}_i$ is the molar partial enthalpy of component i while $\bar{h}$ is the molar enthalpy of the mixture. Let us consider one lumped parameter system as an element of a network of compartments. This element may exchange matter and energy with its neighbours through links designated by the l index. It contains N_i mole of component i and its internal energy is U. The energy and component i balances are written as follows:

$$\frac{dU}{dt} = F_q + F_w + \sum_l F_l \bar{h}_l = F_q + F_w + \sum_{i,l} F_{il} \bar{h}_{il} \tag{3.164}$$

$$\frac{dN_i}{dt} = \sum_l F_l \chi_{il} + \sigma_i V = \sum_l F_{il} + \sigma_i V \tag{3.165}$$

where F_q and F_w are respectively the total heat flux and the total power that are exchanged by the system through its boundary, while F_{il} and χ_{il} are respectively the molar flow rate and the molar fraction of component i through the link l, while F_l is the corresponding total molar flow rate.

3.4.3.2 The port-based approach

The Gibbs equation (3.136) is supposed to be valid for the system at uniform pressure, temperature and composition so that one can derive the entropy balance from (3.136), (3.164) and (3.165):

$$\frac{dS}{dt} = \frac{1}{T}\left[F_q + F_w + \sum_{i,l} F_{il}\bar{h}_{il} - \sum_i \bar{\mu}_i\left(\sum_l F_{il} + \sigma_i V\right)\right] + \frac{P}{T}\frac{dV}{dt} \tag{3.166}$$

According to the definition of the chemical potential per mole unit $\bar{\mu}_i = \bar{h}_i - T\bar{s}_i$, (3.166) can be rearranged in order to exhibit a source term and exchanged terms:

$$\frac{dS}{dt} = \sum_{i,l} F_{il}\bar{s}_{il} + \frac{F_q + F_w}{T} + \frac{P}{T}\frac{dV}{dt} + \sum_{i,l} F_{il}\left(\frac{\bar{h}_{il} - T\bar{s}_{il}}{T} - \frac{\bar{\mu}_i}{T}\right) - \sum_{i=1}^N \bar{\mu}_i \sigma_i V \tag{3.167}$$

Let us consider for example that the heat flux is exchanged with a heat source at T_{ext} and that the volume V varies in contact with a pressure source at P_{ext} with $F_w = -P_{\text{ext}}\frac{dV}{dt}$. Equation (3.167) can be given under the following form:

$$\begin{cases} \dfrac{\mathrm{d}S}{\mathrm{d}t} = \sum_{i,l} F_{il}\bar{s}_{il} + \dfrac{F_q}{T_{\text{ext}}} + \sigma_s V \\[2ex] \sigma_s = \dfrac{1}{V}\left[\left(\dfrac{F_q}{T} - \dfrac{F_q}{T_{\text{ext}}}\right) + \dfrac{P - P_{\text{ext}}}{T}\dfrac{dV}{dt} + \right. \\[2ex] \left. \qquad\qquad + \sum_{i,l} F_{il}\left(\dfrac{\bar{h}_{il} - T\bar{s}_{il}}{T} - \dfrac{\bar{\mu}_i}{T}\right) - \sum_{i=1}^{N}\bar{\mu}_i \sigma_i V\right] \end{cases} \qquad (3.168)$$

The first term in the entropy production is due irreversible heat transfer, the second one is due to mechanical friction, the third one to the irreversible mixing of the inlet fluxes of matter with the matter contained in the system and finally the fourth one is due to chemical reactions.

3.4.4 Constitutive equations

A model only based on balance equations cannot be used if constitutive equations are not available (cf. Appendix B, Sect. B.2.8). These relations constitute a model for the matter properties – i.e. transport, thermodynamic properties (see for example [167]) and chemical reaction rates. In order to calculate these properties of the matter, a great number of models are available, more or less complicated according to the situation. Classical textbooks or references are devoted to this question, which is probably the most important and difficult one in chemical engineering [167, 173, 209].

3.4.4.1 Thermodynamic properties

One has to relate the specific internal energy, entropy, enthalpy of the system to P, T and the composition. As far as the total mass balance is involved, one has also to relate the specific volume or the mass or molar density to the same variables. A thermodynamic model is a set of relations allowing to calculate all these properties (see for example [173, 209]. These relations have been derived by considering equilibrium situations. According to the principle of local equilibrium, they are also assumed to apply at a point, even if the system under consideration is not at equilibrium as a whole. According to the classical way to proceed, we present very briefly this question by separating the case of pure components from the case of mixtures.

Equations of state are generally used to model the specific volume v of a fluid. They are given under the general form $\varphi(P, \text{v}, T, \theta_1, \theta_2, \dots) = 0$, where θ_1, θ_2, ... are parameters. Some of these equations of state can be applied for both liquid and gaseous phases while others are devoted to only one phase. All the properties are calculated by using equation of states. As far as u is concerned, the following expression is derived where u is primarily considered as a function of v and T:

$$du = c_v(v,T)dT + \left(T\frac{\partial P}{\partial T} - P\right)dv \tag{3.169}$$

where $c_v(v,T)$ is the heat capacity at constant volume. In many applications, it is better to consider P and T as the output variables so that the enthalpy $h = u + Pv$ is more convenient. The following relation is then derived:

$$dh = c_P(P,T)dT + \left(v - T\frac{\partial v}{\partial T}\right)dP \tag{3.170}$$

where $c_P(P,T)$ is the heat capacity at constant pressure. If the port-based approach is used, the specific entropy s can be expressed by using the following relations:

$$\begin{cases} ds = \dfrac{c_v(v,T)}{T}dT + \dfrac{\partial P}{\partial T}dv \\ ds = \dfrac{c_p(P,T)}{T}dT - \dfrac{\partial v}{\partial T}dP \end{cases} \tag{3.171}$$

Equations (3.169), (3.170) and (3.171) have to be integrated along calculations paths. To do so, an arbitrary origin has to be defined for u or h and s.

Equations of state can also be used for mixtures. They are given under the general form $\varphi(P,v,T,\theta_{1m},\theta_{2m},\dots) = 0$, where the parameters θ_{1m}, θ_{2m}, ... depend on the composition. As far as the other properties are concerned, in order to be able to define an arbitrary origin for them, one has to consider each component separately and define its contribution to a given property. Let us for example consider the case of the enthalpy H. H is primarily considered as a function of P, T and N_i, the number of mole of component i. As it is a first order homogenous function with respect to N_i, Euler theorem can be applied [173] (cf. Appendix B, Sect. B.2.1):

$$\begin{cases} H(P,T,N_i) = \displaystyle\sum_i N_i \bar{h}_i(P,T,\chi_i) \\ \chi_i = \dfrac{N_i}{\sum_{i=1}^{N} N_i} \end{cases} \tag{3.172}$$

By definition, $\bar{h}_i = \left(\frac{\partial H}{\partial N_i}\right)_{P,T,N_{k \neq i}}$ is the partial molar enthalpy. Within the framework of the port-based approach, it is also better to consider S as a function of P, T and N_i so that Euler theorem can also be applied:

$$S(P,T,N_i) = \sum_{i=1}^{N} N_i \bar{s}_i(P,T,\chi_i) \tag{3.173}$$

with $\bar{s}_i = \left(\frac{\partial S}{\partial N_i}\right)_{P,T,N_{k \neq i}}$ the partial molar entropy.

Another way to model a mixture is to model the excess Gibbs molar free energy $\Delta g^e(P,T,\chi_i)$. This quantity is the difference between g, the Gibbs molar free energy

of a mixture and g^{id}, the Gibbs molar free energy of the same mixture considered as an ideal solution [173, 209].

As far as reactive systems are concerned, the origin for the calculation of $\bar{h}_i$ is the so-called standard enthalpy of formation. This quantity has been chosen to be 0 for atoms or simple components under their more stable state at ambient conditions (H_2, O_2 for example).

3.4.4.2 Transport properties and chemical reaction rates

These properties allow expressing the fluxes as functions of the effort variables according to the expression of the total entropy production (see (3.152)). The main properties that are required are viscosity, thermal conductivity and diffusion coefficients. These coefficients allow to relate respectively the shear stress tensor to the velocity gradient, the heat flux by conduction to the temperature gradient and the fluxes of component i to the chemical potential gradient. Furthermore, source terms in the material balances are given by the rates of chemical reactions. Finally, one has also to consider coupled phenomena if necessary. Let us first consider the way such coupling may occur.

According to the Curie symmetry principle applied to isotropic systems, all the fluxes are not functions of all the effort variables but only of those having the same tensorial order [60]. The total entropy production can be split into three terms, each of them being positive. In order to express the entropy production according to these three terms, one has to consider the entropy production associated to viscous effects. The quantity $\tau : \nabla \mathbf{v}$ can be expressed as follows provided that τ is symmetric [60]:

$$\tau : \nabla \mathbf{v} = \tilde{\tau} : \left(\tilde{\nabla} \mathbf{v}\right)^s + \frac{1}{3} \mathrm{Tr}(\tau) \nabla \cdot \mathbf{v} \qquad (3.174)$$

To derive (3.174), τ has been decomposed as follows:

$$\tau = \tilde{\tau} + \frac{1}{3} \mathrm{Tr}(\tau) \mathbf{I}, \qquad \text{with } \mathrm{Tr}(\tilde{\tau}) = 0 \qquad (3.175)$$

Similarly, $\nabla \mathbf{v}$ has been decomposed according to:

$$\nabla \mathbf{v} = \left(\tilde{\nabla} \mathbf{v}\right) + \frac{1}{3} \mathrm{Tr}(\nabla \mathbf{v}) \mathbf{I} = \left(\tilde{\nabla} \mathbf{v}\right)^s + \left(\tilde{\nabla} \mathbf{v}\right)^a + \frac{1}{3} \left(\nabla \cdot \mathbf{v}\right) \mathbf{I}, \text{ with } \mathrm{Tr}(\tilde{\nabla} \mathbf{v}) = 0 \quad (3.176)$$

where $\left(\tilde{\nabla} \mathbf{v}\right)^s$ and $\left(\tilde{\nabla} \mathbf{v}\right)^a$ are respectively the symmetric and anti-symmetric parts of $\tilde{\nabla} \mathbf{v}$. By combining (3.152) and (3.174), the entropy production can be expressed as follows:

$$\sigma_s = -\sum_{i=1}^{N} \frac{\mu_i \sigma_i}{T} \underbrace{- \frac{\frac{1}{3}\text{Tr}(\tau)\nabla \cdot \mathbf{v}}{T}}_{\sigma_s^{\text{Sc}}} \underbrace{- \frac{\mathbf{f}_q}{T^2}\nabla T - \frac{1}{T}\sum_{i=1}^{N} \mathbf{f}_i^R\left((\nabla \mu_i)_T - \mathbf{g}_i\right)}_{\sigma_s^{\text{Vect}}}$$

$$\underbrace{- \frac{\tilde{\tau} : \left(\tilde{\nabla}\mathbf{v}\right)^s}{T}}_{\sigma_s^{\text{Tens}}} \geq 0 \qquad (3.177)$$

where σ_s^{Sc}, σ_s^{Vect} and σ_s^{Tens} are respectively the scalar, vectorial and tensorial contributions to the entropy production. Coupling between phenomena occurs only within these three sets of phenomena.

Within the so-called "Linear thermodynamics of irreversible processes", the relations between the flow and effort variables are expressed linearly. This does not mean that the resulting models are linear. They are generally non-linear firstly because thermodynamic and transport properties are functions of the state variables as well as the chemical rates [60] and secondly because of the coupling between the phenomena.

As far as we know, coupling between chemical reactions and scalar viscous effects are generally not considered [21] so that we express separately $\text{Tr}(\tau)$ as a function of $\nabla \cdot \mathbf{v}$ on the one hand and σ_i as functions of μ_i on the other hand.

The flow variable $\frac{1}{3}\text{Tr}(\tau)$ is assumed to be a function of the effort variable $\nabla \cdot \mathbf{v}$ only. If the system is not to far from equilibrium, a linear relation can be postulated:

$$\frac{1}{3}\text{Tr}(\tau) = -\kappa\left(\nabla \cdot \mathbf{v}\right) \qquad (3.178)$$

where κ is the dilatational or volume viscosity, which is independent of $\nabla \cdot \mathbf{v}$ within the framework of linear irreversible thermodynamic. This situation corresponds to the so-called Newtonian fluid but κ depends on P, T and the composition of the fluid.

Beyond the linear thermodynamics of irreversible processes, the case of nonlinear chemical kinetics has to be carefully considered. As a matter of fact, the definition of effort and flow variables as well as the relation between them is not evident. For the sake of simplicity, we restrict ourselves to the case of thermally activated chemical reactions. When a mixture is subject to chemical reactions, some species are consumed, some others are produced. Global or apparent chemical reaction rates can be fitted to experimental results but such an approach is empirical. A deep understanding of a global chemical transformation is based on a decomposition of such a global chemical process into independent elementary processes [176]. It is assumed that for an elementary process, the species are really brought into contact one with the others in order the atoms initially present in the reactants can be redistributed in the products. Such elementary processes are assumed to involve a low number of reactants, mainly, one, two or three (mono-, bi- or tri-molecular processes) and their orders are assumed to be equal to the stoichiometric coefficients.

Let us consider the entropy production due to chemical reactions, i.e. $\sigma_s^{\text{Reac}} = -\sum_{i=1}^{N} \frac{\mu_i \sigma_i}{T}$. We assume that the overall chemical process has been decomposed according to a set of R independent elementary processes so that σ_i is expressed by (3.122). Then, σ_s^{Reac} can be expressed as follows:

$$\sigma_s^{\text{Reac}} = -\frac{1}{T} \sum_{i=1}^{N} \sum_{k=1}^{R} \left(v_i^k \mu_i \bar{M}_i \right) r_k = \frac{1}{T} \sum_{k=1}^{R} A_k r_k \qquad (3.179)$$

where

$$A_k = -\sum_{i=1}^{N} v_i^k \bar{\mu}_i = -\Delta_r G_k \qquad (3.180)$$

where A_k is the affinity or the opposite of the Gibbs free energy $\Delta_r G_k$ of the k-th chemical reaction and $\bar{\mu}_i = \mu_i \bar{M}_i$ the chemical potential per mole unit. In (3.179) and (3.180), the stoechiometric coefficients v_i^k are considered to be positive for a product and negative for a reactant. As pointed out in [11, 163] the rate of a chemical reaction, and particularly the rate of an elementary process, is a function of the concentrations. Consequently, it can be given as a function of the affinity, as it is suggested by (3.179), only for an equilibrated reaction and near the equilibrium position [60]. In this case, the overall chemical process is described within the framework of the linear thermodynamic of irreversible processes. Otherwise, one has to consider separately the forward and reverse directions (see also [114]). In order to illustrate this point, let us consider the case of an elementary chemical process described by the following stoechiometric equation:

$$\sum_{i=1}^{N} v_i^f Re_i \quad \leftrightarrow \quad \sum_{i=1}^{B} v_i^r Pr_i \qquad (3.181)$$
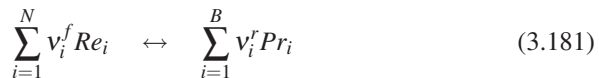
This process is supposed to lead to a possible equilibrium. In order to split more easily a chemical process into forward and the reverse directions, we have defined positive stoechiometric coefficients v_i^f and v_i^r respectively for those directions. As far as the process (3.181) is assumed to be an elementary one, its rate can be expressed as follows:

$$r = r_f - r_i = k_f \prod_{i=1}^{N} C_i^{v_i^f} - k_r \prod_{i=1}^{N} C_i^{v_i^r} \qquad (3.182)$$

where k_f and k_r are the rate constants that are commonly considered as functions of the temperature according to the Arrhenius relation:

$$k_f = k_f^0 e^{-\frac{E_f}{RT}} \qquad\qquad k_r = k_r^0 e^{-\frac{E_r}{RT}} \qquad (3.183)$$

In order to express the rate of the process as a function of the chemical potentials, one has to invert the relation between $\bar{\mu}_i$ and C_i. A thermodynamic model is then necessary. The rather simple but frequently case considered in chemical kinetics has been treated in [11, 163] by assuming the case of an ideal solution. These authors have considered a less usual reference for the expression of $\bar{\mu}_i$ (the component i at

unit concentration) then the one ordinary used in thermodynamic. However, their approach can be used and generalized to non-ideal solutions. As a matter of fact, a more usual but not unique way to derive a calculation path for the chemical potential is to consider $\bar{\mu}_i^*(P,T)$, the chemical potential of the pure component i in the same physical conditions as the reference [173]. The chemical potential is then expressed as follows:

$$
\begin{cases}
\bar{\mu}_i(P,T,\chi_1,\ldots,\chi_{N-1}) = \bar{\mu}_i^*(P,T) + RT\ln(a_i) \\
\qquad\qquad\qquad\quad = \bar{\mu}_i^*(P,T) + RT\ln(\gamma_i(P,T,\chi_1,\ldots,\chi_{N-1})\chi_i) \\
\qquad\qquad\chi_i = \dfrac{C_i}{C}
\end{cases}
\tag{3.184}
$$

where C is the total molar concentration, a_i the activity of i with respect to the state of pure component and γ_i the activity coefficient. γ_i has to be calculated from a thermodynamic excess model. The simplest model is the ideal solution where $\gamma_i^{\mathrm{id}} = 1$. By combining (3.182) and (3.184), one can find that:

$$
r = r_f - r_r = \frac{k_f C^{\sum_{i=1}^N v_i^f} e^{-\frac{A_f^*}{RT}} e^{\frac{A_f}{RT}}}{\displaystyle\prod_{i=1}^N (\gamma_i)^{v_i^f}} - \frac{k_r C^{\sum_{i=1}^N v_i^r} e^{-\frac{A_r^*}{RT}} e^{\frac{A_r}{RT}}}{\displaystyle\prod_{i=1}^N (\gamma_i)^{v_i^r}}
\tag{3.185}
$$

where

$$
A_f = \sum_{i=1}^N v_i^f \bar{\mu}_i \quad A_f^* = \sum_{i=1}^N v_i^f \bar{\mu}_i^* \quad A_r = \sum_{i=1}^N v_i^r \bar{\mu}_i \quad A_r^* = \sum_{i=1}^N v_i^r \bar{\mu}_i^*
\tag{3.186}
$$

A_f and A_r are respectively the forward and reverse affinities while A_f^* and A_r^* are the corresponding quantities calculated at the reference state. The same flow variable r is associated to the two effort variables A_f and A_r so that the entropy production due the elementary process (3.181) is given by:

$$
\sigma_s^{\mathrm{Reac}} = \frac{A_f r - A_r r}{T} = \frac{Ar}{T}
\tag{3.187}
$$

Let us notice that, as far as the process (3.181) can lead to an equilibrium, the latter can be predicted directly from thermodynamic by using the condition:

$$
A^{\mathrm{eq}} = -\sum_{i=1}^N v_i^k \bar{\mu}_i = A_f^{\mathrm{eq}} - A_r^{\mathrm{eq}} = 0
\tag{3.188}
$$

This equilibrium condition also corresponds to the fact that:

$$
r^{\mathrm{eq}} = r_f^{\mathrm{eq}} - r_r^{\mathrm{eq}} = 0
\tag{3.189}
$$

Consequently, k_f and k_r must satisfy a condition that can be derived by combining (3.184), (3.185), (3.188) and (3.189):

$$k_f \frac{(C^{eq})^{\sum_{i=1}^{N} v_i^f} e^{-\frac{A_f^*}{RT}}}{\prod_{i=1}^{N} (\gamma_i^{eq})^{v_i^f}} = k_r \frac{(C^{eq})^{\sum_{i=1}^{N} v_i^r} e^{-\frac{A_r^*}{RT}}}{\prod_{i=1}^{N} (\gamma_i^{eq})^{v_i^r}} = \kappa^{eq} \qquad (3.190)$$

Finally, if the process is considered to be close to the equilibrium conditions, one can linearise (3.185) by evaluating

$$k_f \frac{C^{\sum_{i=1}^{N} v_i^f} e^{-\frac{A_f^*}{RT}}}{\prod_{i=1}^{N} (\gamma_i)^{v_i^f}} \qquad \text{and} \qquad k_r \frac{C^{\sum_{i=1}^{N} v_i^r} e^{-\frac{A_r^*}{RT}}}{\prod_{i=1}^{N} (\gamma_i)^{v_i^r}}$$

at the equilibrium conditions according to (3.190) and by linearizing the results with respect to A_f and A_r. The linearized rate expression of the process (3.181) is then given by:

$$r = r^{eq} + \tilde{r} = \tilde{r} = \kappa^{eq} \frac{e^{\frac{A_f^{eq}}{RT}}}{RT} A \qquad (3.191)$$

according to the linear thermodynamic of irreversible processes.

As far as elementary processes are concerned, a model has been derived by [11, 84] to explain the dependence of chemical reaction rate constants with temperature as given by the Arrhenius relation: this model is based on the concept of activated complex. We give a very simplified presentation of this model since it involves highly detailed calculations based on molecular theories. To this end, we consider the case of an elementary bi-molecular process in the forward direction:

$$A + B \quad \rightarrow \quad Pr \qquad (3.192)$$

If such a process is elementary, it is assumed that the atoms composing A and B are really brought into contact: this elementary amount of matter is called the activated complex and is noted $(AB)^{\mp}$. This activated complex is considered to be an ordinary molecule possessing usual thermodynamic properties. However, at the molecular level, one direction of vibration leads to the decomposition of the activated complex proportionally to its concentration so that the activated complex is "treated as a molecule with one degree of vibrational freedom less than normal" (cf. [84], p. 402). In order to derive the rate of the elementary process (3.192), the activated complex $(AB)^{\mp}$ is considered as if it were in equilibrium with the reactants, according to the following equivalent process:

$$(a) \quad A + B \leftrightarrow (AB)^{\mp} \qquad (b) \quad (AB)^{\mp} \rightarrow Pr \qquad (3.193)$$
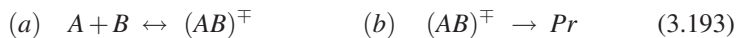
The rate r_f of the process [84, 109] is given by the decomposition rate of $(AB)^{\mp}$ since the quasi-stationary state principle is applied to this entity. From statistical thermodynamic arguments, it is shown that r_f is given by:

$$r_f = \frac{\bar{k}T}{\bar{h}} C_{(AB)^{\mp}} \tag{3.194}$$

where $\bar{k}$ and $\bar{h}$ are respectively the Boltzmann and Planck constants. The derivation of (3.194) is based on the assumption that the rate of decomposition of the activated complex is related the frequency of one vibrational degree of freedom inside this complex. If now the activated complex and the reactants A and B are assumed as if they were at equilibrium, one can expresse $C_{(AB)^{\mp}}$ as a function of C_A and C_B. If $\bar{\mu}_A$, $\bar{\mu}_B$ and $\bar{\mu}_{(AB)^{\mp}}$ are respectively the chemical potential per mole unit of A, B and $(AB)^{\mp}$, the chemical equilibrium condition:

$$\bar{\mu}_{(AB)^{\mp}} = \bar{\mu}_A + \bar{\mu}_B \tag{3.195}$$

can be used to derive the equilibrium constant of the process (3.193)(a) $K_{\mp}$, which is defined by:

$$RT \ln\left(\frac{a_{(AB)^{\mp}}}{a_A a_B}\right) = RT \ln K_{\mp} = -\left(\bar{\mu}^0_{(AB)^{\mp}} - \left(\bar{\mu}^0_A + \bar{\mu}^0_B\right)\right) = -\Delta G^0_{\mp} \tag{3.196}$$

As far as $K_{\mp}$ is a function of the mixture composition, the rate equation (3.194) can be formally expressed as a function of $K_{\mp}$ through its dependence on $C_{(AB)^{\mp}}$. The way this dependency will be expressed depends on the thermodynamic model that is used to represent the mixture. As far as the chemical rates are functions of the molar concentrations:

$$r_f = k_f C_A C_B \tag{3.197}$$

by combining (3.194), (3.196) and (3.197), the rate constant can be expressed as follows:

$$k_f = \frac{\bar{k}T}{\bar{h}} K_{\mp} \frac{\dfrac{C_{(AB)^{\mp}}}{a_{(AB)^{\mp}}}}{\dfrac{C_A}{a_A}\dfrac{C_B}{a_B}} = \frac{\bar{k}T}{\bar{h}} \frac{C_{(AB)^{\mp}}}{C_A C_B} \frac{a_A a_B}{a_{(AB)^{\mp}}} e^{\frac{-\Delta G^0_{\mp}}{RT}} \tag{3.198}$$

After some tedious calculations [57], it can be shown that the entropy production due to vectorial phenomena can be expressed as follows:

$$\sigma_s^{\text{Vect}} = -\frac{\mathbf{f}_q}{T} \cdot \nabla \ln(T) - \frac{1}{T} \sum_{i=1}^{N} \mathbf{f}_i^R \cdot \mathbf{e}_i \tag{3.199}$$

The effort variables $\mathbf{e}_i$ per unit of mass are given by the following relation:

$$\mathbf{e}_i = \frac{CRT}{\rho_i} \mathbf{d}_i = T\nabla\left(\frac{\mu_i}{T}\right) + h_i \nabla \ln(T) - \frac{\nabla P}{\rho} - \mathbf{g}_i + \frac{\displaystyle\sum_{j=1}^{N} \rho_j \mathbf{g}_j}{\rho} \tag{3.200}$$

According to their definitions, $\mathbf{e}_i$ and $\mathbf{f}_i^R$ are not independent since:

$$\sum_{i=1}^{N} \mathbf{f}_i^R = 0 \qquad \sum_{i=1}^{N} \mathbf{d}_i = 0 \tag{3.201}$$

Within the framework of linear irreversible thermodynamic, the flow variables $\mathbf{f}_i^R$ and $\mathbf{f}_q$ are linearly expressed as functions of the effort variables $\mathbf{e}_i$ and $\nabla \ln(T)$. The relation between $\mathbf{f}_q$ and $\nabla \ln(T)$ is analogous to the Fourier relation while the relations between $\mathbf{f}_i^R$ and $\mathbf{e}_i$ is related to classical isothermal diffusion. However, coupling phenomena can exist. The thermal effort $\nabla \ln(T)$ can generate mass fluxes: this is the Soret effect. The Dufour effect is the generation of a heat flux $\mathbf{f}_q$ due to the diffusive effort variables. As far as the flow variables $\mathbf{f}_i^R$ are concerned, the Maxwell-Stefan approach consisting in expressing the effort variables as function of the fluxes [201] is more and more used in chemical engineering. The advantage of this approach is that the physical interpretation of the diffusion coefficients is easiest since they are analogous to drag or friction coefficients. Since coupling between $\nabla \ln(T)$ and $\mathbf{f}_i^R$ is considered, the so-called generalized Maxwell-Stefan equations are derived as follows.

For the sake of simplicity, let us first consider the case of isothermal systems and let us consider the forces acting on component i. A driving force $\mathbf{e}_i$ is assumed to compensate exactly a drag force that is due to the presence of the other components j. This drag force is proportional to the relative velocity of component i with respect to component j. It is usual to express this momentum balance by using $\mathbf{d}_i$ instead of $\mathbf{e}_i$ as follows:

$$\begin{cases} \mathbf{d}_i = \sum_{j \neq i} \dfrac{\chi_i \chi_j}{D_{ij}} (\mathbf{v}_j - \mathbf{v}_i) = \sum_{j \neq i} \dfrac{\chi_i \chi_j}{D_{ij}} ((\mathbf{v}_j - \mathbf{v}) - (\mathbf{v}_i - \mathbf{v})) \\[2mm] \quad = \sum_{j \neq i} \dfrac{\chi_i \chi_j}{D_{ij}} \left(\dfrac{\mathbf{f}_j^R}{\rho_j} - \dfrac{\mathbf{f}_i^R}{\rho_i} \right) \\[2mm] D_{ij} = D_{ji} \end{cases} \tag{3.202}$$

If now the Soret effect is included, one define D_j^{T} as the thermal diffusion coefficient for component j, a modified relative velocity is introduced so that the force equilibrium becomes:

$$\begin{cases} \mathbf{d}_i = \sum_{j \neq i} \dfrac{\chi_i \chi_j}{D_{ij}} \left[\left(\dfrac{\mathbf{f}_j^R}{\rho_j} + \dfrac{D_j^{\mathrm{T}}}{\rho_j} \nabla \ln(T) \right) - \left(\dfrac{\mathbf{f}_i^R}{\rho_i} + \dfrac{D_i^{\mathrm{T}}}{\rho_i} \nabla \ln(T) \right) \right] \\[2mm] \sum_{j=1}^{N} D_j^{\mathrm{T}} = 0 \end{cases} \tag{3.203}$$

Equation (3.203) is an implicit relation between the effort and the flow variables that has to be inverted in order to express the flow variables as functions of the effort variables [201]. As far the heat flux is concerned, its expression is as follows [57]:

$$\mathbf{f}_q = -\left[\lambda_0 + \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{CRT}{\rho_i}D_i^{\mathrm{T}}\frac{\chi_i\chi_j}{D_{ij}}\left(\frac{D_j^{\mathrm{T}}}{\rho_j}-\frac{D_i^{\mathrm{T}}}{\rho_i}\right)\right]\nabla\ln(T)$$

$$-\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{CRT}{\rho_i}D_i^{\mathrm{T}}\frac{\chi_i\chi_j}{D_{ij}}\left(\frac{\mathbf{f}_j^R}{\rho_j}-\frac{\mathbf{f}_i^R}{\rho_i}\right)\quad(3.204)$$

The quantity

$$\lambda_0 + \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{CRT}{\rho_i}D_i^{\mathrm{T}}\frac{\chi_i\chi_j}{D_{ij}}\left(\frac{D_j^{\mathrm{T}}}{\rho_j}-\frac{D_i^{\mathrm{T}}}{\rho_i}\right)$$

is commonly related to the thermal conductivity λ as it has been introduced by Fourier [21]:

$$\lambda = \frac{\lambda_0 + \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{CRT}{\rho_i}D_i^{\mathrm{T}}\frac{\chi_i\chi_j}{D_{ij}}\left(\frac{D_j^{\mathrm{T}}}{\rho_j}-\frac{D_i^{\mathrm{T}}}{\rho_i}\right)}{T}\quad(3.205)$$

As far as tensorial irreversible processes are concerned, there is only one process described here so that no coupling has to be considered. The flow variable $\tilde{\tau}$ is only function of the effort variable $\left(\tilde{\nabla}\mathbf{v}\right)^s$. A linear relation can approximate this function if the system is not to far from equilibrium:

$$\tilde{\tau} = -2\eta\left(\tilde{\nabla}\mathbf{v}\right)^s\quad(3.206)$$

where $\tilde{\tau}$ is assumed to be a symmetric tensor. η is the viscosity of the fluid only depending on P, T and the composition for a Newtonian fluid. One can find for example in [167] the way to calculate η for fluids in many situations.

3.4.5 Port-based modelling examples

Many approaches of computer aided modelling in process engineering are based on the formulation of balance equations (including energy balance), constitutive equations and constraint equations due to the environment. Such approaches have been used to develop structured modelling methodologies for distributed parameter systems such as [83, 132]. Even if these structured modelling approaches can be viewed as classical ones in process (and chemical) engineering, we will rather apply here on two examples the port-based methodology previously developed in Chapter 1. The two chosen examples, a batch gas phase chemical reactor and an adsorption column, will highlight the advantages of the approach. In both cases, the port-based approach is applied, starting from Gibbs equation, using internal energy, material and entropy balance equations, deriving constitutive equations in terms of port variables from classical thermodynamic assumptions, in order to obtain a port-based model of the processes in the form of a generalized Bond Graph.

Fig. 3.14 A closed constant volume chemical reactor.
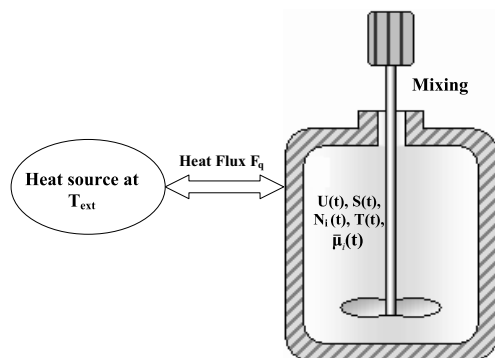
In the reactor example, physical variables are considered as spatially uniformly distributed. As a consequence, a lumped port-based model is derived. It is shown that in this model, two irreversible processes are sources of entropy production: the heat transfer and the chemical reaction.

In the adsorption column case, an isothermal model is considered. The model focuses on mass transfer phenomena (adsorption and diffusion). It follows that a distributed parameters model is derived which points up these transport phenomena are the sources of entropy production. These phenomena (adsorption, diffusion and dispersion) occur at three different scales. Therefore, the model of the adsorption column also provides a nice example of an application of the port-based methodology to multi-scale modelling.

In both examples, the port-based models and their bond graph formulations appear to be easy to re-use and to connect to other process sub-models. This property comes from the use of port variables and is obvious for the lumped parameter model. However, in the adsorption column example, the model is stated independently of the chosen boundary conditions for describing the environment. This "free-boundary" formulation allows to connect the model of the adsorption column to other plant sub-models, if any. This property is a critical advantage of the port-based model on classical partial differential balance equations models. Further readings about modelling and about method of spatial discretization associated to this port based approach can be found in [12–15, 52, 71].

3.4.5.1 Modelling of a batch gas phase chemical reactor

The topic of chemical reactors modelling is very important in chemical engineering (see for example the classical textbook [115]). The situations are very numerous and complex and we give here a rather simple example to illustrate the question of classical - versus port-based approach of their modelling. More complex situations have been described elsewhere ([53]). Let us consider a closed constant volume gas phase chemical reactor as represented on Fig. 3.14. Such a system is a batch reactor because the production is not continuous.

We assume that the system is perfectly mixed: this means that the state variables are uniform. The reactor is initially fed with the reactants and only one reaction is supposed to occur. This reaction is defined by the stoichiometric equation:

$$\sum_{i=1}^{N} v_i B_i = 0 \qquad (3.207)$$

where B_i are considered chemical species, N their number and v_i the stoichiometric coefficients with $v_i > 0$ for a product and $v_i < 0$ for a reactant. During the reaction progress, the reactor is in thermal contact with the surrounding at T_{ext}.

The model is based on components i and internal energy balances (see for example [131]):

- Component i balance:

$$\frac{dN_i}{dt} = v_i rV \ \forall i \in \{1, \ldots, N\} \qquad (3.208)$$

where N_i are the numbers of moles of component i in the mixture, V is the total reactor volume and r the reaction rate. Let us notice that, due to the fact that there is only one reaction, the state of the system is completely defined by only one variable. One can choose the number of moles of one reactant or product. It is also common to define the extent $\chi(t)$ such that

$$N_i(t) = N_i(0) + v_i \chi(t) \qquad (3.209)$$

so that the equations (3.208) become:

$$\frac{d\chi}{dt} = rV \qquad (3.210)$$

- Internal energy balance:

$$\frac{dU}{dt} = F_q \qquad (3.211)$$

where U is the total internal energy and F_q the total heat flux.

One is interested in calculating the evolution of the number of moles N_i as well as the temperature and the pressure. The question of properties then arises. At first, one has to choose a thermodynamic model for the mixture in order to express U and P as functions of P, T and N_i. To calculate the reaction progress, an expression of the chemical rate has to be known as well as an expression of the heat flux F_q. The model will then take the following form:

$$\frac{d}{dt}\left(\sum_{i=1}^{N}N_i\bar{u}_i(P,T,\chi_i)\right) = F_q = \alpha A(T_{ext} - T)$$

$$\frac{d\chi}{dt} = rV \qquad (3.212)$$

$$N_i(t) = N_i(0) + v_i\chi(t)$$

$$\varphi(P,V,T,N_i) = 0$$

where $\bar{u}_i$ denotes the component i specific internal energy, α a heat transfer coefficient (per surface unit) and A the surface area for the conduction. The map φ is given as a thermodynamic state equation for the mixture (see previously). For instance, if the gas can be assumed to be an ideal gas mixture, the thermodynamic model is very simple:

$$\bar{u}_i(P,T,x_i) = \bar{u}_i^{ig}(T)$$

$$d\bar{u}_i^{ig} = \bar{c}_{v,i}^{ig}(T)\,dT \qquad (3.213)$$

$$PV = \left(\sum_{i=1}^{N}N_i\right)RT$$

where the superscript ig stands for ideal gas and where $\bar{c}_{v,i}^{ig}(T)$ is the constant volume specific heat capacity for component i. The model can then be expressed according to the time variation of the temperature:

$$\left(\sum_{i=1}^{N}N_i\bar{c}_{v,i}^{ig}(T)\right)\frac{dT}{dt} = \alpha A(T_{ext} - T) - \left(\sum_{i=1}^{N}v_i\bar{u}_i^{ig}(T)\right)rV$$

$$\frac{d\chi}{dt} = rV \qquad (3.214)$$

$$N_i(t) = N_i(0) + v_i\chi(t)$$

$$PV = \left(\sum_{i=1}^{N}N_i\right)RT$$

where $\Delta_r U := \sum_{i=1}^{N}v_i\bar{u}_i^{ig}(T)$ is called the internal energy of reaction.

The Gibbs equation (cf. Sect. 3.4.2.3) applied to the mixture on a molar basis in the case of a constant volume system gives:

$$dU = T\,dS + \sum_{i=1}^{N}\bar{\mu}_i dN_i \qquad (3.215)$$

where $\bar{\mu}_i$ is the chemical potential for the component i in the mixture. In order to derive the entropy balance, one combines the internal energy balance (3.211), the Gibbs equation (3.215), the material balances (3.208) and the entropy balance:

$$\frac{dS}{dt} = \underbrace{\frac{F_q}{T_{ext}}}_{f_{heat}} + \Sigma_s \tag{3.216}$$

where Σ_s denotes the entropy production per volume unit. Doing so, one finds the entropy production:

$$\Sigma_s = F_q \left(\frac{1}{T} - \frac{1}{T_{ext}} \right) - \frac{\sum_{i=1}^{N} v_i \bar{\mu}_i}{T} rV \tag{3.217}$$

Two irreversible processes are sources of entropy production:

- The entropy production due to heat transfer:

$$\Sigma_{heat} = F_q \left(\frac{1}{T} - \frac{1}{T_{ext}} \right)$$

- The entropy production due to the chemical reaction:

$$\Sigma_{reac} = -\frac{\sum_{i=1}^{N} v_i \bar{\mu}_i}{T} rV$$

The port-based model is then in its final form:

$$\begin{aligned}
\frac{dS}{dt} &= \frac{\alpha A (T_{ext} - T)}{T} - \frac{\sum_{i=1}^{N} v_i \bar{\mu}_i}{T} rV \\
\frac{d\chi}{dt} &= rV \\
N_i(t) &= N_i(0) + v_i \chi(t) \\
\frac{dU}{dt} &= T \frac{dS}{dt} + \sum_{i=1}^{N} \bar{\mu}_i \frac{dN_i}{dt}
\end{aligned} \tag{3.218}$$

In order to compute the pressure and the temperature, one has to relate these variables to the entropy and the number of moles which is unusual because according to the Gibbs equation, one should use relations of the following form:

$$\begin{aligned}
T &= T(S, V, N_i) \\
P &= P(S, V, N_i) \\
\bar{\mu}_i &= \bar{\mu}_i(S, V, N_i)
\end{aligned} \tag{3.219}$$

If such relations were available, the model (3.218) could be expressed in an integral causality form. In fact, the thermodynamic models are generally available in the literature under the following form:

Fig. 3.15 Bond graph representation of the batch reactor.
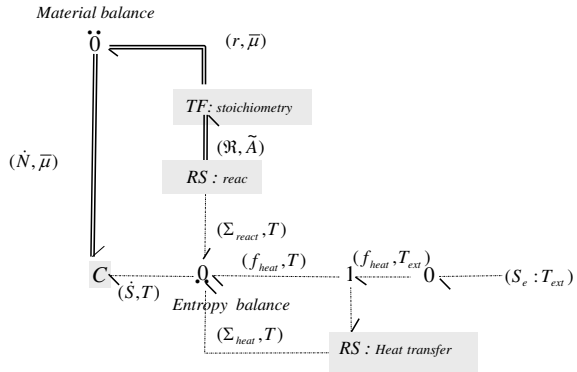
$$S(P,T,N_i) = \sum_{i=1}^{N} N_i \bar{s}_i(P,T,\chi_i)$$

$$\bar{\mu}_i = \bar{\mu}_i(P,T,\chi_i) \tag{3.220}$$

$$\varphi(P,V,T,\chi_i) = 0$$

where $\bar{s}_i$ denotes the specific molar entropy of component i. For instance, in the case of an ideal gas mixture, this model reduces to

$$S^{ig}(P,T,N_i) = \sum_{i=1}^{N} N_i \bar{s}_i^{ig}(P,T,\chi_i)$$

$$\bar{\mu}_i(P,T,\chi_i) = \bar{\mu}_i^{ig*}(P,T) + RT \ln \chi_i \tag{3.221}$$

$$PV = \left(\sum_{i=1}^{N} N_i \right) RT$$

with $\bar{s}_i^{ig}(P,T,x_i) = \bar{s}_i^{ig*}(P,T) - R \ln \chi_i$ and where the exponent * stands for properties of the pure gas.

Finally when dealing with chemical reactions and nonequilibrium thermodynamics, the vector of thermodynamic affinities $\widetilde{A}$ naturally shows up instead of chemical potentials. For thermodynamic equilibrium affinity A is defined as follows: $-\sum_{i=1}^{n} v_i \bar{\mu}_i$. In the case of nonequilibrium thermodynamics, in order to obtain structured model we have to split affinity in two components: the first one corresponds to reactants and the other one to products.

The power conjugate flux associated to $\widetilde{A}$ is

$$\mathfrak{R} = \begin{bmatrix} rV \\ -rV \end{bmatrix}$$

The bond graph model of the batch reactor is given Fig. 3.15.

Fig. 3.16 Schematic representation of an adsorption column.
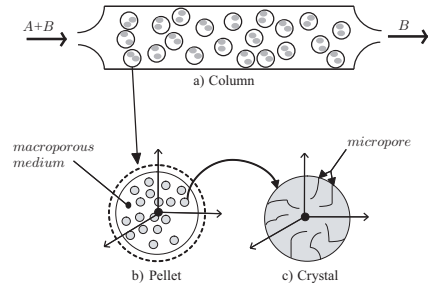
3.4.5.2 Bond graph modelling of an adsorption column

The aim of this example is to present a port-based distributed parameter model of the mass transfer phenomena in an adsorption column. This model is built using Bond Graph language. The main phenomena occurring in the column (dispersion, diffusion) are represented by a dissipative part and an instantaneous power conserving structure named *Stokes-Dirac* structure. This structure is the basis of the infinite dimensional port Hamiltonian models formulation proposed in Chapter 4. These models represent *reversible* systems such as the lossless transmission line, the vibrating string or the eulerian fluid problem. They are hamiltonian with respect to this geometric power conserving structure which is based on Stokes' theorem. This structure then represents a canonical interdomain coupling between two physical domains for reversible systems.

We shall show, in an analogous way, that the port-based model of an adsorption process may be decomposed into a Dirac structure associated with the balance equations and some closure relations applied to some ports of the Dirac structure. These closure equations are the constitutive equations representing storage with the thermodynamical properties or dissipation of energy with the phenomenological model of diffusion. We suggest the reader refer to [12–15, 52, 71] for further details about the port based model.

The adsorption is the phenomenon of deposit of molecules from fluid phase onto solid surface. The adsorption process is based on the ability of a solid to preferentially adsorb constituents present in a fluid phase in order to separate them. This separation is essentially based on the difference of properties that rules the behavior of each constituent in the fluid mixture. For instance, consider a binary gas mixture where one constituent, say *A*, is adsorbed faster than the other one, say *B*. Then, when this mixture is supplied at the inlet of the column, component *A* is adsorbed and the outlet gas is enriched with component *B* during some transition time.

The central part of a plant associated with the separation process by adsorption is constituted by columns packed with adsorbent pellets, themselves constituted by crystals of solid (Fig. 3.16) (see [96, 172]). In our case, zeolite is used as adsorbent medium, so the description of the mass transfer phenomena may be decomposed considering three scales: namely the column scale, the pellet scale and the crystal scale (respectively called extragranular, macroporous and microporous scale), as it

is represented in Fig. 3.16. This is a *classical* approach in Chemical Engineering, justified by the physical sizes of crystals, pellets and the column. For instance according to [58], the radius of a crystal is of an order of magnitude of 1 μm and the radius of a pellet approximately 0.8 *mm* for 13X CECA zeolite. This difference in the size of crystals, pellets and the column gives rise to several levels of porosity and so different resistance to the mass transfer in the adsorption column. *This is why the adsorption process is a multi scale process*. The complexity of modeling such process is that the mass transfer is modeled by partial differential equations in each level.

As already mentioned in Sect. 3.4.1, the system variables are divided into extensive and intensive variables, depending on whether their values depend on the "size" of the system or not. In analogy with mechanical systems, the thermodynamic force is always an intensive variable and the displacement is always an extensive variable, yielding an extensive energy transfer. The internal energy of a system is then expressed in terms of products of pairs of conjugate variables such as (pressure P, volume V), (temperature T, entropy S) and (chemical potential μ_i, mole number n_i (for species i)). In fact all thermodynamic potentials are expressed in terms of pairings of conjugate variables [53]. In the framework of nonequilibrium thermodynamics, let us consider the simple open one phase system with p species. The internal energy U of this system is a function of the extensive variables V, S and n_i. The coupling of the energy with these extensive variables and the expression of the intensive one can be given by the differential of the fundamental equation also called Gibbs equation (3.136), here reported for clarity:

$$dU = T\,dS - P\,dV + \sum_{i=1}^{p} \mu_i\,dn_i \qquad (3.222)$$

with $T = \frac{\partial U}{\partial S}$, $P = -\frac{\partial U}{\partial V}$ and $\mu_i = \frac{\partial U}{\partial n_i}$. The internal energy corresponds to the total energy of the physical system under consideration and is subject to a conservation law.

When systems are considered at constant pressure and temperature, it is common to deal with the Gibbs free energy $G = U + PV - TS$ which is function of mole numbers, T and P. Since the two variables T and P are constant, only the material domain can be represented. So only the pair of power conjugate variables $\left(\mu_i, \frac{\partial n_i}{\partial t}\right)$ are considered.

In the context of distributed parameter systems with three-dimensional spatial domain, it leads to express the time variation of the Gibbs free energy G over a sub-volume Ω of the spatial domain as: $G = \int_{\Omega} \sum_i \mu_i c_i$ where c_i is the molar density of the species i (mol/m³). The variables μ_i and c_i are energy conjugated since their product over the spatial domain yields the energy over the spatial domain.

According to the concepts presented in Chapter 4 (e.g., see Definition 4.3), we have to distinguish between the differential forms of different degrees defined on the spatial domain. The state variables are the molar densities (mol/m³). They are 3-forms on the considered spatial domain, as well as the molar density time derivative. Their

evaluation over any sub-volume gives a mole number or $\mathrm{mol/s}$. The effort variables, intensive ones, are the chemical potentials ($\mathrm{J/mol}$) that are 0-forms. On the other hand, the port variables at the spatial boundary of the domain are the molar flux ($\mathrm{mol/m^{2} \cdot s}$), which are 2-forms, and the chemical potential. We define the molar flux as a 2-form that can be evaluated on any surface of the boundary of the considered domain and the chemical potential as a function that can be evaluated on any point of this boundary. These two latter variables are power conjugated.

Remark 3.1. In the sequel, for simplicity, we shall consider an isothermal isobaric model of the adsorption column. We shall assume that the mixture injected at the inlet of the column is composed of an inert gas and of one adsorbable gas (penetrating the crystals). The mixture is supposed to behave like an ideal gas in the extragranular and macroporous scales. The well known Langmuir model is used for the adsorption equilibrium. Moreover we shall consider the port-based model in spherical coordinates in the microporous and macroporous scales and we shall use the assumption of spherical symmetry for reducing the spatial domains from $\mathbb{R}^3$ to $\mathbb{R}$. z and x will denote the radial coordinate in the microporous scale and in the macroporous scale respectively. In the extra-granular scale, we shall use cylindrical coordinates (r, θ, l). We shall suppose a symmetry about l and an homogeneity with respect to r. This will reduce the spatial domain to $\mathbb{R}$ in this scale.

It is now necessary to give the constitutive equations representing the dissipative phenomena in each scale of the adsorption column model. These closure equations are presented in appropriate coordinates for each scale. These expressions link the physical molar flux to the driving forces (the gradient of chemical potential). Moreover as we previously noticed, these variables are power conjugate through the integral over the considered volume. But since symmetry assumption are made and the coordinate systems are reduced, they are linked through the integral over the considered interval. The integral over the two other variables are implicitly included in the molar flux. It corresponds to taking as the natural pairing of conjugate variables the 0-form representing the linear molar flux and the gradient of chemical potential that are 1-forms. In a same way, it can be seen that the state variable is then a linear density ($\mathrm{mol/m}$) that is a 1-form. In what follows the index i can take two values: 1 will refer to the inert gas and 2 to the adsorbable gas.

In the crystal scale, the assumptions reduce the spatial domain to $Z = [0, R_c] \subset \mathbb{R}$ where R_c is the mean radius of crystals and z is the coordinate. The Maxwell-Stefan's model [201], which expresses the diffusion of p species by setting that the driving force is the chemical potential gradient $\frac{\partial \mu_i^{ads}}{\partial z}$, is used to model the diffusion in the crystal scale. We assume that each molecule which lies in the microporous scale is adsorbed. This means that in the adsorbed phase, there is no possibility of two different molecules undergoing counter-exchange at an adsorption site [201]. In our case, the Maxwell-Stefan's equation is given by:

$$\widehat{N}_2^{ads} = 4\pi z^2 N_2^{ads} = -\frac{\widehat{q_2}^{ads} D_2^s}{RT} \frac{\partial \mu_i^{ads}}{\partial z} \tag{3.223}$$

for the adsorbable species. $\widehat{q_2}^{ads} = 4\pi z^2 q_2^{ads}$ is the linear molar density (mol/m) and q_2^{ads} the molar density (mol/m^3), respectively. D_2^s is the Maxwell-Stefan diffusivity between the adsorbable species 2 and the solid, R is the ideal gas constant and T the temperature. The constitutive relation (3.223) characterizes the dissipation element which relates the pairing of conjugate variables

$$\left(\widehat{N}_2^{ads}, \frac{\partial \mu_2^{ads}}{\partial z}\right)$$

as previously defined.

Considering spherical coordinates in the pellet scale and spherical symmetry lead to consider the spatial domain as $X = [0, R_p] \subset \mathbb{R}$ where R_p is the mean radius of pellets and x is the coordinate. We also use Maxwell-Stefan's law for modelling the diffusion in the macroporous scale. In the pellet, we consider only the friction between the gas molecules, the Maxwell-Stefan constitutive relations of diffusion are written as:

$$-\frac{\widehat{c}_1^{mac}}{RT}\frac{\partial \mu_1^{mac}}{\partial x} = \frac{y_2\widehat{N}_1^{mac} - y_1\widehat{N}_2^{mac}}{D_{1,2}}$$
$$-\frac{\widehat{c}_2^{mac}}{RT}\frac{\partial \mu_2^{mac}}{\partial x} = \frac{y_1\widehat{N}_2^{mac} - y_2\widehat{N}_1^{mac}}{D_{1,2}} \tag{3.224}$$

where $y_i = \frac{\widehat{c}_i^{mac}}{\widehat{c}_T^{mac}}$ is the molar fraction of species i in the macroporous scale, $\widehat{c}_T^{mac}$ is the total linear density, $\widehat{N}_i^{mac}$ is the molar flux of species i. $\widehat{c}_i^{mac}$ is the linear molar concentration of species i (mol/m) with $\widehat{c}_i^{mac} = 4\pi x^2 c_i^{mac}$. $D_{1,2}$ is the Maxwell-Stefan diffusivity between 1 and 2 (m^2/s). This is the *classical* diffusion equation [21, 201]. It is important to notice that, contrary to the case in the microporous medium, this equation does not express explicitly the molar flux as a function of the chemical potential gradient. We obtain an implicit relation to describe the dissipative element.

At the extragranular scale, the spatial domain is reduced to $L = [0, L] \subset \mathbb{R}$ with L the length of the column. l is the coordinate at this scale. The mass transfer phenomenon is slightly different from the two first scales. The mass transfer in this scale is governed by convection and dispersion. The convective flux is given by:

$$\widehat{N}_{i\,conv}^{ext} = \pi R_{cl}^2 c_i^{ext} v = \widehat{c}_i^{ext} v \qquad \text{for } i = 1, 2 \tag{3.225}$$

with v is the mean fluid velocity, c_i^{ext} is the molar density of species i (mol/m^3), $\widehat{c}_i^{ext}$ is the linear concentration of species i (mol/m) where $\widehat{c}_i^{ext} = \pi R_{cl}^2 c_i^{ext}$ and R_{cl} is the radius of the column section.

The dispersion is due to flow inhomogeneity. It is represented by means of an axial dispersion parameter D_{ax} and its corresponding flux expression is analogous to the Fick's relation [21]. The constitutive relation that gives the dispersive flux as function of the gradient of the chemical potential, at constant temperature and pressure, is given by:

$$\widehat{N}_{i\,disp}^{ext} = -\frac{\widehat{c}_T^{ext} D_{ax}}{RT} e^{\frac{\mu_i^{ext} - \mu_i^0(T,P)}{RT}} \frac{\partial \mu_i^{ext}}{\partial l} \tag{3.226}$$

where $\mu_i^0(T,P_0)$ is the reference chemical potential and $\widehat{c}_T^{ext}$ the total linear molar density.

To complete the model of adsorption in each scale we shall add the constitutive equations defining the thermodynamic properties of the mixture in each scale. These closure properties define the energy storing elements C. This leads to express intensive variables (the chemical potential at each scale) as functions of the extensive variables.

In the adsorbed phase at microporous scale, we assume that only the component indexed by 2 is diffusing at the micropores. Moreover we use the Langmuir model to describe the adsorption equilibria. We obtain the following closure equation defining the thermodynamic properties of the mixture in the microporous medium.

$$\mu_2^{ads} = \mu_2^0(T,P) + RT \ln \left(\frac{1}{P\,k} \frac{\widehat{q}_2^{ads}}{\widehat{q}_s^{ads} - \widehat{q}_2^{ads}} \right) \tag{3.227}$$

This closure equation expresses the chemical potential μ_2^{ads}, in the adsorbed phase, of the components 2 at some temperature T and pressure P. $\mu_2^0(T,P)$ denotes the chemical potential of pure component 2 at standard state and k is a function of the temperature T and the Langmuir coefficient b given by $k = \frac{b}{RT}$. $\widehat{q}_s^{ads}$ represents the linear saturation concentration.

In the macroporous and the extragranular media the mixture is a gaseous phase assumed to be an ideal gas. The constitutive equations defining the thermodynamical properties in the two scales is the classical expression of the chemical potential for an ideal gas. So in the macroporous medium (respectively in the extragranular) we have:

$$\mu_i^{mac} = \mu_i^0(T,P) + RT \ln \left(\frac{\widehat{c}_i^{mac}}{\widehat{c}_T^{mac}} \right) \qquad \mu_i^{ext} = \mu_i^0(T,P) + RT \ln \left(\frac{\widehat{c}_i^{ext}}{\widehat{c}_T^{ext}} \right) \tag{3.228}$$

In the remaining part of this section, we shall propose the port-based model describing the mass transfer in the three scales identified in the adsorption column previously described. We shall show that the port-based model at each scale of the adsorption process may be decomposed into a Dirac structure associated with the conservation laws and some constitutive equations coupled to some ports of the Dirac structure. Each one of these constitutive equations represents an energetic phenomenon and the *Stokes-Dirac structure* represents the coupling between these energetic phenomena and also with the external environment (the boundaries of each scale). These port-based models shall also be represented in the bond graph language [53, 98] admitting a slight extension as their port variables are now differential forms. Also the interconnections between the microporous-macroporous and the macroporous-extragranular scales are formulated as power conserving interconnection structures.

Fig. 3.17 Bond Graph representation of the mass balance in the Extragranular scale.
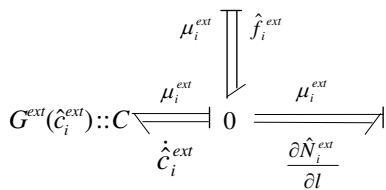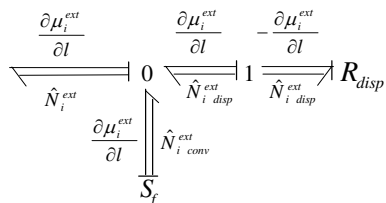
$$G^{ext}(\hat{c}_i^{ext})::C$$

with ports μ_i^{ext}, $\hat{f}_i^{ext}$, $\dot{\hat{c}}_i^{ext}$, $\frac{\partial \hat{N}_i^{ext}}{\partial l}$ and 0-junction.

Fig. 3.18 Bond Graph representation of the convective and dispersive fluxes.

$$\frac{\partial \mu_i^{ext}}{\partial l}, \quad \frac{\partial \mu_i^{ext}}{\partial l}, \quad -\frac{\partial \mu_i^{ext}}{\partial l}$$

with $\hat{N}_i^{ext}$, 0-junction, $\hat{N}_{i\,disp}^{ext}$, 1-junction, $\hat{N}_{i\,disp}^{ext}$, R_{disp}, $\frac{\partial \mu_i^{ext}}{\partial l}$, $\hat{N}_{i\,conv}^{ext}$, S_f.

In the column scale, the model variables are defined on the spatial domain $L \in \mathbb{R} = [0, L]$. The *dynamic model* in the column scale is then given by the mass balance equation including a distributed source term [21]:

$$\frac{\partial \hat{c}_i^{ext}}{\partial t} = -\text{div}(\hat{N}_i^{ext}) + \hat{f}_i^{ext} \qquad (3.229)$$

where $\hat{N}_i^{ext} = \hat{N}_{i\,conv}^{ext} + \hat{N}_{i\,disp}^{ext}$ and $\hat{f}_i^{ext} = \pi R_{cl}^2 f_i^{ext}$ is the flow of species i per unit of lenght. This is a distributed source accounting for the molar flow coming out of a macroporous medium at a point l of the spatial domain L. In the bond graph, this mass balance is represented by the 0-junction connected to the energy storing element C as shown in Fig. 3.17.

The convection and the dispersion phenomena that generate the flux $\hat{N}_i^{ext}$ in this scale are represented in the Fig. 3.18. The R_{disp} element represents the dispersion phenomenon with the constitutive relation (3.226).

Let us briefly show how the Stoke-Dirac structure representing the interconnection structure between storage and dissipative part of our subsystems appears in this model. The variation of the total Gibbs energy into the spatial domain is given by:

$$\int_L d\hat{g}^{ext} = \int_L \left(\sum_{i=1}^{2} d\left(\hat{N}_i^{ext}(t,z) \mu_i^{ext}(t,z) \right) \right)$$

$\hat{g}^{ext}$, the Gibbs power flux on the boundary of the domain, is a 0-form and $d\hat{g}^{ext}$, the linear power density, is a 1-form, on the spatial domain. Using integration by parts this relation leads to the well known Stoke's Theorem:
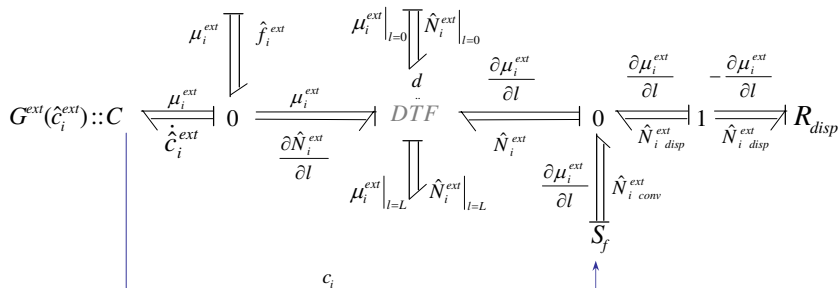
Fig. 3.19 Bond Graph model in the Extragranular scale.

$$\sum_{i=1}^{2}\left(\int_{L}\mu_i^{ext}(t,z)\mathrm{d}\widehat{N}_i^{ext}(t,z)+\int_{L}\widehat{N}_i^{ext}(t,z)\mathrm{d}\mu_i^{ext}(t,z)\right)=$$

$$=\sum_{i=1}^{2}\int_{\partial L}\widehat{N}_i^{ext}(t,z)\mu_i^{ext}(t,z) \quad (3.230)$$

where $\sum_{i=1}^{2}\int_{\partial L}\widehat{N}_i^{ext}(t,z)\mu_i^{ext}(t,z)$ is the total power flux at the boundary ∂L. Now let us define two sets of power conjugate variables,

$$\begin{bmatrix} e_{i1} \\ f_{i1} \end{bmatrix}=\begin{bmatrix} \mu_i^{ext}(t,z) \\ \mathrm{d}\widehat{N}_i^{ext}(t,z) \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} e_{i2} \\ f_{i2} \end{bmatrix}=\begin{bmatrix} \mathrm{d}\mu_i^{ext}(t,z) \\ \widehat{N}_i^{ext}(t,z) \end{bmatrix}$$

and the associated boundary conditions

$$\begin{bmatrix} \mu_i^{ext}|_0 \\ -\widehat{N}_i^{ext}|_0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \mu_i^{ext}|_L \\ -\widehat{N}_i^{ext}|_L \end{bmatrix}$$

Finally with the constitutive relation for the dispersion (3.226), the Dirac structure is finally obtained:

$$\begin{bmatrix} e_{i2} \\ f_{i1} \end{bmatrix}=\begin{bmatrix} 0 & \mathrm{d} \\ \mathrm{d} & 0 \end{bmatrix}\begin{bmatrix} e_{i1} \\ f_{i2} \end{bmatrix}$$

and by the choice of the boundary conditions such that the variation of the internal energy is only due to power flow at the boundary (cf. (3.230)).

The interconnection between the first part, representing the energy storage, and the second part, representing the convection and the dispersion, and also the boundary conditions is represented by the element DTF that symbolizes the Dirac structure. The complete bond graph model is then given in Fig. 3.19. We note that as we consider a fluid moving with a constant velocity, so the Sf represents an energy source coming from another energetic domain.

The mass transfer model in the pellet, macroporous scale, is similar to the model of the adsorption process in the column scale. The variables are defined on the spatial domain $\{l\}\times X=[0,R_p]\subset\mathbb{R}$. This means that the macroporous medium must be indexed by the point of the spatial domain $L=[0,L]\subset\mathbb{R}$. For the sake of clar-

$$\mu_i^{mac}\big|_{x=0} \qquad \hat{N}_i^{mac}\big|_{x=0}$$

$$\mu_i^{mac} \quad \hat{f}_i^{mac}$$

$$G^{mac}(\hat{c}_i^{mac})::C \quad \underset{\dot{\hat{c}}_i^{mac}}{\overset{\mu_i^{mac}}{\rightleftarrows}} \quad 0 \quad \underset{\frac{\partial \hat{N}_i^{mac}}{\partial x}}{\overset{\mu_i^{mac}}{\rightleftarrows}} \quad DTF \quad \underset{\hat{N}_i^{mac}}{\overset{\frac{\partial \mu_i^{mac}}{\partial x}}{\rightleftarrows}} \quad 1 \quad \underset{\hat{N}_i^{mac}}{\overset{-\frac{\partial \mu_i^{mac}}{\partial x}}{\rightleftarrows}} R_{diff}$$

$$\mu_i^{mac}\big|_{x=R_p} \qquad \hat{N}_i^{mac}\big|_{x=R_p}$$
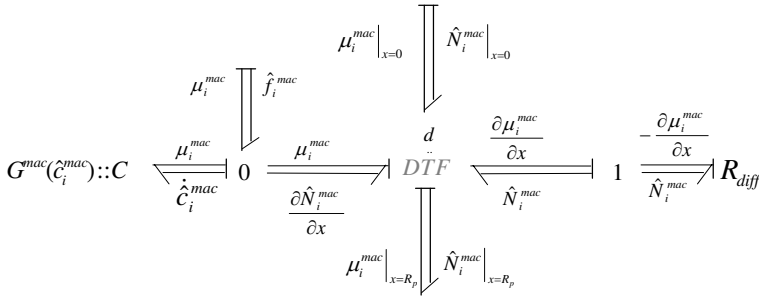
Fig. 3.20 Bond Graph model of the diffusion at the macroporous scale

ity, we will omit this index in the remaining of the section. The *dynamic model* of diffusion process in the pellet is then given by the balance equation:

$$\frac{\partial \hat{c}_i^{mac}}{\partial t} = -\text{div}(\hat{N}_i^{mac}) + \hat{f}_i^{mac} \tag{3.231}$$

where $\hat{N}_i^{mac}$ is the linear molar flux given by the constitutive equation for diffusion (3.224) and $\hat{f}_i^{mac}$ is the flow of species i per unit of domain. This term is a distributed source accounting for the molar flow coming out of a microporous medium at a point x in the spatial domain X. The model is given in Fig. 3.20 where the dissipative element R_{diff} is the diffusion model. Its constitutive equation is given in (3.224). The C element represents the storage phenomenon, its constitutive equation is given in the first part of (3.228). The DTF is the Stokes-Dirac structure associated with this scale.

The model at the crystal microporous scale, is similar to the two previous scales. The variables are defined on the spatial domain $\{l\} \times \{x\} \times Z \subset L \times X \times Z$. This means that the microporous medium is indexed by the point of the macroporous spatial domain X which it self indexed by a point in the spatial domain L. For simplicity these indexes will be omitted. The *dynamic model* in the microporous medium is then simply given by the mass balance equation:

$$\frac{\partial \hat{q}_2^{ads}}{\partial t} = -\text{div}(\hat{N}_2^{ads}) \tag{3.232}$$

and the bond graph model is represented in Fig. 3.21, where the R_{ads} element is the diffusion model that represents the dissipative phenomenon. Its constitutive equation is given in (3.223). The C element represents the storage phenomenon, its constitutive equation is given in the second part of (3.228). The DTF is the Stokes-Dirac structure related with this scale.

Before illustrating the interconnection structures between the three scales, we start presenting the coupling between the macroporous and the extragranular scales. The hypothesis of separation of the two scales amounts to the following assumptions: we assume that in a slice of fluid there is a sufficient number of pellets of
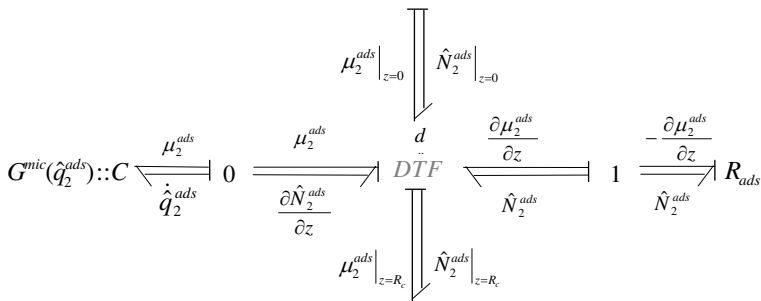
Fig. 3.21 Bond Graph representation of the adsorption process at the microporous scale
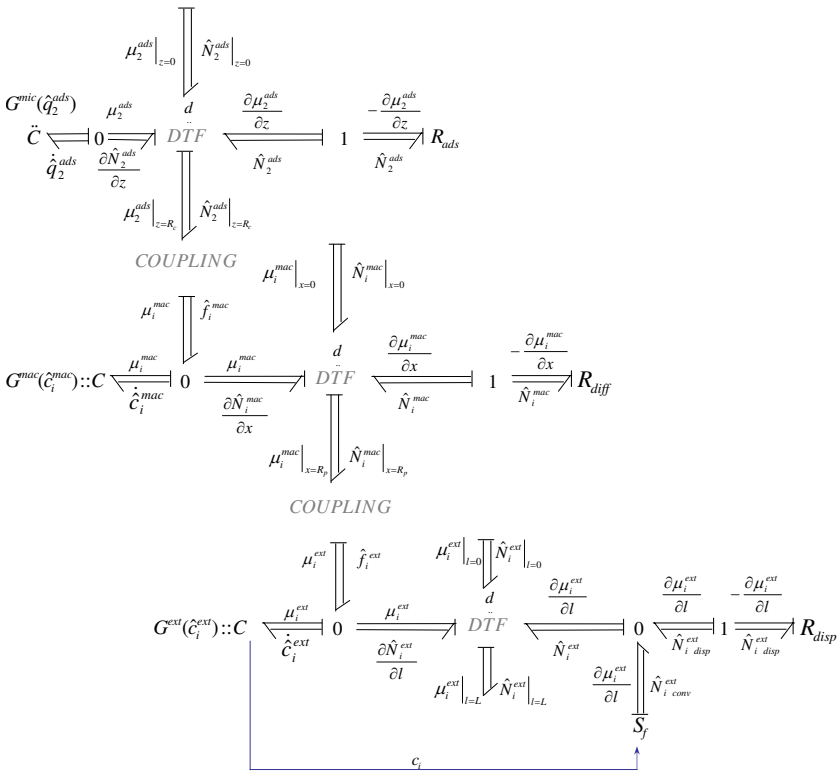

Fig. 3.22 The complete Bond Graph model of the adsorption column.

much smaller size so that a pellet is abstracted to a point. The *concentration* of pellets in the extragranular fluid is denoted by $c_{pellet}(l)$ where l is in L the spatial domain of the extragranular scale. At a point $l_0 \in L$, is attached a spatial domain isomorphic to some domain X and indexed by l_0. Thus the domain of the set of pellets in the fluid is $L \times X$.

Furthermore we use two assumptions, to couple the macroporous and the extra-granular scales by relating firstly the intensive variables consisting of the chemical potential $\mu_i^{mac}(l,x)_{|x=R_p}$ of the macroporous scale restricted to the boundary $x = R_p$ of its domain, and the chemical potential $\mu_i^{ext}(l)$ at the extragranular scale at the point $l \in L$. Secondly a coupling relation is defined on the conjugated extensive variables, the volumetric density flux variable at the extragranular scale $\widehat{f}_i^{ext}(l)$ and the flux variable of macroporous scale $\widehat{N}_i^{mac}(l,x)_{|x=R_p}$ restricted to the boundary of its domain.

The coupling relation between the intensive variables is derived from the assumption of local equilibrium at the interphase between the macroporous and the extragranular fluid. This leads to the equation:

$$\mu_i^{mac}(l,R_p) = \mu_i^{ext}(l) \tag{3.233}$$

The coupling relation between the extensive variables expresses the continuity of molar flux exchanged between between the two scales at the point $l \in L$:

$$\widehat{f}_i^{ext}(l) + \widehat{N}_i^{mac}(l,R_p) \cdot c_{pellet}(l) = 0 \tag{3.234}$$

It can be shown that these relations define an interconnection power continuous structure.

The coupling between the macroporous and microporous scales will be identical as the coupling between the extragranular and the macroporous scales, so we have the following equations that relates the intensive and extensive variables:

$$\mu_i^{ads}(x,R_c) = \mu_i^{mac}(x) \tag{3.235}$$
$$\widehat{f}_i^{mac}(x) + \widehat{N}_i^{ads}(x,R_c) \cdot c_{crystal}(x) = 0 \tag{3.236}$$

where $c_{crystal}(x)$ is the *concentration* of crystals in the pellet.

The complete Bond graph model is represented in Fig. 3.22. In this model are represented the models of the three scales and the interconnection between the scales.