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Modelling and Simulation in Thermal and Chemical Engineering

A Bond Graph Approach

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Springer-Verlag Berlin Heidelberg GmbH

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A Bond Graph Approach

With 134 Figures

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ISBN 978-3-642-08566-6

CIP data applied for

Die Deutsche Bibliothek - CIP-Einheitsaufnahme
Thoma, Jean : Modelling and simulation in thermal and chemical engineering : a bond

ISBN 978-3-642-08566-6 ISBN 978-3-662-04181-9 (eBook)
DOI 10.1007/978-3-662-04181-9

Originally published by Springer-Verlag Berlin Heidelberg **New York in** 2000
Softcover reprint of the hardcover 1st edition 2000

Typesetting: Camera-ready by author
Cover-design: MEDIO, Berlin
Printed on acid-free paper SPIN: 10742329 62 / 3020 hu - 5 4 3 2 1 0

For their Love and Support

To my Wife Souheir and my children Fouzi and Nassim.

Belkacem Ould Bouamama

To my Wife Rose Marie.

Jean Thoma

Foreword

It is a great pleasure for me to introduce this book which has the main ambition to make thermodynamics more directly accessible to engineers and physicists by stressing the analogies with the other physical domains; this science has discouraged more than a few students.

The book comes from the meeting of two persons:

1. Jean Thoma, inventor of hydrostatic machines and transmissions, professor at the University of Waterloo (Canada), expert in simulation and pilgrim for the promotion of bond graphs around the world.

2. Belkacem Ould Bouamama, associated professor at the University of Science and Technology in Lille, France, specialist in industrial control and seduced by the richness and structure of the bond graph method.

Thermodynamics is a difficult subject; its concepts like entropy, enthalpy, etc. are not intuitive and often very abstract. For this reason, it is current practice to neglect the thermal aspects, although they are necessarily there in all physical phenomena, and to use isothermal models. This is equivalent to think that the system is immersed in an infinite temperature reservoir and maintains its temperature constant even if it receives or dissipates electric and other type of energy.

For heat transfer and variable temperature, if it should be included, the classical approach is to study the changes between equilibrium states, and not the process itself, which is more a thermostatic than a thermodynamic approach. This is justified when only the constraints of equilibrium state must be satisfied.

On the other hand, if one needs to know the time behaviour of state variables, one must include the dynamics of the process. Main applications are thermal processes, thermofluids and processes with phase change.

The bond graph language is very suitable for such phenomena because of the following characteristics:

- an energetic viewpoint which gives a structure to the modelling procedure and allows the splitting of the system into sub-systems,
- an unified terminology in all physical domains, based on using the analogy of physical effects,
- a graphical representation to visualize the power transfer, but also to fix the relations between cause and effect,
- an inherent flexibility for completing a model by adding effects that have been before neglected,

- a systematic way of writing the mathematical equations from the bond graph model in the form of differential equations,
- a support for the model structural properties analysis.

The authors have made a remarkable pedagogical effort by siting the principal effects studied in parallel with the electric analogy. Furthermore, they have woven in many personal remarks (the one I prefer is the "striptease of entropy"). There are many examples, partly from industrial practice, in detail, sometimes with simulation included.

This book will in the first place for all beginners in thermal and thermodynamic engineering, where it is an excellent starting point for a sweet introduction. This is especially so if the reader is already acquainted with the bond graph methodology. The book is also a good tool for learning bond graph modelling for the thermal and thermodynamics specialist.

October, 1999
Geneviève DAUPHIN - TANGUY
Professor, Ecole Centrale de Lille, France.

Authors' Preface

The systems in thermal and chemical engineering are governed by many effects of different engineering disciplines and various technological components. Therefore for modelling and simulation of such systems we need an unified approach, using the same signs or language for the entire system. The bond graph method with its interdisciplinary outlook seems best suited to such systems. It allows by its graphical nature to show the exchanges of power in the system, including effects of storage and dissipation of energy.

The principal purpose of this book is to model and simulate energy processes by the bond graph method. We have elaborated the matter in a way that also the reader non familiar with the bond graph can use the method of simulation to a certain extend. In the text, there are many examples, both of simple pedagogical cases as of real and complex systems taken from the industrial experience of the authors.

The work is for students of engineering which would like to know more about modelling energy processes. The specialist of chemical engineering will also find the book interesting with its graphical representation of chemical reactions and of osmosis, which is an enigma, but important in many industrial processes.

The book is also for the teachers and researchers of modelling that desire to introduce new concepts in their teaching. It offers a new approach for explaining more simply the thermodynamics, a discipline which is interesting but poorly understood. Further, even bond graphs as modelling tool needs to be more researched. Therefore, the book is also proposed to post-graduate students.

The book is based on the pedagogical and industrial experience of the authors in France (Several Universities in Lille, France) and in other countries (MIT, Boston, MA, USA, University of Waterloo, (Ontario, Canada), Academy of oil And Gas, Moscow, Russia). The many examples result from the problems encountered by the authors, particularly in thermal engineering and hydrostatic machines. In this sense the contacts with EDF (Electricity of France), Imagine Company and companies like Galdabini, Gallarate, Italy, IIASA (International Institute of Applied Systems Analysis, Vienna, Austria) have given substance to this development.

The researches have executed in the LAIL, laboratory of Automatic Control and Industrial computer, based on a very fruitful cooperation with Jean Thoma.

Energetic problems are based mostly on thermodynamics. We have developed the Bond graph modelling with the three notions: Entropy, Enthalpy and Power, which could also be the title of the book. From the notion of entropy, which not abstract but really very simple, we develop thermodynamics in the first chapter, carefully distinguishing system with and without mass flow. So entropy is in the book not something very abstract, but quite simply a thermal charge, a concept finding its origins with Sadi Carnot in 1824. The motivation to use bond graphs in chemical engineering is also presented.

The second part of the book is devoted to the modelling of thermofluids, with emphasis on the enthalpy as power variable. Practical applications follow of some components like heat exchanger and turbines.

The third chapter concerns the bond graph modelling of chemical systems and phase change of water and other chemical substances. The notions of chemical resistance, capacitance and chemical tension (potential) are introduced, mainly to model chemical reactions. This allows to model condensation of steam or vaporisation and even osmosis.

The fourth chapter gives a pedagogical view of modelling by bond graphs in process engineering, underlining the selection of liaison variables in function of type of modelled process.

The fifth chapter deals with modelling and simulation of real industrial systems like ventilation of buildings, hydropneumatic accumulator, steam boiler, etc.

The base of bond graph methodology and the listings of several simulations, added with a reflection on the value of power, solar energy and the glasshouse effect are given in the appendix. The question of thermal inertia and inverse analogy is also given in the first appendix.

In spite the care in preparing. the manuscript, the authors know the imperfections can remain. Therefore they will be happy to receive pertinent observations from the readers.

Jean THOMA *Belkacem OULD BOUAMAMA*

Acknowledgement

The authors wish to thank professor Geneviève Dauphin-Tanguy, the head of the research group Bond Graph in the Laboratory of Automatic Control and Computer Science in Industry (LAIL, UPRESA CNRS 8021) for the constant encouragement during the writing of this book.

The authors wish also to acknowledge the Professors Marcel Staroswiecki, Mireille Bayart and Jean Philippe Cassar of the research group ASPIC (Analysis and Supervision of Complex Industrial Processes) in the same laboratory for their useful observations.

We also thank Christian Kleijn of Twentesim Company for supplying the simulation of the room ventilation given in section 5.3.

Any extended research task requires considerable dedication and this always leaves less time for family activities. The authors wish to thank their wives, children and friends for their patience and support during the writing of this monograph.

Abstract

The systems in thermal and chemical engineering are governed by many effects of different engineering disciplines and various technological components. Therefore, for modelling and simulation of such systems we need an unified approach, using the same signs or language for the entire system. The bond graph method with its interdisciplinary outlook seems best suited to such systems. The bond graph approach provides a rigorous and systematic methodology for modelling the multi-energy domain embracing in industrial process engineering the mechanical, electrical, thermal and chemical energies. As opposed to classical modelling methods, bond graph methodology helps to understand the basic physical principles and represent them in a graphical way. Furthermore, the bond graph shows up clearly energy storage and dissipation effects and has the advantage of an efficient transition to the computer by causality assignment and power direction.

The principal objective of this book is to model and simulate energy processes by the bond graph method. We have elaborated the matter in a way that also the reader non familiar with the bond graph can use the method of simulation to a certain extend. In the text, there are many examples, both of simple pedagogic cases as of real and complex systems taken from the industrial experience of the authors.

The developed topics include:

- Principles of Modelling of Thermodynamic Systems
- Bond Graph Modelling and Simulation of Thermofluids
- Bond Graph Modelling of Chemical Reactions and Phase Change
- Bond Graph Methodology in Process Engineering
- Industrial Application of Bond Graphs Modelling and Simulation of different types of Processes
- Elements of Bond graph Approach
- Listings of several simulations, added with a reflection on the usual values of the power, solar energy and the glasshouse effect.

This publication will be of interest to students of engineering, which would like to know more about modelling energy processes. The specialist

of chemical engineering will also find the book interesting with its graphical representation of chemical reactions and of osmosis, which is an enigma, but important in many industrial processes. The book is also for the teachers and researchers of modelling that desire to introduce new concepts in their teaching. It offers a new approach for explaining more simply the thermodynamics, a discipline that is interesting but poorly understood. Further, even bond graphs as modelling tool needs to be more researched. Therefore, the book is also proposed to post-graduate students.

Contents

1

Introduction to Thermodynamic Systems Modelling

1.1 Importance of Modelling

1.1.1 Definition

The first problem for a control or systems engineer in front of a process to control is to obtain a precise and easily manipulated model with predictions corresponding to the real observation. The different mathematical equations describing a system and to predict its behaviour is called a mathematical model. The mathematical model can also be defined as an operator giving the relation between input and output signals. It is important to note that input and output variables refer to the model and not to the physical system: for instance the steam flow out of a boiler can well represent the input of a model.

1.1.2 Importance

It is not necessary to insist on the importance of model building as far as in science one has always looked for a suitable model. Indeed, in order to control or simulate any process, we must first describe the phenomena (chemical, physical or others) by such a model. That means that we should find some equations, algebraic or differential, which give results as near as possible to the real system. The same is true for economical systems, for which simulation with or without bond graphs is sometimes used.

It is interesting to note that in automation projects, the modelling requires between 50% and 80% of the total time. Even more, if the classical design tools of control engineering are still much used in industry, it is because the control engineer is incapable to produce the precise models required for modern theories.

Recently, modelling has become more prominent due to the complexity of modern industrial processes: The quest for optimal solutions, helped by powerful computers needs a mathematical model for all types of simulation. This is the reason for the importance of modelling. From simple control of ovens until artificial satellites, all ambitious enterprises need simulation one way or the other. Independent service enterprises for modelling exist today within the framework of research and development.

1.1.3 Levels of Modelling

Nevertheless, its level of language can classify each modelling method. Let us examine the different levels using as example a fluid heating system with a heat exchanger (Fig 1.1). Here, $\dot m$, P, T, $\dot H$ and $\dot Q$ denote respectively mass flow, pressure, temperature, enthalpy flow and heat flow. The indexes a, s, c, m, ex and e give respectively feeding, output, boiler, metal of boiler, exterior and entry of hot fluid to the heat exchanger.

To differentiate the different powers, we denote in future the enthalpy flow by convection in (J/s) by $\dot H$, the thermal flow transported by conduction $\dot Q$ and by $\dot E$ all other forms of power (electric, mechanical...). All symbols of the used variables and their units are given at the end of the book.

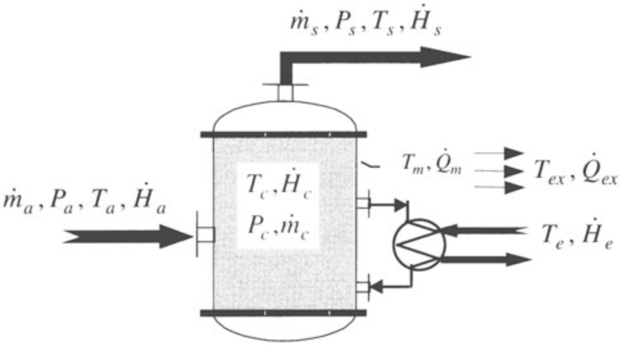

FIGURE 1.1. Heating of fluid, technological level of modelling

According [*Lorenz, 1996*] we can distinguish four levels of modelling:

1. *The technological level.* This level constructs the architecture of the system by assembly of different sub-systems, which are the simple components (heat exchanger, boiler, pipe...). Our figure 1.1 is such an example. On this level, the modelling languages give a normalized description in the form of technological schema. It is easy to carry out but indicates only how the schema is made. In this level of modelling, the adequation of the model is not verified and the physical phenomena are not considered. Consequently, it is a " black box" model.

2. *The physical level.* On this level, the modelling uses an energy description of the physical phenomena. One uses the basic concepts of physics such as dissipation of energy, transformation, accumulation, sources and so on. The variables have physical meaning: like energy, power, effort and flow, and so on. In our example, the boiler receives

a heat flow, given by the heat exchanger and by the feeding water. We have an accumulation of hydraulic and thermal energy in the boiler. There is a dissipation of heat energy in the direction of the metal, which accumulates a part of this thermal energy. One can also suppose that there is dissipation towards a source of external temperature or the environment. The manipulated variables are pressure, temperature, thermal and hydraulic flow.

3. *Mathematical level.* The basic elements are here the mathematical operators such as integrators derivators and algebraic functions. The best-known example is the block diagram of control engineering. The mathematical model is represented by the mathematical equations (algebraic, differential and algebro-differential) which should describe as faithfully as possible the system. Unfortunately, one cannot always be sure of the correspondence of the model with physical reality. The main advantage is that the language used, mathematics is universal and applied to all physical domains. In our example, we must translate the dissipation of energy by the law of linear heat conduction (law of Fourier) and the accumulation of energy in the boiler and the metal by integration of the inflowing powers, and so on.

4. *Algorithmic level.* The algorithmic level is connected directly with information processing and the manipulated concepts are from informatics. So this level indicates how the models are calculated. We consider that this level is almost the same as the mathematical level. The notion of causality or relation between cause and effect has been used first in bond graphs, but is important also in general in computer science. In particular it allows a more robust simulation by using as far as possible integration and not derivations. All researchers know that integration is simpler than derivation. Indeed it is simpler to determine the temperature from the thermal flow by integration than the thermal flow by deriving the temperature.

Our models show the algorithms in the model and the manner how calculation should proceed.

1.1.4 Interest of Bond Graph in Process Engineering

Definition of the Bond Graph Method

The Bond graph tool was first developed since 1961 at MIT, Boston, USA by Paynter [*Paynter,* 1961], Karnopp and Rosenberg. Jean Thoma uses it since 1966. More recent references are [*Karnopp et al., 1975, 1990*] and [*Thoma, 1975*], [*Thoma, 1991*].

Bond graph modelling is based on the exchange of power in a system, which is normally the product of an effort variable and a flow variable. This exchange takes places in bonds, represented by a simple line, but carrying two kinds of additional information, namely power direction and causality. It is then based furthermore on the dissipated and stored quantities, connected by the different junctions. As such, the bond graph allows to write directly the system equations and to discover numerical problems before going near to the computer.

A detailed presentation of the Bond graph method is contained in appendix A. Further information is contained in [*Borne et al., 1992*], [*Thoma, 1975*], [*Thoma,* 1991].

Why use Bond Graph in Process Engineering?

Modelling systems with rigid structure has seen much progress, but thermal and thermodynamic systems, and generally process engineering is still to be done because the phenomena are so complex. Nevertheless, these processes are present in industry with risk such as nuclear and require consequently a precise models.

Industrial processes are very non-linear, principally due to the interaction of different phenomena (mechanical, thermodynamic, chemical...). The behaviour of this kind of system is normally described by non-linear differential equations. Writing equations by classical methods, especially state equations, is therefore complex. Modelling could do with a unified approach that can show the physical nature and the localization of state variables. Bond graphs are such an approach, but here the state variables are associated with a storage of energy, in particular the displacement of C-elements and the moment of I-elements.

The bond graph allows precisely by its graphical nature to display the exchange of power in a system, including storage and transformation. Furthermore, the bond graph model is subject to evolution, meaning the model can be refined by adding more elements like thermal losses or inertia effects, without having to start all over again. The bond graph method is suitable to obtain integrated models of all the physical domains.

The bond graph allows to represent the four levels of modelling. Let us examine our example.

The technological level can be represented by the word bond graph (Fig 1.2). This means that the system is represented as several subsystems. The interconnection is realized by the pair effort and flow. Normally, one calls this pair, effort times flow, a power variable [*Karnopp et al., 1990, Borne et al., 1992*]. Here the authors prefer the term liaison variable, especially in word bond graphs, because in many cases, the pair effort flow has not the physical dimension of a power. For such, it is accepted in practice to call them pseudo bond graphs. In thermal engineering, it goes back to [*Karnopp, 1979*], although the term was probably known and used before. The other case, where effort times flow is a power, are just called true bond graphs.

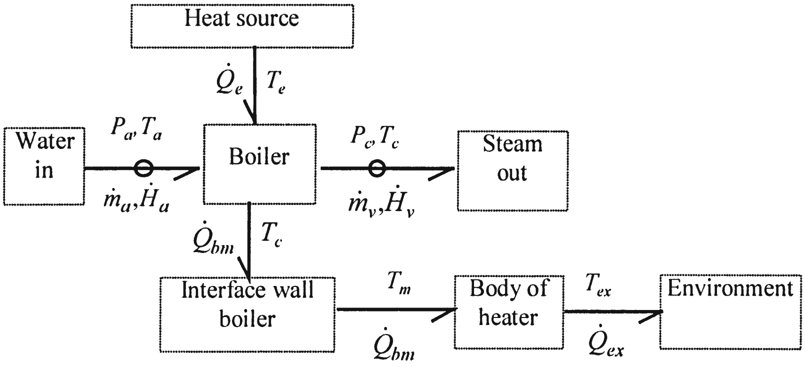

FIGURE 1.2. Technological level by a word bond graph

The liaison variables couple the different subsystems and in particular, the parts of a word bond graph. The choice of the liaison variables is discussed in section 4.3.

The technological representation is already more physical with a word-bond graph, because at the input and output of each component we show the liaison variables with power direction. In bloc diagrams, on the other hand, one uses information variables. In bond graphs, if several powers are coupled in one bond, it will carry a small ring around it.

The physical level implies to consider the phenomena's of physics, which enter the model (inertia, friction, and compressibility...), and to introduce the system graphically. Here, we use a universal language for all domains of physics, the bond graphs, and we see the power exchanges clearly displayed (Fig 1.3).

All phenomena of storing energy and dissipation of power are shown. In particular, the storage of thermal and hydraulic energy is represented by the C-element with two ports called a multiport C. The storage of thermal energy on the other hand is a simple C-element. The dissipation of power is shown by the R-elements. The parameter values K_m and K_{ex} represent respectively the heat transfer coefficient between boiler to the metal and towards the environment. The external temperature is considered constant and given by the effort source Se.

The different junctions, parallel junctions (0-junctions) and series junctions (1-junctions) give connection between the components. The parallel junction connects elements under the same effort, here pressure and temperature, and the series junction the elements subject to the same flow, here mass flow and enthalpy flow.

The mathematical level from a bond graph is obtained by writing the constitutive equations of the components or phenomena, taking into account the causalities. The obtained models can be linear or non-linear and the non-linearity can come from the components or the structure, a fact

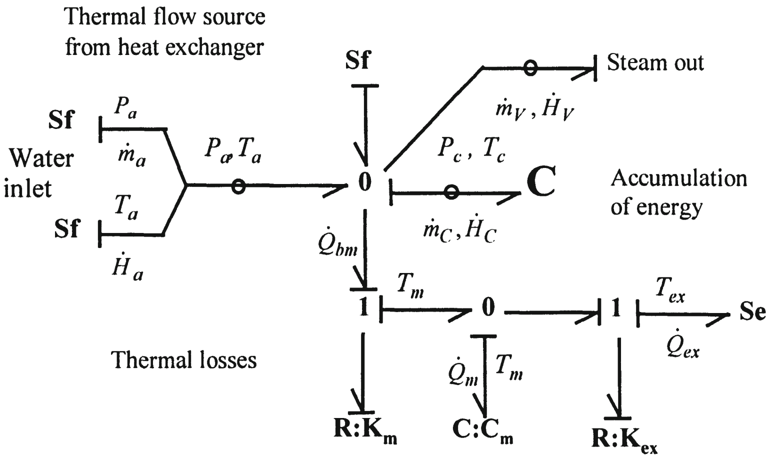

FIGURE 1.3. Bond graph model as example of physical level

allowing introducing a partial linearization. As a difference from classical behavioural modelling, the state equations are determined directly by reading the bond graph. The number of state variables is equal to the number of C- and I—elements in integral causality. In our example (Fig 1.3), we have three state variables, the thermal energy Q_m (image of temperature) stored by the body of the boiler, the enthalpy H_c and the mass m_c accumulated by the boiler.

$$x = \left[\begin{array}{ccc} Q_m & H_S & m_S \end{array}\right]^T \tag{1.1}$$

The systematic method developed in the appendix allows deriving the non-linear state equations in the form:

$$\dot{x} = f(x, u) \tag{1.2}$$

A detailed and pedagogical example is given in chapter 4 and various other examples in chapter 5.

The algorithmic problem is solved in the bond graph method by systematic assignment of causalities, as shown by the perpendicular line on the bond. Analysis of the graphical structure gives knowledge a priory if the problem is solvable mathematically or not.

Concluding, the advantages of bond graph modelling for thermal and other systems are:

- an unique language for all physical domains,
- showing clearly the relations cause and effect in the model,

- possible further development of the bond graph.
- as tool of analysis, one can also have information about the structural properties of the system, such as controllability, observability, [*Sueur and Dauphin 1991, Tagina, 1994*].

1.2 Thermal and Thermodynamics

1.2.1 Degrees of Freedom and Liaison Variables in Thermofluids

The analysis of physical process in process engineering concerns mainly the modelling of systems with circulation of fluid and its thermal and thermodynamics ramifications. We take a term used by bond graphers and say that we want a reticulation of the system. Reticulation means representation by a network of elements in interaction, either by an equivalent circuit or by a bond graph. We desire thus a reticulation of machines, or, in other words, we want a model that gives the principal physical phenomena, but not the details like the stream lines around turbine blades.

One point to note is that we make no difference between thermal and thermodynamics. We use the concepts of thermodynamics as necessary for the reticulation of thermal machines and especially the notion of entropy. The relation of thermal energy and entropy is discussed in section 1.3.

Let us take as example a gas turbine according to the schema or equivalent circuit on figure 1.4. At left there is a compressor, on top a heat exchanger, which augments the temperature (heater), at right a turbine and below another heat exchanger which reduces the temperature again (cooler). This is the Joule cycle, called Brayton cycle in the USA.

The fluid circulating in the system is characterized by several variables, such as: the efforts (pressure P and temperature T), the volume flow $\dot{V}$, the entropy flow $\dot{S}$, the power variables such us internal energy flow $\dot{U}$ or enthalpy flow $\dot{H}$, and other variables like quality of steam X.

Evidently there are more variables then degrees of liberty (DOF) of the fluid. The DOF is the number of variables necessary to describe the process.

In mechanical and electrical systems, the number of liaison variables is equal to the number of DOF. In a thermodynamic system like a flowing fluid, the system is characterized by a number of variables, that is by pressure P and temperature T for the efforts, and volume flow $\dot{V}$ or mass flow $\dot{m}$ (for compressible fluid) for the flows. Further variables can be added such us the quality of steam, internal energy flow etc.. One sees immediately that the number of variables is higher then the number of DOF. Consequently, the selection of liaison variables is not trivial and depends on the type of the modelled process.

For thermofluids, one uses occasionally the pair enthalpy flow-specific

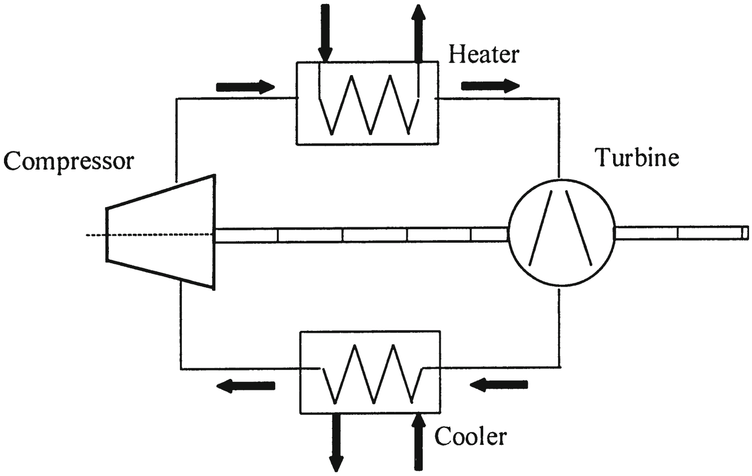

FIGURE 1.4. Principle of gaz turbine

enthalpy instead the natural choice temperature and flow enthalpy (see section 4.3). This choice allows to determine the mixture fraction or quality of steam of two-phase mixture and to use the thermodynamic functions, especially for steam turbines. In the case of matter at rest, one can use the pair temperature, entropy flow for a true bond graph or the pair temperature-heat flow for a pseudo bond graph.

Lagrangian and Eulerian Reference Frame

It is important to well distinguish a model with mass at rest, the Lagrangian Reference Frame, and a model with mass in movement, the Eulerian Frame. This difference is shown on figure 1.5. We have the thermodynamics with matter at rest and with matter in movement, or flow of matter. The matter at rest is subject of classical thermodynamics in the form $T/\dot{S}$ (temperature and entropy flow) and in the form $T/\dot{Q}$ (temperature and heat flow), resulting in true and pseudo bond graphs.

In the Lagrangian frame, the observer travels with the fluid, and one can formulate, as said, in true and pseudo bond graphs. Both forms have their advantages, as we shall see. In the Eulerian point of view, used much in fluid mechanics, the matter flow is described from the point of view of an immobile observer. Thus, we are in the presence of matter in movement or flow of matter. One case is a tube of hot gas, a compressible fluid. Here is necessary to use the coupling capacitors modelled by a multiport C as we shall see in 1.4. In this case, we have conservation of mass flow, and not of volume flow. The liaison variables are $(P, \dot{m})$ for hydraulic power and $(T, \dot{H})$ for thermal power, sometimes also $(h, \dot{H})$ for thermal power. For incompressible fluid, as in the case in automobile radiators, there is

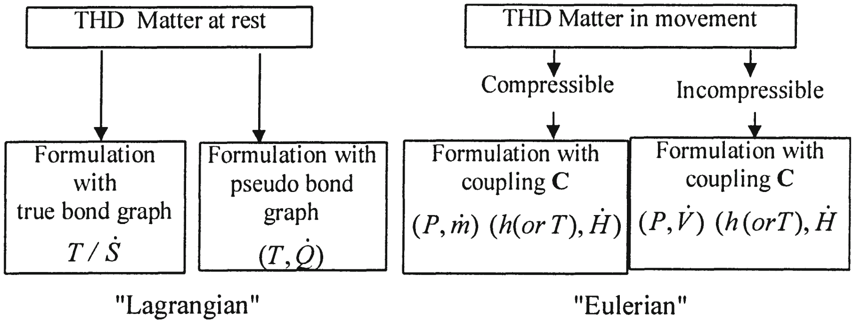

FIGURE 1.5. Eulerian and Lagrangian frames of reference in thermodynamics

conservation of both volume and mass flow, and one can take either one as hydraulic flow variable. For the thermal side one uses almost always the enthalpy flow driven by the circulating fluid.

1.3 Heat Flow and Entropy Flow

1.3.1 Carnot's Equation

We treat in this section the matter at rest with its thermal properties. In analogy with electric and electronic, the heat flow (quantity of heat transmitted per unit of time), is a power resulting from the product of a tension T and of a current $\dot{S}$

$$\dot{Q} = T\dot{S} \tag{1.3}$$

The thermal flow is expressed like any other power in Joules per seconds or Watt, the temperature T has its own unit, called Kelvin (K) and the entropy flow $\dot{S}$ in $J/(K.s)$. This equation is called often the equation of Carnot[1] and represent the foundation of all thermodynamics. It is known since a long time [*Calendar 1911*] [*Thoma, 1971*], [*Falk 1976*] and [*Fuchs 1996*]. The last two authors establish the entire thermodynamics on this

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[1] The equation of Carnot was published in his work "the motive power of fire" (Carnot 1824]. In this work entropy is called caloric and power is called heat. The equation of Carnot defines the entropy, precisely the entropy flow and heat flow. In our conception the entropy must be considered as an accumulation of entropy flow (integral with respect to time), in the same sense as an electric charge has to be considered as an accumulation of current. As electric charge, the thermal charge or entropy is not visible, but its representation becomes very vivid as one studies its properties: the entropy flow accompanies inevitably the transport of heat. This is in the same sense as electric current is always associated with the transport of power.

method. Let us note that the equation is only valid when the matter is at rest or immobile.

The equation of Carnot is analogue to the equation of the electric power: $P = u.i$. As electric current i is the flow of an electric charge, the thermal current is the flow of entropy, and the heat is the flow of power.

All our development of thermal and thermodynamics is based on the equation of Carnot. For matter at rest it is always true, whether for reversible or irreversible process; these notions are defined in paragraph 1.6. For the matter in movement, the equation of Carnot remains approximately true, as we shall see in section 1.8.

Our definition of entropy according Carnot is a little different from the usual definition of Clausius: their relation is given in section 1.4. For matter in movement, as we have said, the definition remains approximately true. In practice it is always to work both formulations, that is $T/\dot{S}$ and $T/\dot{Q}$.

Figure 1.6 represents an ideal gas in a cylinder and subject to variations of temperature as supplied by a thermal source, which can be regulated.

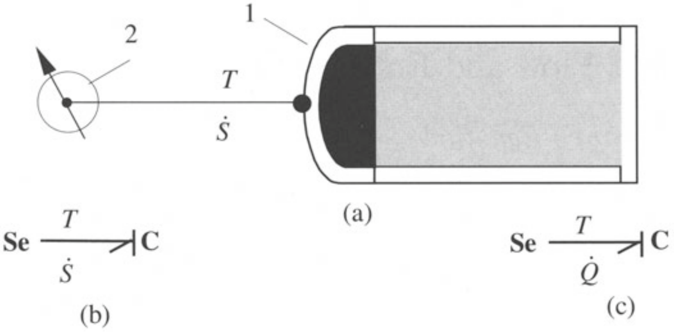

FIGURE 1.6. Thermal Condenser. a. Schema, b. model with true Bond graph, c. model with pseudo bond graph

The thermal source is analogous to a generator of tension in electricity. Any variation of the temperature coming from the source produces a change of temperature of gas. The wall is supposed to be perfectly isolated as indicated by the oblique line. The black part indicates a thermal conduction within the cylinder, or, more precisely, at the end of the cylinder.

The Bond graph model is given by the figures 1.6b and 1.6c. Here both formulations, that is true and pseudo bond graph are possible, with entropy flow or heat flow; they are connected by equation of Carnot. Let us remember that both these variables are conserved in this schema and they can vary only if they are absorbed or are received by the source. As conclusion, the body becomes a thermal condenser, the analog of an electric condenser. Also an electric condenser can be formulated with electric charge flow or electric energy flow.

The condenser stores at the same time internal energy and entropy. The augmentation of temperature is given by equation:

$$dU = c_v m dt \tag{1.4}$$

Which gives by integration

$$U = c_v m \int_{T_{ref}}^{T} dT = c_v m \left(T - T_{ref}\right) = c_v m T_{inc} \tag{1.5}$$

Here m is the mass of the gas and c_v the specific heat per mass at constant volume: one considers effectively the volume of the thermal condenser as constant. T_{ref} is a temperature of reference, $298K$ and the increase of temperature from the reference.

Equation 1.4 is true when c_v depends not on the temperature what is approximately the case. From expression 1.4 followed by integration

$$dU = TdS$$

The entropy S becomes

$$S = c_v m \int_{T_{ref}}^{T} \frac{dT}{T} = c_v m \ln \frac{T}{T_{ref}} \tag{1.6}$$

Let us note, that for T_{ref}, the quantities U and S are equal to zero.

For a small variation of temperature T_{inc} or if c_v is constant, we derive by Taylor expansion and obtain:

$$S \approx c_v m \frac{T_{inc}}{T_{ref}} \tag{1.7}$$

One can than conclude, that the entropy is proportional to the variation of variation of temperature T_{inc}[2]. Let us remark that a body with expansion of volume, mainly a gas, will put in action also hydraulic energy. Effectively, if we heat a body under constant pressure P, the expansion of the volume consumes a part of hydraulic energy. Thus, the entire thermal energy is not stocked, but a part of it is given out as hydraulic energy. To reticulate this correctly we need a double condenser with energy path such as represented on figure 1.7. It is known in the domain of bond graphs as a multiport-C.

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[2] Let us note that in principle there are the absolute quantities for $U$and S, these values are given by theorem of Nernst (third law of thermodynamics). However, these absolute values are not known with sufficient precision. It is as little like the altitude in geography: one gives the altitude in meters over the sea level and not from the center of the earth, because more precisely known [Falk 1976].

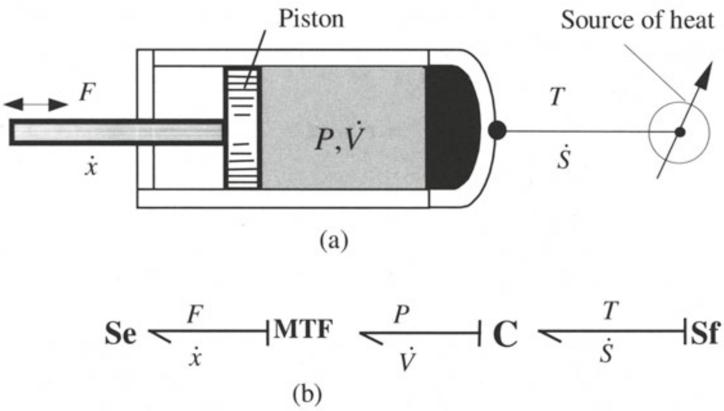

FIGURE 1.7. Thermal Condenser with two energy paths. a. Schema, b. Bond graph

The transformation of hydraulic energy $(P, \dot{V})$ to the mechanical energy is modeled by the modulated transformer MTF. F and $\dot{x}$ represent respectively the force and the speed applied to the piston.

1.3.2 The Principles of Thermodynamics

The principles or laws of thermodynamics are in all manuals, but a summary is given here:

- *First law.* Energy is universally conserved. This law is also called principle of conservation. Energy is represented by bonds and by parallel junctions of bond graphs, either true or pseudo bond graph. If energy enters an accumulator (multiport C or I), its state is changed. If the energy is recovered, the accumulator returns to its original state.

- *Second law.* There is a variable entropy, which is not universally conserved, but only semi-conserved. It is indestructible, but is generated by all sorts of friction. The second law is also called the principle of evolution. Flowing entropy is connected to flowing heat by the equation of Carnot. We also have the generation of entropy by friction including the heat conduction if finite temperature difference. All this takes place in RS elements, which conserve the power, but are irreversible. In other words, dissipation makes new entropy.

- *Third law.* At zero absolute temperature, the entropy content of all bodies is zero. Also called the principle of Nernst, (Berlin, Germany, about 1910) is valid only for slow cooling. With quick cooling, a part of the entropy can remain in the body, because conduction decreases rapidly with temperature. One says also, that a part of entropy is frozen within the body, an important effect in process physics.

1.3.3 Entropy and Disorder

According to the statistical thermodynamics of Boltzmann, entropy is very often assimilated to the disorder and we mention briefly their relation. In this book we will not use the statistic arguments, because all our results can be obtained by the phenomenological thermodynamics using the conception of entropy as thermal charge. However, the concept of disorder is well accepted by many people and we make some remarks at their intention: one speaks almost always about a perfect gas where the disorder means distribution of the molecules on the higher velocities, or more precisely on the higher momentum. Thus, more disorder means to have more molecules with high momenta and consequently more energy. The mean energy of all the molecules is proportional of the temperature (theorem of equipartition). Much entropy means many molecules with high momentum that is more disorder in the space of momenta. We see also that the energy increases with entropy and temperature, parameters often used in this book.

All those ideas come from the kinetic theory of gases, which have nevertheless logic difficulties, which can be resolved only by quantum mechanics. In that mechanics one uses the concept of degree of freedom (DOF) valid for each body in the any form, gas, liquid or solid. The DOF of each molecule are quantified and can take only discrete values according to quantum mechanics. The entropy of each DOF is expressed by the formula of Boltzmann

$$S = -k \sum_i p_i \ln p_i \tag{1.8}$$

Where p_i are the probabilities of the occupation of a state i with a determined energy. The entropy of a complete body is simply the sum of the entropy of all DOF. Since those probabilities are always smaller than one, the logarithm is negative with the minus in front of the entropy.

Two particular cases can be noted:

1. if the DOF is in a determined state, its probability is equal to one and the logarithm is zero. The other probabilities are zero and therefore the entropy of this DOF is also zero. There is no disorder, because one has a certainty about the value of this DOF,
2. if all probabilities are equal, the DOF have a maximum of entropy. According to another formula of Boltzmann this is the case at high temperatures.

The DOF are more or less excited by the temperature, in particular, there is an appreciable probability of excitation for the states with energy comparable to the mean energy. The states of energy much larger will not be occupied, the states with low energy will be occupied: in both cases, the contribution to entropy is zero. Only when the energy is comparable, we have contribution to entropy. These considerations are valid for each DOF.

In general, there is a difference of the microphysics of probability and phenomenological thermodynamics. A continuous transition between both viewpoints should be possible [*Falk, 1976*].

1.4 Matter without Movement as Multiport

1.4.1 General Views

The simple representation of matter as C-element must be completed in general by the coupling of thermal and hydraulic phenomena. For this we introduce a multiport C, that is a network of condensers. This element was called firstly C-field by Henry Paynter [*Paynter, 1961*], but since a certain time we call it multiport C because it implies its function (see appendix A). We shall use this in our book and at the same time use multiport I and multiport R for a network of inductors and resistors.

A multiport C is very simply the network of several condensers in the electric case or of their analogies in the other disciplines. A general law which characterizes a multiport C is a relation between effort e and displacement q as the time integral of flow, in the form:

$$\Phi c(e, q) = 0$$

Other than the electric condenser networks, we have many other types, which fall in the category of multiport C, such as electric condensers with moving plates, even elastic structures.

The multiport C in a true Bond graph verifies always the reciprocity of Maxwell, which is a consequence of the conservation of energy, as we shall soon see.

In thermodynamics, there is always a coupling between thermal and hydraulic or mechanical effects, hence expressed by a multiport C. The typical phenomena is the increase of volume of gas liquids or solids. The variables of liaison of the multiport C are the temperature and the entropy on the thermal side and the pressure and the volume on the hydraulic side. One supposes that the mass of the body is constant.

The coupling between thermal and hydraulic effects is most important for gases. In that case we have as prototype the ideal gas. Let us note, that all matter at large dilution (high temperature and low pressure) verifies the ideal gas equation. It is described by the following equation, the so-called ideal gas equation

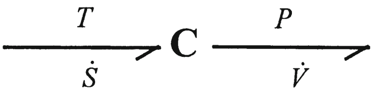

FIGURE 1.8. Thermodynamic body as multiport C

$$PV = mRT \quad \text{and} \quad S = S_{ref} + mc_v \ln\left(\frac{T_1}{T_{ref}}\right) \tag{1.9}$$

Where m is the mass, R is the gas constant referred to mass, P the pressure, V volume, T temperature, S the entropy and c_v the specific heat. T_{ref} and S_{ref} represent the reference value of temperature and of entropy.

Equation 1.9 is called the equation of state of a gas. Equations of this type describe also the liquids and solids. However, liquids or solids have normally a small thermal expansion and therefore the thermal-hydraulic coupling is smaller, but exists in principle. Another example is the mixture of gas and liquid, which is described by thermodynamic tables. The mixture water vapour is a practical case often used in process engineering. It will be treated in the chapters 4 and 5.

The state of all thermodynamic bodies or gases is described by four variables of state, pressure and temperature on one hand and volume and entropy on the other hand. As we have already mentioned in section 1.2.1, a fluid at rest has always two DOF (degrees of freedom) which are normally pressure and temperature. If they are fixed from the outside, the fluid it self fixes then the other variables (volume and entropy). This is well described by the multiport C with two bonds.

Figure 1.8 shows a body with total constant mass as multiport C; the orientation of the powers is indicated by the sense of the half arrows. This sign indicated convention is usual in thermodynamics but gives the unnecessary minus signs in practice.

1.4.2 Equations of Multiport C

Concerning the equations of multiport C, let us write the algebraic sum of the thermal and hydraulic powers is equal to the accumulation of the internal energy U

$$\dot{U} = T\dot{S} - P\dot{V} \tag{1.10}$$

which becomes by multiplying with the element dt and writing $Udt = dU$

$$dU = TdS - PdV \tag{1.11}$$

This is the TdS equation or equation of Gibbs [*Falk, 1976*] and is useful especially if pressure and temperature depend only on entropy and volume. These two variables are displacements in the sense of bond graphs and in the case that U is a function of only S and V and we express the pressure and temperature by derivatives:

$$P = -\frac{\partial U(V,S)}{\partial V} \quad \text{and} \quad T = \frac{\partial U(S,V)}{\partial S} \tag{1.12}$$

The minus sign in the formula (1.10) and (1.11) comes from the orientation power, as we have said, and shows the effect that the hydraulic power (pressure times volume flow) is taken positive when it leaves the multiport C. By deriving both expressions (1.12):

$$\frac{\partial P(V,S)}{\partial S} = \frac{\partial^2 U(S,V)}{\partial V} \quad \text{and} \quad \frac{\partial T(V,S)}{\partial V} = \frac{\partial^2 U(V,S)}{\partial S \partial V}$$

one obtains the important relation of Maxwell:

$$\frac{\partial P(V,S)}{\partial S} = -\frac{\partial T(V,S)}{\partial V} \tag{1.13}$$

This equation is one of the four Maxwell relations. It is a property of the multiport C and valid for all multiports C or I. Multiport R have a similar reciprocity of Onsager described in the third chapter.

Let us note, that the minus signs come from the orientation on the bond graph of the figure 1.8. If the half arrows were oriented towards the multiport C, all the signs would be positive.

The Maxwell reciprocity are true only for true bond graphs and not for pseudo bond graphs. The reciprocities are a consequence of the conservation of energy expressed by equation (1.10) and (1.11). Sometimes they are even considered as expression of the law of energy conservation (first law). Anyway, for simulation of thermal processes one needs both true and pseudo bond graphs, as we shall see later.

Mathematical Formulae and Physical Variables

Physical variables must be well distinguished from mathematical formula. Mathematical formulae give a relation between input variables and output variables, called also independent and dependent variables. Different are physical variables, they can be a function of different inputs. In this sense the expression $U(S,V)$ and $U(T,V)$ describe the same variable (internal energy), but are expressed by different formulas (curves or tables) in function of different entrance variables. The physical variables are equal if the entrance variables are compatibles, that is refer to the same state $S(T,V)$.

Let us take for illustration an electric condenser with a moving plate, separated from the other plate at a distance x. The tension on both plates is given by:

$$u = \frac{q}{C} = \frac{q}{\frac{\epsilon A}{x}} \tag{1.14}$$

Where q is the electric charge, A is the area and ϵ the dielectric constant. The stored internal energy U is given by three following forms:

$$U = q\frac{u}{2} \qquad U = \frac{q^2 x}{2\epsilon A} \qquad U = \frac{u^2 \epsilon A}{2x} \tag{1.15}$$

We have very well the same physical variable, the internal energy, but expressed by different functions. One function gives the energy in function q and x, the other in function of U and x.

1.4.3 Entropy according to Clausius

Rudolph Clausius introduced about 1855 another definition of entropy which is often cited in the literature. This definition is more narrow as ours and refers only to multiport C. One multiplies the equation of Carnot by dt and obtains

$$TdS = dQ, \quad \text{where } S = \int \frac{dQ}{T} \tag{1.16}$$

This equation gives the change of entropy by the change of heat with absolute temperature. Sometimes one gives the suffix “rev” to dQ to indicate that the effect of series resistances is negligible (sec.1.8) and that the process is reversible. One mentions never the effect of parallel resistances such as the conductance of entropy towards the environment. Unfortunately this method with the suffix has troubled many students including author Jean Thoma, who has thought a long time about its signification in 1950. The flow of entropy is different if one measures before or after the resistance which is one prefers a formulation with dQ (see sec.1.6).

1.5 Properties of Multiport C

1.5.1 Properties and Reciprocities of Maxwell.

The multiport C is important and its properties are forming a large part of the books on thermodynamics. In the present book we will limit ourselves to some of these properties.

We shall use the associated energies of the multiport C, which are formulated by adding to the internal energy U the products TS and PV, which both have the dimension of energy. Therefore the variation of internal energy is:

$$dU = dQ + dW \tag{1.17}$$

dU is an exact differential since U a state function of the variables S and V. If the only available energy exchanges are the transfer of heat and of pressure forces we have:

$$dW = -PdV \tag{1.18}$$

In writing $dQ = TdS$ we obtain:

$$dU(S, V) = TdS - PdV \tag{1.19}$$

The equation (1.19),which can be written under following form:

$$d(U + PV) = dH = TdS + VdP$$

allows to enter the notion of enthalpy

$$H = U + PV \tag{1.20}$$

Further variables are derived by adding also the product ST as follows

$$F = U - TS \tag{1.21}$$

and

$$G = F + PV = U - TS + PV \tag{1.22}$$

The energy variable F is called free energy (or Helmholtz free energy) and G the free enthalpy (or Gibbs free energy). These associated energies are state functions of different input variables: $U(S, V)$, $H(S, P)$, $F(T, V)$ and $G(T, P)$.

The transition between the different energies as detailed here is often called a transformation of Legendre in the literature. However, there are therefore different energies and state functions of different input variables.

Especially the free enthalpy will be used very often with chemical reactions in chapter 3.

By deriving expressions (1.20), (1.21) and (1.22), we obtain:

$$\begin{aligned} dU(S,V) &= TdS - PdV \\ dH(S,P) &= TdS + VdP \\ dF(T,V) &= -SdT - PdV \\ dG(T,P) &= -SdT + VdP \end{aligned} \tag{1.23}$$

which is valid if mass remains constant. They are called often the Gibbs relations.

In order to memorize easily these equations or the associated energies we propose the figure 1.9.

Here we have always two input variables corresponding to the two DOF (degrees of freedom), which depend on the associated energy. For example, the free energy dU has very well dV and dS which are connected to dU by designs minus and plus. One obtains the relation of Gibbs relation by multiplying T by dS and P by dV.

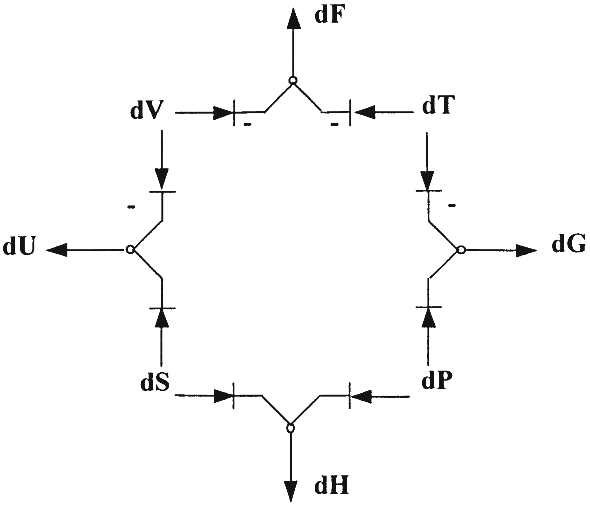

FIGURE 1.9. Graphical representation of Gibbs equations

The bond graph model with the causalities is shown on figure 1.10, where the multiports C are between two appropriate sources. They are pressure and entropy on thermal side and pressure and volume flow on the hydraulic side. The state variables are indicated by the causalities acting on the C-element.

One should note that in the presence of several chemical species, we have to add further pairs of efforts and flows, namely μ (chemical potential) and

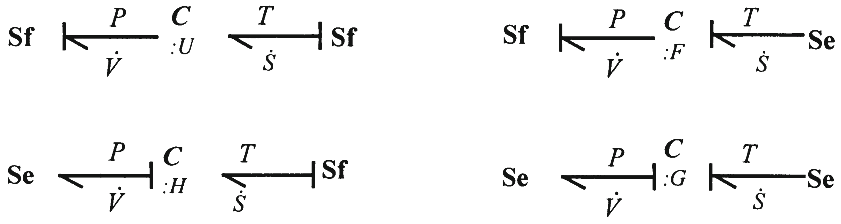

FIGURE 1.10. Multiport C between appropriate sources for the Gibbs equation.

$\dot{n}$ (molar flow). So we obtain for the Gibbs equation of m chemical species in derivative form:

$$dU(S,V) = TdS - PdV + \sum_{i=1}^{m} \mu_i dn_i \tag{1.24}$$

In general, pressure depends principally on volume, but also on what happens on the thermal side: entropy constant or temperature constant or any intermediary case. Similarly, temperature depends principally on entropy but also whether we have constant volume or constant pressure.

In analogy to equation 1.13, we can now obtain the other reciprocities of Maxwell by a deriving twice respectively the expression U, H, F, and G :

$$\begin{array}{ll} \dfrac{\partial P(S,V)}{\partial S} = -\dfrac{\partial T(S,V)}{\partial V} & \dfrac{\partial T(P,S)}{\partial V} = \dfrac{\partial V(P,S)}{\partial S} \\ -\dfrac{\partial S(V,T)}{\partial V} = -\dfrac{\partial P(V,T)}{\partial T} & -\dfrac{\partial S(P,T)}{\partial P} = \dfrac{\partial V(P,T)}{\partial T} \end{array} \tag{1.25}$$

All these differential relations of a body are called the reciprocities of Maxwell and represent the relations between the derivatives of the different variables of a body. Further relations between the chemical potential can be derived similarly from equation 1.24. The equation 1.24 really represents a body or system of variable mass. Here especially the case with constant temperature and pressure is important. These sources can absorb and produce thermal or mechanical energy, as may be required by the constitutive equations of the multiport C. We have then for the variation free enthalpy:

$$dG = \sum_{i=1}^{m} \mu_i dn_i \tag{1.26}$$

which is valid if temperature and pressure are constant.

In thermodynamics, the variable amounts of matter n_1,n_2....n_m are called the phase of a chemical system (Fig. 1.11).

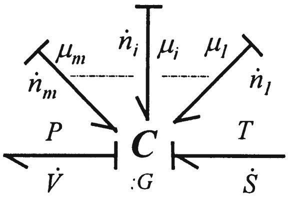

FIGURE 1.11. Chemical System as multiport C

These phases appear like a multiport C, depending on pressure and temperature and also on the matter variables. If they change, we have a system of variable composition

1.5.2 Calculation of Specific Heat

- Case of a real Gas

As said before, the temperature depends both on entropy and on volume. We calculate here these dependencies of entropy and on temperature when volume or pressure is kept constant. A calculation schema, really the block diagram and the corresponding bond graph with the appropriate causalities are shown on figure 1.12.

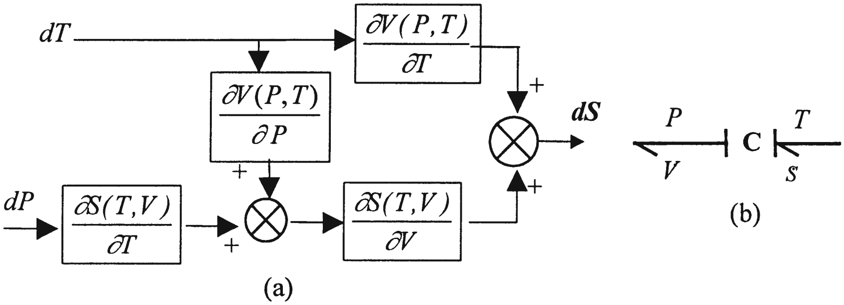

FIGURE 1.12. Calculation of entropy as function of temperature. a. Block diagram, b. Bond graph as multiport

The gains of the blocks are the derivative of volumes and entropy by T and V. Therefore for a constant volume we have simply:

$$dS = \frac{\partial S(T,V)}{\partial T} dT \tag{1.27}$$

since under constant volume V, the expression $\frac{\partial S(T,V)}{\partial V}$ is zero.

The relation 1.27 is connected to the expression of thermal capacity and constant volume:

$$dU = TdS = C_v dT \tag{1.28}$$

thus, we obtain

$$C_v = T\frac{\partial S(T,V)}{\partial T}$$

and

$$dS = \frac{C_v}{T} dT \tag{1.29}$$

Let us note that the thermal capacities C_v is connected to the specific heat by the relation: $C_v = c_v m$.

If on the hand, we keep the pressure constant, we must take the vertical branch of fig. 1.12 into account, we obtain:

$$dS = \frac{\partial S(T,U)}{\partial T} dT + \frac{\partial V(P,T)}{\partial T}\frac{\partial S(T,V)}{\partial V} dT \tag{1.30}$$

This expression can be easily deducted from the relations 1.12, 1.25 and 1.28. It expresses that at constant pressure there is an expansion of volume in function of the temperature, a phenomena, which is present especially in an ideal gas.

Further, the entropy can be transformed by the third reciprocity of Maxwell and we obtain if $dP = 0$:

$$dS = \frac{\partial S(T,V)}{\partial T} dT + \frac{\partial V(P,T)}{\partial T}\frac{\partial P(T,V)}{\partial T} dT \tag{1.31}$$

As said, in formula 1.31 there is an additional term to determine the variation of entropy in function of the temperature at constant pressure. This term is the product of variation of volume at constant pressure and of the pressure at constant volume.

Let us introduce specific heat per unit mass at constant volume $c_v$and c_p as expressed by the equation:

$$\begin{aligned} c_v &= \frac{T}{m}\frac{\partial S(T,V)}{\partial T} \\ c_p &= \frac{T}{m}\frac{\partial S(T,P)}{\partial T} \end{aligned} \tag{1.32}$$

These relations are directly a consequence of the equation of Carnot

$$\begin{aligned} c_v &= \frac{1}{m}\frac{\partial Q(T,V)}{\partial T} \\ c_p &= \frac{1}{m}\frac{\partial Q(T,P)}{\partial T} \end{aligned} \tag{1.33}$$

Combining equation 1.31 and 1.32 we obtain

$$c_p = c_v + \frac{T}{m}\frac{\partial V(T,P)}{\partial T}\frac{\partial P(V,T)}{\partial T} \tag{1.34}$$

- Case of an ideal Gas

We have seen that specific heats are different in general for all bodies as long as they have volume expansion. Let us take now the case of an ideal gas, where this effect is especially strong. Here the state equation can be written in two forms:

$$\begin{aligned} V(P,T) &= m\frac{RT}{P} \\ P(V,T) &= m\frac{RT}{V} \end{aligned} \tag{1.35}$$

Using the relation 1.31 we obtain

$$c_p = c_v + m\frac{R^2T}{PV} \tag{1.36}$$

Replacing PV by the state equation ($PV = mRT$) one obtains one important relation for ideal gases between both specific heats

$$c_p = c_v + R \tag{1.37}$$

There are many relations between the derivatives of a multiport C, which can be calculated in the same manner. The ones here given here are the most important, since the relation between the specific heats is often needed.

1.6 Friction with Entropy Generation

1.6.1 Introduction

Here we shall study the influence of friction in thermal processes. By friction we designate not only the mechanical friction, but also the electrical friction in electric resistance. We have also thermal friction, introduced by the phenomena of heat conduction; it will be analysed in the case of electric heating of a building. We discuss finally the influence of thermal friction on a multiport between two sources.

1.6.2 Types of Friction

We distinguish four types of friction:

1. mechanical friction, including hydraulic and electric friction,
2. conduction of heat with appreciable temperature difference,
3. mixture of different gases,
4. and friction in chemical reactions.

The points 3 and 4 will be treated in chapter 3 and we concentrate here only on the mechanical friction and conduction of heat. The essential properties of the conduction process are the conservation of power in the irreversibility of the phenomena. Thermal power can be generated but not destroyed. Figure 1.13 shows the different friction. First there is simple electric resistance which generates thermal power equal to the electric power according to the equation 1.38.

$$\dot{E} = ui = T\dot{S} = \dot{Q} \tag{1.38}$$

In the hydraulic resistor, we have similarly

$$\dot{E} = P\dot{V} = T\dot{S} = \dot{Q} \tag{1.39}$$

The figure 1.13c represents the mechanical friction by revolving shaft with a disc brake. The heat power appears here on this disc and the brake pads, from where it is very difficult to evacuate in practice.

In bond graphs the symbol R means any kind of resistance. In order to include thermal effects, we add to this one the symbol S for a source of heat: each RS element is in the same time a source of entropy and of heat. These two quantities are connected by the equation of Carnot (1.3). In this way one arrives at an element RS which is power conserving and

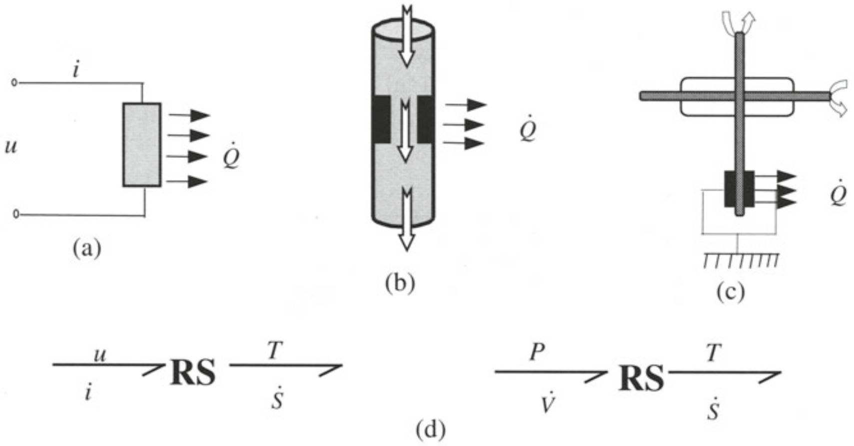

FIGURE 1.13. Different types of the friction. a. Electric, b. Hydraulic, c. Mechanical, d. Bond graph model of the friction.

irreversible (see Fig.1.13d). The symbol *RS* is standardized in the practice of bond graphs that why we accept it here. In principle we need two separate elements, using as example *RSME* for mechanical and *RSTE* for thermal friction studied in section 1.6.3. Some programs of simulation require this difference.

We can also represent the mechanical friction as a sequence of two phases, a friction with high temperature and negligible entropy followed by the thermal friction, which lowers the temperature and generates entropy [*Thoma*, 1971].

1.6.3 Thermal Friction

We have defined the thermal friction as the heat conduction at high temperature. As example let us examine the finite conductivity between two pieces as represented on figure 1.14. If we take T_1 and T_2 the two temperatures of the extremities, the thermal flow is transferred from T_1 and T_2 by equation:

$$\begin{aligned}
&\dot{Q}_1 = \dot{Q}_2 = K_C\,(T_1 - T_2) = \dot{Q} \\
&\dot{S}_1 = \frac{\dot{Q}}{T_1}, \quad \dot{S}_2 = \frac{\dot{Q}}{T_2} \\
&\text{where} \quad \dot{S}_2 = \frac{T_1}{T_2}\dot{S}_1
\end{aligned} \tag{1.40}$$

The thermal power is conserved and an increase of the flow of entropy is $\dot{S}_2 > \dot{S}_1$, since $T_1 > T_2$. Hence the thermal energy goes always from the high to the low temperature and the thermal power goes backwards.

Conduction of heat can be represented by a true bond graph (Fig.1.14b) and by a pseudo Bond graph (Fig. 1.14c). In true bond graphs there is the difference $T_1 - T_2$ which is multiplied by which is dissipated in the element *RS*.

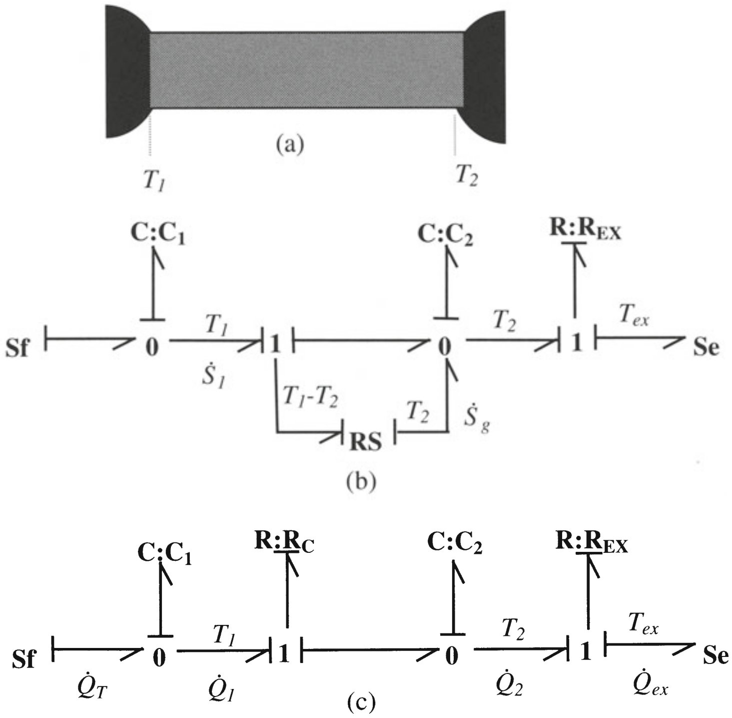

FIGURE 1.14. Thermal friction. a. Schema of thermal conduction, b. True Bond graph, c. Pseudo Bond graph

This is the conservation of power; it generates new entropy, which is injected to the lower temperature by the parallel junction as:

$$\dot{S}_g T_2 = (T_1 - T_2)\dot{S}_1 \tag{1.41}$$

In a pseudo Bond graph (Fig. 1.14c) the thermal flow $\dot{Q}$ is conserved and we have a simple constitutive equation:

$$\dot{Q} = \frac{1}{R_C}(T_1 - T_2) \tag{1.42}$$

Where K_C is the thermal conductance ($K_C = 1/R_C$).

In the building industries, the equation 1.42 is expressed as follows:

$$\dot{Q} = UA\,(T_1 - T_2) \tag{1.43}$$

Where A is the area of the wall. The value of U is in practice of the order of 20 $W/(K.m^2)$ for an well-insulated wall. Let us note, also that this reticulation is valid for both senses of temperature drop because in the formula 1.42 the flow becomes correctly negative. If there is the possibility of $T_1 < T_2$, the element $SWIT$ described in section 1.6.5 will be be added.

In other words, the friction power is always thermal and comes from the multiport RS and is injected at the bond or side with lower temperature. In mechanical and electrical friction, on the other hand, the thermal power or dissipation remains separate in the thermal domain. With thermal friction, the thermal power or dissipation is mixed with the entering thermal power.

Let us suppose that one is interested also by thermal losses because of imperfect insulation. Considering the temperature exterior as an effort source, the stored thermal energy, image of temperatures T_1 and T_2 are directly deduced from the bond graph according the imposed integral causalities as follows:

$$\begin{aligned} T_1 &= \frac{1}{C_1}\int\left(\dot{Q}_T - \dot{Q}_2\right)dt \\ T_2 &= \frac{1}{C_2}\int\left(\dot{Q}_2 - \dot{Q}_{EX}\right)dt \end{aligned}$$

In both equations $\dot{Q}_{EX}$ is the thermal flow dissipated towards the exterior. It is calculated by constitutive algebraic equation of R element:

$$\dot{Q}_{EX} = \frac{1}{R_{EX}\,(T_2 - T_{EX})}$$

$\dot{Q}_T$ is the thermal flow delivered by the source of flow S_f, C_1 and C_2 are respectively the thermal capacities of the rooms including their walls. The simulation schema of similar processes will be treated in detail in chapter 4.

1.6.4 Bond Graph Model of a Building

As example of a simulation from the technology we examine one room heated electrically, where the heat escapes by all the walls (Fig.1.15a).

The thermal capacity of the walls must be considered and accumulate heat. Figure 1.15b shows the corresponding pseudo bond graph. The electric heat becomes a simple flow source, which conserves the power:

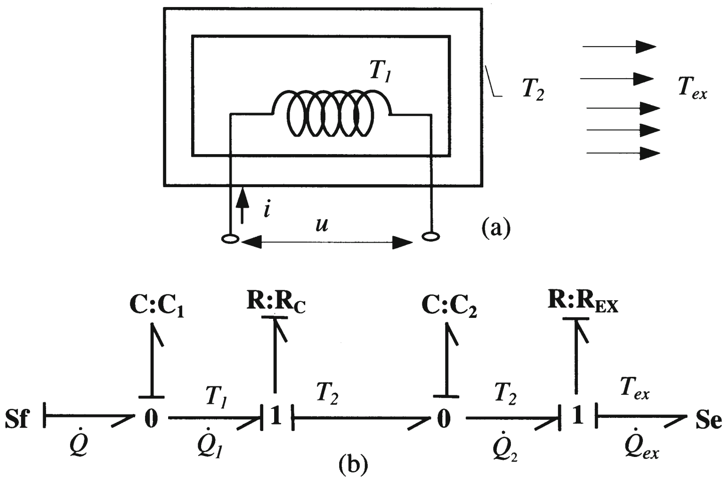

FIGURE 1.15. Heating with conduction. a. schematic, b. pseudo bond graph model

$$\dot{Q} = ui \tag{1.44}$$

The model is a sequence of elements R for heat conduction and of condensers C for thermal capacity. The external environment at constant temperature T_{EX} becomes also an effort source. Let us note that the value of the elements depends on the reticulation, thus on the number of elements. If C_{tot} and R_{tot} are respectively the total resistance and the total capacity of the walls, the equation for the element number i is given by:

$$\begin{aligned} C_i &= \frac{C_{tot}}{n} \\ R_i &= \frac{R_{tot}}{n} \end{aligned} \tag{1.45}$$

where n is the number of elements.

1.6.5 *Thermal Conduction in True Bond Graphs*

The modelling by pseudo bond graphs for the conduction allows showing both directions of heat flow. On the other hand, the use of a true bond graph for the same phenomena needs the precautions if the sense of the temperature difference can change. The dissipated power is always the product of entropy and a temperature drop. This new entropy is injected on the side of low temperature as represented by the junction *SWIT* on figure 1.16.

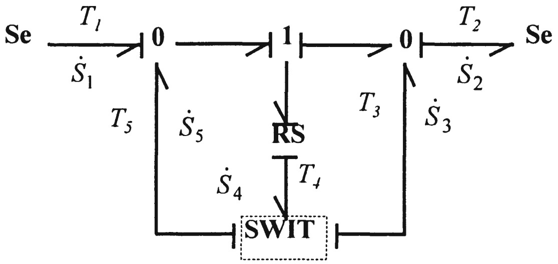

FIGURE 1.16. Generation of entropy by an RS element

This is placed behind the element *RS* and has the purpose to direct the new entropy to the right or to the left according to the sense of the entropy flow.

The element *SWIT* derives from simple switch. It is described by the following equations:

$$\begin{cases} \dot{S}_3 = \dot{S}_4, \quad \dot{S}_5 = 0 \quad \text{if} \quad T_1 > T_2 \\ \dot{S}_5 = \dot{S}_4, \quad \dot{S}_3 = 0 \quad \text{if} \quad T_1 < T_2 \end{cases}$$

It expresses that the new entropy is always injected in the part of lower temperature. Such a junction can be omitted when the direction of the flow does not change as for example on figure1.14 c.

The junction *SWIT* can be built as an instruction of the type *IF*on a computer. Let us note that in other manuals one uses instead of the switch a multiport R modulated by a Boolean variable, that which can take the values 0 and 1.

1.6.6 The Body as Multiport C between two Sources

We discuss here a case similar to heating by conduction, but with thermal friction placed between the body, a multiport C, and the temperature source. We use a true bond graph with temperature and entropy flow. The figure 1.17 represente this multiport C between two sources of effort, which apply pressure and temperature. The sources can be realized by the piston 3 and a temperature source 2. The thermal resistance 1 conserves power and increase entropy. It is shown on fig.1.17b by the bond graph symbol *RS*.

The thermal resistor injects new entropy at the side of low temperature. We can also say that the injection takes place on the side of the multiport C if one increases temperature and on the side of the source if one decreases the temperature; this is done by controlling the temperature source. So the entropy flow depends on the measuring point: before or after the resistance.

On the other hand (see paragraph 1.3.3), heat flow is conserved and does

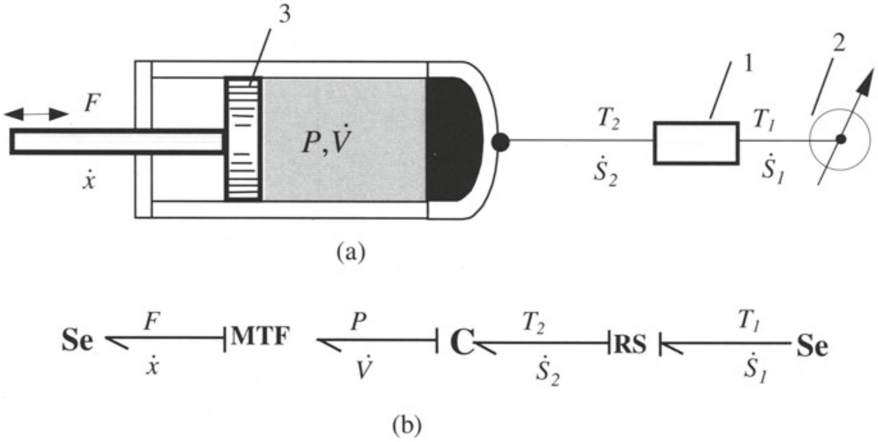

FIGURE 1.17. Body as multiport C between two sources, mechanical and thermal. a. Schema, b. bond graph model

not depend on the measuring point. Therefore a formulation with heat flow, that is a pseudo bond graph is sometimes preferable.

Figure 1.18 is similar but with two thermal friction elements; on top a schema and below a bond graph. Here we have a second resistance in parallel which conducts to another temperature source. This source can be colder and represent the environment; the resistance comes from an imperfect thermal insulation. In that case there is not much change but only the final temperature of the multiport C is calculated by analogy to the Kirchoff law from the values of the resistance. On calls this a resistance in parallel because it makes a parallel path for entropy.

Let us also note, that a change of the hydraulic source, for instance a diminution of the volume provokes an augmentation of the temperature. One says that entropy is pressed out and this proceeding is called entropy squeezing. The entropy must go through the thermal friction RS and generates new entropy in function of the speed of the processes. This law of entropy squeezing is valid for ideal gases, but not universal. Sometimes, pressure increase provokes a decrease of entropy and temperature: the material rubber is a famous example.

Finally, also in the domain of hydraulics, there can be a friction, as the friction of the piston in the cylinder. This friction generates then new entropy, which can be, depending on the arrangement, injected in the multiport C.

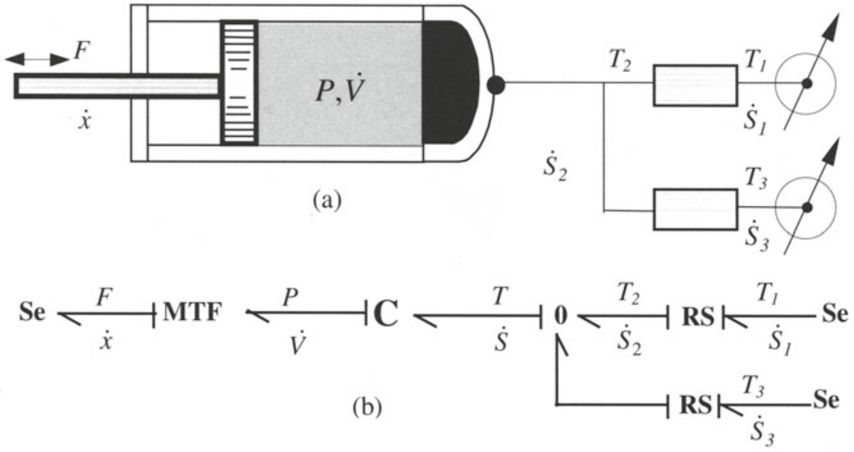

FIGURE 1.18. Body as multiport C between two sources and a parallel resistor. a. schema, b. Bond graph

1.7 Static Processes and Carnot Cycle

We discuss here a small modification of figure 1.18, where we have added a switch with three positions with the hot source T_1, a cold source T_2 and one position without any connection (see Fig. 1.19).

On this figure one introduces in the center a gas and increases the temperature by using the hot source such that its volume increases. In this way the gas delivers its hydraulic or mechanic power by using the piston. At the end of the expansion one can connect to the cold source which results in a reduction on volume. One obtains this way a machine that can produce this cycle several times and furnish a continuous mechanical power. This power is equal to the power supplied at the expansion power minus the power necessary at compression. Compared to figure 1.18a the switch of the figure 1.19 has a third position, which is empty and connected to the air. On the bond graph model this is represented by a flow source as Sf.

Sadi Carnot [*Carnot, 1824*] has studied this process and saw already a long time ago that the change between the two sources produces losses and generation of entropy in the series resistance. In effect at the end of the expansion the gas is still at the temperature T_{1f} and connected the source with temperature T_2. So we have a thermal short circuit with production of entropy, until the gas has temperature T_2. In order to avoid this phenomenon, the connection is kept in air and continued to increase the volume, which allows further decrease of the temperature of the gas. In the moment the gas temperature reaches T_2 , the connection with the cold source is established. The temperatures being equal now there is no short circuit with strong entropy flow and therefore no generation of entropy.

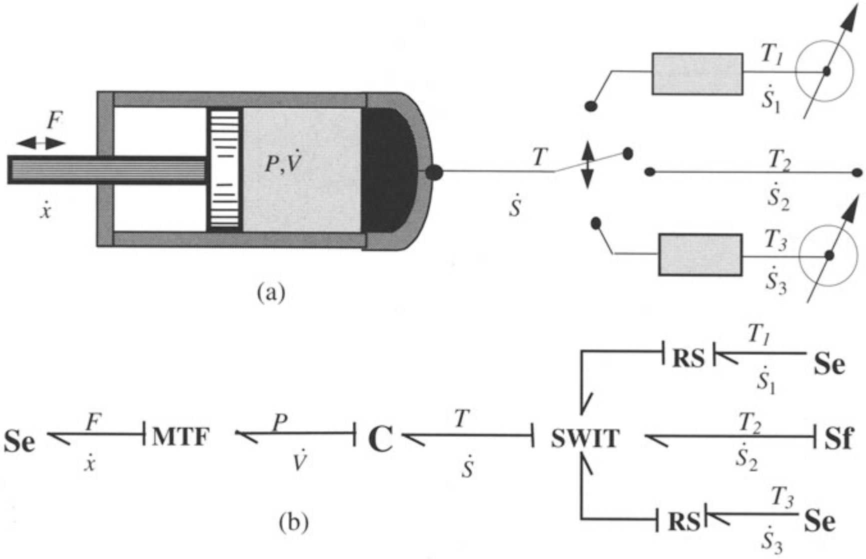

FIGURE 1.19. True bond graph model of thermal conduction at appreciable temperature diference. a. Schema, b. bond graph model.

Naturally the expansion must be sufficiently slow in order to avoid generation of entropy during the connection with the two sources. Today one calls the periods of connection to the thermal sources isothermally, because they run at constant temperatures and the periods without connection the adiabatic (at constant entropy). The process of Carnot is characterized by two isotherms and two adiabatics and avoids, as we have said, generation of entropy in the series resistance.

Nothing is mentioned about parallel resistance (insufficient insulation of the cylinder or multiport C) or is supposed negligible. So the schema of the figure 1.19a does produce entropy as translated by the equation:

$$\begin{aligned} \dot{Q}_1 &= T\dot{S}_1 \\ \dot{Q}_2 &= T\dot{S}_2 \end{aligned} \tag{1.46}$$

The mechanical power is by a power balance

$$\dot{E} = \dot{Q}_1 - \dot{Q}_2 = T_1\dot{S}_1 - T_2\dot{S}_2 \tag{1.47}$$

and the efficiency called the efficiency of Carnot is given by his famous formula:

$$\eta = \frac{\dot{E}}{\dot{Q}_1} = \frac{T_1\dot{S} - T_2\dot{S}}{T_1\dot{S}} = \frac{T_1 - T_2}{T_1} \tag{1.48}$$

As said, the conduction of the cylinder towards the environment is ignored: The value of that resistance is considered infinite. We have also to underline that during expansion hydraulic energy is produced but during compression a good part of it is used for compressing the gas. The ratio of the net mechanical energy recovered divided by the energy of the heat source is called the work ratio. In the Carnot cycle this ratio is very bad, that is small, and that is why one uses other cycles in the practice. Interesting is also the realization of a Carnot cycle in the so called Stirling engine with intermediate storage of entropy; *[see Falk, 1976, page 229]*. This intermediate storage is also the reason, why such an engine is economical in theory, but voracious in practice.

1.8 Process with Moving Matter

1.8.1 Matter in Movement

Until now we have treated matter at rest, taking Lagrangian viewpoint. Here we take now the Eulerian viewpoint with matter in movement. Let us for this examine the dynamics of a mass flowing in a conduit according to the schema on figure 1.20.

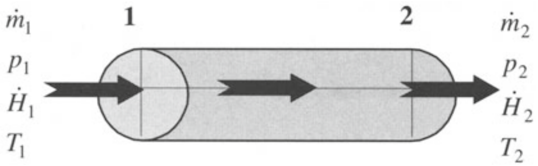

FIGURE 1.20. Moving matter in a insulated conduit

The mass or matter it self, mostly a gas, has two degrees of freedom. Therefore, as we have said, two variables, the pressure and the temperature can be imposed from the exterior and the gas assumes then the volume and the entropy. The mass of the gas remains constant. In principle, we could also fix the other variables like volume and entropy and the gas determines the pressure and the temperature.

In the Eulerian viewpoint appears a new DOF, the mass flow through the conduit. We have therefore thee DOF in total for the movement of the fluid in the conduit. We calculate the power driven through the conduit, which is equal to the flow of internal energy plus the hydrostatic power:

$$\dot{U} + P\dot{V} = \dot{m}\,(u + Pv) = \dot{m}h = \dot{H} \tag{1.49}$$

with $\dot{U}$ the flow of internal energy, P the pressure, $\dot{V}$ the volume flow, $\dot{m}$ the mass flow and $\dot{H}$ the enthalpy flow. We have also the specific quantities, u the internal energy by mass and h the specific enthalpy per mass, both with dimension (J/kg) and finally v the volume unit per mass (m^3/kg).

Globally, there is conservation of the mass flow enthalpy flow, which can be translated as:

$$\begin{aligned} \dot{m}_1 &= \dot{m}_2 \\ \dot{H}_1 &= \dot{H}_2 \end{aligned} \tag{1.50}$$

In the equation (1.50) we have supposed that the conduit is thermally insulated but the fluid may be compressible or incompressible. The first hypothesis is expressed by equality of the enthalpy flow at the entrance and at the output and the second by the equality of the mass flow. If the fluid is compressible, the mass flow is always conserved but not the volume flow. About the entropy flow we cannot say much, only that it can merely increase, because there may be frictions in the conduit.

Let us suppose now, that the insulation of the conduit is not perfect, that there are thermal losses towards the exterior. This is shown on figure 1.21a.

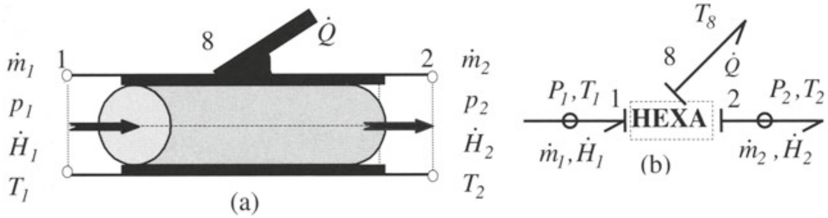

FIGURE 1.21. Matter in movement in a non insulated conduit a) schematic, b) Bond graph model with the word HEXA

The conduit acts like a heat exchanger and is surrounded by a mantle of high thermal conductivity. The heat exchanger is modelled by the element $HEXA$ further studied in section 2.2.1. The direction of the half arrow indicates the sense of the thermal losses.

We have conservation of the mass flow, but flow of enthalpy changes:

$$\begin{aligned} \dot{m}_1 &= \dot{m}_2 \\ \dot{H}_1 &\neq \dot{H}_2 \\ \dot{H}_2 &= \dot{H}_1 - \dot{Q}_8. \end{aligned}$$

Consequently, temperature and entropy become lower. The volume flow becomes also less if there is thermal contraction. Therefore it is necessary to distinguish clearly between the mass flow $\dot{m}$ (kg/s), which remains constant and the volume flow (m^3/s) which varies in function of the density of the gas, therefore with the temperature.

We have on figure 1.21 one DOF more, the heat flow. One can for instance write:

$$\dot{Q}_8 = K_C \left(T_1 - T_8\right) \tag{1.51}$$

where K_C is the coefficient of heat exchange. This function is in the general case not linear and can depend also on other variables for instance the mass flow or the velocity of the fluid.

It is also just to note that we use here the pseudo bond graph and in consequence the temperature T_1 can be easily determined from the mass flow and the enthalpy flow with the specific heat c_p.

$$T_1 = \frac{\dot{H}_1}{\dot{m}_1 c_p} \tag{1.52}$$

The two further flows, namely volume and entropy flows at the extremity of the conduit associated are determined as follows:

$$\begin{aligned} \dot{V} &= \dot{m}v \\ \dot{S} &= \dot{m}s \end{aligned} \tag{1.53}$$

where v and s are respectively the volume and the specific entropy per mass. The relation 1.53 is valid for compressible and for incompressible fluids.

1.8.2 Ratio between Conduction and Convection

It is important to distinguish the phenomena of conduction and of convection. In conduction the entropy flow $\dot{S}$ and heat flow $\dot{Q}$ are connected by the equation of Carnot, which is pushed by the temperature difference. This is shown by a resistance, which dissipates energy and the generated entropy is added to the outgoing entropy flow as we have seen in paragraph 1.6.

In the phenomena of convection, the entropy flow and enthalpy flow are carried by a mass flow which is pushed by the pressure difference. So the convection is reversible and entropy conserving, unless there are resistances.

An interesting property is that a ratio of enthalpy to entropy is approximately equal to the temperature of the flow. We choose a reference and measure the variation of enthalpy and entropy by the expressions:

$$\dot{H} - \dot{H}_{ref} = \dot{m}c_p\,(T - T_{ref}) \tag{1.54}$$

and

$$\dot{S} - \dot{S}_{ref} = \dot{m}c_p \int_{T_{ref}}^{T} \frac{dT}{T} = \dot{m}c_p \ln \frac{T}{T_{ref}} \tag{1.55}$$

The ratio between variation of enthalpy and the entropy compared to a reference value is best expressed by a quantity T_{HS} with the dimension of a temperature:

$$T_{HS} = \frac{\dot{H} - \dot{H}_{ref}}{\dot{S} - \dot{S}_{ref}} = \frac{T - T_{ref}}{\ln \frac{T}{T_{ref}}} \tag{1.56}$$

In (1.56), the quantity T/T_{ref} is the temperature expressed in multiple of the temperature of reference. Introducing $\delta = (T - Tref)/Tref$, (the difference of temperature as multiple of temperature of reference), one obtains:

$$T_{HS} = \frac{T\delta}{(1+\delta)\ln(1+\delta)} \tag{1.57}$$

The figure 1.22 shows the comportment of the function $T_{HS}(\delta)$. It is equal to 1 with small value of δ and has a value of 0,721 for $\delta = 1$.

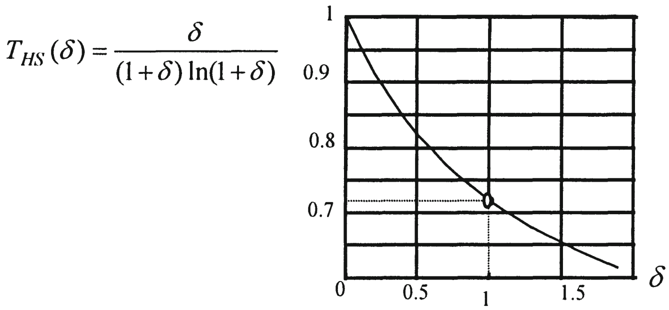

FIGURE 1.22. Behavior of the function δ.

For a value of $\delta = 1$ we have the following equation:

$$\dot{H} - \dot{H}_{ref} = 0,721\left(\dot{S} - \dot{S}_{ref}\right) \tag{1.58}$$

It means that the enthalpy carried by the fluid corresponding only to 72 % of the product temperature by entropy flow, while it is equal to a 100% in the case of conduction. Let us remind that $\delta = 1$ corresponds to a temperature $T_{ref} = 596K$ with a reference of $298K$. This is already a hot gas and if the temperatures are lower, the difference between convection and conduction becomes less.

So we can conclude that the equation of Carnot is approximately valid also for convection, if one refers entropy and enthalpy to the same temperature.

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2

Modelling of Thermofluids

2.1 Conservation of Power in Multiports

2.1.1 Multiport R:Reco

Figure.2.1 represents the flow of a compressible liquid through a resistance. Since it is compressible, the volume flow and entropy flow change in the passage of the resistance which we have represented by the word bond graph (Fig. 2.1b) *RECO* or REsistance of COnvection. We have shown this multiport by the symbol *RECO* instead of the usual *R* for resistance in the other manuals. We use here a pseudo bond graph with multibonds to model the coupling of thermal and hydraulic energy. Further, the bonds carry a ring around in order to indicate that it is a multibond. Until now, the bond graphers [*Karnopp, 1979*] used another symbolism, to distinguish bonds, a hydraulic in full line and a thermal bond in dotted lines. This representation is not practical for the modelling of complex systems.

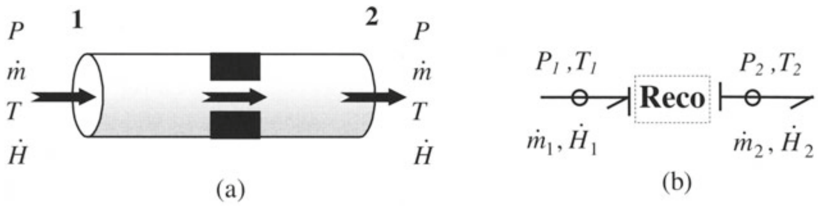

FIGURE 2.1. Transport of internal and hydrostatic energy in a compressible flow. a. Schema, b. bond graph.

The hydraulic resistance is also called restrictor and is a multiport since the laws in action are not a scalar but matrix form (see appendix A).

The multiport *Reco* is thus a multivariable system; called “MIMO“ which means Multiple Input Multiple Output. In our case, the choice for entries and outputs is seen from of the causalities affected to this element. If one imposes for instance the effort, one obtains a bond graph model and a block diagram as shown in figure 2.2.

The volume flows and the entropy flows are not conserved. Therefore, in compressible fluids systems, like industrial pneumatics, these flows can not be used as variables. However, mass flow and the enthalpy are conserved and serve often as bond graph variables:

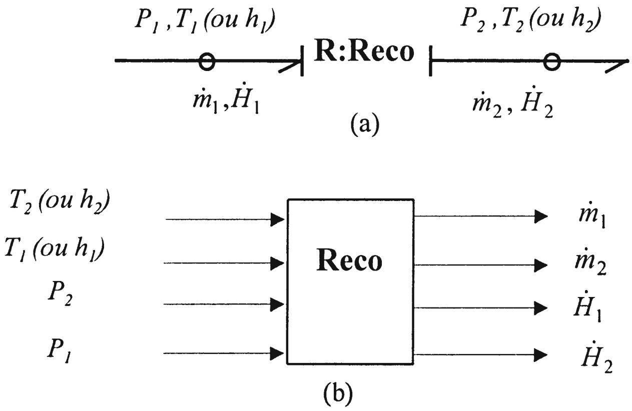

FIGURE 2.2. Simulation of the multiport Reco. a: bond graph model, b: Block diagram model for simulation

$$\begin{aligned} \dot{H}_1 &= \dot{H}_2 = \dot{H} \\ \dot{m}_1 &= \dot{m}_2 = \dot{m} \end{aligned} \tag{2.1}$$

For causalities, the efforts upstream and downstream that are pressure and temperatures are imposed and we determine in the *Reco* the mass flow and enthalpy flow. This is more natural causality than some others often used for simulation. We need some capacitors, called coupling capacitors between the elements *Reco*, to produce our causalities, as we shall see in section 2.1.2. This is also true for the more complex elements we introduce in section 2.3.

Pressures and temperatures at the both ends *Reco* are designated respectively by the point P_1, P_2, T_1 and T_2. Hence we have matrix relation as follows:

$$\begin{bmatrix} \dot{m} \\ \dot{H} \end{bmatrix} = \begin{bmatrix} \Phi_{R1}(P_1, P_2, T_1, T_2 \\ \Phi_{R2}(P_1, P_2, T_1, T_2 \end{bmatrix} \tag{2.2}$$

In chemical engineering, the relations are non-linear. The thermal flow that is the transported enthalpy flow is given by two forms:

$$\begin{aligned} \dot{H} &= \dot{m} \\ \dot{H} &= \dot{m} c_p T_1 \end{aligned} \tag{2.3}$$

with P_1 the upstream pressure and T_1 or h_1 the temperature or the specific enthalpy upstream. The choice between these efforts is discussed in section 4.3. Also, c_p is the specific heat at constant pressure.

The downstream pressure influences also the flow, but not the downstream temperature. This is a general principle of physics: Downstream temperature has no influence, downstream pressure has.

The constitutive equations depend on the details of *Reco*, and widely used form is [*Prandtl 1952*], [*Borel 1984*]:

$$\begin{aligned} \dot{m} &= \frac{K_d A}{2}\frac{P_1}{\sqrt{T_1}} \quad \text{if} \quad P_2 < 0.5P_1 \\ \dot{m} &= K_d A\sqrt{(P_1 - P_2)\frac{P_2}{T_1}} \quad \text{if} \quad P_2 > 0.5P_1 \end{aligned} \tag{2.4}$$

where K_d is the coefficient of hydraulic losses and A the area at the most narrow point.

This equation is given by two formulae which connect at one point in the middle. There, both formulae give the same result and even their derivatives are the same. It follows from equation 2.4 that the flow becomes zero if both pressures are equal ($P_1 = P_2$). If the flow is reversed, we have ($P_1 < P_2$) the mass flow naturally reverses and can be calculated by the similar formulae:

$$\begin{aligned} \dot{m} &= \frac{K_{d1} A}{2}\frac{P_2}{\sqrt{T_2}} \quad \text{if} \quad P_1 < 0.5P_2 \\ \dot{m} &= K_{d1} A\sqrt{(P_2 - P_1)\frac{P_2}{T_1}} \quad \text{if} \quad P_1 > 0.5P_2 \end{aligned} \tag{2.4a}$$

Here the hydraulic coefficient K_{d1}can be different if the pipe is not symmetrical. Normally the flow reversal is not needed, because one has a definite flow direction. If reversal is needed, it can be implemented by a *SWIT* element as discussed above.

According to these expressions, the mass flow depends on upstream and downstream pressure but depends only on the upstream temperature. The downstream temperature has no influence on the flow, as we have seen.

The reticulation given here is valid only if the fluid on the interfaces goes relatively slowly. If the speed is high, there must be a term corresponding to the kinetic energy of the fluid stream. Within the components, here the restrictor, speed or velocity may become large. So we can calculate restrictors and turbomachines, but the interaction of a jet with a turbine wheel is excluded: It requires a special bond graph.

2.1.2 Multiport C

As mentioned before, we need coupling capacitors between *Reco* elements and others. They represent the conservation of energy in the conduits upstream and downstream. These energies are represented by a multiport for the compressible fluid, which always conserves energies. The equations for the coupling capacitor are different, whether we have incompressible fluid (hydraulics) or compressible fluid (pneumatics).

As an example, let us take restrictor or nozzle with conserved mass flow according figure 2.3.

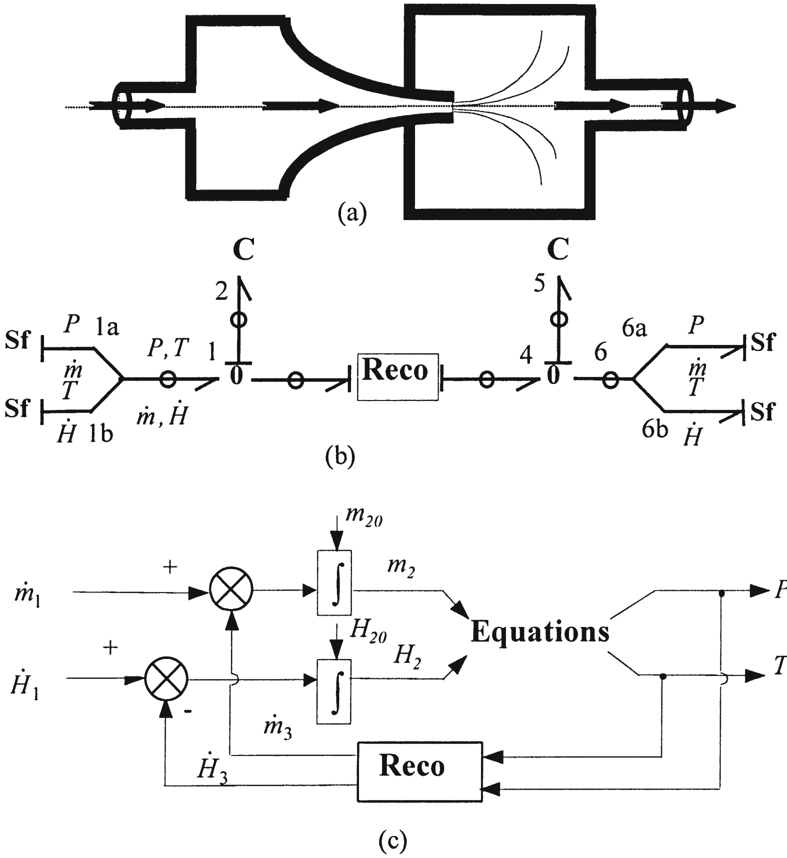

FIGURE 2.3. Coupling of hydraulic and thermal energy in a jet. a. Schema, b. Bond graph model, c. Structure of calculation or block diagram.

The volume flow will not be conserved, as said, because the volume of the fluid increases with reduction of pressure. Concerning the entropy we have no specific information except the fact that it can only increase. Since we have a resistance, this increase will be substantial. The enthalpy which represents the total energy will also be conserved.

The bond graph of the restrictor is represented on the figure 2.3b and a block diagram for calculation on figure 2.3c. The bond graph can be shown as coupled multibond with the ring (bond 1a and 1b) or be split up as two single bonds (bond 6a and 6b). Here the restrictor is highly asymmetric, it is almost a jet and therefore the flow coefficients (equation 2.4) will be very different.

If the causalities are integral, the coupling capacitors allow calculating the efforts, pressure and temperature, which will be used by the element *Reco* as inputs.

The mass and accumulated energy are calculated in the multiport C by the constitutive equations and the both junctions:

$$\begin{aligned} m &= \int (\dot{m}_1 - \dot{m}_3)\, dt \\ H &= \int \left(\dot{H}_1 - \dot{H}_3\right) dt \end{aligned} \tag{2.5}$$

Similar equations allow to calculate m_5 and H_5:.

$$\begin{aligned} m_5 &= \int (\dot{m}_4 - \dot{m}_6)\, dt \\ H_5 &= \int \left(\dot{H}_4 - \dot{H}_6\right) dt \end{aligned} \tag{2.6}$$

The effort (P and T) in the coupling capacitors are calculated from the integral of the flows by relations which depend on the physics of the system, whether it is incompressible or compressible. These equations correspond to the element “Equations“ in figure 2.3c.

For incompressible fluids or hydraulics we have:

$$\begin{aligned} T_2 &= \frac{H_2}{m_2 c_v} \\ H &= \frac{\beta}{\rho V} m_2 \end{aligned} \tag{2.7}$$

with β the compressibility modulus, has a dimension of pressure. The value is of $1200 MPa$ for industrial hydraulic oil but depends on the inclusion of air. Consequently it varies very much from $1500 MPa$ for oil without air until $10 MPa$ for the blood in the arteries where this last value includes the dilatation of the tube walls with pressure [*Thoma, 1971*].

V is the volume of the coupling capacity, a geometric quantity that is known from the dimension of the tube or of the reservoir. This geometric variable does not depend on the fluid: gas fills completely the offered volume.

For compressible fluids or pneumatics we take an ideal gas and the efforts are:

$$\begin{aligned} T_2 &= \frac{H_2}{m_2 c_v} \\ P_2 &= \frac{mRT}{V} = \frac{RT}{c_v} \frac{U}{V} \end{aligned} \tag{2.8}$$

The algorithms of the calculus equation (2.7) and (2.8) are designated by the word "equations" on the figure 2.3c. These equations give the pressure and the temperature in function of the mass m and the accumulated energy by the coupling capacitors C_2. In equations (2.5) and (2.6) the mass flow and enthalpy flow in the bonds 1 and 6 is imposed by an external member, while in the bonds 3 and 4 they are calculated from the constitutive equations of *Reco* according to the relations (2.3) and (2.4). The initialization of the algorithms is of course given by the initial conditions m_{20} and H_{20} of the integrators.

The constitutive equations of the element C_2 are identical to the ones given earlier.

2.1.3 Dissipation of Energy in a Resistance

Hydraulic Losses

Let us calculate now the hydraulic flow in the case where the fluid is almost incompressible. We take as example the flow of oil of dynamic viscosity between the walls of a piston and the cylinder. It is called the Poisseuille equation. The figure 2.4 shows such a typical gap of a height of about $e = 10 microns$, and of a with l and of a length L of some centimetres.

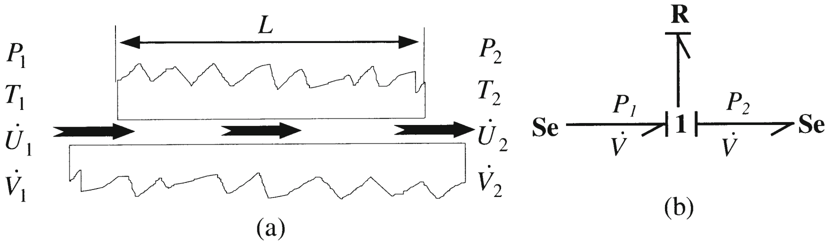

FIGURE 2.4. Hydraulic resistance with the losses of an incompressible fluid. a. Schematic of the losses of oil between the piston and cylinder, b. Bond graph model.

Since the oil is incompressible one uses sometimes for the flow variable the volume flow which is connected to the mass flow by the density ρ.

We suppose first that the thermal effects are negligible, and the bond graph model is then shown by figure 2.4b. The volume flow is given by a well-known formula of hydraulics, and the mass flow by multiplying with ρ.

$$\dot{V} = \frac{1}{12}\frac{(P_1 - P_2)}{\mu}e^3\frac{l}{L}$$
$$\dot{m} = \rho\dot{V} \tag{2.9}$$

Dissipation of thermal energy in the resistance

Let us examine the flow in a conduit through the same hydraulic resistance which dissipates its energy by heating as shown on figure 2.5.

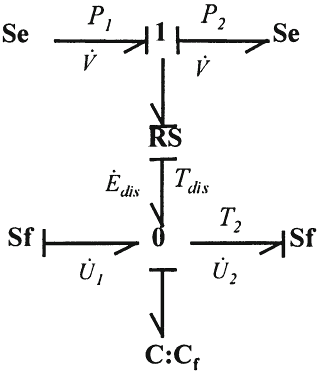

FIGURE 2.5. Bond graph of energy dissipation in a resistance

The dissipated power $P\dot{V}$ gives a heating of the fluid of density ρ. On the bond graph the element R becomes then a multiport RS and the dissipated energy $\dot{E}_{dis}$will directly be added to the internal energy of the fluid $\dot{U}_1$. The average temperature T_2 is calculated by C element of global thermal capacity C_f. The constitutive equations are as follows:

$$\begin{aligned} \dot{E}_{dis} &= (P_1 - P_2)\,\dot{V} \\ T_2 &= \frac{1}{C_f}\int\left(\dot{E}_{dis} + \dot{U}_1 - \dot{U}_2\right)dt \end{aligned} \tag{2.10}$$

with $\dot{U}_2$ the output internal energy flow.

If one neglects the thermal part, the multiport RS becomes a simple element R and we are returning to the classic hydraulic system. Nevertheless the thermal bond exists and can often not be neglected, because of the increase of temperature is often very important. In hydraulics, the heating of oil is for instance about $5.5K$ for $10MPa$ (100bar) and of $16.5K$ for $30MPa$ (300 bar).

Other Thermal Effects

Naturally with the heating of the oil, the viscosity becomes less along the gap. We obtain a hydraulic film, normally called adiabatic hydraulic film, which can be calculated analytically [*Thoma, 1975*]. With constant viscosity, according to formulae (2.9), we have an isothermal oil film. A first approximation to adiabatic oil films is to take the isothermal oil film, but with the viscosity at the mean temperature before and after the gap; this viscosity is given by a curve or table from the oil manufacturer. In the practice, author measures both temperatures and calculates the mean viscosity and estimates the gap height, that is the half play between the piston and the cylinder. In a hydraulic pump, this variable can not be directly measured. This estimation is therefore useful in spite of the many perturbations that can come.

2.1.4 Combined Hydraulic Resistance

In the preceding paragraph we have neglected the inertia force, which is normally justified for a narrow gap. However these forces exist and can become important when the height and the length of the gap are of the same order. Also it is important if the gap is round which is normally called an orifice. So, if we have a pressure drop due to the inertia, the flow is calculated by the equation:

$$\dot{m} = A\rho\sqrt{|P_1 - P_2|}\,sign\,(P_1 - P_2) \tag{2.11}$$

The flow coefficient K_d is about 0.71 and depends very much on rounding of the entry of the orifice. A is the area and ρ the density of fluid. The expression sign signifies the sign of $(P_1 - P_2)$. This last one is very often suppressed if the difference of pressure can not become negative.

In practice it is relatively simple to chose which of the formula, (2.9) or (2.11) to take. Nevertheless, there are certain cases where both pressure drops are appreciable. A hydraulic servovalve according to figure 2.6 is a typical example. Here the flow of the fluid is regulated by the passage section which is variable in function of the position x of the valve stem, and the other variables.

So the flow passage or the position x of the valve steam is normally taken as information bond, which means that the forces on the valve stem are negligible.

Let us suppose now, that we have two hydraulic restrictors, one due to viscosity and the other due to inertia, which are appreciable. Both these restrictors are in series, coupled by a series junction (1-junction). Therefore one is in resistance causality and the other in conductance causality as shown by the figure 2.7. This introduces an algebraic loop; in other words, for *Rvisco* the cause is the effort and the effect is the flow and for $R_{inertia}$

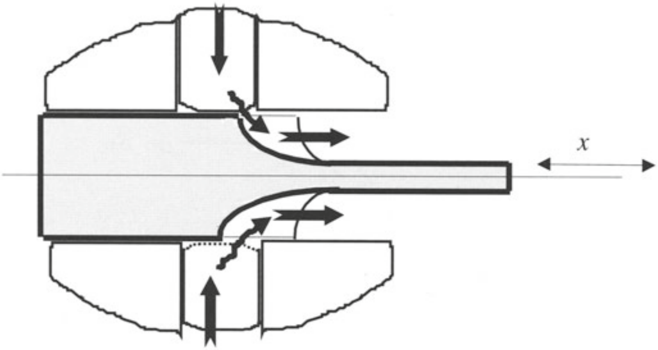

FIGURE 2.6. Schematic of a hydraulic servovalve

the cause is the flow and the effect is the effort. We have therefore during the simulation algorithmic problems, because tie loop conducts to implicit equations.

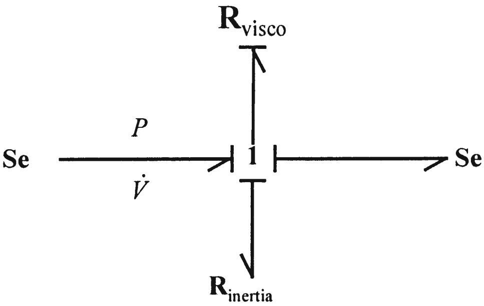

FIGURE 2.7. Introduction of an algebraic loop by the series circuit of two resistances, one in a resistance causality and the other in conductance

In order to avoid the algebraic loop, an I-element (inertia) is added on the 1-junction, as shown on the figure 2.8. This brings both R-elements to resistance causality as indicated by the bond graph. The element I is introduced mainly for avoiding the algebraic loop, but one can give it a physical sense: it is the inertia due to the kinetic energy of the flow.

The corresponding bond graph for servovalve is given on figure 2.9.

The speed of the valve stem is integrated to give the position, which then is amplified by a gain G. As explained before, the force on the valve stem is neglected and this indicated by the signal bonds.

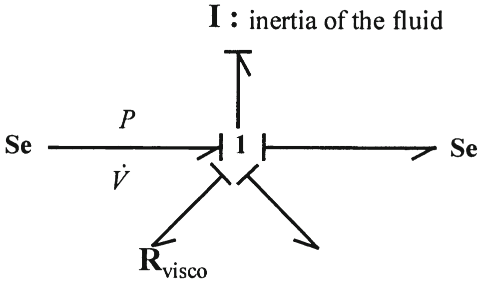

FIGURE 2.8. Two hydraulic resistances: one viscous, the other due to inertia. To avoid the algebraic loop, we have added an I-element, which represents the kinetic energy of the jet. It forces both restrictors in resistance causality

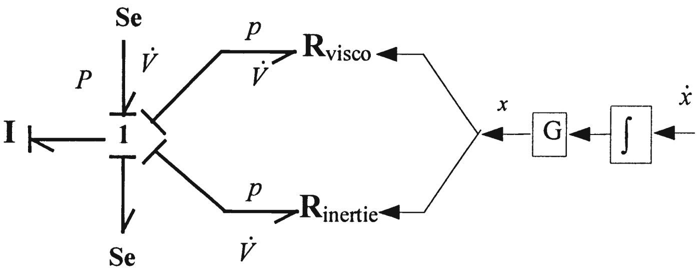

FIGURE 2.9. Bond graph model of the servovalve with two resistances in serial connection

2.1.5 Patching Formulae in Restrictors

A resistor, restrictor or gap, both compressible and incompressible, introduces a very important concept in simulation technique. As a physical device, the restrictor has an absolutely continuous characteristic, from high forward pressure over zero the high reverse pressure. For incompressible fluid and a thin gap, this is given by formula (2.9). If one is sure that the pressure difference never becomes negative in a given simulation, the sign function can be left out for simplification.

With compressible flow, we have equation (2.4) and (2.4a). Here we have both for forward and reverse flow two formulae, which are patched, up the middle. So we have in total four formulae to describe a completely smooth characteristic. Again, if some part of the characteristic is not needed, the corresponding formula can be omitted for brevity. The general principle of patching different formulae for a given characteristic, and the omission if not needed, is also used elsewhere in simulation technique.

2.2 Heat Exchanger

2.2.1 *The Element Hexa*

For a fluid going through a resistance we have conservation of the enthalpy flow. In a heat exchanger, enthalpy is not conserved but increased by the flow of conduction . We propose to model the exchange of heat by an element which we call *HEXA* (heat exchanger) instead of doing it by resistive elements for the reason we show below [*Ould Boumanma, 1997*]. The heat exchange between two fluids as shown by the figure 2.10a is modelled by the elements R (Fig. 2.10b) or by the heat exchanger HEXA (Fig. 2.10c).

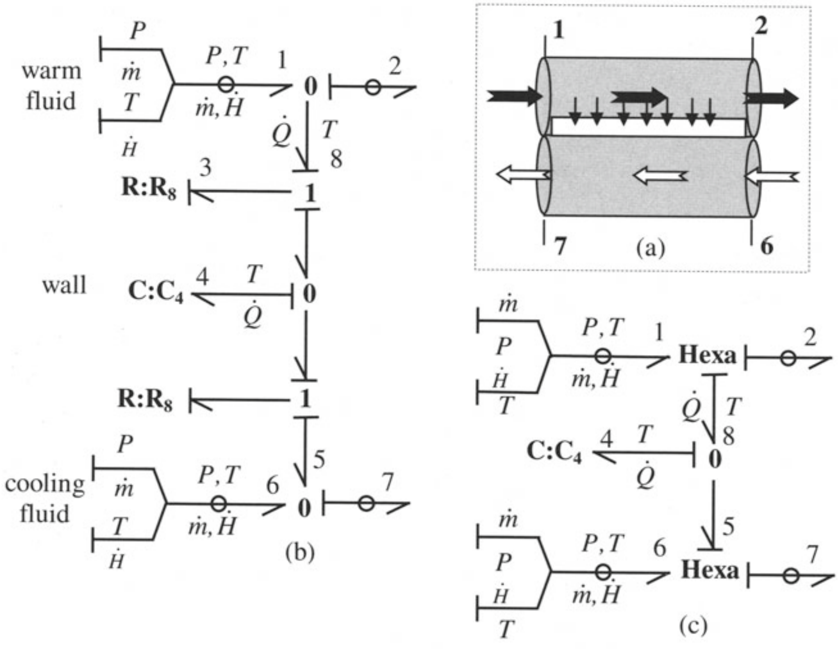

FIGURE 2.10. Bond graph of a heat exchanger. a. Schema, b. Modelling by elements R, c. Modelling by an element HEXA.

In the heat exchanger according to figure 2.10 there is the same mass flow ($\dot{m}_1 = \dot{m}_2$), but a variation of temperature and of thermal enthalpy ($T_2 \neq T_1$, $\dot{H}_2 \neq \dot{H}_1$). So, on the bond graph of figure 2.10b, T_1 would be equal to T_2, which is contrary to physical reality. Hence, displaying this process by a parallel junction (or 0 junction) alone is not adequate because of the temperature increase.

To avoid this, we replace the parallel junction by a *HEXA* bloc as shown on figure 2.10c. This bloc has the following constitutive equations:

$$\begin{aligned} \dot{m}_1 = \dot{m}_2, \quad \dot{H}_2 = \dot{H}_1 - \dot{Q}_8, \quad T_2 = \frac{\dot{H}_2}{\dot{m}_2 c_p} \neq T_1 \\ \dot{m}_6 = \dot{m}_7, \quad \dot{H}_7 = \dot{H}_6 + \dot{Q}_5, \quad T_7 = \frac{\dot{H}_7}{\dot{m}_7} \end{aligned} \tag{2.12}$$

c_p is the specific heat determined from the properties of the fluid.

In order to avoid the inconvenience with the parallel junction, some bond graphers [*Paul Ove et al., 1995*] insert an R-element to impose the relation 2.12.

The temperature stored by the wall of the heat exchanger, is calculated by the C-element C_4 :

$$T_4 = \frac{1}{C_4} \int \left(\dot{Q}_8 - \dot{Q}_5 \right) dt \tag{2.13}$$

where the heat flow transferred by conduction are calculated by constitutive equations of R elements:

$$\dot{Q}_8 = \frac{1}{R_8} \left(T_2 - T_4 \right)$$

$$\dot{Q}_5 = \left(T_4 - T_7 \right)$$

Where $\frac{1}{R_8} = K_8$ and $\frac{1}{R_5} = K_5$ are the thermal conductances and C_4 the global thermal capacity of the wall.

2.2.2 An Element Hexa between two Multiports C

The bond graph of a heat exchanger with the symbol $HEXA$ is placed between two coupling capacitors as shown on figure 2.11. It exchanges heat through the wall. According to the indicated causalities, it receives the effort variables, pressure and temperature by the bonds 2 and 4 calculates the mass flow and enthalpy flows according equation 2.12.

The principal constitutive equations are seen on the bond graph (Fig. 210c) and are:

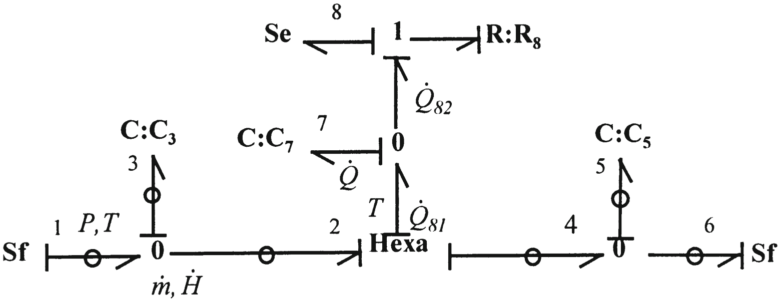

FIGURE 2.11. Bond graph of a heat exchanger placed between a fluid and a wall

$$
\begin{aligned}
T_3 &= \frac{1}{m_3 c_p} \int \left(\dot{H}_1 - \dot{H}_2\right) dt \\
m_3 &= \int \left(\dot{m}_1 - \dot{m}_2\right) dt \\
T_5 &= \frac{1}{m_5 c_p} \int \left(\dot{H}_2 - \dot{Q}_{81} - \dot{H}_6\right) dt \\
m_5 &= \int \left(\dot{m}_4 - \dot{m}_6\right) dt \\
T_7 &= \frac{1}{C_7} \int \left(\dot{Q}_{81} - \dot{Q}_{82}\right) dt \\
\dot{Q}_{81} &= \frac{1}{R_{81}} \left(T_3 - T_7\right) \\
\dot{Q}_{82} &= \frac{1}{R_{82}} \left(T_7 - T_8\right) \\
\dot{m}_4 &= \dot{m}_2 \\
\dot{H}_2 &= \dot{m}_1 c_p T_3
\end{aligned}
\tag{2.14}
$$

T_8 is the effort source which represents the temperature of the environment. R_{81} and R_{82} are the resistances for the global heat exchange and are imposed by the external flow sources Sf.

2.3 Turbomachines

2.3.1 Introduction

We call a turbomachines any machine for compressible gas. The steam turbines do not belong to this category because the working fluid is a mixture of gases, that is the vapour and water. On the other hand the positive displacement machines or machines with cylinders are considered turbomachines. On figure 2.12 are shown a turbine and a piston machine. The turbine is characterized by a working fluid with input enthalpy flow $\dot{H}_1$ and output enthalpy flow H_2 , a mechanical shaft and possibly heat conduction $\dot{Q}_8$. In the cylinders the working fluid is enclosed during the cycle.

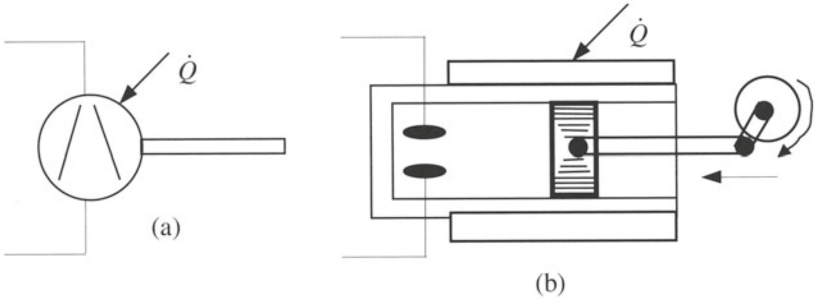

FIGURE 2.12. Representation of turbomachines. a. Turbine, b. Piston machine.

There are two ways of seeing the working of a turbomachines, first as simple turbomachines analogue to the one shown in section 1.2 or on the figure 2.12a. It can also be considered as a piston machine (Fig. 2.12b) having a Carnot cycle or other. In this last case the fluid must return to its initial state which is in practice done by an exchange of the fluid through valves: The used fluid is driven out and new fluid is entering through the valves from the exterior. Therefore the fluid is without movement during the closure of the valves.

Nevertheless, for the analysis one uses the Eulerian viewpoint (see section 1.2) and assimilates a piston machine to a turbomachines.

To the power balance, which comprises already thermal and hydraulic power, comes a third member, the mechanical power of the shaft. Therefore one must know the torque in function of the rotation frequency of the shaft.

$$M = M(\omega) \tag{2.15}$$

The torque can depend also on other measurable variables in the turbomachine (mass flow, temperature...):

$$M = M(\omega, T, \dot{m}) \tag{2.16}$$

The power balance becomes then:

$$\dot{H}_2 = \dot{H}_1 - \dot{Q}_8 + \dot{E}_9 \tag{2.17}$$

2.3.2 Element TEFMA

The figure 2.13a shows the bond graph of a turbomachine. We remind that the word *TEFMA* (Thermofluid) Machine, like *HEXA* is an arbitrary designation. Technically it is a word-bond graph.

2.3.3 Simulation of the Dynamic of a Turbomachine

The figure 2.13b shows the block diagram of a simulation corresponding to figure 2.13 with the same causalities. We have not shown the integration of the elements C, which allows to calculate the efforts in bonds 1, 8 and 2 in function of the flow sources Sf and the I-element.

We use the same designations as the *TUTSIM* program. *GAI* for a gain, *FNC* for any function of one variable and *MUL* a multiplication. It follows from the causality on the bond graph that the efforts P_1, T_1 and P_2 are given for block *FNC* which calculates the mass flow (equal to $\dot{m}_2$). The downstream temperature T_2 has no effect on a turbine as we have already underlined with the restrictor.

The enthalpy flow $\dot{H}_1$ is calculated by the *MUL* block in function of the specific heat at constant pressure, c_p and the mass flow $\dot{m}_1$:

$$\dot{H}_1 = \dot{m}_1 c_p T_1$$

The block *GAI* shows the heat flow $\dot{Q}_8$ in the casing of the turbine. This last one can be taken as a function of the temperature difference $(T_8 - T_1)$, where T_8 is calculated by the C-element. In the same way we have indicated that the mass flow can be a function of the rotation frequency ω_9 of a shaft especially with compressors. In the lower part of the figure 2.13, the block *FNC* gives the torque M_9 in function of ω_9 as given by the machine. The product of these two quantities, realized by the *MUL* block, gives a mechanical power $\dot{E}_9$. The output enthalpy $\dot{H}_2$ is determined according to equation 2.16.

This block diagram is valid for all thermal turbomachines, let it be turbine piston machine or compressor. Let us note, also that the flow velocities on the frontiers of the model (bond graph or block diagram) must be small because the kinetic energy must be small compared to the static enthalpy.

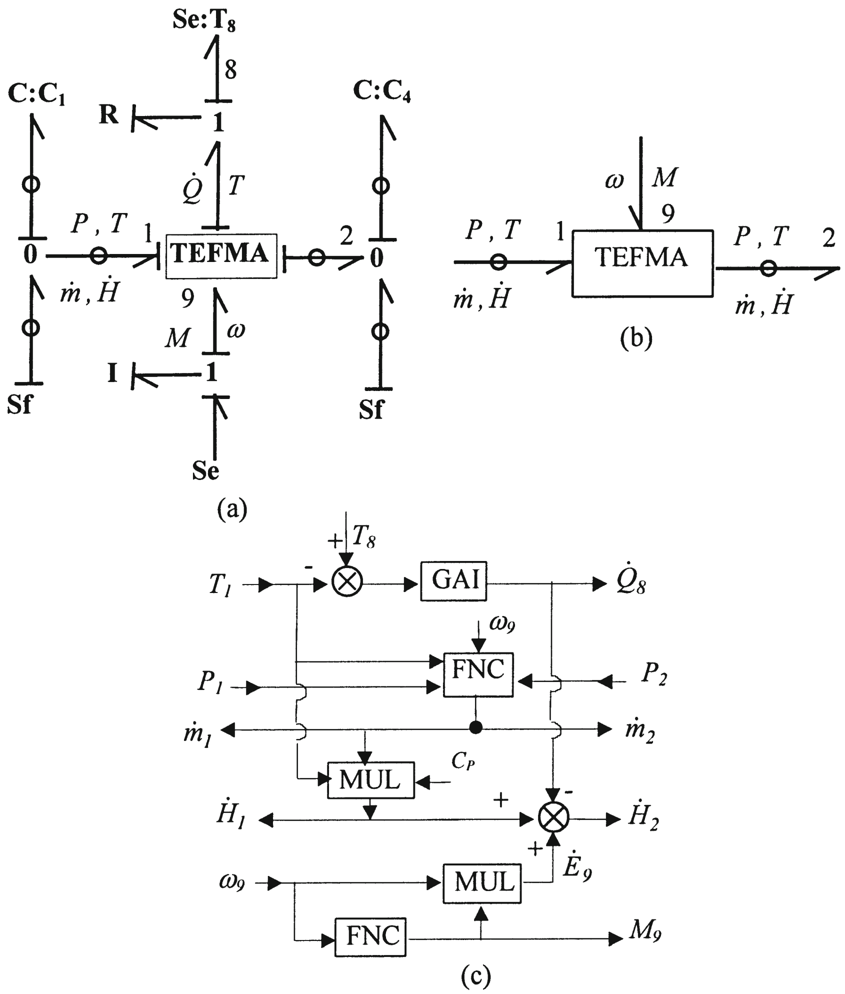

FIGURE 2.13. Simulation of turbomachine. a. bond graph model, b. TEFMA element, c. bloc diagram of simulation.

Inside the turbomachine, or other components, on the other hand, the speeds can be high as we have seen.

2.4 Hydropneumatic Accumulator

The hydraulic accumulator can be considered as an intermediary system by its hydraulic and thermodynamic elements. It is a standard component of oil hydraulics and has many applications such as the cylinders of turning railway wagons and the hydropneumatic suspension of cars.

In this last case, the working fluid is a compressible stationary gas. Let us examine such a system as represented on figure 2.14.

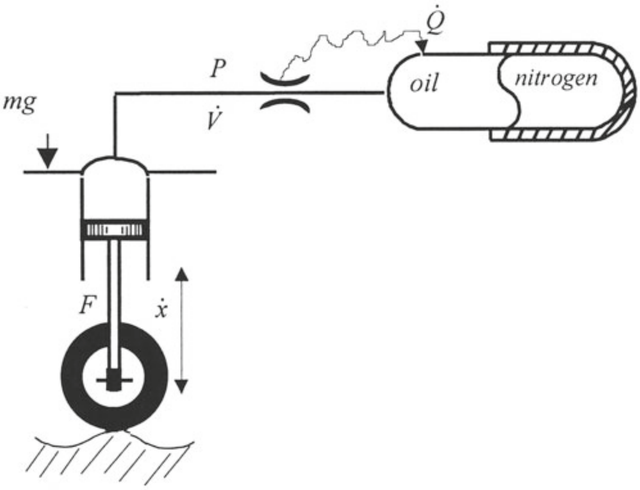

FIGURE 2.14. Hydropneumatic suspension

The vertical movement of the car in function of the road profile is transmitted to a cylinder filled with oil. This oil goes through a resistance by heating itself and produces thermal fluid $\dot{Q}$, which is evacuated for a gas accumulator, a nitrogen gas, which is compressible. There is a physical separation between oil and nitrogen in the form of an elastic membrane. Therefore the movement of the wheel is well damped by this nitrogen cushion, which replaces the springs.

The bond graph model shows this multiple energy system on figure 2.15.

The mechanical part is represented by the flow source $Sf12$ that shows the height variations of the road. The I-element showing the inertia is due to the mass of the chassis and a gravity force modelled by $Se15$.

The transformation of mechanical energy of vertical movement into hydraulic energy by a piston is modelled by the element TF. The hydraulic

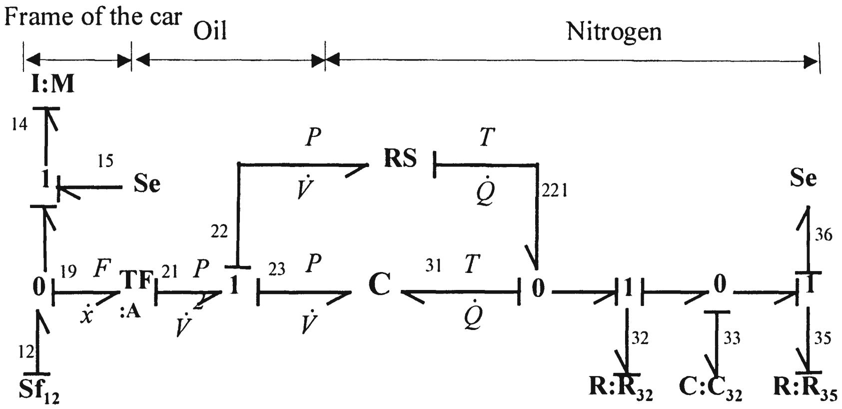

FIGURE 2.15. Bond graph model of hydropneumatic Suspension

resistance represented by the element RS has the effect of a damper and generates a heat flow $\dot{Q}_{221}$. The part of this thermal energies is accumulated by the multiport-C. This elementis consist of a true bond graph at the hydraulic side ($P_{23}, \dot{V}_{23}$) and a pseudo bond graph at the thermal side number 31 ($T_{31}, \dot{Q}_{31}$).

On the thermal side, we have R_{32} and then a partial storing in C_{33} and partial dissipation to the environment by element R_{35}. The external temperature is given by an effort source $Se36$.

2.4.1 Simulation of Hydropneumatic Suspension

The bond graph modelling with $TUTSIM$ program is given in annex B.1. The two ports C in integral causality allows to calculate the pressure and the temperature from the volume flow and the heat. The idea of the calculus consists to calculate first the hydraulic energy (work) as product of the pressure by variation of the cylinder volume (relation valid for perfect gas):

$$\dot{E} = P_{23}\dot{V}_{21} = \dot{U}_{41} \tag{2.18}$$

The internal energy U_{411} is determined by simple integration of the algebraic sum of $\dot{U}_{411}$, the heat flow $\dot{Q}_{221}$ coming from the resistance RS_{22} and the heat flow absorbed by the wall $\dot{Q}_{32}$:

$$U_{411} = \int \left(\dot{U}_{41} + \dot{Q}_{221} - \dot{Q}_{32} \right) dt \tag{2.19}$$

The temperature is determined from the thermal capacity at constant volume and the mass of the gas:

$$T_{31} = \frac{U_{411}}{mc_v} \tag{2.20}$$

Contrary to the problems with mass flow, here the mass of nitrogen is constant and it is a parameter. The pressure becomes then:

$$P_{23} = \frac{mRT_{31}}{V_{212}} = \frac{R}{c_v}\frac{U_{411}}{V_{212}} \tag{2.21}$$

R is the constant of gas and V_{212} is the effective volume:

$$V_{211} = V_0 - V_{211}$$

V_{211} shows the variation of the volume from the piston displacement and is calculated by integration of the volume flow:

$$V_{211} = \int \dot{V}_{21} dt$$

V_0 is the initial volume given by the geometric dimensions of the cylinder, $\dot{V}_{21}$ is given by the transformer TF in function of the piston cross-section and the vertical speed of the wheel $\dot{x}$ (m/s):

$$\dot{V}_{21} = A\dot{x} \tag{2.22}$$

The pressure P_{22} is calculated from the volume flow according to the expressions (2.7) or (2.8).

The differential equation for the dynamic of the thermal systems in the accumulator and the mechanical movement of the wheel are easily deducted from the bond graph of figure 2.15. It can have the following elegant form:

$$C_{33}\dot{T}_{33} + (K_{35} + K_{32})\, T_{33} = K_{32}T_{31} + K_{35}T_{36} \tag{2.23}$$

for the thermal phenomena, and

$$\dot{x}_{19} = F_{12} - \frac{1}{M}\int (AP_{21} + Se15)\, dt \tag{2.24}$$

for the frame of the car.

Let us note that $\dot{x}_{19}$ shows the relative velocity of the frame or body and the wheel:

$$\dot{x}_{19} = \dot{x}_{whell} - \dot{x}_{frame} \tag{2.25}$$

In these equations K_{32} and K_{35} represent the global coefficient of heat exchange, or thermal resistance. C_{33} is the global thermal capacity of the wall of the accumulator and I the inertia or mass of the frame of the car.

The thermal resistance is generally calculated by the following equation:

$$\frac{1}{R} = \lambda \frac{A}{L} \tag{2.26}$$

where A is the surface of the heat exchanger, λ is the coefficient of thermal conductivity and L the thickness of the wall.

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3

Modelling of Chemical Systems and Phase Change

3.1 Potential or Chemical Tension

3.1.1 Introduction

We have considered until now the modelling of thermodynamic systems with constant mass. In this chapter we shall develop the modelling of chemical and thermodynamic systems by bond graph at variable mass. Let us consider first the chemical system of just one species. The variables that describe this phase are T, S, P, V, and n. Comparing to constant mass of the first chapter we have in that case two supplementary variables: the chemical tension and the number of moles n.

We call the chemical potential the chemical tension, following a proposition of [*Falk,1976*] and [*Job,1981*]. It is almost like electrical tension, although the physical meaning is quite different. For bond graphers, it is simply an effort, and the complementary flow is the molar flow.

The internal energy accumulated by the system is described by the Gibbs equation:

$$dU = TdS - PdV + \mu dn \tag{3.1}$$

The relation 3.1 is represented on a bond graph by a multiport C as shown on figure 3.1. It has three ports : two ports associated with thermal and hydraulic power and an additional bond of the chemical power.

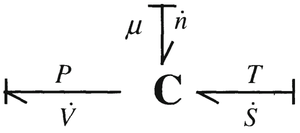


FIGURE 3.1. Bond graph model of chemical system with a variable mass

This power is the chemical tension μ as effort and the molar flow $\dot{n}$. The product is a chemical power, hence here we have a true bond graph. The molar flow is simply the normal mass flow divided by z, the molecular mass number.

In order to familiarize us let us say that the chemical tension shows the tendency of one chemical constituent to become larger or more important.

As Job [1981] argues, chemical tension is not a complicated concept, derived from the free enthalpy (see equation 3.5), but quite simple and defined by equation (3.1) and (3.2). It increases with pressure and decreases with temperature (equations 3.6) and always increases with concentration of a chemical substance.

In order to distinguish the chemical tension from the pressure let us examine the movement of a fictive piston, which presses on a chemical substance in a cylinder (Fig 3.2). The pressure P will act on the piston and tends to displace it entirely, whilst the chemical tension will penetrate the fluid or the substance in the interstices (pores of the permeable piston). This is to say in the space between the molecules. Nevertheless there is a little layer on the surface, where the fluid adheres by surface tension. In thermodynamics, the pressure has as prime consequence a variation of volume and the temperature a variation of entropy. The chemical tension is associated in chemistry to the transfer of matter. The electric tension is associated to the transfer of electrons.

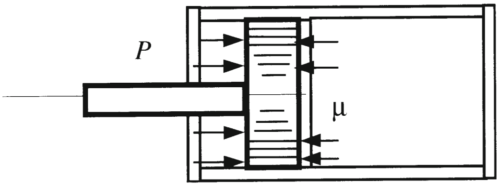


FIGURE 3.2. Schematic of a piston pressing on a chemical substance

There is a similarity between pressure and chemical tension, In particular if the pressure becomes larger, the chemical tension becomes larger as well. On the other hand, contrary to the pressure the chemical tension becomes less with increasing temperature, as we shall demonstrate further on (equation 3.6).

To repeat, the chemical tension is a fundamental quantity of physics and chemistry, although many authors will not recognize it as such. According to the bond graph of figure 3.1, it depends on the molar mass n, on the volume V and on the entropy S. Therefore the chemical tension at constant entropy and volume is:

$$\mu = \left(\frac{\partial U(S,V,n)}{\partial n} \right)_{S,V} \tag{3.2}$$

The chemical tension is influenced by the presence of other substances, in addition to the influence of pressure and temperature. In this sense the chemical tension of one substance depends on the concentration of another substance present.

$$\mu_1 = \mu_1(T, V, n_1, n_2) \tag{3.3}$$

As said, the influence goes in the sense of a decrease of chemical tension by the presence of other substances. For instance the chemical tension of water is decreased by a dissolved salt, which is very important for the osmosis, as we shall see in chapter 3.4. The bond graph model of one phase with two chemical species at variable composition is given by the figure 3.3. The multiport C is associated to the accumulation of energy as given by :

$$dU = TdS - PdV + \sum_{i=1}^{2} \mu_i \dot{n}_i$$

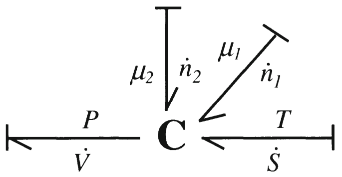


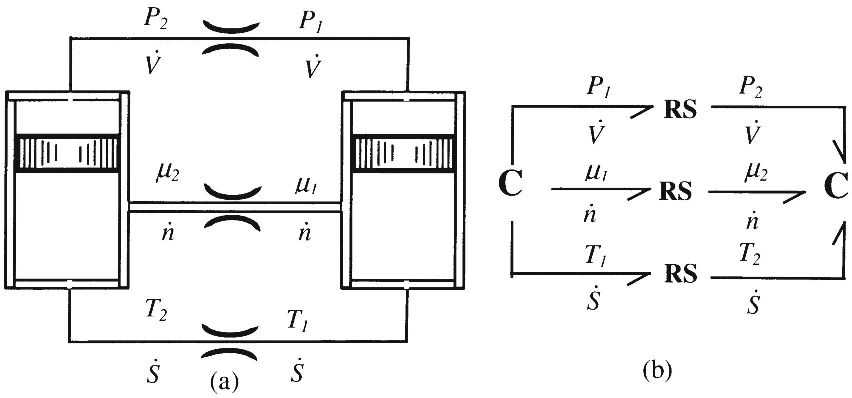
FIGURE 3.3. Bond graph of a chemical two phases system with variable mass

The chemical tension is a fundamental quantity of physics and it is present in many different phenomena [*Job 1981]*. We consider by definition that for a homogeneous mixture, the chemical tension of one constituent equal to free enthalpy divided by quantity of matter. In the system *S.I.* it is therefore expresses in *Joule/Mole*. Its units is called the Gibbs (G) proposed by Wiberg [*Wiberg, 1972*] We have therefore:
The unit kiloGibbs (kG) gives very comfortable values [*Job, 1981*].

3.1.2 Chemical Thermal and Hydraulic Equilibrium

In order to establish an analogy with other energy domains let us consider the exchange of energy between two different substances which are contained in two cylinders (Fig 3.4]. Between the two cylinders, there are three different exchanges.

1. Exchange of volume flow under the influence of pressure, by the upper bond. If pressures are equal, we have hydraulic equilibrium.
2. Exchange of chemical species or substance, that is a chemical reaction, indicated by the middle bond. It is obtained when the chemical tensions are equal and is chemical equilibrium.



(a)

(b)

FIGURE 3.4. Thermal, hydraulic and chemical equilibrium in two cylinders containing different substances. a. Schematic, b. Bond graph model

3. Exchange of heat by thermal contact in the lower bond. This is the thermal bond with ceases when the temperatures are equal. So it is thermal equilibrium.

So we have the three conditions of equilibrium: hydraulic, chemical and thermal. The two cylinders come to complete equilibrium or rest only when all the appropriate efforts are equal. An example is the equilibrium between water and vapour, usually called steam in turbine practice. Here pressure and temperatures are equal by contact, and the chemical equilibrium is given by the equality of chemical tensions.

The difference between chemical tension is also the origin of the dynamics of chemical reactions. Further, the chemical tension in each phase in a chemical system depends on pressure and temperature and further on the concentration of the other substances. All chemical reactions can produce themselves in one direction or the other direction, depending on temperature and pressure. As said, [J*ob,1981*], we can describe the chemical reactions and their dependence on the temperature as the interaction of chemical potential and this without looking on the deep nature of the phenomena of this reaction. It is also a good way to teach chemistry in secondary schools.

3.1.3 Properties of Chemical Tension

We take the expression of free enthalpy in order to study the properties of chemical tension.

$$G(P,T) = U - TS + PV$$

If we keep the pressure P and the temperature T constant we have

$$\mu = \frac{\partial G(P,T,n)}{\partial n} \tag{3.4}$$

The condition of homogeneity of substances shows that certain physical quantities are proportional to their molar mass. These variables are called extensive variables and the enthalpy is one of them. We remind that the extensive variables are proportional to the substance while, on the contrary, the intensive variables are independent of the amount of substance (there is also substances, which are neither extensive nor intensive like the pressures). The transmitted energy is always the product of an intensive variable multiplied by the differential of an extensive variable. With the density of enthalpy g we have then:

$$G(P,T,n) = ng(P,T)$$

Combining this expression and from (3.4) we obtain:

$$\mu = \frac{dng(P,T)}{dn} = g(P,T) \tag{3.5}$$

The chemical tension is the derivative of the free enthalpy with respect to molar mass only if pressure and temperature are constant. This is true at least for homogeneous substances. Under these conditions, the chemical tension is equal to the free enthalpy by unit of mass. Many chemical engineers confound the notions of chemical tension (potential) and enthalpy density and publish tables of free enthalpy density, also called Gibbs free energy. For more details let us recommend the Job [1981].

In introducing the molar density of energy $u = U/n$, of entropy $s = S/n$ and the volume density $v = V/n$ one can write:

$$\mu = u - Ts + Pv = h - Ts = \frac{G}{n} = g$$

where we have for the density of enthalpy $h = H/n$. From this last equation we can deduce:

$$\begin{aligned} \left(\frac{\partial \mu}{\partial T}\right)_{(P,V)} &= -s \\ \frac{\partial \mu}{\partial P}_{(T,S)} &= v \end{aligned} \tag{3.6}$$

Since the variables entropy per mole and volume per mole are positive, the chemical tension increases with the volume and decrease with the temperature. In this way our qualitative remarks on the dependence of chemical tensions of the temperature and the pressure are substantiated.

$$\begin{aligned} \frac{\partial \mu}{\partial T} &< 0 \\ \frac{\partial \mu}{\partial P} &> 0 \end{aligned}$$

3.1.4 Constitutive Equations for Gas and Liquids

Let us determine the dependence of chemical tension from the pressure and the temperature. For gases and liquids one determines first the entropy from the global specific heat C_p

$$S(T,P) - S(T_{ref},P_{ref}) = \int_{T_{ref}}^{T} \frac{C_p}{T} dT = C_p \ln \frac{T}{T_{ref}} \tag{3.7}$$

By inserting (3.7) in equation (3.6) one obtains

$$\mu(T,P) - \mu_{ref}(T_{ref},P_{ref}) + \int_{T_{ref}}^{T} \frac{C_p}{T} \ln \frac{T}{T_{ref}} dT - S = C_p \ln \frac{T}{T_{ref}} \tag{3.8}$$

In this case the variable $S(Tref, P_{ref})$, the reference entropy is important. Now we must distinguish between gas and liquid as follows

1. For a gas we have

$$\frac{\partial \mu(T,p)}{\partial V} = v = \frac{V}{n} = \frac{R(T+T_{ref})}{P} \tag{3.9}$$

By integrating we obtain:

$$\mu_{gaz}(T,P) - \mu_{gaz}(T,P_{ref}) = \int_{P_{ref}}^{P} R(T+T_{ref}) \frac{dP}{P} = R(T+T_{ref}) \ln \frac{P}{P_{ref}} \tag{3.10}$$

2. For the liquids, equation (3.6) remains valid. The influence of temperature on the chemical tension is given by the specific entropy. The influence of pressure on the chemical tension is given by the specific volume, which is practically constant, because the compressibility of liquids is very small. So we obtain:

$$\frac{\partial \mu(T,P)}{\partial P} = v = cste$$

from which one has:

$$\mu_{liq}(T,P) - \mu_{liq}(T,P_{ref}) = v(P - P_{ref}) \tag{3.11}$$

Since v is generally small for the liquid (water) compared to gases, one can neglect the dependence of the pressure. One admits therefore, that the chemical tension of the liquid is independent of pressure.

3.2 Coupled Powers and Entropy Stripping

In order to analyse the mass transfer caused by chemical tension, let us look at the communication between two substances contained in two cylinders through a membrane. The main action comes from the movement of the pistons. (Fig 3.5).

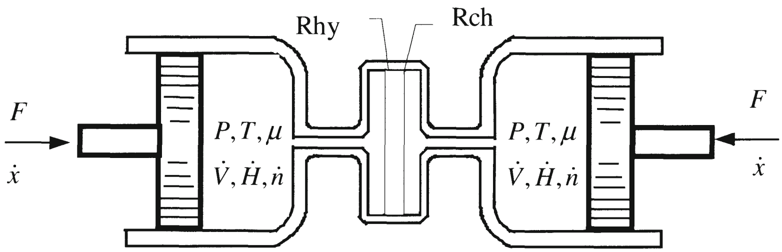


FIGURE 3.5. Two substances communicating through a membrane pushed by the pistons

The membrane is characterized by a chemical resistance R_{ch} sensible to the chemical tensions and by a hydraulic resistance R_{hy} sensible to the pressure difference. In practice the chemical resistance will be in preponderance if the diameter of the pores of the membrane is less than $10nm$. We see that the schema is similar to figure 2.1 but we have on more energy, the chemical energy. It drives fluid through an extra resistor, the chemical R.

The corresponding bond graph model is represented by figure 3.6.

The power bonds are coupled by the pairs of variables $(P, V.)$, $(T, U.)$ and $(\mu, \dot{n})$ which belong respectively the hydraulic, thermal and chemical power. We will mention later the choice of variable effort and the simulation in function of the DOF of the system. Let us note that on the piston faces

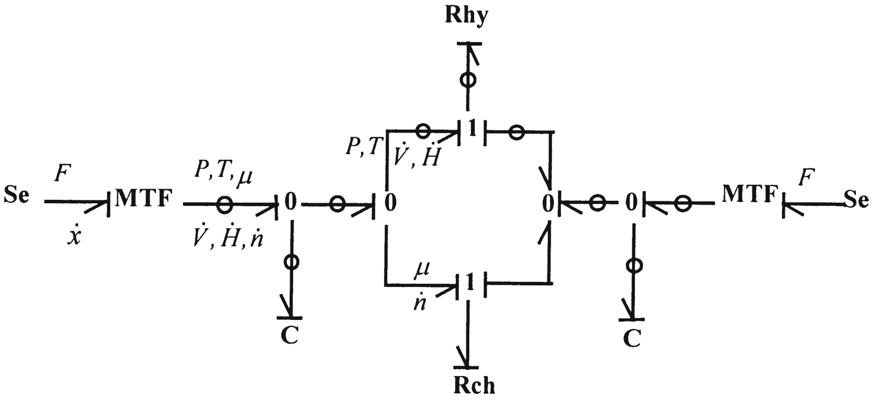


FIGURE 3.6. Bond graph model with chemical and hydraulic

the chemical tension is also acting, but has no effect since the pistons are supposed without pores.

In order to conform to chemical literature, we replace the mass flow by the molar flow; these variables are connected by $\dot{n} = \dot{m}/z$, where z is the molar mass.

Let us study now more in detail the phenomena of change of entropy and of volume change which will be produced by mass transfer from phase 1 to phase 2 on figure 3.5 and 3.6. The bond graph model is given by figure 3.7 and the system is subject to two effort sources, of pressure and of temperature.

The transformers TF are modulated by the densities of entropy s and volume v. Like all transformers they have equations between two efforts and two flows. In our case they are:

$$\begin{aligned} P_4 &= vP_3 \\ T_9 &= sT_8 \\ \dot{V}_3 &= v\dot{V}_4 \end{aligned} \tag{3.12}$$

The parameters of the transformers are entropy density s and specific volume v. They allow also passing from the flux of entropy or volume to the molar flux by the following relations:

$$\begin{aligned} \dot{S}_8 &= s\dot{n}_{10} \\ \dot{V}_3 &= v\dot{n}_{10} \end{aligned} \tag{3.13}$$

In general in the physical chemistry, the variables s and v are expressed by the partial derivatives as follows:

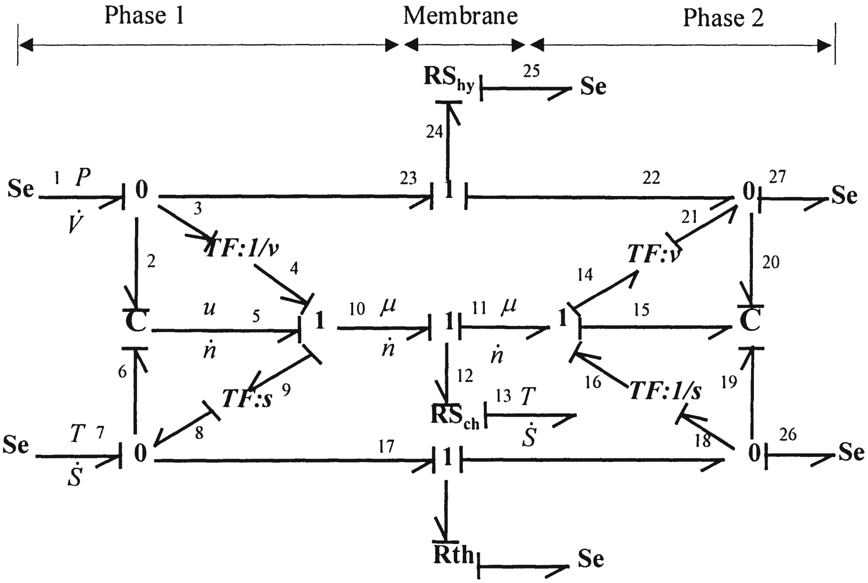


FIGURE 3.7. Bond graph of mass exchange between two substanc

$$s = \frac{\partial S(P,T,n)}{\partial n}$$

$$v = \frac{\partial V(P,T,n)}{\partial n}$$

The transformers at the left of figure 3.7 have two functions.

1. The constitutive equations of the series junctions shows that entropy and volume are taken away their bonds and consequently are not going the chemical resistance. Then, they are any way added again on the other (right) side of the bond graph. This state is obtained by the flow relations of the transformer, equation (3.13). Let us note the flow in the bond 8 is the flow entropy, but the parameter of the transformer changes it into the chemical flow.

2. The effort equation of the transformers show the transition between the internal energy per mole ($u = U/n$) and the chemical tension. based on relations (3.12), the constutive equation of parallel junction 1 gives:

$$\mu_{10} = u_5 - sT_8 + vP_3 \tag{3.14}$$

The transformers at the right side of figure 3.7 have exactly the same function in reverse. The relation (3.14) is a transformation of Legendre and represented by the transformers. The series junction 4, 5, 9 and 10 on figure 3.7 assures the equality of flows and the passage from internal energy per mass to chemical tension. Furthermore, the entropy from the disappearing phase 1, will go through the bonds 9, 8 and 17 towards the phase 2 via the further bonds 18, 19 and 16 where it is needed to produce the structural entropy in phase 2. Any excess or deficit is taken from the entropy generated by chemical friction.

If there is a no variation of temperature, the entropy in the multiport C changes only trough bond 8. If there is variation, it changes also through the conduction bond 6. Consequently at constant temperature the conduction bonds transport no flow.

The relation 3.14 shows an interesting natural phenomena which we explain as follows : the chemical tension which generates the change of mass depends on the internal molecular energy U. To this one must added the hydrostatic pressure vP. Further, and this is important, one must deduct the term Ts from the internal energy; this signifies that the entropy S accumulated in one phase reduces the chemical tension and consequently the force, which pushes the substance to change its phase. We must note in particular, the term Ts which must be deducted, or stripped, from the internal energy U. We call this effect “entropy stripping“ [*Thoma, 1977*].

In bond graph, entropy and the volume are stripped by the transformer on thermal and hydraulic side. Then, only the chemical tension is responsible for the running of the reaction or generally the transformation of matter. On the right side of the bond graph, these two variables must be recovered again, we speak then of “unstripping “. We call this entire proceeding the entropy stripping or, with humour the striptease of entropy.

In the spirit defined by our introduction we accept this as a natural law, discovered by Gibbs at the end of the 19th century. What this law has in common with a cabaret show is as follows: the matter behaves like a striptease girl, before dancing she must first get rid of the entropy Ts in the phase 1 and take the hydraulic energy PV. After the dance, she takes the necessary entropy Ts, and releases the volume before leaving.

In order to fix the ideas, let us cite as example the boiling of water or the condensation of steam. In condensing in particular, that is in changing the phase, the vapour must first get rid of the heat and entropy of evaporation. This is called the latent heat and entropy of evaporation. The example will be treated below.

Let us note that if the dimensions or diameter of the pores of the membrane are small, the equilibrium is established by the equality on chemical tensions. On the other hand, if they are large, the equilibrium is established by the equality of pressures. These two conditions introduce in general a contradiction, which conducts to the enigma of osmosis, treated in section 3.4.

In principle the stripping and the transformers would not be necessary and could be absorbed in the multiport C. Nevertheless, it is useful in practice to leave them to show the entropy flow coupled with the mass flow. In this way the temperature will stay constant if one takes the entropy away from the external source. The vertical bonds of conduction will become active only if one changes the source adjustment.

The detailed reticulation of the figure 3.7 shows therefore the entropy stripping and it is important for the osmosis and the chemical reactions. Sometimes one uses a more compact notation as shown on figure 3.8.

On figure 3.8, the transformers and the series junctions are replaced by the word coupler or "coupl", but the causalities will not change. They produce no entropy. All the irreversibilities reside in the resistance R_{hy} and R_{ch}. We use this compact representation in the future. Sometimes even, the couplers can be neglected, but this is an approximation that must be justified because entropy stripping is always there in the chemical resistance. The hydraulic resistance on the other hand, does not know entropy stripping and is subject only to pressure.

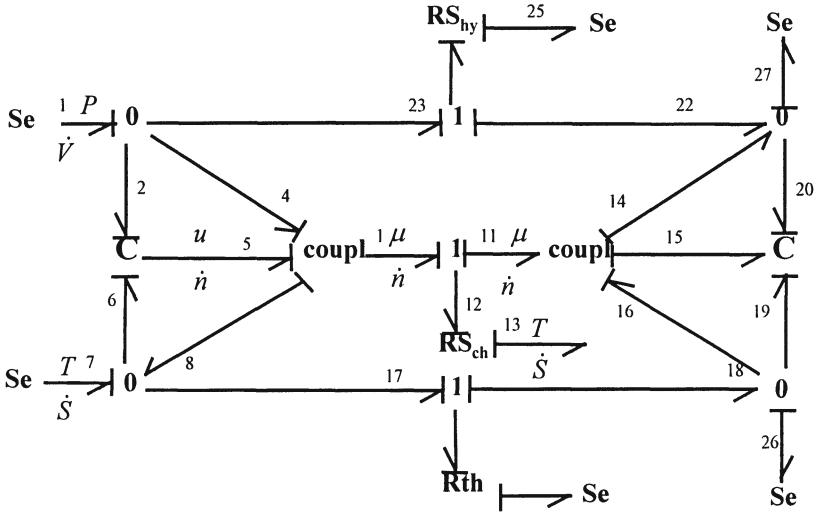


FIGURE 3.8. The transformers and the series junctions are replaced by the word coupler or "coupl"

Let us note that the process of entropy stripping is perfectly reversible and generates no entropy, as indicated by the transformers and the junctions. Only the resistances are irreversible, that is with generation of entropy.

The chemical processes are thus characterized by two resistances.

1. The hydraulic resistance which is sensible to the pressure and entrains

entropy and volume.

2. The chemical resistance which is sensible only to chemical tension and where entropy and volume are stripped.

As said, these concepts will be applied further on the phenomena of osmosis and the chemical reactions.

3.3 Chemical RC Circuit and Phase Change

3.3.1 Analogy between Electric and Chemical Circuit

For the study of chemical reactions we introduce firstly the analogy with electrical circuits. The figure 3.9 a represents a simple electric circuit with a resistance R and two condensers C. The capacity of one condenser is variable, by variation of the distance between the plates.

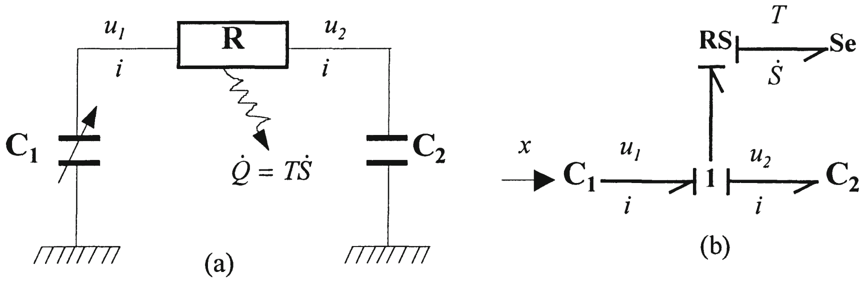


FIGURE 3.9. Electric circuit with variable capacitor. a. schema, b. Bond graph

The electric system is in equilibrium when both voltages of the capacitors are equal which means that no current flows through the resistor. This state is analogous in chemistry by the equality of chemical tensions. In electricity (like in chemistry), if the voltages are not equal, a current will flow from the higher to the lower voltage. The corresponding power $\dot{Q} = i\,(u_1 - u_2) = T\dot{S}$ is dissipated as heat in the resistance R, as indicated by the arrow in "zigzag".

The corresponding bond graph appears on figure 3.9b. The electric resistance becomes a multiport RS that generates a flow of entropy. If we change the capacity of the condenser C_1, this will give a variation of voltage and consequently a perturbation of the electric equilibrium. This generates an electric current, which produces again heat. As an example, if one increases the capacity of C_1 (by approaching the plates), the tension u_1 diminishes and the current circulates from C_2 to C_1. The dissipation of energy is always positive and produces heat according to the equation of Carnot. Let us remind that power flow out of the resistor is irreversible which is one aspect of the second law of thermodynamics: Dissipation is always positive.

We now consider a similar chemical circuit shown on figure.3.10. It represents a chemical reaction between two substances contained by two recipients and acting on each other by the intermediary of a membrane. A variable pressure P allows instead the separation of electric plates, the change the capacity and therefore the chemical tension without varying the molar flow. The molar flow $\dot{n}$ that through the membrane takes the role of a resistor with dissipation. The molar flow is analogue to the electric current. The bond graph model is shown on figure. 3.10b.

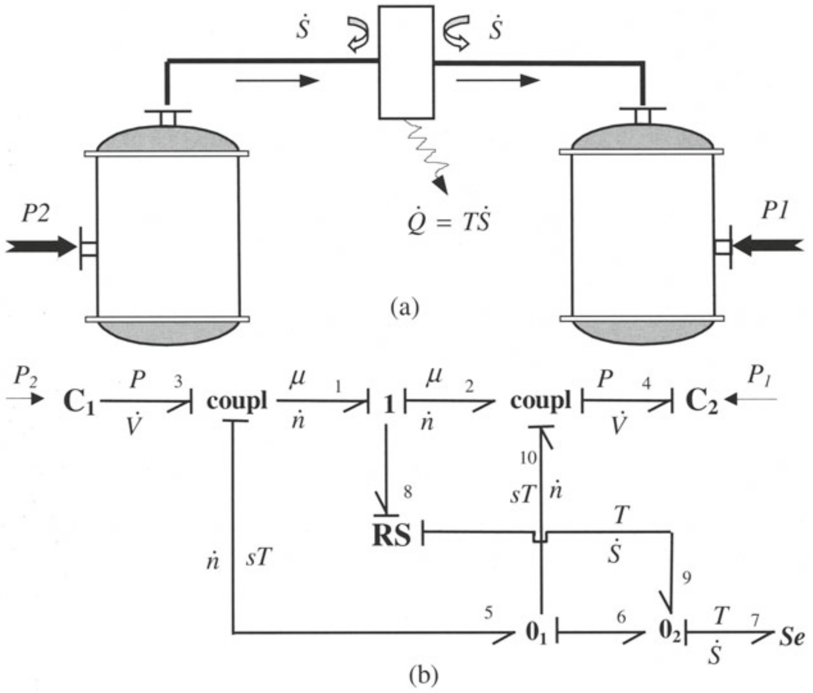


FIGURE 3.10. Chemical RC circuit. a. Schematic with two tanks for reactants and products, b. Bond graph with coupler

The difference between electric and chemical case is the entropy stripping of the reactants and the unstrippng of the products. There exist consequently the couplers introduced in section 3.2 shown by the curved arrows in the schematic on figure 3.10a and by the word "coupl" on the bond graph 3.10. So on this figure we have stripped entropy in bond 5, then unstripped in bond 10. The excess is added to the dissipated entropy in bond 9.

Consequently we have structural entropy and entropy of dissipation. The difference of stripped entropy of reactants and products is called the structural entropy of the reaction. From equation (3.12) and (3.13) we have for it and the corresponding energy.

$$\begin{aligned}\dot{S}_{strip} &= \dot{n}\,(s_5 - S_{10}) \\ \dot{E} &= \dot{n}T\,(s_5 - S_{10})\end{aligned} \tag{3.15}$$

Structural Entropy, Enthalpy of Reaction and Endothermic and Exothermic Reactions

The structural entropy can be positive or negative and is given together with the entropy from dissipation to the environment. Naturally, the dissipation is always positive. So there we have two entropy currents which are entirely different:

1. The net structural entropy of the chemical reactions which can be positive or negative.
2. The resulting entropy from the dissipation in the resistance which is always positive.

The dissipation is always given as

$$\dot{E}_{dis} = \dot{n}\,(\mu_1 - \mu_2) = T\dot{S}_{gen} = \dot{Q}_{gen} \tag{3.16}$$

where $\dot{S}_{gen}$ and $\dot{Q}_{gen}$ generate respectively the entropy and the generated heat.

The sum of these two components multiplied by the absolute temperature corresponds to the enthalpy flow of the reaction:

$$\begin{aligned}&\dot{E}_{strip} + \dot{E}_{dis} = \dot{n}\,(h_1 - h_2) \\ &\text{where: } h = \mu + sT\end{aligned} \tag{3.17}$$

From the enthalpy flow of the reaction we obtain by time integration the enthalpy of reaction.

The entropy of the final product depends on the temperature, because those products behave like a multiport C. Following a suggestion of Wiberg [*Wiberg,1972*], we can compare the entropy capacity to a glass filled with entropy until a certain level. This level represents the temperature. By the chemical reaction, the dimension of the glass changes, its diameter increases in the case of endothermic reaction. It is then necessary to supply from the environment some entropy in order to maintain the constant level or temperature. If this is prevented, the temperature decreases. Thus in chemical reactions, the entropy capacity of the products may be larger, and the temperature becomes lower. This augmentation of capacity is the reason why certain reactions produce a cold that is they are endothermic. This is the case as long as the entropy produced by the dissipation, carried by bond 9 of figure.3.10b is not sufficient to produce the deficit of structural entropy. Then, as we have said, the reaction is endothermic.

Nevertheless the majority of chemical reactions produce entropy at constant temperature, which must be transmitted to the environment. One says then that they are exothermic.

Let us return to the chemical circuit of figure.3.10a. If one establishes a contact between both tanks, the equilibrium will establish itself by the equality of chemical tensions. The entropy stripping of the reactants does first supply the needs of unstripping of the product (parallel junction 5, 6 and 10). Then what is left will be combined with the dissipation entropy (bond 9) in the parallel junction at end. This gives, as we have said, the enthalpy of reaction.

3.3.2 Evaporation of Water in a Boiler

Modelling byTrue Bond Graph

The evaporation of water can be considered as a chemical reaction. We have really a change of phase: the liquid phase disappears and the vapour phase appears; it is a gas. The chemical tension is the important parameter in this proceeding. In particular, in the equilibrium of water with vapour, there is the equality of chemical tension. If this equality or equilibrium is disturbed, for instance by more heat in the water, its chemical tension of water increases and the evaporation will start again.

On figure 3.11a we have the process of evaporation of water in a boiler heated by the external source $\dot{Q}_{ex}$. This is a true bond graph, only the two couplers of figure. 3.8 are combined in one. Also, the pipes for water and for vapour are not represented. We have therefore a closed tank with the equilibrium water vapour, heated by an external source. Later we show that with the conduits a pseudo bond graph is simpler.

In true bond graphs, the condition of equilibrium between the phases of vapour and of liquid is that the variation $d\mu_1$ and $d\mu_2$ of the chemical tensions should be equal. Knowing that:

$$\begin{aligned} d\mu_1 &= -S_1 dT + V_1 dP \\ d\mu 2 &= -S_2 dT + V_2 dP \end{aligned} \tag{3.18}$$

we have the following condition of equilibrium

$$\frac{dT}{dP} = \frac{V_2 - V_1}{S_2 - S_1} \tag{3.19}$$

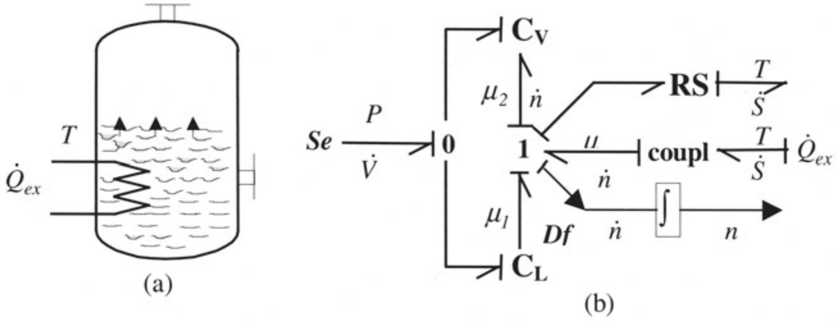


FIGURE 3.11. Modeling of the Process of Evaporation in a boiler. a. Schema, b. True bond graph model

This allows calculating the temperature in function of the pressure of vapour or steam and is known as the equation of Clausius Clapeyron. Next we consider that the volume per mass of the water is negligible compared to that vapour and the vapour as an ideal gas ($V_2 = RT/P$). Then with the evaporation (latent) entropy and heat $L = T(S_2 - S_1)$ one obtains as differential equation for the temperature as function of pressure

$$\frac{dT}{dP} = \frac{RT^2}{LP} \tag{3.20}$$

Integration of (3.20) gives:

$$\log \frac{P}{P_0} = \frac{L}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)$$

The couplers of figure.3.11 control the evaporation

$$\dot{n}\,(s_2 - s_1)\,T = \dot{Q}_{ev} = T\dot{S}_{ev} \tag{3.21}$$

where $s_2 - s_1$, the specific entropy of evaporation is calculated by following equation:

$$s_2 - s_1 = \frac{L}{T}$$

Also the expression 3.21 contains the evaporation enthalpy, but a part of the introduced heat will be transformed into mechanical energy because at constant pressure one has

$$dQ = Tds = du + Pdv = d(u + Pv) = dh$$

As already said, one uses normally the expression “latent“ heat L of evaporation which is important in phase change. It is defined by the quantity of heat that should be supplied to the mass of $1kg$ of liquid , at a pressure P and a temperature of saturation T, for transforming it completely into vapour; it depends on temperature and pressure.

Let us remind that to bring $1kg$ of water to the saturated temperature T_s is

$$H_{LS} = C_p T_S \tag{3.22}$$

as measured from zero$°C$ (the temperature and pressure reference, Sec 1.8.2). The enthalpy of saturated vapour H_{VS} is the sum of the enthalpy of water and of the latent heat:

$$H_{VS} = H_{LS} + L \tag{3.23}$$

For superheat, one requires another quantity of heat H_{SUR} by the equation:

$$H_{SUR} = \int_{T_S}^{T} C_{ps} dt \tag{3.24}$$

where C_{ps} is a specific heat of the superheated steam. Strictly, it is a function of the temperature but the dependence is often neglected.

We have here the three equilibrium conditions:

1. the equilibrium of pressure assured by the movement of the surface of the water,
2. the equilibrium temperature between both phases and influenced by an external source $\dot{Q}_{ex}$ which maintains the boiling temperature constant,
3. and the chemical equilibrium assured by the equal chemical tensions of water and vapour.

For this last point let us note, that to each temperature corresponds a certain saturation pressure. If the external pressure is below the saturation pressure there will be formation of vapour until this pressure is attained or until all the water is transformed in vapour.

As long as there is simultaneously water and vapour, for each temperature corresponds a certain pressure independent of the volume of water and vapour. Reciprocally, for each pressure there is a certain temperature, which has nothing to do with an external entropy flow. When the external pressure corresponds to atmospheric, the evaporation takes place at $100°C$ or $373K$ and takes the name of boiling. The proceeding of a boiling is described by the ensemble of the characteristics which given as "thermodynamic tables" in all specialized textbooks. The heated water goes then from the liquid to the dry vapour state. Between the two states, we have a mixture of liquid and vapour: it is called saturated humid vapour. The saturated humid vapour is defined by the quality or mixture ratio X. Hence the mass of $1kg$ of mixture with the quality X contains $(1-X)kg$ of liquid and Xkg of gas. The specific volume ν_M and the specific enthalpy h_M of the mixture are calculated as follows:

$$\begin{cases} \nu_M = (1-X)\nu_L + X\nu_V \\ h_M = (1-X)h_L + Xh_V \end{cases} \tag{3.25}$$

where ν_V, ν_L, h_L and h_V are respectively specific volume and the specific enthalpy of the vapour and liquid. Let us repeat that with $X = 0$ we are in the liquid state and with $X = 1$ we have only saturated dry vapour usually called dry steam. Equation (3.25) is very important for the simulation of mixtures of two phases as we shall see later.

Returning to the bond graph of 3.11b, a detector of flow Df delivers an information-bond to calculate a water quantity remaining by integration of the molar flow.

The reticulation of a evaporation system with a true bond graph, that is with the power variables $(T, \dot{S})$, $(P, \dot{V})$ and $(\mu, \dot{n})$ allows to model phase change but does not include the power in the mass flow on entrance and exit of the boiler. These bonds carry both mass flow and enthalpy flow and consequently a pseudo-bond graph is preferable. To repeat, the pseudo-bond graphs show better the phenomena with entering and leaving water and steam. We have nevertheless wanted to show the model with a true bond graph for establishing a connection between evaporation and chemical reaction.

Evaporation of two Phases by Pseudo-Bond graph

1. Vapour as Real Gas

The reticulation of a steam boiler by pseudo bond graphs is more comfortable, using pressure and temperature as efforts and mass flow and enthalpy flow as flows. The reason is mainly that they obey more simple conservation principles.

The evaporation process in a boiler feed by water is reticulated by a pseudo-bond graph (figure.3.12). We consider the precise case where the phases of water and of vapour are completely separated.

The storage and dissipation of energy in the system are represented by the coupled bonds of thermal energy $(h, \dot{H})$ and hydraulic $(P, \dot{m})$. The

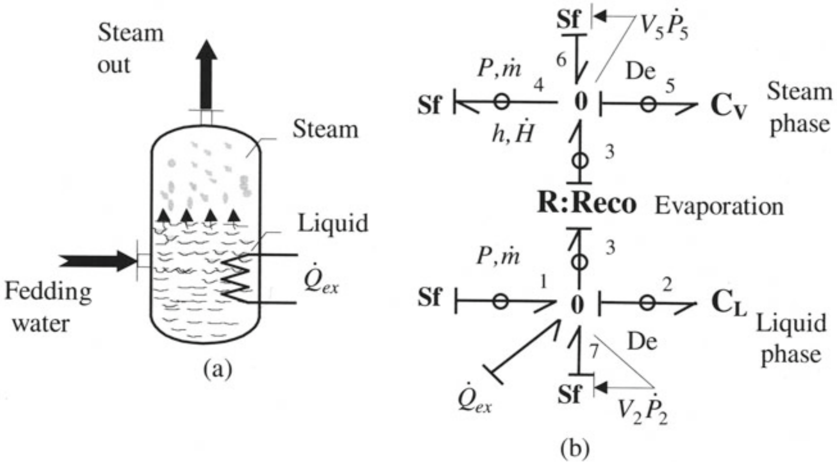


FIGURE 3.12. Bond graph model of evaporation process. a. Evaporation in a boiler, b. Bond graph model (vapour as real gas)

two phases of water and vapour are connected by the multiport $R : Reco$, which represents the entire evaporation. The phases vapour and water are respectively shown by the multiport C_V and C_L which associate the storage of thermal energy and hydraulic energy in their phases.

The quantities of mass and enthalpy m_2, H_2, m_5 and H_5 refer respectively to the vapour and water phase. They follow from the constitutive equations of the multiports C_V and C_L in integral causality:

$$
\begin{aligned}
m_2 &= \int (\dot{m}_1 - \dot{m}_3)\, dt \\
H_2 &= \int \left(V_L \dot{P}_2 + \dot{Q}_{ex} - \dot{H}_3 \right) dt \\
m_5 &= \int (\dot{m}_3 - \dot{m}_4)\, dt \\
H_2 &= \int \left(V_V \dot{P}_5 + \dot{H}_3 - \dot{H}_4 \right) dt
\end{aligned}
\tag{3.26}
$$

The efforts specific enthalpy of steam h_2 and of liquid h_5 are calculated in function of accumulated enthalpy H and mass m:

$$
\begin{aligned}
h_2 &= \frac{H_2}{m_2} \\
h_5 &= \frac{H_5}{m_5}
\end{aligned}
$$

The vapour comes out with the same enthalpy as the stored vapour and we can write then that:

$$\dot{H}_4 = \dot{m}_4 h_5$$

The flow sources Sf on bonds 6 $V_5\dot{P}_5$ and 7 $V_2\dot{P}_2$ represent the mechanical energy of pressurization due to the variation of those pressures. The flow sources are calculated by an information bond on the pressure P given by effort detector De and appear if one chooses enthalpy flow instead of the internal energy, as we shall see in chapter 4. V_L and V_V are the volumes occupied by liquid and vapour, respectively. In this way the volume of the vapour will be determined from vapour density ρ_V and mass occupied by the vapour m_2 and the volume of liquid is deduced from geometric volume of the boiler V_C :

$$\begin{aligned} V_V &= \frac{m_2}{\rho_V} \\ V_L &= V_C - V_V \end{aligned} \tag{3.27}$$

The vapour density ρ_V is easily determined from thermodynamic table in function of vapour pressure or enthalpy [*Ordys 1994*].

At the interface the liquid will come to evaporation, modelled by an resistive element $R : Reco$. The constitutive equation of this multiport, which associates evaporation and dissipation of energy are empiric [*Ordys 1994*]:

$$\begin{aligned} \dot{m}_3 &= K_{ev}\left(P_2 - P_5\right) \\ \dot{H}_3 &= \dot{m}_3\left(h_2 - h_5\right) = \dot{m}_3 L \end{aligned} \tag{3.28}$$

Let us consider that the evaporated mass flow $\dot{m}_3$ is proportional to the difference between the pressures (or temperatures) of the liquid phase P_2 and the vapour phase P_5., where the coefficient of proportionality K_{ev} is determined by experience. While the mixture is under saturation, the pressure P_2 and P_5 are calculated from tables or thermodynamic functions. The flow of enthalpy $\dot{H}_3$ equals the mass flow $\dot{m}_3$ times the latent heat of evaporation L, where $L = h_2 - h_5$.

The block diagram of the model is shown on figure.3.13. Let us remind in the equation that H and h designate respectively the total enthalpy in *Joules* and the specific enthalpy *Joule/kg*. The quantities H_{20}, m_{20}, H_{50} and m_{50} are the initial conditions.

2. Vapour as ideal Gas

We have supposed that the vapour in the superior part of the boiler behaves like an ideal gas. As said, we uses the ideal gas laws to determine the steam pressure:

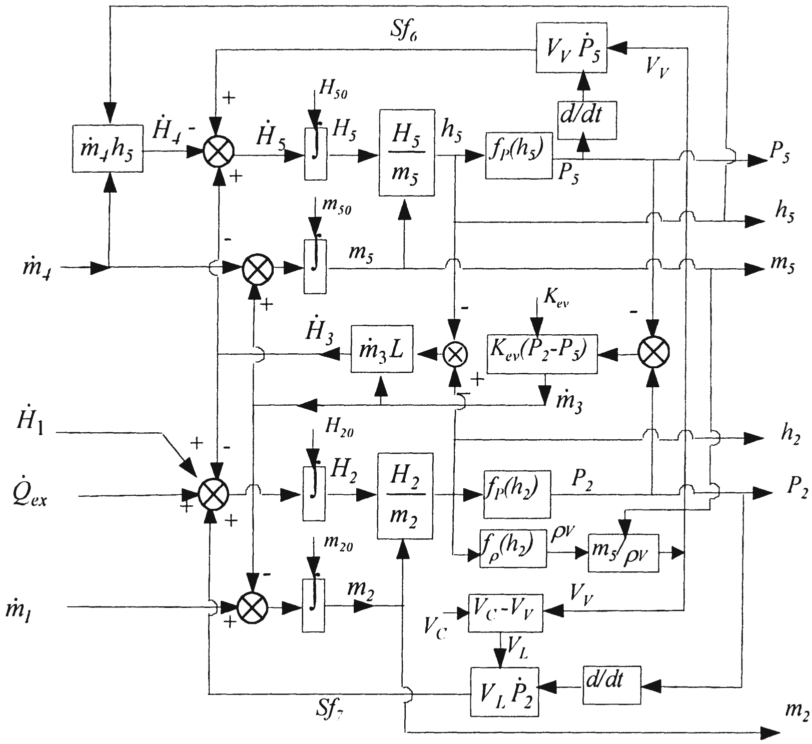


FIGURE 3.13. Block diagram of the simulation of evaporation in two phases

$$P_5 = m_5 \frac{RT_5}{V_V} = \frac{R}{c_v} \frac{U}{V_V}$$
$$T = \frac{U}{m_5 c_v} \tag{3.29}$$

with R the gas constant, U the internal energy and c_v the specific heat at constant volume.

These simplifications introduce some simulation problems:

- c_v is not constant and must be calculated in function of the temperature,
- selecting for power variable the internal energy U (instead of the enthalpy H) introduces a supplementary power bond $P\dot{V}$ [*Ould Bouamama et al. 1997*].

Bond Graph Model of a Mixture of two Phases

We consider here a two phases mixture, namely water and steam. There is not a net separation between the two phases and there may be steam bubbles. The accumulator is modelled by two ports C-element. This multiport is associated with storage of thermal and hydraulic energy of a mixture in the tank.

On figure. 3.14 are represented the bond graph and the block diagram simulation.

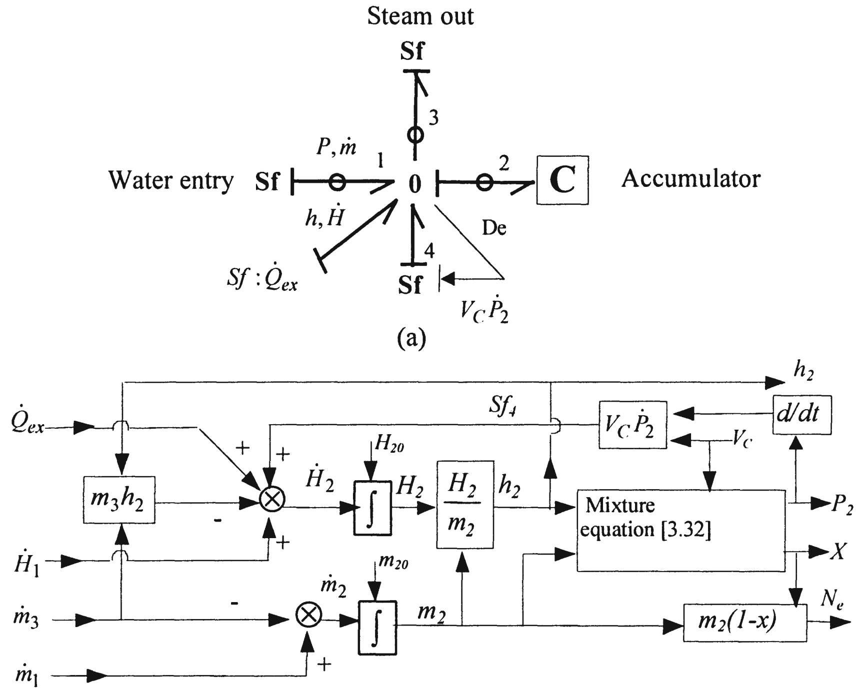


FIGURE 3.14. Modelling of a mixture with two phases. a. Bond graph model, b. Block diagram simulation.

The constitutive equations of the multiport C are given as usual by:

$$
\begin{aligned}
m_2 &= \int (\dot{m}_1 - \dot{m}_3)\, dt \\
H_2 &= \int \left(V_C \dot{P}_2 + \dot{Q}_{ex} - \dot{H}_3 \right) dt
\end{aligned}
\tag{3.30}
$$

together with a system of two phase equation of the mixture,

$$
\begin{cases}
h_2 = \dfrac{H_2}{m_2} = h_v(P_2)X + h_L(P_2)\,(1 - X) \\
v_2 = \dfrac{V_C}{m_2} = v_v(P_2)X + v_L(P_2)\,(1 - X)
\end{cases}
\tag{3.31}
$$

where $h_L(P_2)$, $h_v(P_2)$, $\nu_L(P_2)$ and $\nu_v(P_2)$ represent respectively the enthalpy and volume per mass of liquid and vapour in the vapour phase. They are determined by the method of least squares from the table of equilibrium of water and vapour (see appendix C). V_C is the geometric volume of a boiler and it is equal to the volume of the mixture steam and water.

The solution of 3.31 allows to determine not only the effort P_2 , but also the relative steam/water ratio which is an important parameter in industrial boilers. It allows to calculate the water remaining , which means the water level in the boiler Ne:

$$Ne = m_2(1 - X) \tag{3.32}$$

3.3.3 Condensation of Vapour

In industrial processes, condensation of steam to water is often needed, and is the reverse of evaporation in a boiler. So there must be cooling water for the latent heat. The liquid or condensate, is then cooled down to a temperature inferior to saturation. In the present chapter we study one simplified example such a condenser, while a complete simulation of such a condenser with the Matlab-Simulink program will be given in chapter 5.

Figure. 3.15.a shows the schema and the bond graph model of the condenser. The superheated steam is condensed by contact with the vertical tubes of the cooling circuit in which cold water circulates. The circuit wets the surface of the cold tube and forces therefore a continuous film of condensate which flows downwards under the effect of gravity.

On figure 3.15 we have two separate phases, liquid and vapour. We consider that the mean temperature of the part of tubes immersed in the vapour phase is the same; and the condenser is perfectly thermally insulated. A more refined model appears in Chapter 5.

The constitutive equations of the multiport C_V associated with the storage of energy in the steam phase allows to determine the quantity of enthalpy and of mass. Nevertheless, vapour being a compressible fluid, we choose as variables of state rather the mass per volume ρ_3.

$$\begin{aligned} H_3 &= \int \left(\dot{H}_1 - \dot{Q}_{81} - \dot{H}_7 + V_3\dot{P}_3\right) dt \\ \dot{m}_3 &= \dot{m}_1 - \dot{m}_7 = \frac{d\left(V_3\rho_3(t,T)\right)}{dt} \\ \text{where } \rho_3 &= \frac{1}{V_3\left(\dfrac{\partial\rho_3}{\partial T}\right)_{T=T_{sat}}} \int \left(\dot{m}_1 - \dot{m}_7\right) dt \end{aligned} \tag{3.33}$$

Since the vapour is at saturation, the variation of mass per volume at

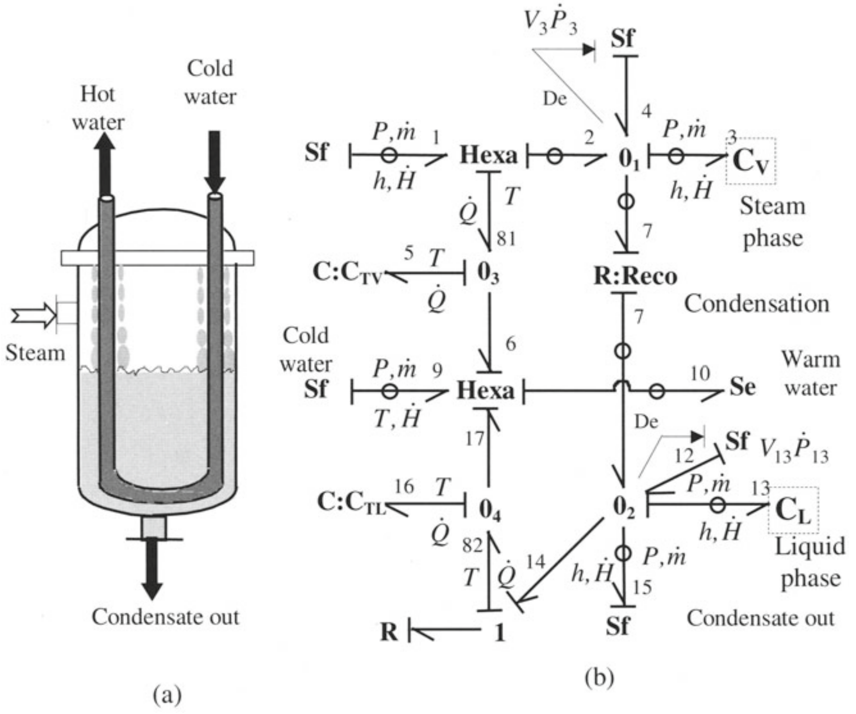


FIGURE 3.15. Bond graph model of condensation of vapour. a. Scheme of a condenser, b. Bond graph model of the condensation process

saturation temperature T_{sat} $\left(\frac{\partial\rho_3}{\partial T}\right)_{T=T_{sat}}$ is taken from thermodynamic tables (in appendix C). V_3 is the volume occupied by the vapour and $\dot{H}_7$ the latent heat given out by condensation. P_3 is the pressure in the steam phase. $\dot{m}_1$, $\dot{H}_1$, $\dot{m}_7$ and $\dot{H}_7$ are the mass flow and enthalpy flow respectively in the entrance of condenser and of condensation. The elements $C : C_{TV}$ and $C : C_{TL}$ associate the thermal energies by the cooling tube with the capacities C_{TV} and C_{TL} in integral causality:

$$\begin{aligned} T_5 &= \frac{1}{C_{TV}} \int \left(\dot{Q}_{81} - \dot{Q}_6\right) dt \\ T_{16} &= \frac{1}{C_{TL}} \int \left(\dot{Q}_{82} - \dot{Q}_{17}\right) dt \end{aligned} \tag{3.34}$$

The thermal flow by conduction on the vapour and liquid side are determined by the following equations:

$$\begin{aligned}
\dot{Q}_{81} &= K_{81}\left(T_3 - T_5\right) = K_{81}\left(f_T(P_3) - T_5\right) \\
\dot{Q}_6 &= K_6\left(T_5 - T_9\right) = K_6\left(T_5 - \frac{\dot{H}_9}{\dot{m}_9 c_w}\right) \\
\dot{Q}_{82} &= K_{82}\left(T_{14} - T_{16}\right) = K_{82}\left(\frac{H_{13}}{m_{13} c_L} - T_{16}\right) \\
\dot{Q}_{17} &= K_{17}\left(T_{16} - T_{10}\right)
\end{aligned} \tag{3.35}$$

where K_{81}, K_6, K_{82} and K_{17} are the coefficients of global heat exchange. c_w and c_L are specific heat of cooling water and of condensate. They are usually taken of a constant because they vary only weakly with temperature. The vapour is at saturation and its temperature T_3 comes from the pressure of vapour P_3 according the equation of Clausius-Clapeyron. The flow of condensation of this vapour around the tubes is calculated by the resistive multiport $R : R_{ECO}$. It is a function of the difference of following variables and parameters: the temperature between the vapour T_3 and the mean value of the tubes T_T, the mass per volume of the vapour 3 and of the liquid 13 , the dynamic viscosity L, the latent heat L_V of the vapour, and finally of the number n_T and the dimensions (diameter D, length L_T) of the tubes.

If one considers that the thickness of the film of condensation will remain sufficiently small in order that the film remains laminar, the flow can be given by an empiric law of Nusselt:

$$\dot{m}_7 = \frac{\rho_{13}\left(\rho_{13} - \rho_3\right) g}{3\mu_L} e_x^3 \Pi D_T n_T \tag{3.36}$$

where :

$$e_x = \left(\frac{4\mu_L l_T \left(T_3 - T_T\right) \lambda_L}{g\rho_L \left(\rho_L - \rho_V\right)\left(L_V + 0{,}68 C_T \left(T_3 - T_T\right)\right)}\right)^{\frac{1}{4}}$$

Here λ_L is the thermal conductivity of the liquid and C_T the thermal capacity of the tubes. The constitutive equations of the multiport $C : C_L$ allows to determine quantity of the enthalpy and the mass of the condensate, where the mass per volume is constant.

$$\begin{aligned}
H_{13} &= \int \left(\dot{H}_7 - \dot{Q}_{82} - \dot{H}_{15} + V_{13}\dot{P}_{13}\right) dt \\
m_{13} &= \int \left(\dot{m}_7 - \dot{m}_{15}\right) dt
\end{aligned} \tag{3.37}$$

$\dot{m}_{15}$ and $\dot{H}_{15}$ are the mass and enthalpy flows at the exit of the condenser. The pressure P_{13} of the liquid is determined by the hydrostatic law which is a function of the level N_{13} of the condensate and of the steam pressure P_3. In particular the condenser has a cylindric form with section A_C, we obtain:

$$P_{13} = P_3 + g\frac{m_{13}}{A_C} \tag{3.38}$$

This completes our description of the condenser, but a more elaborate model will be given in chapter 5.

3.4 Osmosis

3.4.1 Principles and Bond Graph of Osmosis

The research on osmosis that we shall describe here has been suggested by Henry Atlan and executed in France and Israel [*Thoma, 1985*].

Osmosis is half way between physical and chemical phenomena. It allows generating a pressure in two cells or compartments separated by a membrane. One part contains pure water and the other part water with dissolved salt.

We have seen before, that a system tends always to go to a state with three equilibriums: thermal, hydraulic and chemical; the last one is called also diffusion equilibrium. For osmosis this is modified as will be demonstrated below.

The figure 3.16 shows the principle of osmosis. Two compartments of water are separated by a membrane, which allows passing the water, or generally the solvent, but keeps back the salt, generally the solute. Such a membranes is called a selective or semi-permeable. They exist but have sometimes leakage. We can say that they have hydraulic resistance in parallel connection with chemical resistance.

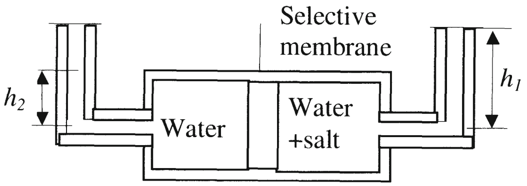


FIGURE 3.16. Principle of osmosis

On figure 3.16 the right compartment contains the salt, the pressure goes up as indicated by the level h_l the vertical tube, because of the membrane is under the influence of the chemical resistance. Hence equilibrium establishes itself by the equality of chemical tensions (chemical potential) which is different from the equilibrium of pressures. There is a transfer of water through the membrane because of the reduction of chemical tension at right due to the presence of dissolved salt. In order to compensate, the pressure of water must increase.

The osmosis is important in biophysics, because it controls many biological phenomena. As an example, the water goes up under osmosis in trees against the gravity force where it is evapourated by the leafs: about 400 liters per day for a big tree. There are also many other applications of osmosis but the interesting thing is that it can also be treated by bond graphs.

The bond graph for water in the osmotic cell of figure 3.16 is given on figure 3.17 [*Thoma, 1985*]. In principle one can present the same bond graph for the salt but we suppose that in our case the membrane blocks the passage of a salt.

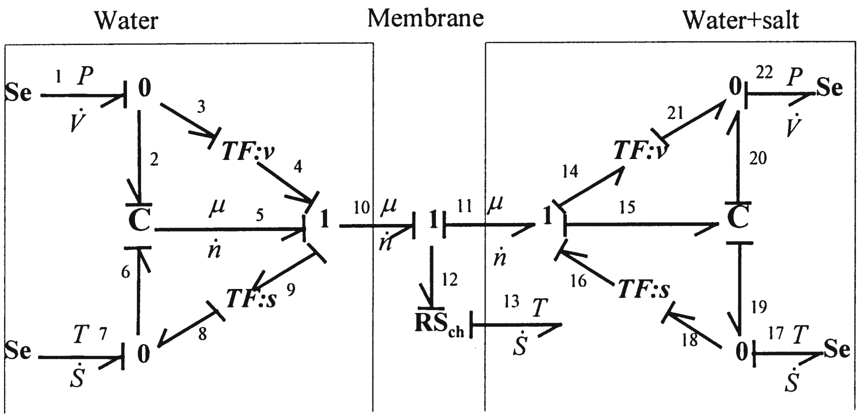


FIGURE 3.17. Bond graph for water and dissolved salt in two compartments separated by a selective membrane

3.4.2 Influence of Pressure and Temperature on Chemical Tension

The model allows particularly to show the influences of pressure and temperature on chemical tension. It comes from the constitutive equation of series junction (1-junction) that has only one common flow:

$$\mu_4 + \mu_5 - \mu_9 - \mu_{10} = 0$$

With the relations (3.12) and (3.13) one obtains again the relation:

$$\mu_{10} = \mu_5 - sT_8 + vP_3$$

This relation shows that the chemical tension becomes less with increasing temperature and becomes more with increasing pressure, because both s and v are positive.

3.4.3 Osmotic Pressure and Boundary Layer

We have seen that at first the pressures in the solvent and in the solution are equal. Then the chemical resistance, rather the conductivity, will be active and transport the solvent through the membrane. So finally, the chemical tensions will be equal and finally the pressure in the solution will be superior to the pressure in the solvent (water). This difference of pressure is called the “osmotic pressure“, which is caused by the initial difference of the chemical tension.

To say again, in chemical equilibrium we have the equality of chemical tensions in of both compartments, water and solution of salt in water

$$\mu_{10} = \mu_{11}$$

While in hydraulic equilibrium we would have equality of hydraulic pressure.

Replacing μ_{10} by equation 3.14 and considering that

$$\begin{aligned} &\mu_{11} = \mu_{15} - sT_8 + vP_{21}, \\ &P_{21} = P_{27}, \\ &\text{and } P3 = P1, \end{aligned}$$

we derive that:

$$\Delta P = P_{22} - P_1 = \frac{(\mu_5 - sT_8) - (\mu_{15} - sT_{18})}{v} \tag{3.39}$$

where v is the specific molar volume which is equal in both compartments.

We introduce here the boundary layer, a concept known from aerodynamics. If the pores of the membranes are large, there is a volume flow due to the difference of pressure between both compartments tending towards hydraulic equilibrium. This is represented by the addition on figure 3.18 of one series and one parallel junction and the bonds 23 to 26. The lead to a hydraulic resistance RS which, as all resistances, generates entropy.

The direction of the half arrows of the power bonds indicate that the hydraulic power goes from right to left, that is from the salted water to

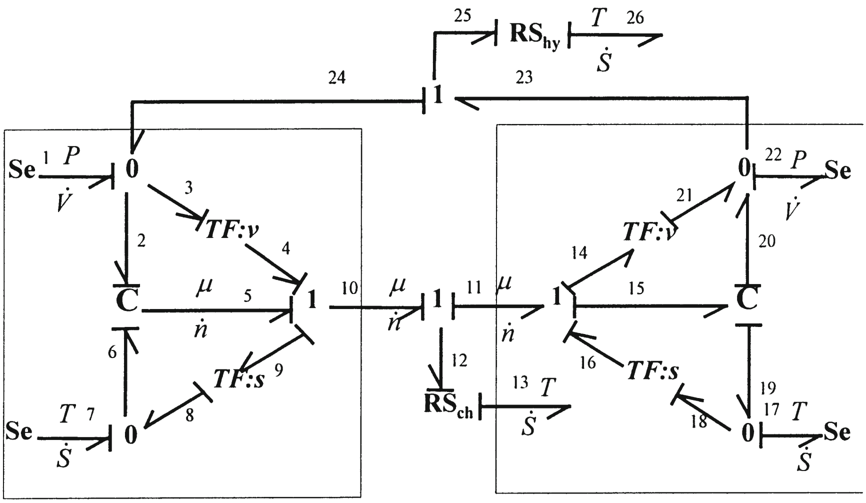


FIGURE 3.18. Bond graph model of the water in the osmosis phenomenon with a permeable membrane

pure water. We have therefore two actions in parallel, chemical action and hydraulic action. The first action belongs to a chemical equilibrium and the second one to a hydraulic equilibrium. The core of the pores is subject to the difference of hydraulic pressure and the part nearer to the walls is subject to chemical tension.

For a pore of circular radius r_p, the speed $u(r)$ in function of its hydraulic radius r_h and the volume flow $\dot V_{25}$ going through RS is calculated according Hagen Poisseuille

$$\begin{aligned} u(r) &= \frac{\Delta P \left(r_p^2 - r_h^2\right)}{4\eta L} \\ \dot V_{25} &= \frac{\pi \Delta P r_p^4}{8\eta L} \end{aligned} \tag{3.40}$$

with L the length of the pores and η the viscosity of the fluid.

It results from equation (3.40) that the hydraulic conductance (inverse of the resistance) diminishes rapidly with the radius of the pores and the hydraulic flow becomes negligible for small pores. On the other hand, as we shall show further on, the chemical flow is much less sensible to the radius.

To summarize, each membrane has a hydraulic resistance, which is subject to the hydraulic pressure for equilibrium, and a chemical resistance, which requires the equality of chemical tension. For the pores of intermediate dimensions both phenomena are active. In that case, the difference of the chemical tension between both gives a flow of solvent (the water), through the separating membrane.

The matter is adhering to the boundary layer of the pores as indicated in figure 3.19, similarly as the boundary layer in aerodynamics.

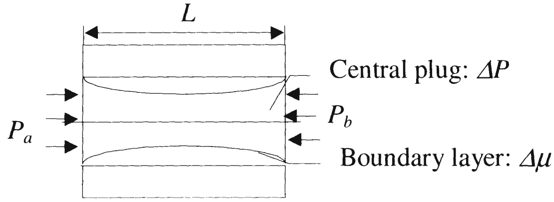


FIGURE 3.19. Longitudinal cross section of a pore

In order to fix the ideas the diameter of a pore has the magnitude of 150 nm. Here it should be noted that this adhesion is not due to action of the viscosity near to the wall and the liquid flow is not influenced by viscosity elsewhere. Further to the boundary layer, which represents the chemical resistance, we have a central plug under the influence of the difference of pressure according to equation 3.40; it represents the hydraulic resistance. Both resistances are in parallel action.

3.4.4 Estimation of Thickness of Boundary Layer

In order to quantify the thickness of the boundary layer driven by the chemical tensions, one calculates first the velocity $u(r)$ according equation (3.40) and then the velocity of the chemical flow. One defines then the thickness of the boundary layer as the distance, which both velocities are equal.

In order to determine the chemical flow and therefore the velocity, one applies the law of diffusion of Fick for the salt. According to this the molar flow of the salt $\dot{n}_S$ is:

$$\frac{\dot{n}_s}{A} = \frac{-D\Delta C_S}{L} \tag{3.41}$$

and the corresponding linear speed

$$u_S = \frac{\dot{n}_s}{\bar{C}_S A} = \frac{-D\Delta C_S}{\bar{C}_S L} \tag{3.42}$$

where D is the diffusion coefficient, L the length of the pores, A the section of the pores and $\bar{C}_S$ the mean concentration of salt in both compartments of the cell. If one designates by A and by B both compartments one writes the equations:

$$
\begin{aligned}
\bar{C}_S &= \frac{C_{SA} + C_{SB}}{2} \\
\Delta C_S &= C_{SB} - C_{SA}
\end{aligned}
$$

from which one obtains for a small concentration C_{SA} :

$$
\begin{gathered}
\frac{\Delta C_S}{\bar{C}_S} = 2 \\
u_S = -\frac{2D}{L}
\end{gathered}
\tag{3.43}
$$

The sign minus in equation (3.43) indicates the direction of passage of salt: From the compartment A (at right) to B (at left). The speed of water will be identical to the one of the salt but in opposed sense:

$$
u_W = \frac{2D}{L} \tag{3.44}
$$

The hydraulic speed $u(r)$ can be written with the distance of the wall δ:

$$
u(r) = \frac{\Delta P.2r_p\delta\left(1 - \dfrac{\delta}{2r_p}\right)}{4\eta L} \tag{3.45}
$$

and then on equalizes the hydraulic and chemical speeds

$$
\frac{2D}{L} = \frac{\Delta P.2r_p\delta\left(1 - \dfrac{\delta}{2r_p}\right)}{4\eta L}
$$

If one supposes that $\dfrac{\delta}{2r_p} \rightarrow 0$, we have the thickness of the boundary layer :

$$
\delta = \frac{4D\eta}{r_p\Delta P} \tag{3.46}
$$

The thickness of boundary layer is of the order of 25 nm.

3.4.5 Estimation of Chemical Resistance

In analogy with Ohms law in electricity, we can define the chemical resistance as the ratio of the chemical tension to the molar flow, which goes through the membranes

$$R_{ch} = \frac{\Delta\mu_W}{\dot{n}_W} \tag{3.47}$$

One determines first the molar flow of the water

$$\dot{n}_W = C_W u_W A = C_W \frac{D\Delta C_S A}{\bar{C}_S L} \tag{3.48}$$

where C_W is the water concentration. The difference of chemical tensions can be determined with approximation by the relation of ideal gas:

$$\begin{aligned} \mu_S &= \mu_{S0} + RT \ln C_S \\ \text{where: } \Delta\mu_S &= \frac{RT\Delta C_S}{\bar{C}_S} \end{aligned} \tag{3.49}$$

with T, the temperature in Kelvin and R the gas constant. Starting from the Gibbs Duhem relation *[Katchalsky, 1965]* one obtains the difference of chemical tensions

$$\Delta\mu_W = \frac{N_S \Delta\mu_S}{N_W} = \frac{C_S RT \Delta C_S}{C_W \bar{C}_S} \tag{3.50}$$

where C_S is the concentration of salt in the compartment B. The combination of both relations (equations 4.48 and 3.50) gives the chemical resistance:

$$R_{ch} = \frac{\Delta\mu_W}{\dot{n}_W} = \frac{C_S RTL}{C_W^2 AD} \tag{3.51}$$

The unit of chemical resistance is ($J.s.mole^{-2}$) and the value about 300 ($J.s.mole^{-2}$).

3.4.6 Inverse Osmosis

An interesting application of osmosis is the so-called inverse osmosis, which is used for desalinating of sea water, that is to separate the water from the salt and to obtain a pure water at high pressure. A schematic principle appears on figure 3.20. Salted water is under high pressure to equalize the chemical tensions and to run the pure water through the membrane.

The corresponding bond graph appears on figure 3.21. A practical membrane for inverse osmosis must then have a minimal resistance for water and a maximal resistance for salt.

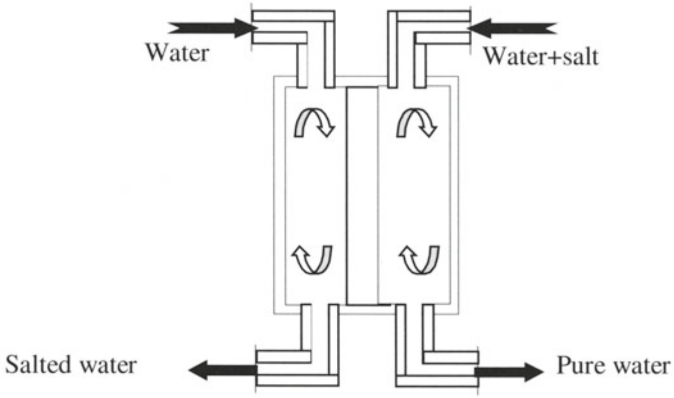


FIGURE 3.20. Principle of inverse osmosis

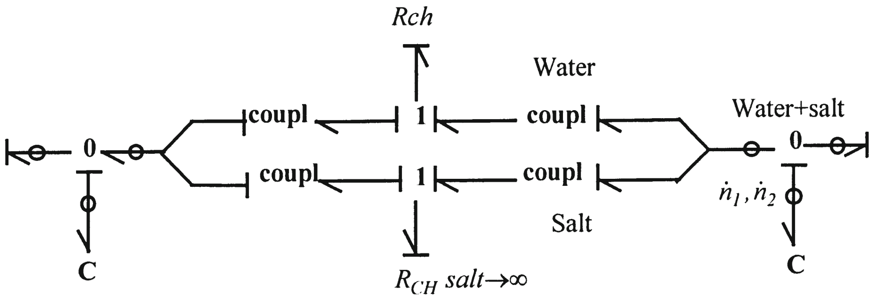


FIGURE 3.21. Bond graph of inverse osmosis

3.5 Chemical Reactions

3.5.1 Bond Graph Model of a Chemical Reaction

As already introduced in section 3.1 and 3.2, chemical reactions can be very well represented by bond graphs where the chemical tension has the role of an effort. Contrary to electric and mechanical systems the bond graphs for chemistry and chemical reactions are not well developed.

In this part we compare chemical reaction to the reaction of change of phase and therefore we shall repeat a little from the preceding paragraphs. A static chemical reaction that is without moving matter is very well reticulated by bond graphs and the model of figure 3.7 can be applied. Only there is no hydraulic resistance, it has an infinite value. If there is a chemical reaction between two substances or reactants A and B which produce two products C and D according to the following equation

$$v_A A + v_B B \overset{K_f}{\underset{K_r}{\rightleftarrows}} v_C C + v_D D$$

An example is the burning of hydrogen and oxygen according to the equation.

$$H_2 + 0,5.O_2 \overset{K_f}{\underset{K_r}{\rightleftarrows}} H_2O$$

This gives $v_A = 1$, $v_B = 0,5$, $v_C = 1$ and $v_D = 0$. These are the stochiometric coefficients and K_f and K_r are the velocity constants of the direct (forward) and inverse (reverse) reactions.

We shall consider in the following that the components are well mixed, that means the concentration does not vary in the reactor, which is then a system of localized parameters. These conditions are generally obtained in the reactors called CSTR (Continuous Stirred Tank Reactor).

For a introduction of the representation of chemical reactions by bond graphs, we show the reaction above considering only the phenomena of chemical transformation. The reaction can be represented by the true bond graph given by the figure 3.22.

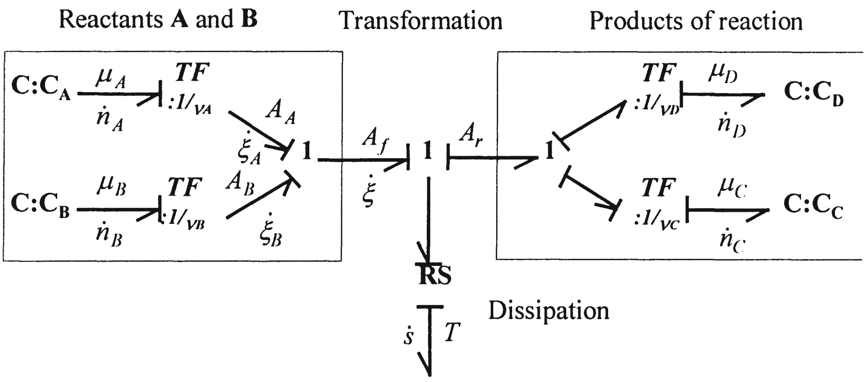


FIGURE 3.22. Bond graph model of chemical reaction

According to the bond graph of figure 3.22 one can define a chemical reaction from a phenomenological point of view with a dissipative multiport RS, which has at its entry the reactants and as exit the products weighted by the stoichiometric coefficients. We neglect here the couplers of figure 3.7 and 3.8, although they are always present and can conduct to endothermic reactions, as we have seen.

According to figure 3.22 the elements $C(C_A$, C_B, C_C, and $C_D)$ are the capacitors representing the storage of matter. Including variable temperature and pressure, they would really be multiports C, a fact neglected here.

The direction of the half arrows corresponds to the run of the reaction, going out by the reactants C_A and C_B towards the products C_C and C_D. Each product is represented by two power variables $(\mu_i\,,\ \dot{n}_i)$. Then we have the transformers to arrive at the power variables of the chemical reactions proper, which are chemical affinity A_i $(inJoule/Mole)$ for effort and the speed of reaction $\dot{\xi}_i$ (in mole/second) for flow. The transformers TF show the transformation from reactants to product and the corresponding module$(1/v_i, i = A, B, C, D)$ denote the stoichiometric coefficients. The central multiport RS controls the speed of reaction and is the subject of chemical kinetics.

According to the assigned causalities (μ_i and $\dot{\xi}_i$ known) the transformers constitutive equations between efforts and the equations between flows are,

$$\begin{cases} A_i = v_i \mu_i \\ \dot{n}_i = v_i \dot{\xi}_i \end{cases} \quad \text{where } i = A, B, C,\ D \tag{3.52}$$

We would like to note about the relation 3.52:

1. The efforts relations of transformer element TF transform the chemical tension μ_i of the species i in its chemical affinity A_i $(A_i = \mu_i v_i)$. Sometimes it is useful to group the affinities in forward affinity (A_f) and reverse affinity (A_r):

$$A = A_f - A_r = (v_A \mu_A + v_B \mu_B) - (v_C \mu_C + v_D \mu_D) \tag{3.53}$$

Let us remind that the chemical affinity A is an effort variable, which represents the force driving the reaction. It is zero in equilibrium, which means that the reaction runs until the affinity A becomes zero.

2 The flow relations of the transformers divide the molar flow $\dot{n}$ by the stoichiometric coefficient v to obtain the velocity of the of reaction:

$$\dot{\xi}_i = \frac{\dot{n}_i}{v_i} (i = A, B, C, D)$$

Let us note, that

$$\xi = \int \dot{\xi}_i dt$$

is called the degree of advancement of the reaction in chemical kinetics.

If we are relatively near to the chemical equilibrium, the velocity of reaction is a function of temperature and only of the difference of affinities

$$\dot{\xi} = \Phi\left((A_f - A_r), T\right) \tag{3.54}$$

This relation is the constitutive equation of the multiport RS in figure 3.22. Furthermore in the same conditions the chemical potential of the species i is connected approximately to its concentration C_i:

$$\begin{aligned} \mu_i &= \mu_{i0} + RT \ln C_i \\ \text{where: } C_i &= \frac{1}{a_i} e^{\frac{\mu_i - \mu_{i0}}{RT}} \end{aligned} \tag{3.55}$$

where $C_i = \frac{n_i}{V}$ is the molar concentration and μ_{i0} the chemical tension independent of the concentration, taken at $T = constant$.

From equation (3.55), we obtain for the condition of equilibrium ($A = 0$):

$$\frac{(C_A)^{\nu A} . (C_B)^{\nu B}}{(C_C)^{\nu C} . (C_D)^{\nu D}} = K \tag{3.56}$$

Equation 3.56 is the well-known law of mass action, which has been directly derived here from our bond graph.

The velocity of the reaction is given by empirical relation:

$$\dot{\xi} = K_f(T) \left[\left(\frac{n_A}{V}\right)^{\nu_A} \left(\frac{n_B}{V}\right)^{\nu_B} \right] - K_r(T) \left[\left(\frac{n_C}{V}\right)^{\nu_C} \left(\frac{n_D}{V}\right)^{\nu_D} \right] \tag{3.57}$$

In the equilibrium the constant of velocity $K(T)$ is

$$K_f(T) e^{\frac{-A_{f0}}{RT}} = K_r(T) e^{\frac{-A_{r0}}{RT}} = K(T) \tag{3.58}$$

where A_{f0} and A_{r0} are the affinity forward and reverse calculated at constant temperature. Taking into account the relations (3.53), (3.55), (3.57) and letting $A_i = \nu_i \mu_i$, we obtain:

$$\dot{\xi} = K(T) e^{\frac{A_f - A_R}{RT}} = \Phi(A_f,\, A_r, T) \tag{3.59}$$

$K(T)$ is the speed constant which varies with the thermodynamic temperature according to the relation of Arrhenius:

$$K(T) = K_0 e^{\frac{-E}{RT}}$$

with E energy of activation, k_0 a frequency factor and R the gas constant. The parameters E and k_0 are determined in practice experimentally by the method of Least square method between minimizing the logarithm of the model (to make it linear) the experimental data:

$$J(\theta) = \min \left[\sum_{i=1}^{N} \left(\ln\left(K_{ex}(i)\right) - \ln\left(k_0 e^{\frac{-E}{RT(i)}}\right) \right)^2 \right] \tag{3.60}$$

Here i and N are respectively the number of species and the number of experiments and $\theta = \begin{bmatrix} \ln k_0 & E \end{bmatrix}^T$ the parameter vector, which is to be estimated. $K_{ex}(i)$ (with $i = 1$ to N) are the given experimental points; they give the speed of reactions at different temperatures. It should be noted that the determination of K_{ex} from experimental results requires the conversion ratio of the reactants which is not directly accessible. One writes therefore any law between the conversion ratios and a measurable quantity such as the efficiency of a product and applies this parameter estimation.

Far from equilibrium the relation of speed of the reactants is more complex and depends singly on forward and reverse affinities, $\dot{\xi} = f(A_f, A_r)$. In this case the central series junction is replaced by a multiport RS indicated on figure 3.23.

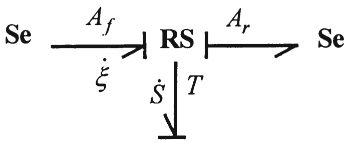


FIGURE 3.23. Representation of chemical resistance far from equilibrium

This distinction between near and far the equilibrium is very important in biophysics.[*Oster, 1973*]. The speed of reaction if governed by the resistance RS, for which different theories are known from chemical kinetics [*Denbigh, 1971*], *[Thoma, 1977*].

This problem was examined by authors. We were disturbed by the fact, that in a so-called theory of the Transition State, the real reaction rate is the difference of molecules going forward and molecules going backwards. This is not possible in the R-element of bond graphs, were flow goes always from the higher to the lower effort, so we could not write a bond graph for it. The transition state theory takes a different viewpoint, a molecular one. The relation between bond graphs and transition state theory must be connected with electrical noise, of which much theory exists; Thoma has written a doctoral thesis on it in 1957. We wanted to investigate further by did not get around to.

3.5.2 Chemical Resistance

The quantity of matter transported by diffusion of species i can be expressed by the law of Fick:

$$\dot{\xi}_i^d = -D_i \frac{dC_i}{dx} \tag{3.61}$$

where $\dot{\xi}_i^d$ is the diffusion flow, D_i the diffusion coefficient and x the space variable. The force or effort driving the diffusion is the chemical tension (potential) and not the concentration. If one expresses the concentration from equation 3.55, there is a constitutive equation of the element R of the type $R(e, f) = 0$:

$$\dot{\xi}_i^d = -D_i \frac{C_i}{RT} \frac{d\mu_i}{dx} \cong \left(\frac{D_i C_{i,l}}{RTW_l}\right) \Delta\mu_i$$

where $\Delta\mu_i$ is the difference of chemical tension of the species i over section l, of the width W_l. The resistance of diffusion for the species i in this region is then:

$$R_{i,l}^d = \frac{RTW_l}{D_i C_{i,l}} \tag{3.62}$$

The chemical resistance determines the speed of reaction, which can go from duration of practically zero (an explosion) until infinite (no reaction).

3.5.3 Chemical Capacity

Knowing that the concentration C_i is equal to the integral of the molar flux $\dot{n}$, equation (3.55) can be written as:

$$\Phi_C \left(\mu, \int \dot{n} dt\right) = 0$$

This is a constitutive equation of a chemical capacity in a bond graph. Nevertheless in general the equation is of the form $n = \Phi(\mu_i)$ which gives the following on derivating in:

$$\dot{n}_i = \frac{\partial \Phi(\mu_i)}{\partial \mu} \frac{d\mu_i}{dt} \tag{3.63}$$

Noting that the capacity is

$$\frac{\partial \Phi(\mu_i)}{\partial \mu} \triangleq C_i$$

From equation (3.63) is deduced the classical relation of a C-element. It connects the efforts to the integral of the flow or displacement by :

$$\mu_i = \frac{1}{C_i} \int \dot{n}_i dt$$

where $\dot{n}_i$ is the molar flux entering the capacity.

Note that one can also use a pseudo bond graph for the reaction, where the effort is the concentration of substance and not the chemical tension; both are connected by equation 3.55. As flow we still have the derivation of concentration. This approach is largely used [*Lefevre, 1985*] because it allows to manipulate a more easily measured variables for simulation.

3.5.4 Thermodynamic Model of Chemical Reactions

Let us analyze the thermodynamic aspects of a chemical reaction. The global bond graph model appears on figure 3.24. This bond graph includes the couplers and shows the thermal and hydraulic effects. The product of chemical affinity A by the speed $\dot{\xi}$ is a power, which is dissipated in the central multiport RS and generates entropy. This multiport absorbs chemical power and produces a equivalent quantity in thermal power; only the absolute temperature must be used

$$T\dot{S}_{gen} = \dot{\xi}\,(A_f - A_r) = \dot{\xi}\,\left(v_A\mu_A + v_B\mu_B - v_C\mu_C - v_D\mu_D\right) \tag{3.64}$$

Let us note that only this entropy is irreversible. Indeed, $A_f - A_r$ becomes negative, $\dot{\xi}$ is also negative, so that their product stays positive. This is similar to the chemical resistance treated in section 3.2, particularly figure 3.7.

The other flows of power comes from the difference between the stripped entropy of reactants and unstripped entropy of products

$$T\dot{S}_S = \dot{\xi}\,(v_A s_A + \mu_B s_B - s_C\mu_C - s_D\mu_D) \tag{3.65}$$

From equations (3.64) and (3.65) conduct to the observable power of a chemical reaction which is also called the enthalpy of reaction, sometimes heat of reaction $\dot{Q}$.

$$\dot{Q} = T\dot{S}_S + T\dot{S}_{gen} = \dot{\xi}\,(v_A h_A + v_B h_B - v_C h_C - v_D h_D) \tag{3.66}$$

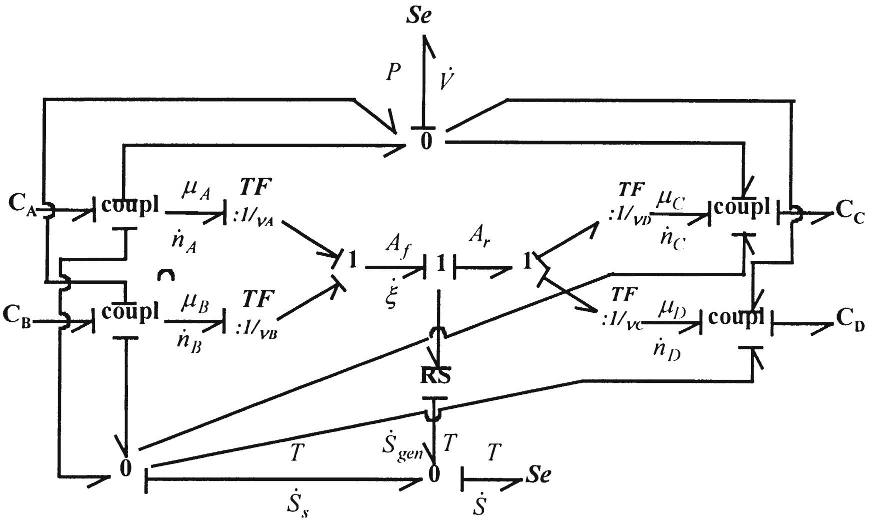


FIGURE 3.24. Global bond graph Model of the chemical reaction including thermodynamic and hydraulic effects

where $h = \mu + sT$ is the molar enthalpy of reaction (J /mole).

The entropy capacity of the products may be at the given temperature larger than the entropy capacity of the reactants

$$s_C\mu_C + s_D\mu_D > \mu_A s_A + \mu_B s_B \tag{3.67}$$

In this case the entropy must come from the dissipation generated by the multiport *RS* or the environment. In this last case, the products will become colder and we have an endothermic reaction. So the strange phenomena of endothermic reaction have a simple explanation by bond graphs.

3.5.5 Parallel and Competitive Chemical Reactions

If a simple chemical reaction, such as represented by the figure 3.22, also other chemical bonds can appear, these reactions are called parallel and competitive because they go forward in parallel to the main reaction, or are an alternative to it. In practice these reactions are undesirable. On the bond graph model such as figure 3.25 a parallel reaction is formed by combination of reactants B with the reactant E to build another product F according to the reaction:

$$B + EF \rightarrow F$$

It is coupled to the principle reaction here ($v_A A + v_B B \longleftrightarrow v_C C + v_D D$) above by a parallel junction.

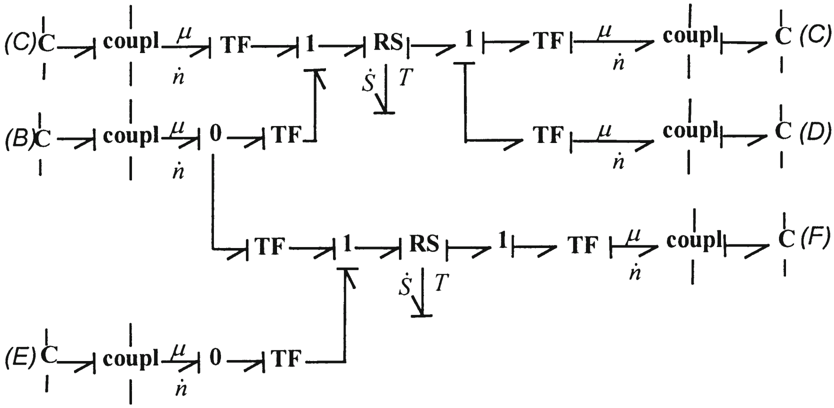


FIGURE 3.25. Bond graph model of parallel (in the parallel junction) and competitive (the series junction) reactions

Brusselator of Prigogine

There exists a system of chemical reactions known under the name of Brusselator [*Haken, 1978*], which has interesting properties, especially the possibility of oscillation of concentration. The reactions are given by the following equations:

$$
\begin{aligned}
&A \longleftrightarrow B \\
&B + 2X \longleftrightarrow 3X \\
&B + X \longleftrightarrow Y + D \\
&X \longleftrightarrow E
\end{aligned}
$$

The simplified bond graph, which is without couplers, model shown on figure 3.26. The reactions are coupled by series junctions.

This example is given only to show how one can represent graphically more complex reactions. As said, we have suppressed the different couplers, because our purpose was only to show the principle. Our module of the transformers assures the stoichiometric coefficients and are expressed by small entire numbers. From this bond graph the reader can find the equation of reaction shown above.

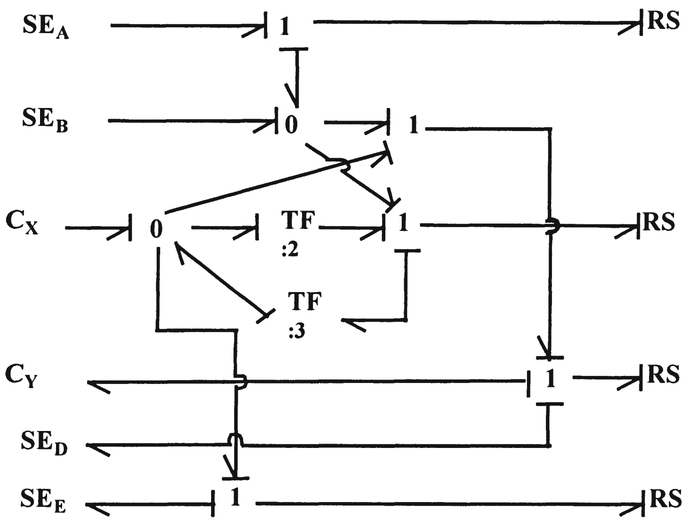


FIGURE 3.26. Example of bond graph for the reactions of Prigogine

3.6 Static Electrochemical Reactions

3.6.1 Electrochemical Coupling

Many chemical reactions are coupled with the transport of electric charges as for instance the dissolution under the form of ions of certain metals in electrolysis. This is the foundation of batteries, accumulators and fuel cells. Figure 3.27 shows a bond graph model of a chemical reaction with a electric bond in series. The coupling is assured by a transformer TF that exchanges molecular mass with the production of electric current according to the equations:

$$\begin{aligned} \eta &= \mu + Fu \\ i &= \dot{n}F \end{aligned} \tag{3.68}$$

The modulus of the transformer TF is Faraday's constant (96.5 $kCb/mole$) and η the electrochemical tension, which differs from the chemical tension as indicated in equation 3.68. This electrochemical tension is then a combination of the chemical tension and of the electric voltage and represents the driving force of the electrochemical reaction: if the driving force becomes zero, we have electrochemical equilibrium, which controls all electrochemical reactions and no chemical flow. If there is no electric charge, the electrochemical tension becomes equal to the chemical tension.

There are many applications of electrochemistry since the time of Mr. Faraday in 1840, like the electrodeposition of metal on the electrode of

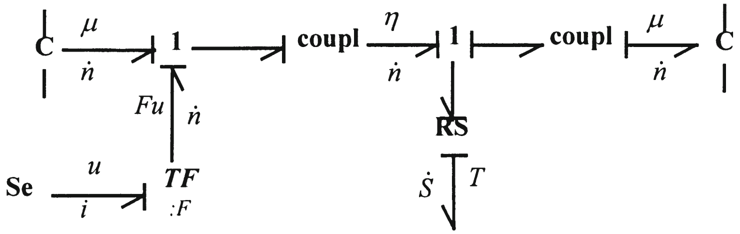


FIGURE 3.27. Bond graph model of a electrochemical reaction

an electrolytic tank. As an example we can also take an electric battery and observe that on the electrodes we have an electric voltage and the charge wants to pass from the positive pole (+) towards the negative pole (-). The electrodes thus create an electric field from the positive pole to the negative pole. Inside the battery there is the same electric field, and the charge is conserved. Hence the charge goes from the negative electrode against the positive electrode against the electric field under the drive of some agent. This agent is the chemical tension of the ions. So it ions which go from large from the large to the small chemical tensions, taking the electric charge with them from the minus electrode to the plus electrode against the voltage drop.

3.6.2 Bond graph Model of Electrolysis

From the figure 3.27 we can develop the bond graph of a battery shown on figure 3.28.

On this figure we introduce a new element *IONI* which assume the coupling of electric current to the ionized molar flow. In electrolysis of water there are ions of hydrogen (H_2). This element is introduced to show the ionization: Loss of one electron of hydrogen and production of the ion H^+. The phenomenon is difficult to show as a model, we have therefore represented it under the form of a word *IONI* (in a word bond graph sense), which shows again the flexibility of bond graphs.

The electrochemical reactions are interesting because they allow to transform chemical energy ($\Delta\mu\dot{n}$) into electric energy ui without generating entropy or heat: their efficiency is not limited by Carnot factor.

The action of a battery corresponds to a discharge a C-field with the exchange of ionized mass for the electric current. If the external electric voltage is higher than what corresponds to the difference of chemical tension, matter will be exchanged in the inverse sense: the battery is then charged. As example let us consider an electric tank with two electrodes of figure 3.29. It is a reaction of hydrogen with oxygen with two electrodes of platinum. One uses often the carbon electrodes with a layer of platinum, since this material is permeable to ions of hydrogen. It is applied in a very

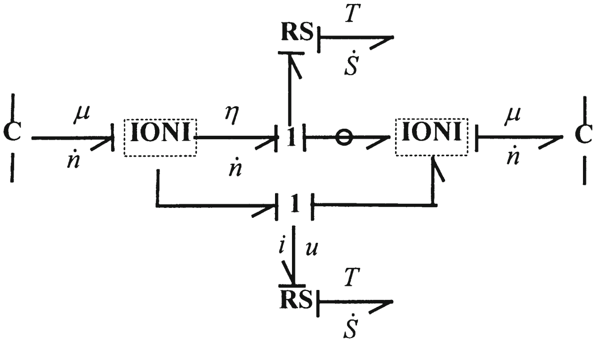


FIGURE 3.28. Bond graph of a battery with two elements IONI for the coupling of electric current on the molar flow

thin layer about $0.1 gr/m^2$. One electrode is surrounded by hydrogen and the other by oxygen as indicated by the bubbles.

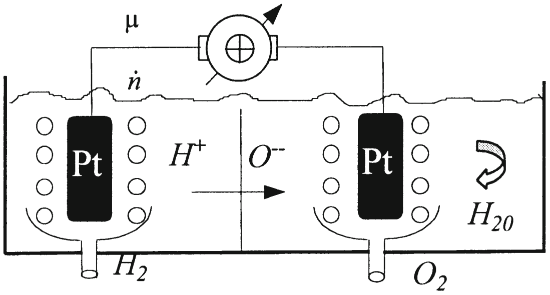


FIGURE 3.29. Schematic of electrolysis of water

Figure 3.30 shows the corresponding bond graph with the sources Se, used because the capacities are very large: they are really external bottles.

The coupled bonds on the elements $IONI$ indicate that a flow of ions is coupled to the electric charge: the ions transport both chemical and electric power. On the other hand, neutral atoms transport only chemical power. In principle we have a coupling between entropy and volume also, but this is neglected. We find the element $IONI$ also on other occasions. The two elements C have been added to have a computationally more robust system, because the two elements $IONI$ impose electrical flow proportional to molar flow. This is because the series junctions have only one flow. In the electrolyte the friction of the ions during their migration through the water is modeled by resistance RS. At the left of figure 3.30 the hydrogen H_2 takes an electron and is transferred as ions towards electrolyte while the electron comes in the electric part. At right the ions of hydrogen H_2 will

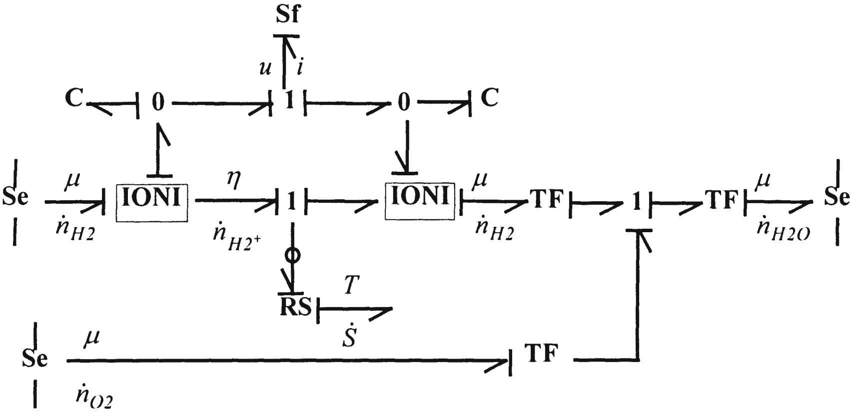


FIGURE 3.30. Bond graph of water electrolysis

be combined with the molecules O_2 in order to form the water. There must be a flow of electrons, that means an electric current after the transformer. The modulus of this last one is normally called the constant of Faraday.

The arrangement of the figure 3.29 works as fuel cell absorbing hydrogen and oxygen and producing water. The tension on the electrodes is 1.23 Volt without electric current, but becomes half this amount with an electric current of 3000 A/m^2 due to the friction. One can also increase the voltage which reverses the electric current and the system dissociates the water in hydrogen and oxygen. That means with a tension of more then 1.23 volts, the system produces the two gases from the water., which is used industrially.

One way to say is that you have two selective membranes for ions and electrons: the first allows migration of the ions from the interface electrode-electrolyte into the electrolyte, but not in the electrons. The second one allows the electron to travel from the electrodes to the wire, but not the ions. The essential property of the membrane is not that it is a thin layer but that it allows to pass one substance but not another. The selective membrane is found here again after osmosis and will be found in reversible mixture, which we will treat in the appendix F.

The reactions take place in a very thin layer at the surface. Only electrodes should have as much surface as possible. Consequently the electrodes are porous, but one has already used fractal geometry [*Le Mehauté, 1990*] to describe them. An interesting review (in German) of fuel cells and batteries is found in Falk 1976, chapter 4.

In this paragraph we wanted simply to sketch the problem and the solution to show that thermodynamics by bond graphs is also good for these problems. Let us remind also that the couplers are always present and can produce temperature and entropy in addition to the many friction elements.

Some fuel cells and batteries actually become hot or cold during operation due to the effect of the couplers. Also one uses often high temperature in order to reduce the ion friction about (450 K).

3.6.3 Reversible and Irreversible Thermodynamics and Dissipation

Since we have already mentioned the notion of near and far the equilibrium in section 3.5 it is worth while to discuss this point in more detail. The three notion dissipation, reversibility and irreversibility are in reality very near. They refer first of all to chemical reactions represented by multiports C and R. Since temperature and pressure effects are coupled, we have really multiports. Firstly, to distinguish, the reversible thermodynamics creates effects in the multiport C and in irreversible thermodynamics creates effects in multiport R. In other words, in reversible thermodynamics one neglects the resistance multiports R, while in irreversible thermodynamics the multiports C are neglected. So a dissipation is generally presented in the multiport R which is really a multiport of type RS. Figure 3.31 shows a bond graph with reversible thermodynamics in the multiport C and irreversible thermodynamics in the multiport RS; our figure 3.26 was an example of this, except for the added transformers.

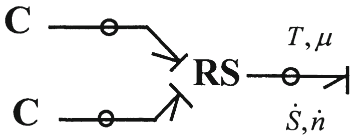


FIGURE 3.31. Representation of reversible multiports C and irreversible multiports RS.

Let us remind that the multiports C have a constitutive equation between the effort (the chemical tension), and integral of flow (molar flow). The multiports RS on the other hand are described by an algebraic relation between the chemical tensions (effort) and the molar flow.

The constitutive equation of the multiport RS is in general non-linear

$$f_i = f_{ij}\left(e^{\frac{\mu_j}{RT}} - 1\right) \tag{3.69}$$

where f_i is the coupling coefficient between the reactions expressed by a matrix. This matrix can be linearized around a certain point of operation near to the normal value of chemical tension μ. In this case, the equation can be written in the form:

$$f_i = L_{ik} e_k \tag{3.70}$$

which gives in the case two reactions

$$\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \end{bmatrix} \tag{3.71}$$

The dissipation and the production of entropy is given by the expression

$$T\dot{S}_d = \sum_i \dot{n}_i \mu_i \tag{3.72}$$

The matrix of coefficients L_{ij} in equation (3.70) and (3.71) is symmetrical, the famous symmetry of Onsager. We can deduct this symmetry by a statistical argument according to Kammer [*Kammer,1985*]. As already underlined in paragraph 3.5 on sees that with the linear relation the reaction is stable while with non-linear relations it is unstable: oscillations can appear. We have mentioned already the Brusselator of Prigogine on figure 3.26.

According to Prigogine one considers that in irreversible thermodynamics the entropy production according equation (3.72) is minimal at constant temperature. This is equivalent to the minimal dissipation of Maxwell [*Maxwell, 1873*] known since many years. According to this old author, a network of electrical resistances driven by voltage sources adjusts its currents in such a way that the total dissipation should be a minimum compatible with the sources. Each new setting of the sources entrains another new dissipation.

It is finally interesting that the notions of near and far from equilibrium and of chemical oscillations can be consulted in [*Oster, 1973], [Haken 1978*] and *[Kammer 1985*]. Finally the bond graph representation of the multiports C and RS and with coupled bonds allow to represent the concept of irreversible and reversible equations much clearer then a system of complex equations.

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4

Bond Graph and Process Engineering

4.1 Overview

4.1.1 Introduction

There is no miracle recipe for the modelling faithfully a complex system and it is necessary to take a spiral approach. The dilemma can be expressed like this: a simple model is false and a complex model cannot be used, in spite of modern computer science. A witness of this fact is the gap between the modern automatic control engineering, which always requires a good model and the practical application in chemical engineering processes.

We have underlined in the first chapter the importance of bond graph modelling in chemical engineering. They have a unified approach, which is good, because in industrial systems occur always phenomena of different nature and technological components from different disciplines (mechanical, thermal, chemical...). Furthermore, as opposed to classical modelling, one can always add to the model further bond graph elements, or simplify them by using simplifying assumptions. This property is particularly important, because chemical and thermal processes are really non-stationary: the heat exchange coefficients, the velocity constants of reaction and thermal conductivity depend on factors like dirt accumulation, aging of catalysts, etc.. To adapt the model one can simply add R-elements (or really RS-elements) to thermal losses and hydraulic restrictions. Furthermore, C and I-elements can be added for thermal capacities, mass storing and inertia effects.

Another point is that one has both static adaptations by R-elements and dynamic adaptation by C and I elements. Here, bond graph modelling allows also to anticipate the problem of solvability by a selection of causalities. The physical process are characterized by a strong mutual coupling of the parameters. Consequently it is necessary to distinguish the causes and effects in the model, depending on its destination. Finally, derivative causalities and algebraic loops can be seen on the bond graphs model and eliminated, for instance by modifying the model.

4.1.2 Methodology

The methodology or the different steps of a bond graph modelling can be seen on figure 4.1.

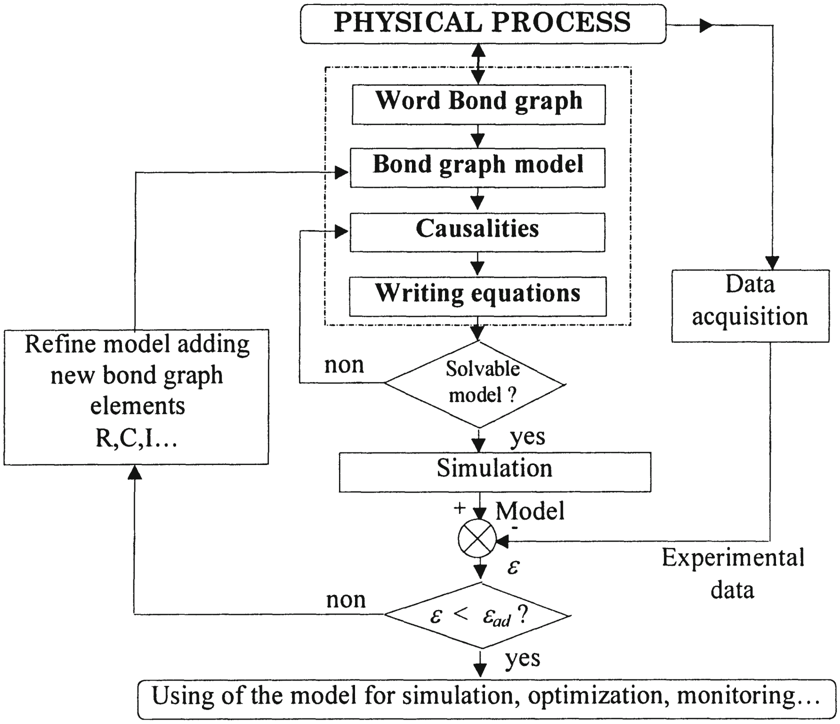
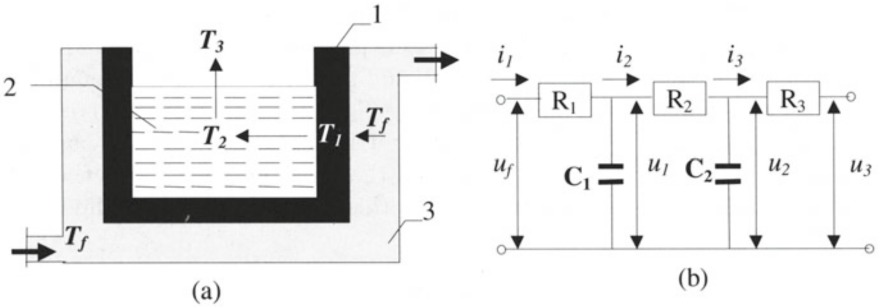


FIGURE 4.1. Different steps of a bond graph modelling

We will illustrate the method by a simple example given by the figure 4.2a. The process is a heating of a thermal bath 2 by exchanging heat flow through the metallic walls 1 with a warm fluid 3 kept at given temperature T_f. Heat is leaving also through the free surface to the environment supposed at the temperature T_3. So, the bath 2 is in contact over a resistor with the external temperature T_3.

Figure 4.2b gives the analogous electrical schema, based on the $(T, \dot{Q})$ analogy, that is a pseudo bond graph. So voltage u takes the place of temperature T and current i the place of heat flow $\dot{Q}$. We are interested here only in thermal phenomena.



(a) (b)

FIGURE 4.2. Steps in modelling a bath heated by hot fluid. a. View of the thermal system, b. Electrical analogy

4.2 Steps in Writing a Bond Graph Model

4.2.1 Word Bond Graph

We have seen that the word bond graph represents the technological level of modelling. There, one splits the entire system into simple subsystems given by words, as shown on figure 4.3.

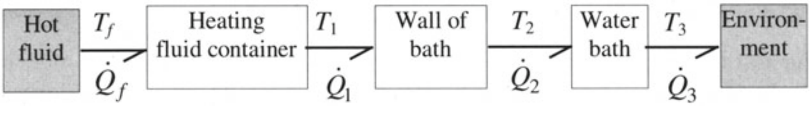


FIGURE 4.3. Word bond graph of the thermal process

We represent at the entry of each subsystem the liaison variables and not the signals as in classical block diagrams. In our case the liaison variables are temperature T and thermal flow $\dot{Q}$. We discuss below the reasons for such a choice. Let us note that therefore we have a pseudo bond graph and we neglect the hydraulic energy as very small.

4.2.2 Bond Graph Model

Here take a physical step, which allows to represent graphically all the important effects. This means to enumerate the modelling hypothesis or to explicit which effects to include, and which ones to neglect. So we consider the system with lumped parameters, that has a evenly distributed temperature. Suppose at first, that the thermal capacity of the wall C_1 is negligible. On the other hand, the thermal capacity of that bath C_2 is included.

The bond graph model is constructed from an energetic consideration of the process. The effort (temperature) source Se with T_f is imposed, and there is a thermal transfer by conduction (modelled by R_{12}) from the hot fluid T_f through the wall to the bath. One part of the heat is accumulated in the thermal capacity of the water C_2, and the other part goes through R_3 to the environment with the temperature T_3. All these effects are coupled by the parallel and series junctions (0-and 1-junctions). Here the parallel expresses the conservation of energy and the series junction shows the addition of efforts, that is temperatures. In this way one constructs the bond graph of figure 4.4.

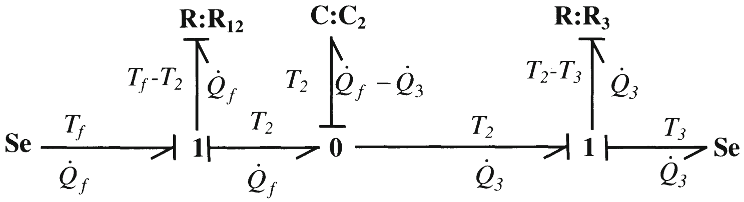


FIGURE 4.4. Thermal bond graph of the process neglecting the thermal capacity of the wall

4.2.3 Assignment of the Causalities

The notion of causalities in bond graphs allows to resolve the algorithmic level of the model building (those rules are shown in appendix A). The assignment of causalities is often imposed by the necessity to resolve numerical problems, but in thermal engineering there is a natural causality, which one uses if possible. It means to impose the efforts, pressure and temperature on the different elements, which then calculate the flows, mass flow and thermal flow.

In our example, we start first by the compulsory causalities, the efforts of the sources of temperature, temperature of the fluid T_3 and of the environment T_f. This gives integral causality in C_2. Next one gives the remaining causalities to the elements R_{12} and R_3, which turn out to be effort in, flow out.

Sometimes are added spurious elements in order to avoid a derivative causality. wherever, in practice a physical justification are given for them. This is the equivalent of an approximation in simulation and a very powerful method. Naturally, the spurious elements give a different system dynamics, and one has to check that the difference is not too large.

As an example, if the thermal resistance R_{12} were absent, we would have derivative causality on a C-element. One could avoid this by a flow source instead effort source, or by adding a thermal resistance and to keep in this way the effort source. These problems require the ingenuity and experience of the human simulator.

4.2.4 Writing Mathematical Equation

According assigned causalities, we have the constitutive equations of each element:

$$\begin{aligned}
&\text{Element } R\text{: } f = \Phi_R^{-1}(e) \;\Rightarrow\; \dot{Q}_f = \frac{T_f - T_2}{R_{12}} \text{ and } \dot{Q}_3 = \frac{T_2 - T_3}{R_3} \\
&\text{Element } C\text{: } e = \frac{1}{C}\int f dt \;\Rightarrow\; T_2 = \frac{1}{C_2}\int \left(\dot{Q}_f - \dot{Q}_3\right) dt
\end{aligned} \tag{4.1}$$

Writing the State Equation

It is sometimes interesting, as for the needs of control engineering, to write the state equations directly from a bond graph. In our system we have only one C-element in integral causality and therefore only one state variable. The state variable is the accumulated thermal energy. Since we have neglected hydraulic energy and suppose the mass of the fluid constant, we can designate the state variable by T_2.

We have thus two inputs, the temperature of the fluid T_f and the ambient temperature T_3. Let us note that the physical sense of the state variable is directly visible on the bond graph.

From the constitutive equations of the C-element, is deduced the state equation. In our first case there is only one state variable, in the linear form, $\dot{x} = Ax + Bu$:

$$\dot{T}_2 = -\left(\frac{1}{R_{12}C_2} + \frac{1}{R_3C_2}\right) T_2 + \left(\frac{1}{R_{12}C_2} + \frac{1}{R_3C_2}\right) \begin{bmatrix} T_f \\ T_3 \end{bmatrix} \tag{4.2}$$

Let us note that the thermal resistances R are equal to the inverse of heat exchange coefficient K_c or conductance ($R = 1/K_c$). The thermal resistance R_{12} is the sum of the resistance R_1 for the transfer fluid - wall and of R_2 for wall-bath.

Refinement of the Model by adding Bond Graph Elements

We suppose that the maximum error of the modelling between the model and the real, process is bigger than the admissible error which is usually about at 5%. We must therefore refine the model by adding further elements. As an example, we can include the thermal capacity of the wall of the bath 1. In this case, the energetic description is as follows: there is a thermal transfer by conduction, modelled by R_1 from the hot fluid T_f to the wall of the heat bath, one part of this energy is accumulated by the thermal capacity of the wall, modelled by C_1. The other part is dissipated by R_2 into the bath. We add thus two effects to the bond graph of the figure 4.4 and arrive at the bond graph of figure 4.5.

Now the system has two state variables, which come from energy storing in the wall of the heat bath and from the heat bath itself. The dynamics is easily deducted from the constitutive equations of two C-elements and three R-elements.

$$
\begin{aligned}
T_1 &= \frac{1}{C_1}\int \left(\dot{Q}_f - \dot{Q}_2\right) dt \\
T_2 &= \frac{1}{C_2}\int \left(\dot{Q}_f - \dot{Q}_3\right) dt \\
\dot{Q}_f &= \frac{T_f - T_1}{R_1} \\
\dot{Q}_2 &= \frac{T_1 - T_2}{R_2} \\
\dot{Q}_3 &= \frac{T_2 - T_3}{R_3}
\end{aligned}
\tag{4.3}
$$

This gives the following state equation:

$$
\begin{bmatrix} \dot{T}_1 \\ \dot{T}_2 \end{bmatrix} = \begin{bmatrix} -\left(\frac{1}{R_1C_1} + \frac{1}{R_2C_1}\right) & \frac{1}{R_2C_1} \\ \frac{1}{R_2C_2} & -\left(\frac{1}{R_3C_2} + \frac{1}{R_2C_2}\right) \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \end{bmatrix} + \begin{bmatrix} \frac{1}{R_1C_1} & 0 \\ 0 & \frac{1}{R_3C_2} \end{bmatrix} \begin{bmatrix} T_f \\ T_3 \end{bmatrix}
\tag{4.4}
$$

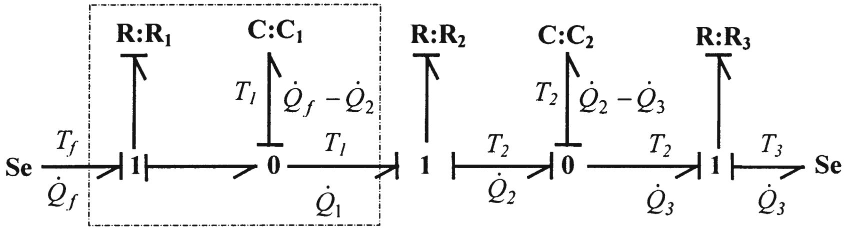


FIGURE 4.5. Bond graph model with added thermal capacity of the wall

4.3 Selection of Liaison Variables in Process Engineering Systems

4.3.1 Introduction

The bond graph method is perfectly well suited to mechanical and electric systems. For them the flows are velocity and electric current, and the effort is force and voltage (the so called inverse analogy will by treated quickly in the appendix, but is not important in practice). This gives a true bond graph, where the product of effort and flow is equal to the power transferred in the bond.

True bond graphs in thermal and chemical engineering introduce complex variables like entropy and chemical potential, which do not obey simple conservation laws. Therefore one uses pseudo-bond graphs where the product effort and flow is no longer a power. On the table 4.1 are shown the liaison variables for the true and the pseudo variables in process engineering.

Field	True Bond Graph		Pseudo Bond Graph	
	Effort (e)	Flow (f)	Effort (e)	Flow (f)
Chemistry	Chemical tension μ $(J/mole)$	Molar flow $\dot{n}$ $(mole/s)$	Concentration C $(mole/m^3)$	Molar flow $\dot{n}$ $(mole/s)$
Hydraulic	Pressure P (pa)	Volume flow $\dot{V}$ (m^3/s)	Pressure P (pa)	Mass flow $\dot{m}$ (kg/s)
Thermal	Temperature T (K)	Entropy flow $\dot{S}$ $(J/(K.s)$	Temperature T (K) or specific enthalpy h (J/kg)	Heat flow $\dot{Q}$ (w) or enthalpy flow $\dot{H}$ (w)

TABLE 4.1. Liaison variables for true and pseudo bond graph in process engineering

As noted above, the choice of the liaison variables is not fixed and depends on the system.

Let us define the choice of liaison variables for several systems used in process engineering.

4.3.2 Liaison Variables for Thermodynamic Systems

Thermal Conduction

With matter at rest, that is heat conduction like trough the wall of heat exchanger and one can use both a true bond graph with the pair entropy flow - temperature $(\dot{S}, T)$ or the pseudo bond graph with heat flow - temperature $(\dot{Q}, T)$. In practice, the last one is more convenient, because it leads to a simple constitutive equation, also called law of Fourier or thermal Ohm's law:

$$\dot{Q} = K_C (T_1 - T_2)$$

On the other hand, the use of entropy flow needs to modulate the thermal conductance by the temperature as shown by the equation (4.5), deducted from equation (1.40) and the corresponding bond graph of the figure 4.6a.

$$\dot{S}_2 - \dot{S}_1 = K_C \frac{(T_1 - T_2)^2}{T_1 T_2} \tag{4.5}$$

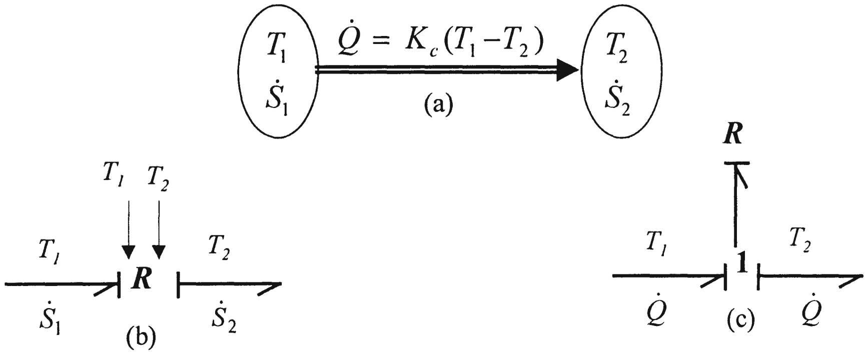


FIGURE 4.6. Liaison variables for thermal conduction a. Schematic b. Modulated resistance for the pair

Convection in Fluid Flow

In convection of fluid, we have two coupled energies, hydraulic and thermal. For the hydraulics, we use as liaison variables the pair $(\dot{m}, P)$. For thermal, the enthalpy flow $\dot{H}$ is used, which represents the total energy per time unit transported by the fluid and therefore the total power transported. As effort variable, one uses always the pressure P, and the temperature T or the specific enthalpy h. The enthalpy flow is calculated by the expressions:

$$\begin{aligned} \dot{H} &= \dot{m} c_p T \\ \dot{H} &= \dot{m} h \end{aligned} \tag{4.6}$$

Using specific enthalpy as effort variable instead of temperature appears at first more involved, but it can be determined easily from the state variables m (mass) and global enthalpy H :

$$h = \frac{H}{m}$$

The determination of temperature requires also the specific heat c_p:

$$T = \frac{H}{mc_p}$$

However, this variable is measurable by the sensors, therefore suitable for control system.

As mentioned above, the choice of the effort thermal variable depends on the state of modelled fluid. Let us examine for the main process engineering phenomena, the choice of the variable of thermal effort (h or T). Regarding the hydraulic power variables, one always uses the pair ($\dot{m}$, P) because in thermofluids, the energies being coupled, the enthalpy flow $\dot{H}$ is calculated from mass flow $\dot{m}$ using the equation (4.6).

In function of thermodynamic state of the mixture water-vapour, one distinguish. In thermal engineering the following cases:

- Fluid at normal temperature below its saturation state

Here one has advantage to use the temperature as effort variable, because the specific heat c_p depends only very weakly on the temperature: as example, for water, the specific heat varies only from $4,185\,kJ/(kg.^\circ C)$ to $4,217\ kJ/(kg.^\circ C)$ between a temperature of 15 to $100^\circ C$ [*Positello, 1982*]. Also, manipulation of temperature is very comfortable for control engineering and appears natural for the human operator.

- Fluid at saturated temperature

Since the liquid is at saturation, one can determine at each temperature the corresponding enthalpy. But the specific heat varies with temperature, so it is difficult to calculate the enthalpy flow. Therefore, it is better to use the pair enthalpy flow - specific enthalpy ($\dot{H}, h$). Furthermore, this choice allows to find other variables like mixture ratio X in a two phases (water and vapour) and to use in this way the thermodynamic tables.

Choice of Flow Variables for an Accumulator

Next we discuss the choice of variables for an accumulator of a mixture water- vapour as shown by the bond graph (Fig. 4.7) with a multiport C.

Neglecting kinetic energy and gravity and supposing perfect thermal insulation, the variation of internal energy stored by a thermodynamic system:

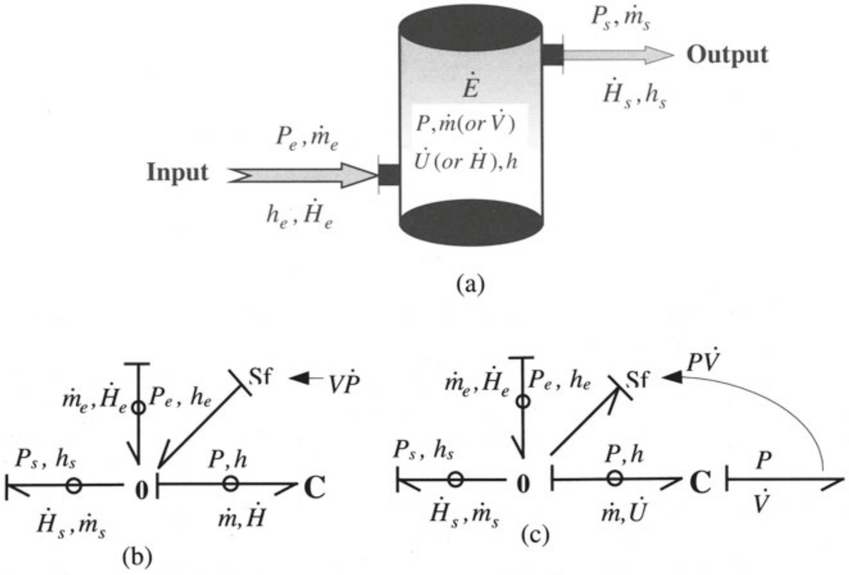


FIGURE 4.7. Choice of flow variables for an accumulator. a. Schema, b. $\dot{H}$ as flow variable, c. $\dot{U}$ as flow variable.

$$\dot{U} = \dot{E} + \dot{H}_e - \dot{H}_s \tag{4.7}$$

where $\dot{H}_e$ and $\dot{H}_s$ are the enthalpies entering and leaving of the accumulator. $\dot{E}$ is the power of due to pressure and is equals to the product of pressure P and variation of vapour volume $\dot{V}$:

$$\dot{E} = -P\dot{V}$$

Equation (4.7) becomes:

$$\dot{U} = -P\dot{V} + \dot{H}_e - \dot{H}_s \tag{4.8}$$

We see that the choice of $\dot{U}$ as flow variable makes appear a state variable V. Hence we need an additional bond $(P, \dot{V})$ of which the hydraulic power $P\dot{V}$ modulates this flow source. This is the price to pay for connecting a pseudo to a true bond graph [*Karnopp, 1979*].

On the other hand, if one takes as flux variable $\dot{H}$, as shown on figure 4.7b, one obtains from equation (4.8) by replacing U by $H - PV$:

$$\dot{H} = V\dot{P} + \dot{H}_e - \dot{H}_s \tag{4.9}$$

Summarizing, in equation 4.9 we have a fictitious power, which is calculated from the volume V, a geometric quantity, and from the pressure P of the accumulator. The structure of the calculation is analogous to the block diagram on the figure 3.14b.

Steam Expansion

In process engineering, one encounters often expansion of vapour through hydraulic resistors, also called restrictors, which are described by a multiport R as shown on figure 4.8. This expansion is normally under constant enthalpy, as shown by the vertical arrow on figure 4.8b. Exceptionally, the expansion can be under reduction of enthalpy, with the multiport R cooled from the outside, as shown by the oblique arrow.

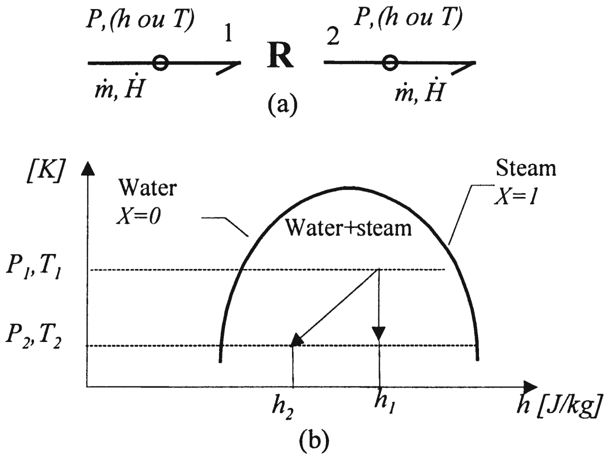


FIGURE 4.8. Steam expansion through a restriction. a. Bond graph model, b. simplified Mollier chart

- Isenthalpic steam expansion

Under constant enthalpy (isenthalpic expansion), pressure, temperature and mixture ratio X varies

$$\begin{gathered} h_1 = h_2 \\ T_1 \neq T_2 \\ P_1 \neq P_2 \end{gathered}$$

but mass flow and enthalpy flow remains constant:

$$\begin{gathered} \dot{m}_1 = \dot{m}_2 = \dot{m} \\ \dot{H}_1 = \dot{H}_2 = \dot{H} \end{gathered} \tag{4.10}$$

where the indices 1 and 2 correspond to upstream and downstream the resistor.

With saturated fluid and using equation (2.4) for the mass flow, and with the relation between pressure and temperature $T_1 = f_T(P_1)$ as shown in appendix C, we calculate

$$\begin{aligned}
\dot{m} &= \frac{K_d A}{2} \frac{P_1}{\sqrt{0,459P_1^2 + 12,7243P_1 + 99,005}} \quad \text{if } \; P_2 < 0,5P_1 \\
\dot{m} &= K_d A \sqrt{(P_1 - P_2) \frac{P_2}{0,459P_1^2 + 12,7243P_1 + 99,005}} \quad \text{if } \; > 0,5P_1 \\
\dot{H} &= \dot{m} h_1
\end{aligned} \tag{4.11}$$

The bond graph model and bloc diagram, are given by figure 4.9.

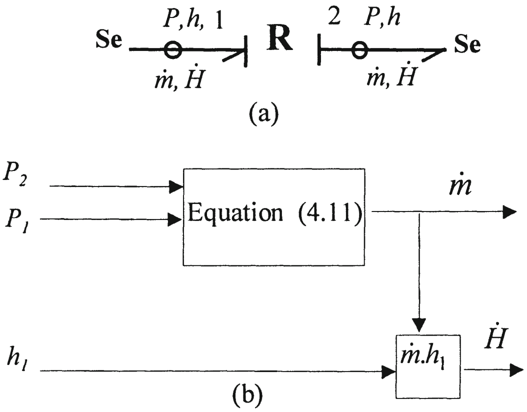


FIGURE 4.9. Steam expansion under constant enthalpy. a. Bond graph model, b. bloc diagram

- Real steam expansion

In the case of a real expansion with thermal losses, we have:

$$\begin{aligned}
h_1 &\neq h_2 \\
T_1 &\neq T_2 \\
P_1 &\neq P_2
\end{aligned}$$

and for the flows,

$$\begin{aligned}
\dot{m}_1 &= \dot{m}_2 \\
\dot{H}_1 &\neq \dot{H}_2
\end{aligned}$$

This is modelled by the bond graph given by figure 4.10. The multiport R represents the dissipation of hydraulic and thermal energy in the restrictor. The heat conduction toward the environment $\dot{Q}_{ex}$ is shown by a simple bond. The corresponding bloc diagram appears on figure 4.10b.

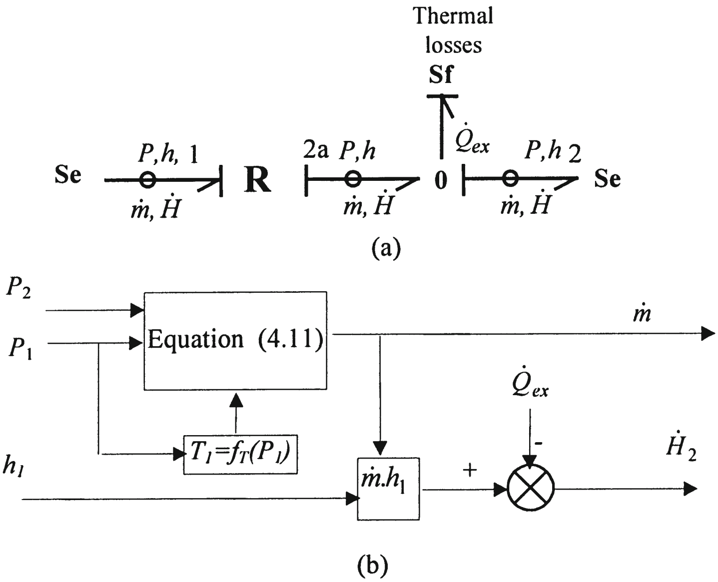


FIGURE 4.10. Real steam expansion. a. Bond graph model, b. Block diagram

The enthalpy flow downstream is calculated by:

$$\dot{H}_2 = \dot{H}_{2a} - \dot{Q}_{ex} = \dot{m}h_1 - \dot{Q}_{ex} \tag{4.12}$$

The mass flow comes from equation (4.11). The block diagram is given by the figure 4.10b.

The conclusion is that for isenthalpic and real expansion, one uses for thermal energy the couple $(h, \dot{H})$ as effort and flow and for the hydraulic power the couple $(P, \dot{m})$.

It follows from equations (4.11) and (4.12) the determination of flows in an expansion requires only the enthalpy and the pressures upstream and downstream. The temperature can always be calculated as function of pressure since the mixture is at saturation. Furthermore, since the specific heat is variable, using temperature as effort would not allow to calculate the thermal flows.

These liaison variables allow to calculate the mass and thermal flow and further the quality or mixture ratio in a two phase fluid as water–steam.

Vapour and Phase Change

Here we have to distinguish evaporation and condensation.

- Evaporation

We have seen that using a pseudo bond graph with the pair of variables $(P, \dot{m})$ and $(h, \dot{H})$ allows access on another important variable, the quality X by using thermodynamic tables.

- Condensation

Condensation of vapour goes with exchange of heat with a cold body. We have seen in section 3.3.3 that we have two thermal effects simultaneously: heat conduction towards the coolant and convection of the condensate.

We use for this the pairs of variables $(T, \dot{Q})$ for the thermal power and $(p, \dot{m})$ for the hydraulic power. As said, those variables are strongly coupled. The mass flow of condensate depends also on both hydraulic and thermal efforts, it is really a function of latent heat, determined from the specific enthalpy h. Other parameters are vapour temperature and more.

4.3.3 Choice of Liaison Variables for Chemical Systems

In the chemical systems one could distinguish the liaison variables modelling the chemical transformation of the reaction and those modelling the kinetic phenomenons of the reaction.

Regarding transformation phenomenon of the reaction, the effort is the chemical potential μ which form with the molar flow $\dot{n}$ a true bond graph. In a pseudo bond graph, as effort variable, is used the concentration C instead of the chemical potential. As flow variable, is used the molar flow $\dot{n}$. Note that in the same conditions, the chemical potential μ of the species i depends on its concentration as given by the equation (3.55).

In other research works, as effort variable is used the concentration of the substance instead of the chemical potential and as flow variable is used the derivative of the concentration. This approach is extensively used [*Lefèvre, 1985*] because it allows to manipulate more intuitive variables and easily measurable (concentration) therefore easy to simulate.

Regarding the liaison variables of the kinetic phenomenons of the reaction are used, for the effort, the chemical affinity A in $(J/mole)$ and for the flow the speed of reaction $\dot{\xi}$ in $(mole/s)$.

We resume the selection of liaison variables in process engineering and chemical system in the table 4.2.

Physical domain	Liaison variable		Power	
	Effort (e)	Flow (f)	Thermal $\dot{H}$	Hydraulic $\dot{m}$
Conduction	T	$\dot{Q}$	$\dot{Q} = K\Delta T$	
Convection (non saturated)	h (*or* T), P	$\dot{H}$, $\dot{m}$	$\dot{H} = \dot{m}h$ $\dot{H} = \dot{m}c_pT$	$\dot{m} = K\Delta P$
Convection (saturated)	h, P	$\dot{H}$, $\dot{m}$	$\dot{H} = \dot{m}h$	equ. (2.4)
Steam expansion	h, P	$\dot{H}$, $\dot{m}$	$\dot{H} = \dot{m}h$	equ. (2.4)
Evaporation	h, P	$\dot{H}$, $\dot{m}$	$\dot{H} = \dot{m}h$	equ. (3.29)
Condensation	h (and T), P	$\dot{H}$ and $\dot{Q}$, $\dot{m}$	$\dot{H} = \dot{m}h$ $\dot{Q} = K\Delta T$	equ. (3.36)
Chemical systems	Effort	Flow	Chemical power	
(transformation)	μ or C	$\dot{n}$	$\dot{E} = \dot{n}\mu$	
(kinetic)	A	$\dot{\xi}$	$\dot{E} = A\dot{\xi}$	

TABLE 4.2. Selection of liaison variables in process engineering

4.4 REFERENCES

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5

Industrial Application of Bond Graph Modelling

5.1 Filling of Pneumatic Automobiles

5.1.1 Bond Graph Model

This chapter is devoted to bond graph modelling and simulation of real industrial systems. We shall not follow the different stages of model building of chapter 4 since we have the practical problem to design, model and simulate different processes by a bond graph.

Our first example concerns a pneumatic automobile, which is supposed has as fuel tank an air reservoir, that is filled up to $20MPa$ while empty it still has a pressure of $5MPa$. Such automobiles have better performances than electric cars. The problem is of course to design a pneumatic motor working with this high pressure range, much higher than the usual pneumatic systems of $0.7MPa$.

Naturally, from time to time these cars must approach a service station to fill up air. The filling up time as of the order of 2 minutes, much shorter than with electric cars. We shall simulate here the dynamics and thermals of the filling process.

The service station is shown on the schema of figure 5.1 with a large reservoir of 3000 litres and a small reservoir in the car of 300 litres. The valve R indicated by an oblique arrow indicates that this resistor is regulated and opened after connection. As said, the car has 5 MPa empty and should be connected to the 20 MPa at the station.

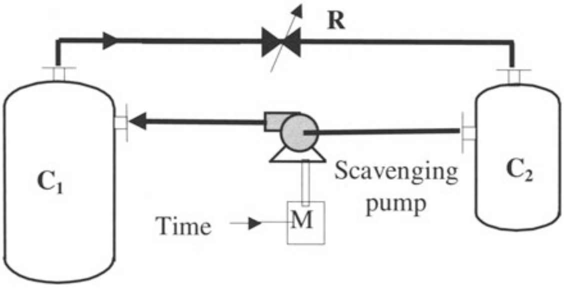


FIGURE 5.1. Circuit for the pneumatic filling station

The air in the small reservoir is compressed and its temperature increases, while the big reservoir becomes a little cooler. So, after filing, one interposes a scavenging process, that delivers air from the small to the big reservoir by means of a scavenging pump. Since the pressures are then equal, the pump consumes little power.

Figure 5.2 shows the bond graph model with an R element for the valve and a transformer TF for the pump. It is driven by a small electric motor turning at constant frequency represented as a flow source Sf.

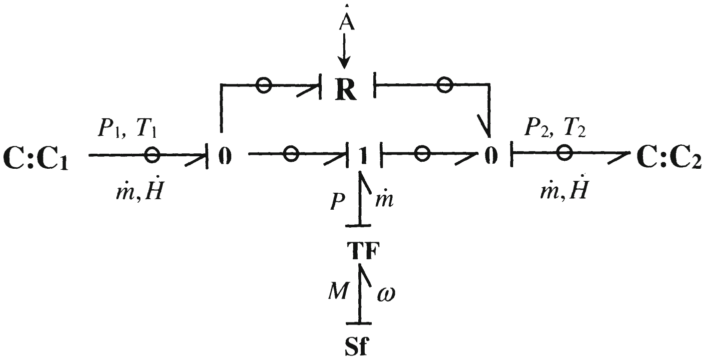


FIGURE 5.2. Bond graph for filling and scavenging of pneumatic automobiles

5.1.2 Simulation by TUTSIM Program

Our interest is the evolution and dynamics of the pressures and temperatures in both reservoirs, and the mass flow $\dot{m}_{31}$ through the resistor R. The corresponding bloc diagram is shown on figure 5.3. The referentials are those used by the program TUTSIM and the listing is given in appendix B.2.

The mass flow $\dot{m}_{31}$ is calculated according to relations 2.4 as mentioned in chapter 2.

$$\dot{m}_{31} = \frac{K_d A}{2} \frac{P_{13}}{\sqrt{T_{14}}} \tag{5.1}$$

The enthalpy flow is determined by multiplying $\dot{m}_{31}$ by specific heat at constant pressure c_p and temperature T_{14} of the reservoir C_1.

$$\dot{H}_{32} = \dot{m}_{31} c_p T_{14} \tag{5.2}$$

The figure 5.3b shows the block diagram for calculation of mass flow and enthalpy flow of the pump. The pump for scavenging is started after 15 s and stopped after 90 s by the logic bloc, FNC46 as shown in appendix B.2.

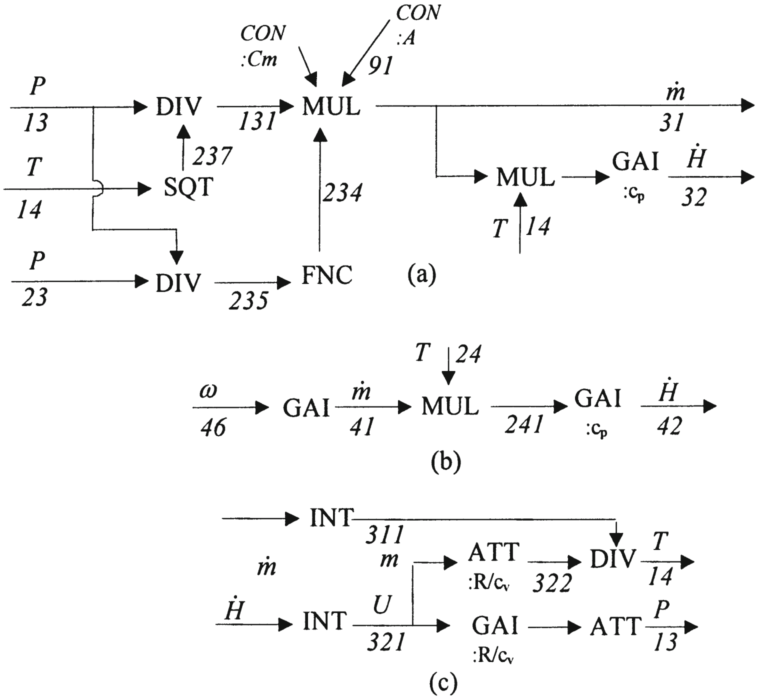


FIGURE 5.3. Block diagram corresponding to the principal parts of the bond graph. a. Resistance Reco, b. Pump, c. Coupling capacitors.

The figure 5.3c shows the block diagram for calculation of pressure and temperature of the multiport C_1, which has the volume V_{13} . using ideal gas law, $PV = mRT$ in with $U = mc_vT$, one obtains:

$$\begin{aligned} T_{14} &= \frac{U_{321}}{m_{311}c_v} \\ P_{13} &= \frac{U_{321}R}{V_{13}c_v} \end{aligned} \tag{5.3}$$

Similar expressions are valid for C_2, the small reservoir in the car.

Simulation results

For the choice of parameters, namely to avoid too large or too small parameters, one must choose the units. Generally, it is necessary to avoid parameters over a million and below one million. Other specialists are stricter and limit the values to one thousand and one divided by one thousand. This is obtained in our simulation by taking as pressure unit $1MPa$, mass flow in kg/s and enthalpy flow in kW. The mass will then be in kg and the energies in kJ.

It is convenient to write all parameters together in a checklist. This appears as table 5.1 for simulation of filling pneumatic automobiles.

Element	**Designation**	**Value**	**Unit**
FNC234	Characteristic of air jet	table	-
INT311	Accumulated mass in tank C_1	770	kg
INT611	Accumulated mass in tank C_2	$19,3$	kg
INT321	Internal energy stored by C_1	150	kJ
INT621	Internal energy stored by C_2	$3,75$	kJ
ATT322, 622	Specific heat at constant volume c_V	$0,78$	$kJ/(k.kg)$
GAI323, 623	$R/\ c_v$	$0,4$	–
GAI41	Mass flow of pump	–	kg
ATT13	Volume of tank C_1	3000	$litre$
ATT23	Volume of tank C_2	300	$litre$
CON132	Flow constant	$0,060$	$\frac{kg\sqrt{K}}{s.Mpa.m^2}$
A91	Flow area of valve Reco	113	m^2
GAI32, 42	Specific heat at constant pressure c_P	$1,005$	$kJ/(K.kg)$

TABLE 5.1. Parameter checklist for air fuelling

Figure 5.4 shows the simulation results made on a PC. As expected by theory, in figure 5.4b we see that the pressures in both reservoirs become equal after $15s$ but the temperature in the automobile goes from 300 to 380 K. Then we scavenge until 90 s.

5.2 Cooling of Diesel Fuel

5.2.1 Bond Graph Model

Here we treat a thermal bond graph for an industrial application, the cooling of fuel between a reservoir and the injection pump for a diesel passenger car. The circuit appears in figure 5.5 with the fuel going from the tank to the injection pump through the heat exchanger $Hexa$ 6. There a part goes to the injectors, while the overflow goes trough $Hexa$ 2 and 3 to another reservoir, called canister; it is arranged inside the tank 5. Between canister and tank we have thermal conduction. From the canister the fuel returns through $Hexa$ 6 to the injection pump.

All heat exchangers bring heat to the environment. The purpose of the study is to dimension the heat exchangers $Hexa$ 3 and 6 so that the temperature of the fuel does not exceed 80°C.

The bond graph of the system, which is a pseudo multi-bond graph with pressure and temperature as efforts and mass flow and enthalpy flow as

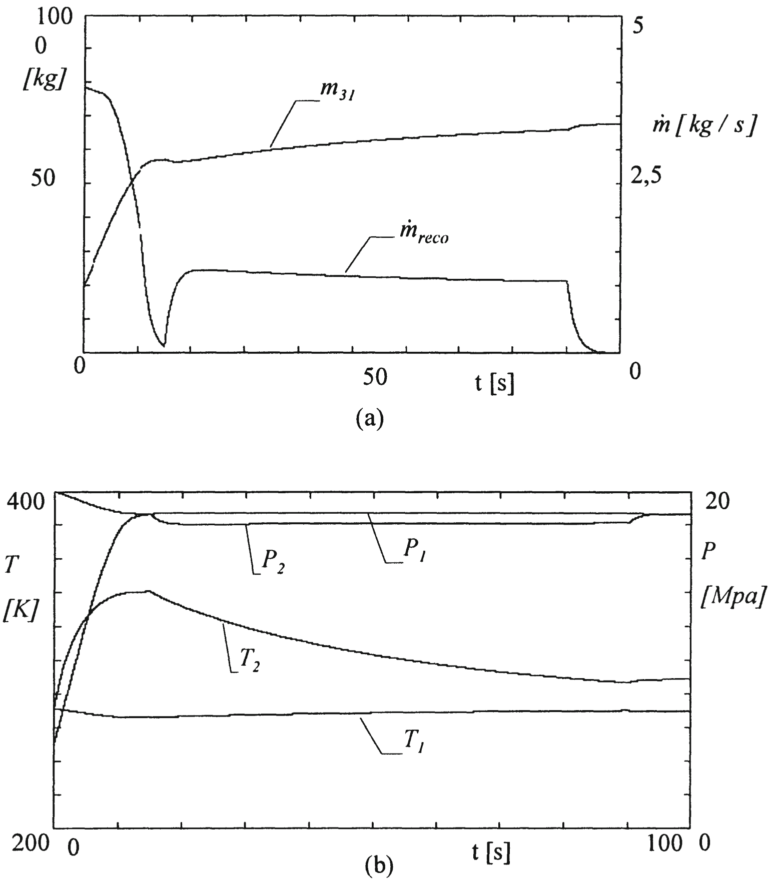


FIGURE 5.4. Simulation results of filling pneumatic automobiles, a. Evolution of mass of air and mass flow through the resistance R, b. Evolution of efforts, pressure and temperature

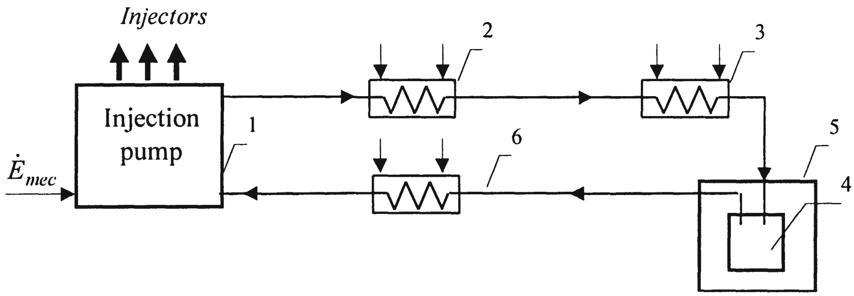


FIGURE 5.5. Fuel circuit in the passenger car

flow variable is given by the figure 5.6. The accumulation of energy comes in the multiports C, which can be associated to the real volumes (canister 4 and tank 5) or to the dead volumes in the conduits. The simple bonds, not multibonds show thermal conduction between canister 4 and tank 5. The exchange of heat with the environment takes place in the elements $Hexa$, it is represented by a thermal effort source $Se28$. The mechanical power $\dot{E}_{mec}$ of the injection pump can be considerable and heat the fuel; therefore it is shown by the flow source $Sf610$, which increase the enthalpy flow in the fuel.

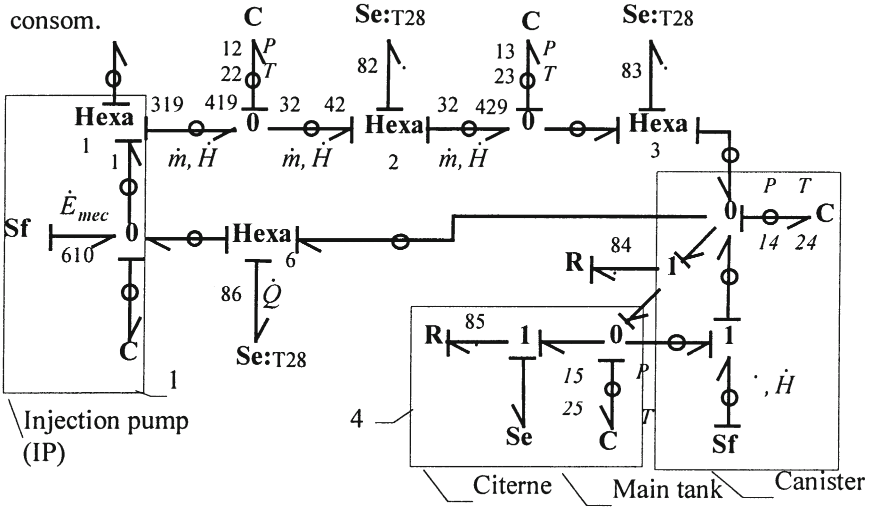


FIGURE 5.6. Bond graph model of the coupling circuit for the diesel fuel

The enthalpy flow comes from multiplying the mass flow, specific heat and temperature upstream. For liquids, specific heat at constant pressure c_p and constant volume c_v are practically equal.

The mass flow $\dot{m}_1$ and enthalpy flow $\dot{H}_1$ in an injection pump are given by:

$$\begin{aligned} \dot{m}_1 &= \dot{m}_6 (1-\varphi) \\ \dot{H}_1 &= \left(\dot{H}_6 + \dot{E}_{mec}\right)(1-\varphi) \end{aligned} \tag{5.4}$$

where φ is the fraction of fuel used and $(1-\varphi)$ the excess returned to the tank.

The thermal flow is transmitted by conduction from the canister 4 to the tank and from the tank to the environment respectively by the following equations:

$$\begin{aligned} \dot{Q}_{84} &= \frac{1}{R_{th84}} \left(T_{24} - T_{25} \right) \\ \dot{Q}_{85} &= \frac{1}{R_{th85}} \left(T_{24} - T_{28} \right) \end{aligned} \tag{5.5}$$

Where R_{th84} and R_{th85} are the corresponding thermal resistances. T_{24} is the temperature in the tank 4 determined by constitutive equation of C element in integral causality:

$$T_{25} = \frac{1}{C_4} \int \left(\dot{Q}_{84} - \dot{Q}_{85} \right) dt \tag{5.6}$$

C_4 is the global heat capacity of tank 4.

Mass and enthalpy flow of the fuel returning from tank 5 to canister 4 are shown by a coupled flow source $Sf34$ and $Sf44$. The constitutive equations of $Hexa$ 2 are:

$$\begin{aligned} \dot{m}_{32} &= \frac{1}{R_{hy}} \left(P_{12} - P_{13} \right) \\ \dot{H}_{42} &= c_v \dot{m}_{32} T_{22} \end{aligned} \tag{5.7}$$

and the enthalpy flow out is

$$\dot{H}_{429} = \dot{H}_{42} - \dot{Q}_{82} \tag{5.8}$$

where $\dot{Q}_{82}$ is the thermal flow dissipated to the environment and calculated as follows:

$$\dot{Q}_{82} = \frac{1}{R_{th82}} \left(T_{22} - T_{285} \right) \tag{5.9}$$

5.2.2 Simulation Results

This work was done for Canadian Industry and the listing is given in appendix B.3. The results of one simulation is given by figure 5.7.

We have brought this as an example of the use of simulation in automobile industry, where the question was the required size of the various heat exchangers. In principle, we have a very simple model, consisting of heat exchangers and coupling capacitors. A part of these capacitors is given by the volume of the canister and the tank. The heat conduction between those two elements and to the environment comes in simple thermal elements R.

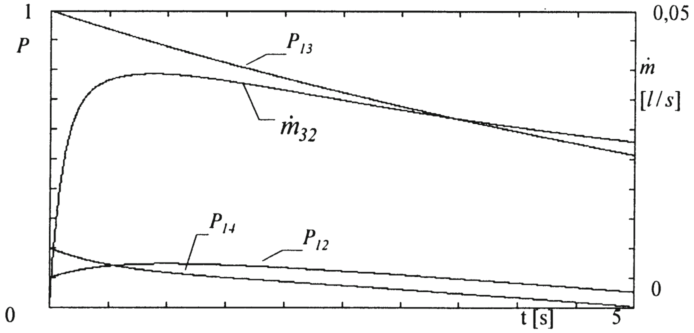


FIGURE 5.7. Simulation result of cooling of diesel fuel

5.3 Ventilation of Buildings

5.3.1 Bond Graph Model

The ventilation of buildings is another application of thermodynamic bond graphs, which is characterized by very low pressures. Indeed, the overpressure (over the atmosphere) is about $1kPa$ (100 mm water column in the old system), while the atmospheric pressure is about $100kPa$ or $10000mm$ water. This requires different units of measurement, as we shall see below, in order to facilitate the working of the computer. The use of bond graphs for problems of such kind shows graphically the dynamics of thermal phenomena in houses and buildings and the subsequent optimization of the heat transfer coefficients.

Like all thermal cases, we have thermal pseudo bond graphs with mass flow and enthalpy flow. The coupling capacitors, as known before from the gas turbines, are here given by the compressibility of air in the rooms and by its heat capacity.

We explain the process on the examples of two rooms in a building as shown on figure 5.8. For simplicity, we take electric heating which delivers simply heat flow.

The corresponding multi bond graph for the heating of the building appears on figure 5.9.

We have designated by VENT the aeration or leakage through the walls. The conduction through the walls is represented by the group WALL. There is also the group FANX, which represents the fan, similar to VENT, but with a mechanical power source.

The pseudo bond graph is given by the figure 5.10.

On figure 5.10 the multibond are decoupled in two single bonds: thermal bond $(T, \dot{H})$ and hydraulic one $(P, \dot{m})$. The wall is modelled by two elements in parallel connection: one is a simple resistor, the other a combination of thermal resistors (thermal tranfer by conduction to the wall

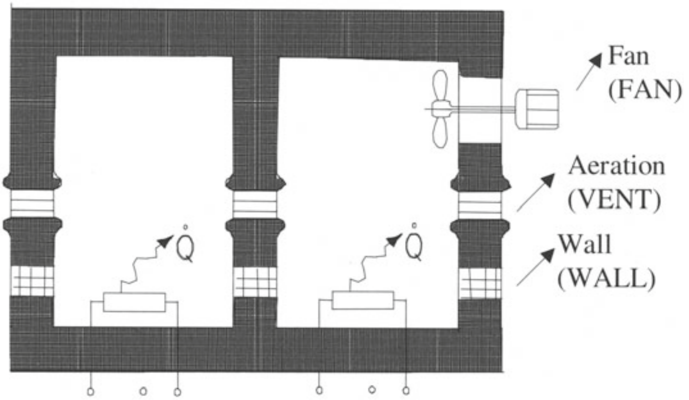


FIGURE 5.8. Scheme of two rooms in a building heated by electricity

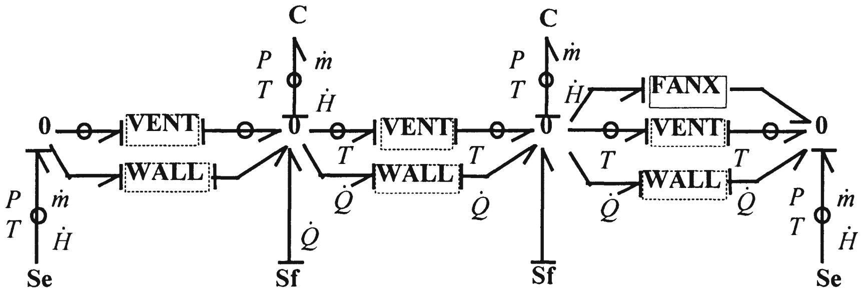


FIGURE 5.9. Bond graph of the heating of the building

and to environment) and capacitors for the heat capacity of the wall. In the trade, one calls these wall light and wall heavy, where the total heat capacity of the wall is in the wall heavy. The environment is represented by two effort sources, one for pressure (above) and the other for temperature (below). We expand each in two separate sources, to avoid having to draw long lines; both have the same pressure and temperature.

The accumulation of the air is modelled by the two ports *C* (Fig. 5.9), the upper part for hydraulics and the lower part thermal. As known from thermodynamics, it is simply energy stored in these capacitors, the distinction of thermal and hydraulic energy belongs only to the bonds. Further energy is stored in the *C*-elements belonging to the walls. The VENT and FANX are represented by a multiport *R* (Fig. 5.11).

The constitutive relations are:

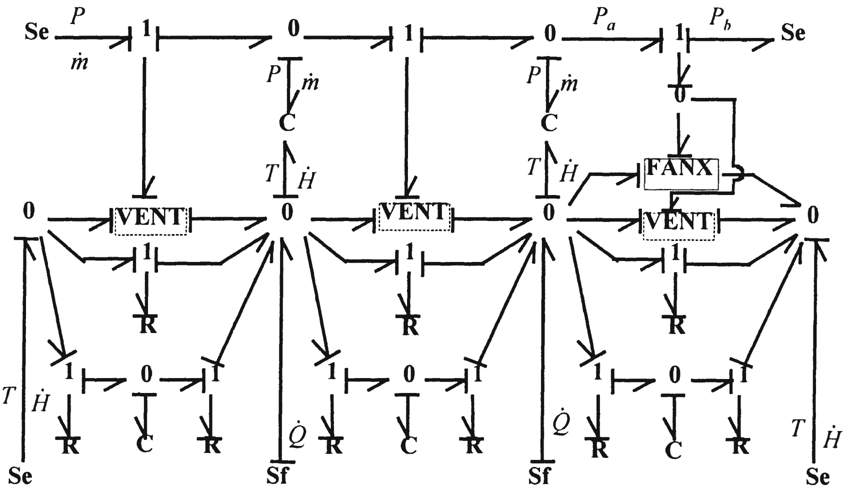


FIGURE 5.10. Detailled bond graph model of the two rooms

$$\dot{m} = \frac{1}{R}\left(P_a - P_b\right) \tag{5.10}$$

for the mass flow, and

$$\begin{aligned} \dot{H} &= \dot{m} c_p T_a \quad \text{if} \quad \dot{m} > 0 \\ \dot{H} &= \dot{m} c_p T_b \quad \text{if} \quad \dot{m} < 0 \end{aligned} \tag{5.11}$$

for enthalpy flow.

The enthalpies are calculated at absolute temperature, thus in simulations, the referential temperature T_{ref} is added to absolute value T.

The element FANX differs from the elements VENT only by an additional effort source P_{fan}:

$$\dot{m} = \frac{1}{R}\left(P_a - P_b + P_{fan}\right) \tag{5.12}$$

The effort variables pressure and temperature are calculated in multiport C. Here it is important to distinguish between the absolute values and the over pressures and over temperatures.

Let P_{ab} and T_{ab} be the absolute values ($100kPa$ and $273K$) and the over pressure and P_{ob} and T_{ob} temperature. The air is governed by the ideal gas law:

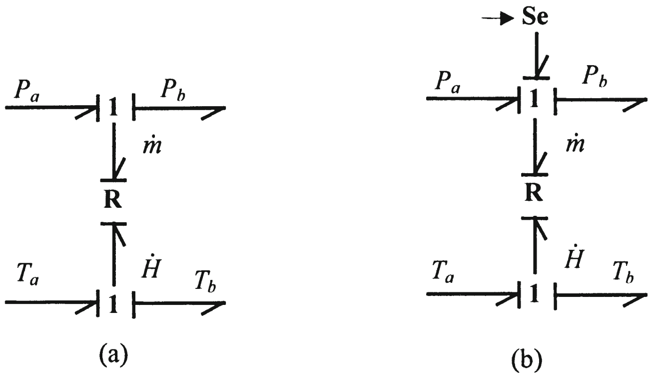


FIGURE 5.11. Bond graph model of the elements VENT (a) and FANX (b).

$$\begin{aligned}
P_{ab} &= \frac{mRT_{ab}}{V} \\
P_{ref} &= \frac{mRT_{ref}}{V} \qquad (5.13) \\
P_{ob} &= P_{ab} - P_{ref} = \frac{mR}{V}\left(T_{ab} - T_{ref}\right) = \frac{mRT_{ob}}{V}
\end{aligned}$$

The absolute internal energy is calculated by

$$\begin{aligned}
U_{ab} &= mc_v T_{ab} \\
U_{ref} &= mc_v T_{ref} \qquad (5.14) \\
U_{ob} &= U_{ab} - U_{ref} = mc_v T_{ob}
\end{aligned}$$

which leads to

$$\begin{aligned}
P_{ob} &= \frac{U_{ob}}{V}\frac{R}{c_v} \\
T_{ob} &= \frac{U_{ob}}{mc_v} \qquad (5.15)
\end{aligned}$$

The simulation of equation 5.15 is shown by the block diagram of figure 5.12. This figure carries also the physical dimensions of some variables, which are helpful to check the calculation.

Physical Dimensions of the Variables

The proper dimensions of variables are important, because it allows to avoid too large and too small numerical values. As said, all variables should be

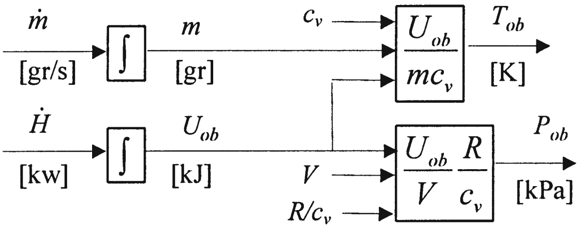


FIGURE 5.12. Block diagram of building ventilation

in the range of one divided by a million and one million, which can be obtained choosing the dimensions appropriately. We always start from the S. I. units and uses simple multiples such as one thousand or a million: So it is then a slight modification of S. I. units.

In ventilation, it is good to use the gram (gr) instead the kilogram (kg) to give the mass flow in gr/s and the kW for the power and the kJ for the energy. From this follow the other units: $kJ/(K.gr)$ for specific heats, m^3 for the volume, the kPa (Kilopascal) and the K (Kelvin) or $°C$ (Celsius) for pressure and temperature.

5.3.2 Simulation by Twentesim

This simulation was executed in Twentesim [*Twentesim, 1996*], and the bond graph given by figure 5.13 shows the bond graph drawn with program and having the typical cercles (really ellipses). They show that the program is in equations, not in bond graph; all appear as listing in appendix B.4

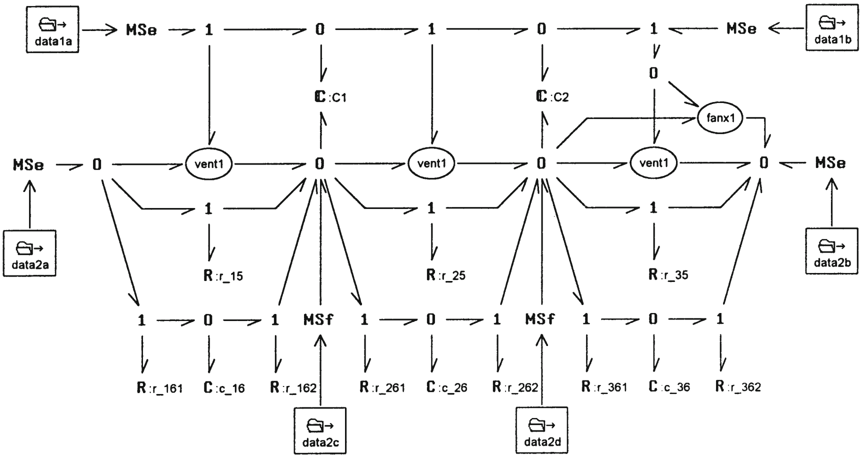


FIGURE 5.13. Bond graph model executed by Twentesim program

The figure 5.12 is similar to figure 5.10, but drawn in Twentesim. It has the typical circles indicating that this part is defined by an equation, while the other parts are defined by a bond graph.

As always, we have used the parameter checklist for the simulation, as given on table 5.2. The paracheck is a little adapted to Twentesim. In order to analyse the dynamics of building ventilation, we have simulated the start of the fan after 25s of normal working. The temperatures T_{22} and T_{32} and the pressure in room 1 decrease suddenly and the enthalpy flow increases by the additional flow of air.

Element	Designation	Value	Used unit
Data 1a, 1b	Pressure Text file		
Data 2a, 2b	Temperature Text file		
Vent 1, 2, 3			
R13	Hydraulic resistance	0.01	$kPa * s/gr$
Tref	Reference temperature	273	K
Cp	Specific heat at constant pressure	1.005	$kJ/K * gr$
Fanx			
R37	Resistance in Fanx	0.01	$kPa * s/gr$
Tref	Reference temperature	273	K
Cp	Specific heat at constant pressure	1.005	$kJ/K * gr$
Data 3	Pressure from table	Table	kPa
R161, R261, R361	Thermal resistance heavy wall 1	25	K/kW
R162, R262, R362	Thermal resistance heavy wall 2	25	K/kW
R15, R25, R35	Thermal resistance light wall	50	K/kW
C16, C26, C36	Heat capacity heavy wall	36	$kW * s/K$
C1, C2			
Cv	Specific heat at constant volume	0.718	$kJ/K * gr$
Tref	Reference temperature	273	K
R	Gas constant	0.287	$kJ/K * gr$
Pref	Reference pressure	0	kPa
V	Volume of room	60	m^3

TABLE 5.2. Parameter checklist for room heating

The simulation was executed on a PC and is shown on figure 5.14. The listings of twentesim programs are given in appendix B.4.

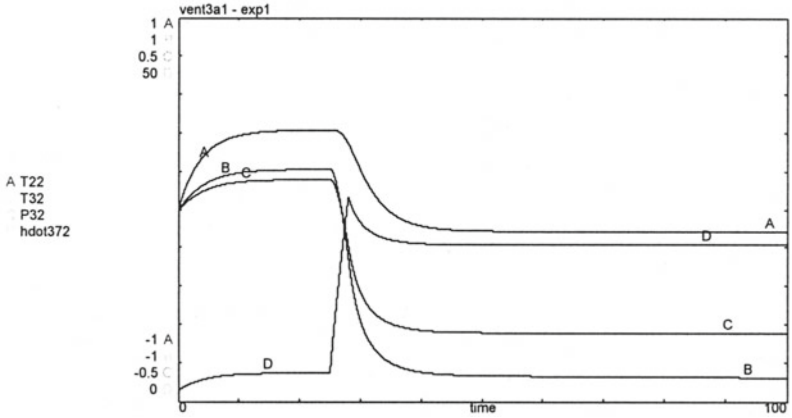


FIGURE 5.14. Simulation results of building ventilation

5.4 REFERENCES

[Twentesim, 1996] Users manual of Twentesim (20sim), Comtollab Products Inc, Box 217 NL-7500AEEnschede, Holland, 1996, fax +31 53 489 2223.

5.5 Installation of Steam Generator

5.5.1 *Description of the Process*

This installation whose overall view is shown on figure 5.15 is a pilot process in reduced scale for a nuclear power plant. It is located at the University of Lille, France in the laboratory of Automatic Control and Industrial Computer (LAIL, unit CNRS UPRESA 8021).

The test plant designed to be a scale-model of part of a power station is a complex non linear system which reproduces the same thermodynamic phenomena as the real industrial process. As shown on figure 5.15, this installation is mainly constituted of four subsystems: a receiver with the feedwater supply system, a boiler heated by a $60kW$ resistor, a steam flow system and a complex condenser coupled with a heat exchanger. The feed water flow $F3$ is circulated via two feed pumps in parallel connection. Each pump is controlled by an on-off controller to maintain a constant water level $L8$ in the steam generator. The heat power $Q4$ is determined based on the available accumulator pressure $P7$. When the accumulator pressure drops below a minimum value, the heat resistance delivers maximum power, when the accumulator reaches a maximum pressure the electrical feed of the heat resistance is cut off. The expansion of the generated steam is realized by

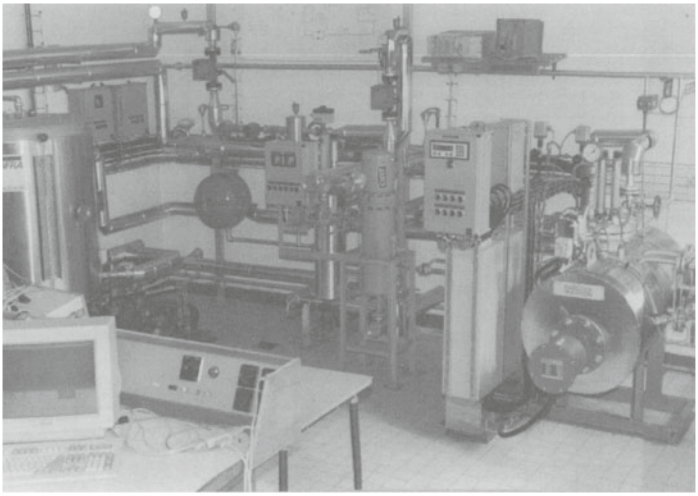


FIGURE 5.15. General view of the steam generator installation

three valves in parallel connection. $V4$ is a manual bypass valve, simulating the pass around of the steam flow to the condenser. $V5$ is a controlled position valve. $V6$ is automatically controlled to maintain proper pressure $P15$ to the condenser. In an industrial plant, the steam flows to turbine for generating power, but at the test stand, the steam is condensed and stored in a receiver tank and then returns to the steam generator.

The operating parameters of the studied pilot installation are visualized on a PC, and the sensor specifications are given in appendix B.5.

The mathematical models of a steam generator are different according the hypothesis and equations used methods of resolution and the available programs. They can be classified in linear or linearized models, non linear models and models with or without calculation of the water volume. The dynamics of the water, that is the water volume, is important, because the water height can increase and decrease and needs to be monitored. This effect is due to variation of the density of the steam and introduces a non-minimum phase elements which is very bad for stability of the system.

This effect called "shrink and swell phenomenon" will not developed in our book because it is important mainly for industrial steam boilers of large dimensions. A bond graph approach which shows the variation of water level and bond graph modelling of "shrink and swell phenomenon" in an industrial steam boiler appears in [*Rimaux, 1996*].

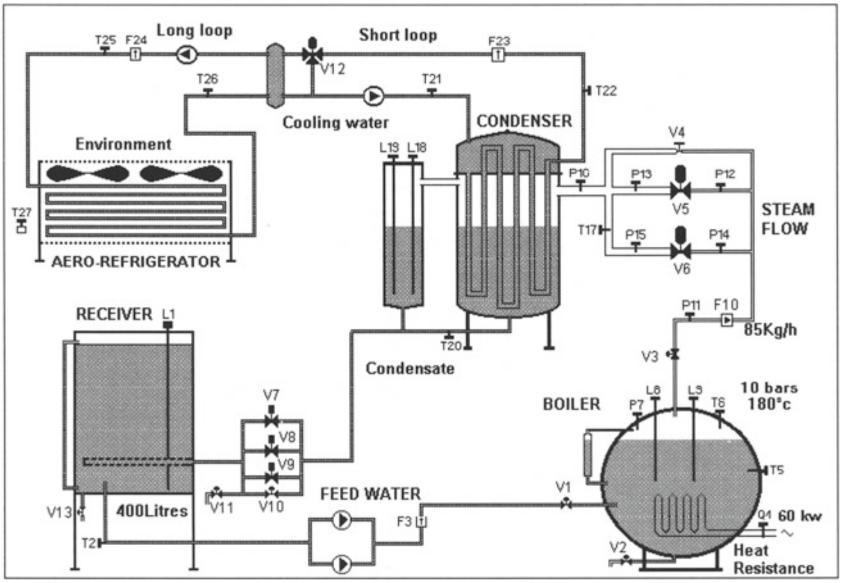


FIGURE 5.16. Scheme of the pilot installaton to be modelled

5.5.2 *Word Bond Graph of the Global Installation*

Hypothesis of Modelling

The system boiler is strongly nonlinear because of the coupling of phenomena of different nature. In effect we have different energies, electric for the heater, hydraulic for the fluid flow, thermodynamic for production of steam and mechanical for pump and valve.

We shall study separately the following subsystems: feeding installation with pump and valve; the steam boiler, expansion of steam. This last one consist of several modulating valves, the condenser with its discharge valve and finally the tank.

We have the following simplifying hypothesis:

1. For the feeding circuit the liquid, water at room temperature is incompressible.

2. In the steam boiler, denoted by GV, water and steam are in thermodynamic equilibrium, which allows to calculate the thermodynamic properties. This is justified by the fact that we have a good homogenous mixture of the emulsion water-steam. The mixture is at uniform pressure P_{GV}, which means that we neglect surface tension of the steam bubbles. The boiler has then a thermal capacity and is subject to heat losses towards the environment.

3. All variables are described by lumped parameters.

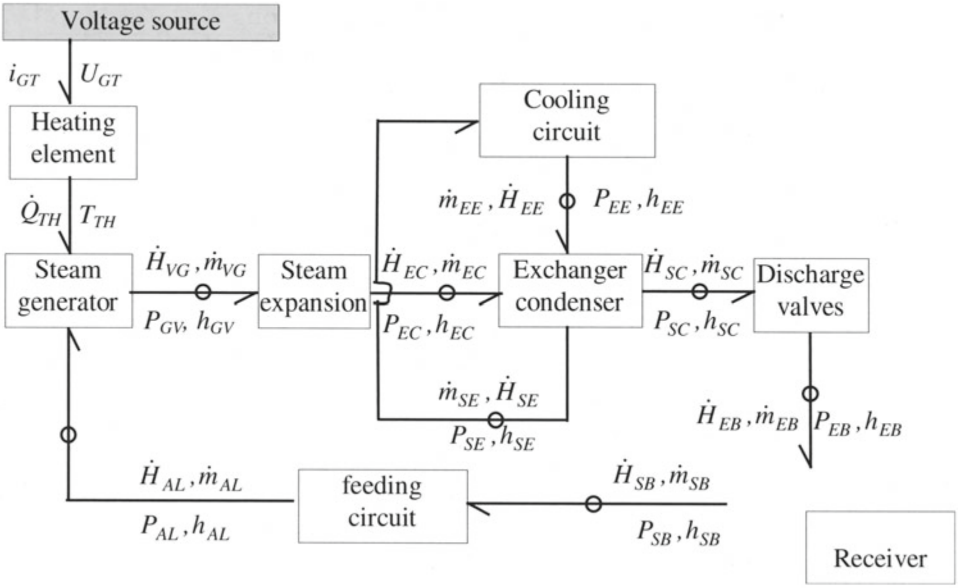


FIGURE 5.17. Word bond graph of steam generator installation

Firstly the word bond graph appears on figure 5.17, where we have given the variables, especially the powers involved. Table 5.3 gives the meaning of the different indices

5.5.3 Bond Graph Model of the Electrical Heater

Heating of the steam generator is realized by an electric element of a power of $60kW$, as represented on figure 5.18. Part (b) of this figure shows the schema of the heater and of exchanged energy. This element can be the core of a industrial nuclear reactor.

Part (a) is the bond graph model with on-off control of the electric heater as function of the steam pressure, with a relay with a dead zone ΔP_{GV}. The control is modelled by the transformer MTF modulated by Boolean variable b_2 (0,1). Since the electric heater is immerged in the steam generator, its temperature T_{TH} is practically equal to the one of the boiler T_{GV}. The system behaves like an integrator and the transmitted power will be proportional to the generator $\dot{Q}_{TH}$. The thermal capacity of the heater element will then be added to the capacity of the mixture in the interior of the steam generator.

Constitutive equations of the electric heater

- RS and MTF elements

Element	Designation	Observations
AL	Feeding circuit	Pump, valve and pipe
GV	Steam generator	Accumulator of steam
TH	Heating element	Electric resistance
GT	Electric power source	Supply the heating element
VG	Steam leaving boiler	Input of steam expansion system
EC	Entry of condenser	Comes from steam expansion
SC	Output of condenser	Goes into discharge valves
EB	Entry of receiver	Output of discharge valves
SB	Output of receiver	Input of feeding circuit
EE	Entry of exchanger	Inlet of the cooling circuit
SE	Output of exchanger	Outlet of the cooling circuit

TABLE 5.3. Meaning of the indexes in the word bond graph of the process

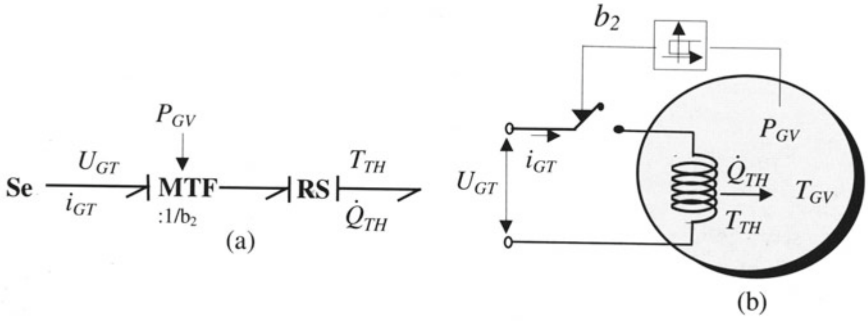


FIGURE 5.18. Electric Heater. a. Bond graph model, b. schema

The multiport RS shows the transformation of electric power $U_{GT}.i_{GT}$ into thermal power $\dot{Q}_{TH}$, as all dissipative elements RS do. The modulated transformer MTF is modulated by the Boolean variable b_2, which shows the switching on and off of the electric heater, controlled by an on-off pressure relay. The constitutive equation is

$$\dot{Q}_{TH} = b_2 \frac{u_{GT}^2}{R_{TH}} = b_2 P_{TH} \tag{5.16}$$

where R_{TH}, P_{TH} and u_{GT} are respectively electric resistance of the heater (in Ohm), heating power in J/s (or W) and the voltage u. The equation of the dead zone of the relay is:

$$b_2 = \begin{cases} 0 \text{ if } P_{GV} > P_{GVref} + \Delta P_{GV} \\ 1 \text{ if } P_{GV} < P_{GVref} - \Delta P_{GV} \end{cases} \tag{5.17}$$

where ΔP_{GV} is the dead zone and P_{GVref} is the desired pressure.

5.5.4 Modelling of Feed Water Supply System

Description of the System

The feeding circuit is built of a water conduit with a number of elbows, of a hydraulic restriction and manual valve. The water is delivered by a pump driven by an electric motor controlled by on-off relay. The regulated variable is the mass of the water N_{GV} in the steam generator. The schema appears in the figure 5.19.

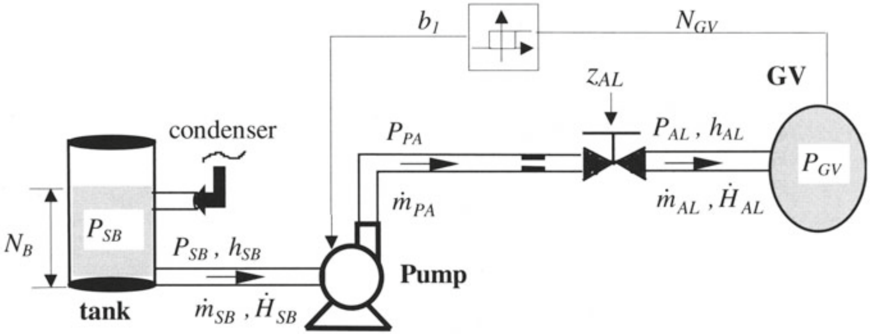


FIGURE 5.19. Schema of feed water supply system

Bond graph model of Feed Water Supply System

The hydraulic model allows to find the mass flow $\dot{m}_{AL0}$ in the feeding circuit. The mass flow is delivered from the intersection of the pump $\dot{m}_{PA}$ and of the conduit $\dot{m}_{AL}$, as shown on figure 5.20.

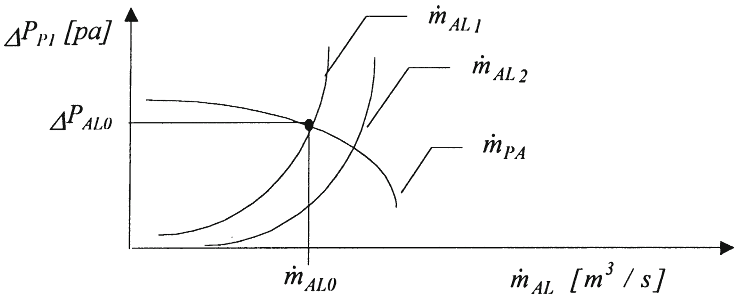


FIGURE 5.20. Determination of mass flows of the feeding circuit

The characteristic of the pump is given by the supplier as curve between the delivered hydraulic height (pressure) ΔP_{PA} (in Pa or meters water height) and the mass flow $\dot{m}_{PA}$. The bond graph model of the feeding circuit appears on figure 5.21. The pump itself is shown as an effort source in parallel with a resistor and allows to find the mass flow $\dot{m}_{PA}$.

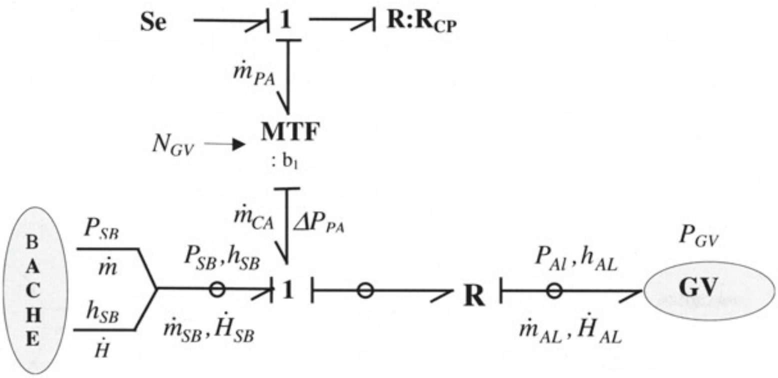


FIGURE 5.21. Bond graph model of feed water supply system

According to the selected causalities one deducts the following equations for each element.

Constitutive equations

- Element $R : R_{CP}$, pump characteristics and series junction:

$$\dot{m}_{PA} = \Phi_{RCP}(\Delta P_{PA}, Se, b_1)) \tag{5.18}$$

To illustrate, the pump characteristic for our process is given by:

$$\dot{m}_{PA} = -8,4948 * 10^{-10} \Delta P_{PA} + 9,722 * 10^{-4} \text{ (in } m^3/s)$$

- MTF element

The transformer MTF is modulated by a Boolean variable b_l coming from the relay with $b_1 = 0$ for high level and $b_1 = 1$ for low level of water in the steam accumulator. According to the selected causalities, we have the relations:

$$\begin{aligned} \dot{m}_{CA} &= b_1 m_{PA} \\ \Delta P_{PA} &= P_{SB} - P_{PA} \end{aligned} \tag{5.19}$$

where $\dot{m}_{CA}$, P_{SB} and P_{PA} are respectively, the mass flow, the out pressure of the tank and the feeding pressure from the pump.

- R Multiport and series 1 junction

The mass flow in the feeding pipe is calculated by Bernoulli law. It is non linear function of the pressure difference of the pump P_{PA} of the output pressure P_{SB}, from the tank, and of the pressure of the steam generator P_{GV} and finally of the flow coefficient $K_{D(ZAL)}$.

$$\dot{m}_{AL} = \sqrt{\frac{\rho_{AL}\left(\Delta P_{PA} + P_{SB} - P_{GV}\right)}{K_D(z_{AL})}} \tag{5.20}$$

where ρ_{AL} is the mass density of the water ($1000 kg/m^3$).

The flow coefficient depends on the details of the tubing and is function of the opening of the valve Z_{AL}. It can be calculated or determined experimentally, as we have done.

The determination of the flow towards the steam generator comes from solving the system of equations:

$$\dot{m}_{AL} = \dot{m}_{CA} \tag{5.21}$$

The output of the relay is:

$$b_1 = \begin{cases} 0 \text{ if } N_{GV} < N_{GVref} - \Delta N_{GV} \\ 1 \text{ if } N_{GV} >_{GVref} + \Delta N_{GV} \end{cases} \tag{5.22}$$

with ΔN_{GV} the dead zone of the relay and N_{GVref} the control signal of water level.

The thermal energy transported by the flow is then:

$$\dot{H}_{AL} = \dot{H}_{SB} = \dot{m}_{AL} h_{AL} \tag{5.23}$$

The enthalpy of the water becomes

$$h_{Al} = c_{pe} T_{AL} \tag{5.24}$$

The specific c_{pe} is practically constant and depends only weakly on the temperature. The temperature of the feeding water varies between 30 and 60 °C. Neglecting any thermal losses, enthalpy flow can be calculated by:

$$\dot{H}_{AL} = \dot{m}_{CA} h_{AL} = \dot{m}_{CA} h_{SB} \tag{5.25}$$

where h_{AL} is the specific enthalpy of the water, equal to the enthalpy leaving the tank. ($h_{AL} = h_{SB}$).

5.5.5 Bond Graph Model of the Boiler

Description of the Steam Accumulator

The schema of steam accumulator is given by the figure 5.22.

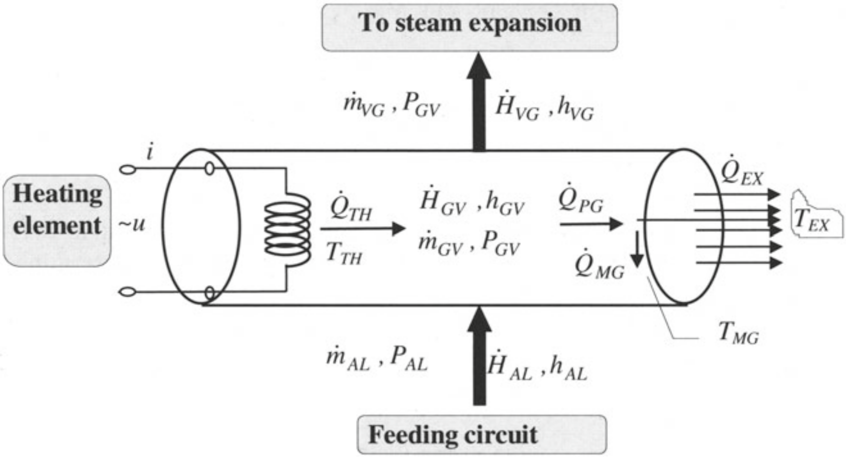


FIGURE 5.22. Scheme of accumulator of vapor

Bond Graph Model of the Boiler

The bond graph of the accumulator is shown on figure 5.23, where the storage of hydraulic and thermal energy is modelled by the two ports C. So it produces a coupled energy. The storing of heat energy by the metal of the boiler is modelled by a simple (one port) C element, while the exchange of heat goes trough R-elements. The heat transfer by conduction from the reservoir to the metal and from the metal to the environment are modelled respectively by The R elements $R : K_{Gm}$and $R : K_{EX}$. K_{Gm} and K_{EX} represent the heat exchange coefficients. External temperature is a constant effort source Se.

Temperature is used as effort in the heater, whilst the steam generator uses specific enthalpy as effort. In order to connect these models, one uses a multiport R, modulated by an anti symmetric matrix [*Tylee, 1983*]. This makes the Legendre transformation between the variables $(T_{TH}, \dot{Q}_{TH})$ and $(h_{GV}, \dot{Q}_{TH})$. The same transformation is used for going from the thermal variables of the mixture of the steam generator to the variables of the wall of the reservoir; this gives the energy losses.

The mixture is at saturation state, so the temperature T_{GV} is a thermodynamic function of the enthalpy and the pressure. Such function is given in appendix C.

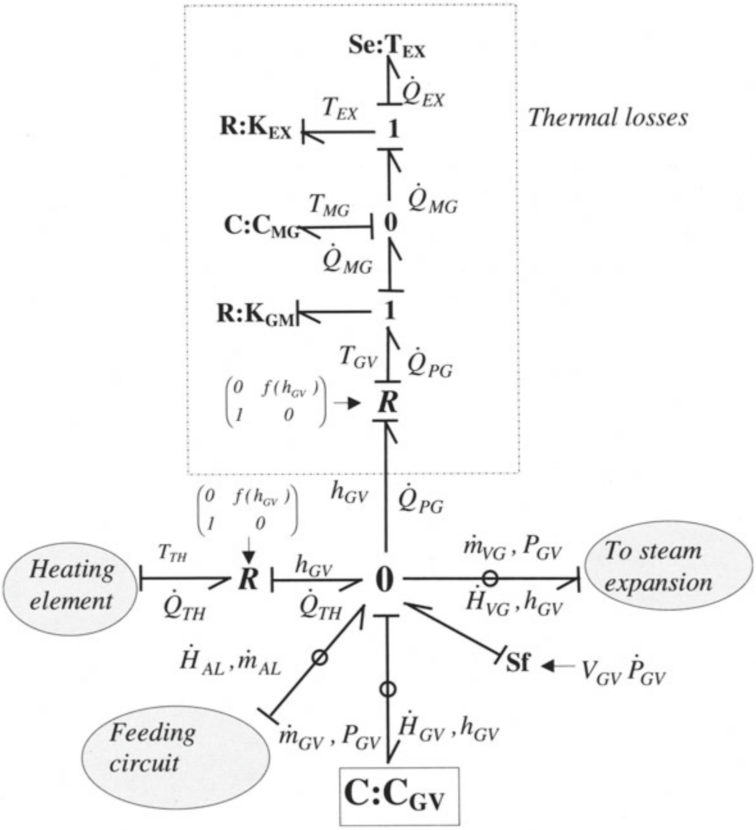


FIGURE 5.23. Bond graph model of the accumulator of steam

$$\begin{aligned} T_{GV} &= f_T(h_{GV}) \\ T_{GV} &= f_P(P_{GV}) \end{aligned} \tag{5.26}$$

Constitutive Equations

- Pseudo element R : Legendre transformation

$$\begin{bmatrix} T_{GV} \\ \dot{Q}_{TH} \end{bmatrix} = \begin{bmatrix} 0 & f(h_{GV}) \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \dot{Q}_{TH} \\ h_{GV} \end{bmatrix} \tag{5.27}$$

- Parallel Junction (0 junction): energy conservation in the steam generator

$$\begin{aligned} \dot{H}_{GV} &= \dot{Q}_{TH} + \dot{H}_{AL} - \dot{Q}_{PG} - \dot{H}_{VG} + V_{GV}\dot{P}_{GV} \\ \dot{m}_{GV} &= \dot{m}_{AL} - \dot{m}_{VG} \end{aligned} \tag{5.28}$$

where the term $V_{GV}\dot{P}_{GV}$ is the power supplied by the energy of pressurization. The volume V_{GV} is the geometric volume of the accumulator.

Since the enthalpy of steam h_{GV} and water mixture in the output of the generator is equal to the to the enthalpy of steam h_{VG} ($h_{GV} = h_{VG}$), and using the above equations, we obtain:

$$\dot{H}_{GV} = b_2 P_{TH} + \dot{m}_{AL} h_{AL} - \dot{Q}_{PG} - \dot{m}_{VG} h_{GV} + V_{GV}\dot{P}_{GV}$$

- R-elements: heat transfer from the boiler to the metal and from the metal to the environment

$$\begin{aligned} \dot{Q}_{PG} &= K_{GM}\left(T_{GV} - T_{MG}\right) \\ \dot{Q}_{EX} &= K_{EX}\left(T_{MG} - T_{EX}\right) \end{aligned} \tag{5.29}$$

- C-element: storage of thermal energy by the metal of the steam generator

$$T_{MG} = \frac{1}{C_{MG}} \int \left(\dot{Q}_{PG} - \dot{Q}_{EX}\right) dt + T_{MG}(0) \tag{5.30}$$

The global heat capacity of the metal is

$$C_{MG} = V_{MG}.\rho_{MG}.c_{metal} \tag{5.31}$$

with V_{MG} the volume, ρ_{MG} mass density and c_{metal} the specific heat of the metal.

The heat exchange coefficients K_{GM} and K_{EX} are complex, nonlinear function as given in appendix E.

- Equations of the two phase mixture

In the case of mixture water and steam, the temperature and pressure are not independent. Hence, if one chooses one parameter, the others are then determined. Equations 3.25 allows to determine the mixture ratio X, the pressure of the mixture and from this to find the corresponding temperature T_{GV}.

Appendix E.2 gives the simulation schema on MATLAB SIMULINK and the MATLAB function listing for the two phase equation 3.25.

- Water level in the steam generator

Basing on calculated mixture ratio X, the water quantity N_{GV} in the two phase mixture is determined as follows:

$$N_{GV} = (1 - X)m_{GV} \tag{5.32}$$

5.5.6 *Bond Graph Model of the Steam Expansion System*

Schema of the Steam Expansion

The steam expansion of figure 5.24 simulates the technical working of a turbine in an electric power plant. It has the purpose of creating a pressure drop after the steam boiler. This is done by several modulated valves as shown on the given figure.

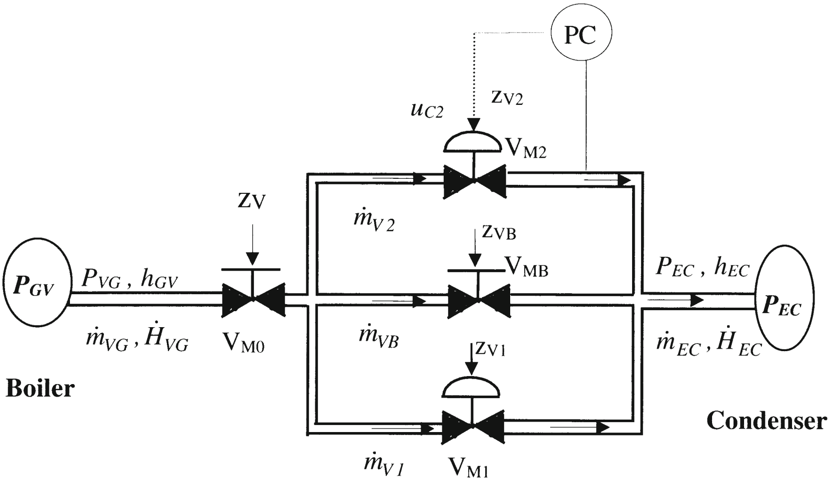


FIGURE 5.24. Schema of the steam expansion system

The valve V_{M1} is controlled from the computer in open loop control. The command value z_{ref} is the percentage of opening $(0 - 100\%)$. It simulates the skirting of steam in a real power plant. The valve V_{M2} has a closed loop as function of the pressure of the condenser P_{EC} and gives the working of the turbine. A manual bypass valve V_{MB}, closed in normal operation, allows to increase or decrease the load on the installation.

Bond graph Model of the Steam Expansion System

The global bond graph model is given by the figure 5.25. The bypass circuit V_{MB} is represented by a transformer MTF, modulated by the Boolean variable b_b. In normal operation we have $b_b = 0$, that is closed valve. The pressure P_{EC} is maintained constant by a control loop PC (pressure control).

V_{M2} is the regulating valve. V_{MB0} is normally opened and has negligible hydraulic losses.

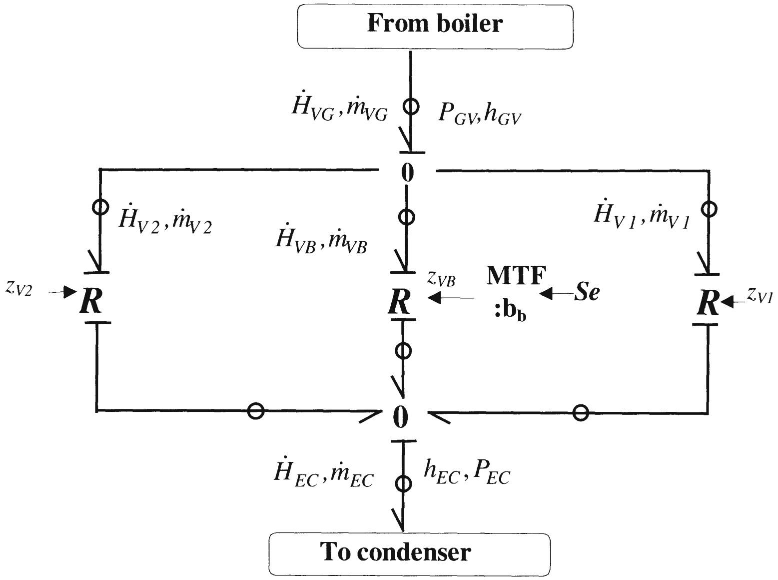


FIGURE 5.25. Bond graph model of the steam expansion system

Constitutive Equations

- Parallel Junction (0-junction)

$$\begin{aligned} \dot{m}_{VG} &= \dot{m}_{V1} + \dot{m}_{V2} + b_b \dot{m}_{VB} \\ \dot{H}_{VG} &= \dot{H}_{V1} + \dot{H}_{V2} + \dot{H}_{VB} = h_{GV} \left(\dot{m}_{V1} + \dot{m}_{V2} + b_b \dot{m}_{VB} \right) \end{aligned} \tag{5.33}$$

where $\dot{m}_{V1}$, $\dot{m}_{V2}$ and $\dot{m}_{VB}$ represent the mass flow through the valves V_{M1}, V_{M2} and V_{MB} and $\dot{H}_{V1}$, $\dot{H}_{V2}$ and $\dot{H}_{VB}$ are the respective enthalpy flows.

The mass flow in each branch is calculated by :

$$\begin{aligned} \dot{m}_i &= K_{Vi}(z_{Vi}) \frac{P_{GV}}{\sqrt{T_{GV}}} \text{ if } P_{EC} < 0.5 P_{GV} \\ \dot{m}_i &= K_{Vi}(z_{Vi}) \sqrt{(P_{GV} - P_{EC}) \frac{P_{EC}}{T_{GV}}} \text{ if } P_{EC} > 0.5 P_{GV} \end{aligned} \tag{5.34}$$

where the index i takes the value 1, 2 and B. The quantities $K_{V1}(z_{V1})$, $K_{V2}(z_{V2})$ and $K_{VB}(z_{VB})$ are the loss coefficients in the corresponding branches. These coefficients are non linear function of the position z of the valve and are determined from experimental data.

The temperature T_{VD} is equal to T_{GV} and comes from the thermodynamic relation 5.26.

The Boolean variable b_b is fixed in function of the state of the bypass valve:

$$b_b = \begin{cases} 1 \text{ if bypass valve is opened} \\ 0 \text{ if bypass valve is closed} \end{cases} \tag{5.35}$$

- Dynamics of the valve $\mathrm{V_{M1}}$

The valve $\mathrm{V_{M1}}$ is represented by a modulated resistor, which is controlled by a signal bond corresponding to the position z of the stem . The position of the valve is controlled by a relay. Therefore, the speed of displacement of the stem $\dot{z}_{V1}$ can be expressed as follows:

$$\dot{z}_{V1}= F_{V1}(sign(z_{V1ref} - z_{V1}), \tau_V) \tag{5.36}$$

where τ_V is the time time delay, about $0.2\,s$ and z_{V1ref} the set value of the bypass valve, given in % and finally F_{V1} the relay function with hysteresis.

- Dynamics of the turbine valve $\mathrm{V_{M1}}$

The valve of the turbine allows closed loop control of the pressure at the entrance of the condenser to a value P_{EC_ref} , obtained from a relay:

$$\dot{z}_{V2}= F_{V2}(sign(P_{EC\_ref} - P_{EC}), \tau_V) \tag{5.37}$$

where τ_V is a pure delay and P_{EC_ref} the set point value of pressure at the entrance of the condenser.

The transfer functions W_V of the two valves have been identified on the pilot installation. Their transfer function has been found as pure integrator with a delay:

$$W_V(p) = \frac{k}{p} e^{-\tau p}$$

The variables p and k are the Laplace operator and the gain.

The bypass valve is normally closed to allow to simulate leakage for surveillance. This is done by opening a valve and setting $b_b = 1$ on the model.

The flow at the input of the condenser equal the output of the boiler or steam generator:

$$\begin{aligned} \dot{m}_{EC} &= \dot{m}_{EC1} + \dot{m}_{EC2} + \dot{m}_{ECB} = \dot{m}_{VG} \\ \dot{H}_{EC} &= h_{EC}\left(\dot{m}_{EC1} + \dot{m}_{EC2} + \dot{m}_{ECB}\right) \end{aligned} \tag{5.38}$$

where $\dot{m}_{EC1}$, $\dot{m}_{EC2}$ and $\dot{m}_{ECB}$ represent the mass flows respectively in the three branches. h_{EC} is the specific enthalpy and the input of the condenser. The efforts variables P_{EC} and h_{EC} are imposed by the dynamics of the condenser modelled below.

5.5.7 Bond Graph Model of the Condenser

Description of the Process

The schema of the condenser is shown by the figure 5.26. The steam arrives from the steam expansion system to the condenser, where it becomes water by contact with the vertical serpentines of the cooling circuit. The change of phase steam - water liberates the latent heat and the water is cooled below its saturation temperature. The liquid, that is the condensed water flows in a continuous film on the cold serpentines or tubes downwards under the influence of gravity. It becomes the condensate of which the level controlled by three valves in parallel connection, by an on-off controller and flows then towards the tank.

Word Bond Graph of the Condensation Process

The technological level of the condenser model is represented by the word bond graph which is given by figure 5.27.

In the presented word bond graph, we have given the indices 1 the variables coming from the expansion (EC in the word bond graph) and 27 at the inflow of the tank (EB).The tubes or serpentines have three sections: on the condenser input in contact with the vapour, in the liquid condensate and finally again in the outflow of the condenser. The condenser is thermally insulated, there are lumped parameters and the steam (vapour) in the condenser is at saturation.

Bond Graph Model of the Condenser

The Bond graph of the condenser is given by the figure 5.28, where we have distinguished the different thermal energies as $\dot{H}$ the flow of enthalpy associated with fluid flow and as $\dot{Q}$ the thermal flow transferred by conduction.

In the presented bond graph model, the multiport capacitors are indicated by small rings around the bonds C_V and C_L. Each of them uses the mass m and the enthalpy H as state variables.

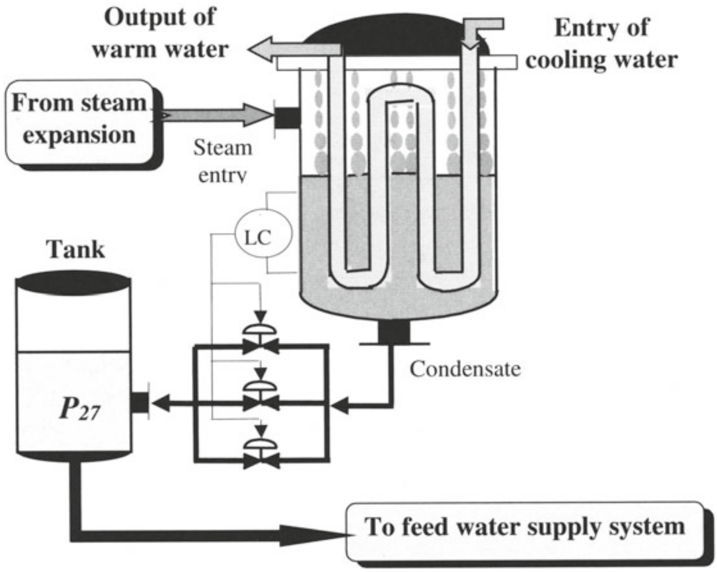


FIGURE 5.26. Schema of the condenser coupled with heat exchanger

In addition, three heat exchanges can be distinguished, in three different sections :

1. between incoming steam and cooling water inflow,
2. between condensate and cooling water,
3. between inlet steam and cooling water outflow.

Each of these heat exchanges is modellized by two elements *Hexa* and a simple, bond capacitor with stored thermal energy Q between them.

Thus, the state equations obtained from the bond graph can be written under the following non linear form:

$$\dot{x} = f(x, u)$$
$$y = C(x, u)$$

where u is the input vector, x the state vector and y the output vector.

From the bond graph, we determine the dimension and the physical nature of the state vector. In the studied system we have seven state variables:

1. The thermal energies Q_5, Q_{10} and Q_{17} stored in the three sections of the serpentines. They are modelled by one port C-elements C_5, C_{10} and C_{17}.

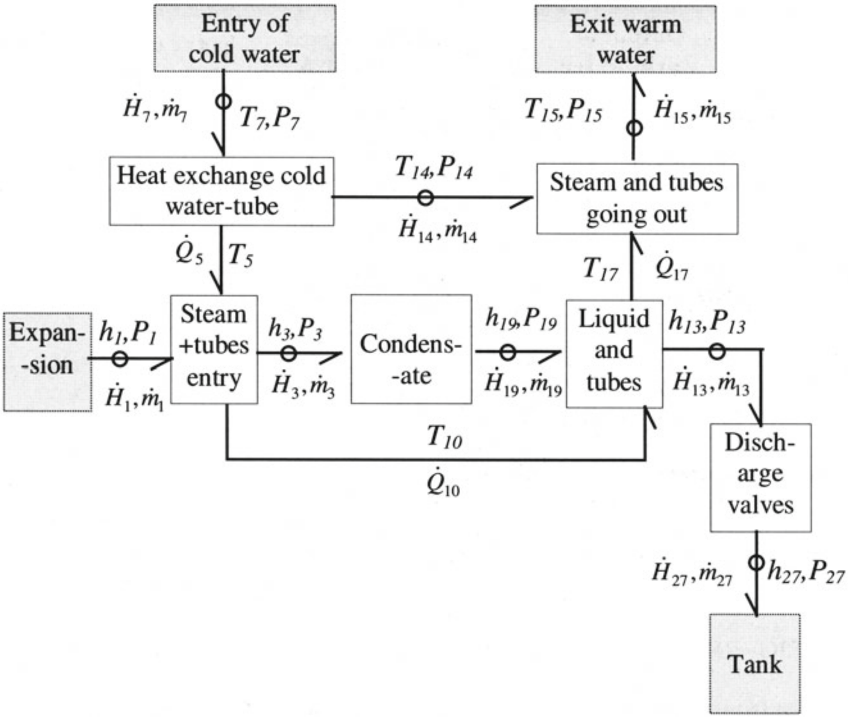


FIGURE 5.27. Word Bond graph of the condenser and cooling serpentine

2. The thermal and hydraulic energies accumulated by the steam and the condensate in the two ports C_V and C_L. They are H_3, H_{13}, m_3 and m_{13}.

The state vector x and the input vector x are thus:

$$x = \begin{bmatrix} Q_5 & Q_{10} & Q_{17} & m_3 & H_3 & m_{13} & H_{13} \end{bmatrix}^T$$
$$u = \begin{bmatrix} \dot{m}_1 & \dot{H}_1 & \dot{H}_7 & \dot{m}_7 & b_1 & b_2 & b_3 & P_{27} \end{bmatrix}^T$$

The flow sources (Sf) on the bonds 28 and 29 represent the mechanical energy of pressurization equal to $V\dot{P}$

The condensation on the serpentine is modelled by the R-element R : *Reco* introduced in the second chapter. It is modulated by the steam density ρ_V and liquid ρ_L. The discharge valves are represented by the multiport R modulated by the Boolean variables b_1, b_2 and b_3. These logic variables with the possible values 0 and 1 are coming from the on-off controller of liquid level. Heat exchange between two fluids through a metal wall is shown in elements *Hexa*. The constitutive equations of this element are:

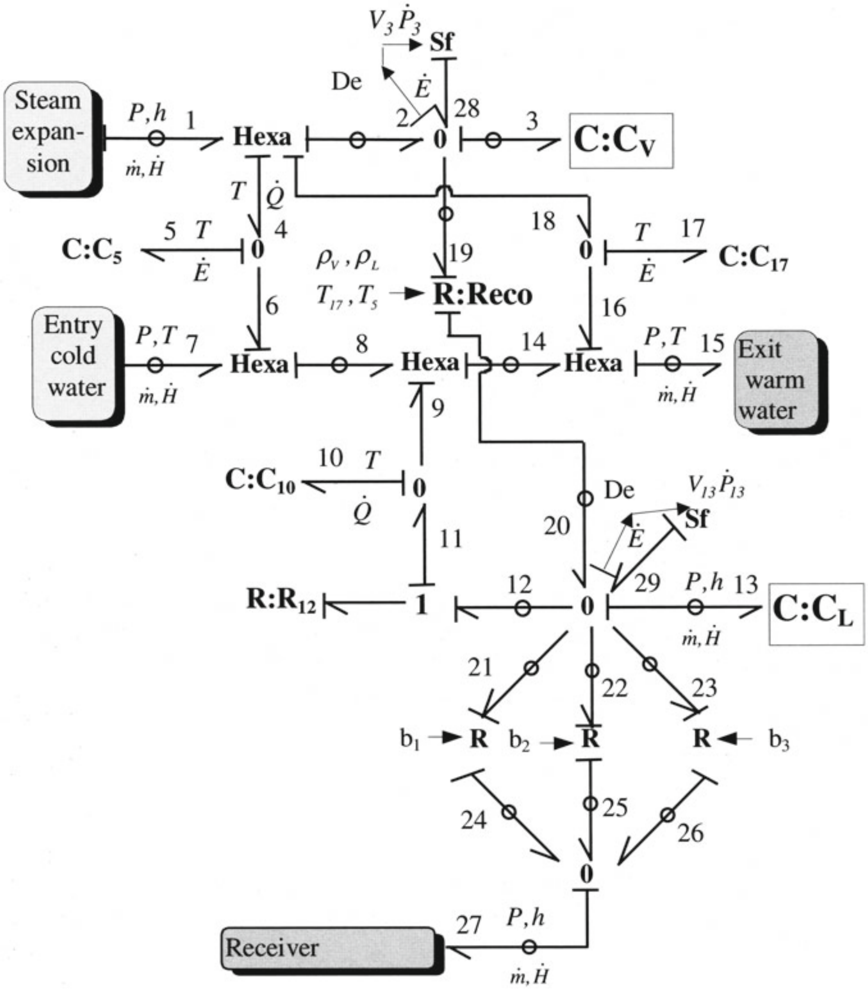


FIGURE 5.28. Bond graph for the condenser and cooling serpentine

$$\begin{aligned} \dot{m}_2 &= \dot{m}_1 \\ \dot{H}_2 &= \dot{H}_1 - \dot{Q} \end{aligned} \tag{5.39}$$

Constitutive Equations

- Multiport $C : C_V$: This shows hydraulic and thermal. energy storing. With steam compressible, we have:

$$\begin{aligned} \dot{m}_3 &= \dot{m}_1 - \dot{m}_{19} = V_3 \left(\frac{\partial \rho_3}{\partial T}\right)_{T=T_{SAT}} \\ \rho_3 &= \int \frac{1}{V_3 \left(\frac{\partial \rho_3}{\partial T}\right)_{T=T_{SAT}}} (\dot{m}_1 - \dot{m}_{19})\, dt \\ H_3 &= \int \left(\dot{H}_1 - \dot{H}_{19} + V_3 \dot{P}_3 - \dot{Q}_4 - \dot{Q}_{18}\right) dt \end{aligned} \tag{5.40}$$

The partial derivative of mass density ρ_3 at saturation temperature T_{SAT} is given from thermodynamic tables as given in appendix C.

- Supplementary Equations

The mixture ratio steam - water X and the pressure P_3 are a function of thermal energy H_3 and mass m_3 of the steam and are determined by the two phase equation 3.25. In our case, the mixture ratio is not very important, one can calculate the efforts as follows:
Firstly, the specific enthalpy is

$$h_3 = \frac{H_3}{m_3}$$

And then, temperature T_3 and pressure P_3 at saturation are determined by the thermodynamic function, given in appendix C.

$$P_3 = f_P(h_3) \text{ and } T_3 = f_T(h_3)$$

The volume of steam V_3 is given as the difference between the geometric volume of the condenser V_C and the volume of the water V_{13} :

$$\begin{aligned} V_3 &= V_C - V_{13} \\ V_{13} &= \frac{m_{13}}{\rho_L} \end{aligned} \tag{5.41}$$

- The one ports C-elements called C_5 , C_{17} and C_{10} represent the thermal energy in the three sections of the serpentines:

$$T_5 = \frac{1}{C_5}\int\left(\dot{Q}_4 - \dot{Q}_6\right)dt$$

$$T_{17} = \frac{1}{C_{17}}\int\left(\dot{Q}_{18} - \dot{Q}_{16}\right)dt \tag{5.42}$$

$$T_{10} = \frac{1}{C_{10}}\int\left(\dot{Q}_{11} - \dot{Q}_9\right)dt$$

The thermal conduction flow is given by, sometimes called the law of Fourier:

$$\begin{aligned} \dot{Q}_4 &= K_4\left(T_3 - T_5\right) \\ \dot{Q}_6 &= K_4\left(T_5 - T_7\right) \\ \dot{Q}_{18} &= K_{18}\left(T_3 - T_{17}\right) \\ \dot{Q}_{16} &= K_{18}\left(T_{17} - T_{15}\right) \\ \dot{Q}_{11} &= K_{11}\left(T_{13} - T_{10}\right) \\ \dot{Q}_4 &= K_{11}\left(T_{10} - T_8\right) \end{aligned} \tag{5.43}$$

where K_i are the heat exchange coefficients. T is the temperature of the liquid condensate determined from the state variables m_{13} and H_{13} and from the thermal capacity c_{13} of the non saturated liquid (considered constant):

$$T_{13} = \frac{H_{13}}{m_{13}c_{13}}$$

The *Hexa* elements in the cooling circuit are modelled as follows: the thermal flow as output of each element is the sum of the thermal flow at the input, but the temperatures are different. This gives:

$$\begin{aligned} &T_6 = T_7, \quad \dot{H}_8 = \dot{Q}_6 + \dot{H}_7 = \dot{m}_8 c_8 T_8 && \Longrightarrow T_8 = \frac{\dot{Q}_6 + \dot{H}_7}{\dot{m}_8 c_8} \\ &T_8 = T_9, \quad \dot{H}_{14} = \dot{Q}_9 + \dot{H}_8 = \dot{m}_{14} c_{14} T_{14} && \Longrightarrow T_{14} = \frac{\dot{Q}_9 + \dot{H}_8}{\dot{m}_{14} c_{14}} \\ &T_4 = T_{16}, \quad \dot{H}_{15} = \dot{Q}_{16} + \dot{H}_{14} = \dot{m}_{15} c_{15} T_{15} && \Longrightarrow T_{15} = \frac{\dot{Q}_{16} + \dot{H}_{14}}{\dot{m}_{15} c_{15}} \end{aligned} \tag{5.44}$$

The mass flow $\dot{m}_W$ and the thermal capacities c_w of the cooling water are constant, also the enthalpy flow carried by the cooling liquid:

$$\dot{m}_7 c_7 = \dot{m}_8 c_8 = \dot{m}_{14} c_{14} = \dot{m}_{15} c_{15} = \dot{m}_W c_W$$

The temperature T_7 is calculated as follows:

$$T_7 = \frac{\dot{H}_7}{\dot{m}_7 c_7} = \frac{\dot{H}_7}{\dot{m}_W c_W}$$

- Multiport R : *Reco* for steam phase

The mass flow of condensation around the serpentines $\dot{m}_{19} = \dot{m}_{20}$ is calculated in a multiport R : *Reco*. It is calculated by an empiric Nusselt formula given above by equation 3.36. The condensed mass flow is then:

$$\dot{m}_{19} = \frac{\rho_{13}\left(\rho_{13} - \rho_3\right) g}{3\mu_{13}} \left(\frac{4\mu_L l_T \left(T_3 - T_T\right) \lambda_L}{g \rho_L \left(\rho_{13} - \rho_3\right)\left(L_V + 0,68 c_T \left(T_3 - T_T\right)\right)}\right)^{\frac{3}{4}} \Pi D_T n_T \tag{5.45}$$

The thermal flow of the condensate is:

$$\dot{H}_{19} = \dot{m}_{19}\left(h_3 - h_{13}\right)$$

- $C : C_L$: Multiport C called C_{13} for thermal and hydraulic accumulation of the condensate:

$$\begin{aligned} m_{13} &= \int \left(\dot{m}_{19} - \dot{m}_{27}\right) dt \\ H_{13} &= \int \left(h_3 \dot{m}_{19} - \dot{Q}_{11} - h_{13}\dot{m}_{27} + V_{13}\dot{P}_{13}\right) dt \end{aligned} \tag{5.46}$$

The liquid pressure P_{13} is a function of the condensate level ($N_{13} = m_{13}/(Ac\rho_{13})$) and of steam pressure P_3 :

$$P_{13} = P_3 + g\frac{m_{13}}{A_C} \tag{5.47}$$

where A_C is the cross section, (in m^2) of the cylindrical condenser.

- Hydraulic resistances R in the discharging valve

We take the inertia of the discharging valves negligible and they behave then as multiports R.

The three branches are constituted by three valves on identical conduits and have the same loss coefficient K_{DC}. The flow in each branch is given by Bernoulli's law for incompressible liquids:

$$\begin{aligned} \dot{m}_{27} &= \sum_{i=1}^{3} b_i K_{DC} \sqrt{P_{13} - P27} \\ \dot{H}_{27} &= h_{13} \dot{m}_{27} = \frac{H_{13}}{m_{13}} \dot{m}_{27} \end{aligned} \tag{5.48}$$

P_{27} is the pressure of the tank, that we shall treat below.

$$b_i = F(N_{13}) \tag{5.49}$$

The Boolean variables b_i come from a logic control system with the level of the condensate N_{13}.

5.5.8 *Bond Graph Model of the Receiver*

The tank is simple energy accumulator. It is at free air and the liquid at ambient temperature. The bond graph model appears on figure 5.30.

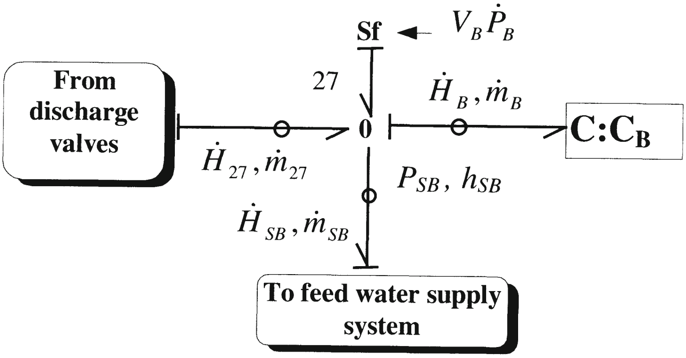


FIGURE 5.29. Bond graph model of the receiver

The quantity of mass m_B and enthalpy H_B stored in the receiver are calculated by the constitutive non linear equations of the multiport C.

$$\begin{aligned} m_B &= \int (\dot{m}_{27} - \dot{m}_{SB})\, dt \\ H_{13} &= \int \left(\dot{H}_{27} - \dot{H}_{SB} + V_B \dot{P}_B \right) dt \end{aligned} \tag{5.50}$$

where V_B is the water volume in the tank ($V_B = m_B / A_B$) and $\dot{m}_{SB}$ the outflow, which equals the flow of the feeding pump $\dot{m}_{SB} = \dot{m}_{AL}$.

The pressure in the tank is calculated as follows:

$$P_{27} = P_{SB} = \frac{m_B \cdot g}{A_B} \tag{5.51}$$

5.6 REFERENCES

[Rimaux, 1996] Rimaux, S. B, Ould Bouamama, and Dauphin Tanguy, G., "Bond Graph model of the shrink and swell phenomena in a PWR Nuclear Power Plant", IEEE-SMC IMACS Multiconference CESA 96, Lille, France PP 288-293.

[Tylee, 1983] Tylee, L., "A Bond Graph description of U-tube Steam Generator" Dynamics, J. of Franklin Institue., Vol. 315, N° 3, pp 165-178, 1983.

Appendix A

Elements of Bond Graph Modelling

A.1 Definition

Bond graph modelling is based on considering the exchange of power between the elements of a system. A bond graph is a collection of multiport element bonded together. In the general sense it is a linear graph whose nodes are multiport element and whose branches are bond. The key of bond graph modelling is the representation (by a bond) of power as the product of efforts and flows with elements acting between these variables and junction structures to put the system together.

The product of effort and flow is then a power, as well known in electricity, where power is voltage times current. This is used in most disciplines, like hydraulics, where power is pressure times volume flow and mechanics where power is force times effort or torque times rotation frequency.

In thermodynamics, power, that is heat flow is also temperature times entropy current. This is much less known but very important and that is why we put it at the beginning of thermodynamics as Carnot equation 1.3.

In some bond graphs the product effort-flow does not have the physical dimension of a power. There are called pseudo bond graphs and need to be used in chemistry, thermodynamics and thermal engineering.

An important example of pseudo bond graphs is thermal and thermodynamics engineering. Here we have both the true Bond graph, with temperature and entropy current, whose product is a power, and the pseudo bond graph with temperature as effort and heat flow as flow. So in this latter formulation effort times flow is not a power and has no physical meaning, but is used for the practical reasons as explicating above in the fourth chapter.

The construction of a bond graph model of a given system is realised in three steps:

1. The first stage is to split up a system into a subsystems or the coupling of different selected phenomena in function of imposed hypothesis. The interconnection is realized by the pair effort and flow. One can say this the technological level of model building or word bond graph.

2. The second step is to reproduce the physical effects, including simplifying hypothesis. Here the interdisciplinary nature of bond graphs is very useful, and shows the exchange of power in a system. It also shows the storing, the transmission and dissipation of energy. Fur-

ther, the mathematical order and the type of dynamics are directly seen on the bond graph. Finally, the bond graph model obtained on a paper or computer screen can modify by adding more elements, like frictions, and inertia's compressibility's. This is the physical level of model building and analysis.

3. The third step is to write the constitutive equations of the elements or components according the selected causalities. This is the mathematical and algorithmic representation.

A.2 Bond Graph Elements with one Port

A.2.1 Representation

The bond graph elements can be classified by their number of ports, from one to three, whilst multiport appear in the next section.

In each closed system, there is both conservation of energy and a continuous flow of power. The exchanged power between two connected systems A and B is represented by a power bond as shown on the figure A.1.

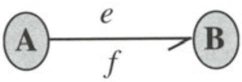


FIGURE A.1. Representation of bond graph one port element

From this comes the term bond graph. The sense of the half arrow gives the direction of the power. If the power flux is sometimes backwards, it is described by negative power.

A.2.2 Used Variables in Bond Graph Modelling

The used variables in bond graph can be classified as follows:

1. *Power or liaison variables.* Here the exchanged power equals effort e times flow f, which are in general function of time:

$$P = ef$$

2 *Energy variables.* These are defined by the following integrals equations:

$p(t)$ *the momentum* or impulse of a movement

$$p(t) = \int_0^t e(\tau)d\tau, \quad p(0) = 0 \tag{A.1}$$

and $q(t)$ *the general displacement*

$$q(t) = \int_0^t f(\tau)d\tau, \quad q(0) = 0 \tag{A.2}$$

The following table A.1 gives the meaning of the variables in the different domains.

Domain	Effort	Flow	Momentum	Displacement
	[Unit]	[Unit]	[Unit]	[Unit]
	$e(t)$	$f(t)$	$p(t)$	$q(t)$
Electric	Tension	Current	magnetic flow	Electric charge
	$[Volt]$	$[Ampere]$	$[Weber]$	$[Coulomb]$
Mechanics of rotation	Torque	Frequency	Angular momentum	Angle
	$[N.m]$	$[Rad/s]$	$[N.s]$	$[Rad]$
Mechanics of translation	Force	Velocity	Momentum	Volume
	$[N]$	$[m/s]$	$[N.s]$	$[m^3]$
Hydraulics	Pressure	Volume flow	Momentum of	Volume
	$[Pa]$	$[m^3/s]$	pressure $[Pa.s]$	$[m^3]$
Thermal	Temperature $[K]$	Heat flow [J/s]	-	Heat energy [J]
Thermodynamics	Temperature $[K]$	Entropy flow $[J/(K.S)]$	-	Entropy $[J/K]$
Chemistry	Chemical tension	Molar flow	-	molar mass
	$[J/mole]$	$[Mole/s]$		$[Mole]$
Economy	Unit price of product	Flow of product	Economic momentum	Inventory

TABLE A.1. Meaning of power and energy variables

Describing now the different elements according to their number of ports.

A.2.3 Passive Elements

These elements store or dissipate energy. The half arrow is usually entering the element. These elements are designated by R, C and I.

- *Resistance* R. This is the generalized friction and connects effort and flow. It gives the dissipation of power (see below) and is found in all disciplines: electric resistors, hydraulic resistors, linear or not, mechanical friction, thermal friction in pseudo bond graphs. The law is of the form:

$$\Phi_R(e,f) = 0 \tag{A.3}$$

Examples are the electric law of Ohm, $U = Ri$ or the hydraulic law of Bernoulli $P = K_D \dot{V}^2$ or Fouriers thermal law $\Delta T = K_C \dot{Q}$.

The graphical representations are given by figure A.2.

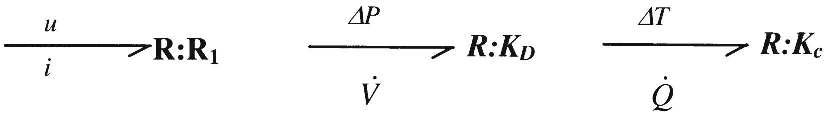


FIGURE 6.2. Graphical representation of R element

- *Capacitance* C. It connects all effects connecting effort and displacement: spring, condenser, accumulator, storage reservoir and compressibility. So we have here storage of energy and the equation is

$$\Phi_C\,(e,q) = 0 \quad \text{or} \quad \Phi_C\left(e, \int f(\tau)d\tau\right) = 0 \tag{A.4}$$

Examples are $u = \dfrac{1}{C}\int idt$ or $u = \dfrac{q}{C}$ in electricity, $P = \dfrac{V}{C}$ or $P = \dfrac{1}{C}\int \dot{V}dt$ in hydraulics and $T = \dfrac{1}{C}\int \dot{Q}dt$ in thermic.

- *Inertia* I. This element is used for mass action, moment of inertia in rotary mechanics, inductance and inertance of a liquid. Its equation is:

$$\Phi_I\,(p,f) = 0 \quad \text{or} \quad \Phi_I\left(f, \int e(\tau)d\tau\right) = 0 \tag{A.5}$$

Example: $u = L\dfrac{di}{dt}$ or $\phi = Li$ in electricity and $P = \dfrac{\rho l}{A}\dot{V}$ in hydraulics. l, A and ρ represent respectively the length and the cross area of the pipe and the density of the fluid circulating in the pipe.

Both C and I elements are associated to storing energy. But in opposite to C element, In the I element, the energy is not conserved when the flow variable disappears: the energy is stored because of dynamic of the system.

A.2.4 Active Elements

These elements supply power to the system. Naturally, this power must come from somewhere, but this is outside our range of interest. One distinguishes:

- *Effort source (Se)*, imposing an effort, which can be function of time but independent of required flow. Examples is the electric voltage generator, pressure, force generator or simply weight force generator.
- *Flow source (Sf)*, imposing a flow independent of required pressure. Examples are electric current generator and imposed velocity in mechanics. They are designated as given by the following figure.

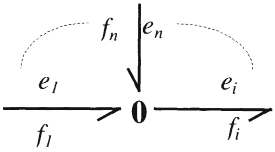
FIGURE A.3. Representation of effort and flow sources in bond graph

Here the orientation of the half arrow is normally out of the sources.

A.2.5 Junctions

Some times called three ports, the junctions allow to couple the elements of a system, particularly R, C, and I-elements. They conserve power.

- *Parallel junctions (0-junctions)*. They associate elements under the same effort, which means parallel circuit in electricity and oil hydraulics, and series circuit in mechanics. This corresponds to the Kirchhoff voltage law in electricity. The constitutive equation and representation of such junction are described by figure A.4.

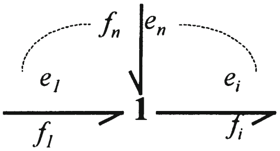


$$e_1 = e_2 = \ldots e_n$$

$$\sum_{i=1}^{n} a_i f_i = 0$$

FIGURE A.4. Parallel junction or 0-junction with $a_i = 1$ for entering power and $a_i = -1$ for leaving power

- *Series junctions (1-junctions)*: They associate elements under the same flow , which means series circuit in electricity and oil hydraulics. In mechanics, this means circuit in parallel, and corresponds to the Kirchhoff current law in electricity. They are described by figure A.5.



$$f_1 = f_2 = \ldots f_n$$
$$\sum_{i=1}^{n} a_i e_i = 0$$

FIGURE A.5. Serial junction or 1-junction with $a_i = 1$ for entering power and $a_i = -1$ for leaving power

In both junction we have power conservation, which can be expressed as:

$$\sum_{i=1}^{n} e_i f_i = 0 \tag{A.6}$$

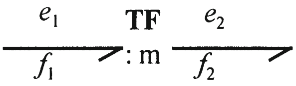
Formerly, the junctions have been called *p*- and *s*-junctions by author Jean Thoma. This is better for generating computer code but has been abandoned for international standardization.

A.3 Bond Graph Elements with two Ports

These elements have two bonds or ports and comprise the transformer and the gyrator, a kind of over crossed transformer.

A.3.1 Transformer TF

This element with two ports makes a model of an electric transformer, a gear reducer in rotary mechanics or simply a lever in rectilinear mechanics. The modulus of the transformer may not be constant, but depend on the time (or any other parameter). One calls it then *MTF* (modulated transformer) and the transforming variable can be continuous or Boolean.

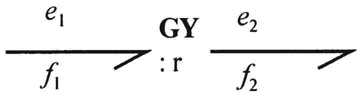


$$e_1 = m\, e_2$$
$$f_2 = m f_1$$

FIGURE A.6. Transformer *TF* and its constitutive equation

A.3.2 Gyrator GY

Called also transducer *TD*, this two ports element is shown with the constitutive equations by the figure A.7.



$$e_1 = r f_2$$
$$e_2 = r f_1$$

FIGURE A.7. Gyrator and its constitutive equation

Examples are the gyroscope, electric motor. There exists also the modulated gyrator *MGY*, which is the electric motor with variable excitation.

Let us note that transformer and gyrator are power conserving but can transform this power from one domain to the other. An example is the electric motor, that transforms from electric into mechanical rotary power.

A.3.3 Carrousel of Thoma

The constitutive relations for different elements are well illustrated by the Thoma carrousel [*Thoma, 1990*] as presented by figure A.8. So a resistor or an -*R*-element gives an algebraic relation between effort and flow, an *I*-element between flow and integral of effort (or momentum *p*), and *C*-element between effort and integral of flow (or displacement *q*). Going around clockwise, we obtain only derivations, anti-clockwise integration's. Since all computers prefer integrations, we should always go anti-clockwise. Note that in the literature exist also the tetragon of Paynter, which is the same, but the name is not right, because it means the simplest body in three dimensions, limited by four triangles.

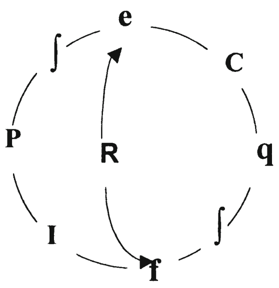


FIGURE A.8. Carrousel of Thoma

A.3.4 Information Bonds

When one variable in a bond is very small it can be neglected, and the transmitted power is also negligible. We have then an information bond, which is the same as in all block diagrams. It is shown as a full arrow on the bond and can represent the transmitted signal by a sensor, integrator, sum member, etc.. Figure A.9 represents also the effort sensor De and the flow sensor Df.

FIGURE A.9. Information bond. a. transmitted signal, b. detector of effort and flow

A.4 Multiports Elements or C, I and R Fields

The bond graph elements so far have scalar constitutive laws. There exist also multiport elements, where each bond has several strands just like a vector (We avoid the name component, because this has an other meaning, the part of a machine). They have been treated in Karnopp 1975 and in the older book of Thoma 1975 and appear on figure A.10.

Multiport C

This element shown by the figure A.11 and called also formerly C-field is associated as energy storing by displacements and associated efforts.

The stored energy is

$$\begin{aligned} E &= \int_{t_0}^{t} \sum_{i=1}^{n} (e_i f_i)\, dt = \int_{t_0}^{t} \sum_{i=1}^{n} (e_i \dot{q}_i)\, dt \\ &= \int_{q_0}^{q} \sum_{i=1}^{n} e_i(q) dq_i = \int_{q_0}^{q} \sum_{i=1}^{n} e(q) dq = E(q) \end{aligned} \tag{A.7}$$

where :

$$\begin{aligned} q &= \begin{bmatrix} q_1 & \dots & q_n \end{bmatrix}^T \\ e &= \begin{bmatrix} e_1 & \dots & e_n \end{bmatrix}^T \end{aligned}$$

Note that here the efforts e_i depend on all displacements. The relation can be linear, given by a matrix, or non linear, given by set of functions.

As an example, the energy stored in a thermodynamic and chemical system having n chemical components is shown as figure A.12.

This multiport C corresponds to the equation of Gibbs. This equation gives the stored energy U as follows:

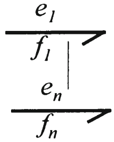
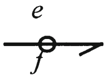
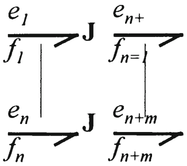
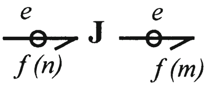
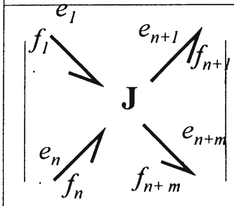
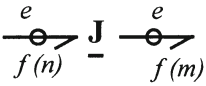
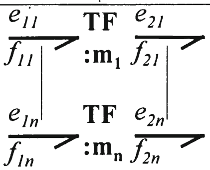
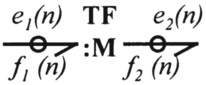
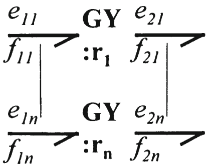
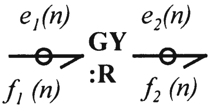
System	Representation	constitutive equation
		
		
		$e_i{}^T f_i - e_k{}^T \cdot_k = 0$
		$\begin{cases} e_1{}^T f_1 = e_2{}^T f_2 \\ e_1 = me_2 \\ f_1 = mf_2 \end{cases}$
		$\begin{cases} e_1{}^T f_1 = e_2{}^T f_2 \\ e_1 = Rf_2 \\ e_2 = Rf_1 \end{cases}$

FIGURE A.10. Multiport elements

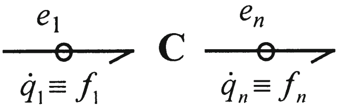


FIGURE A.11. Multiport C

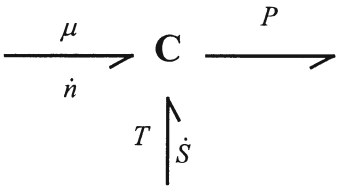


FIGURE A.12. Thermodynamic and chemical example of a multiport C

$$dU = TdS - PdV + \sum_{i=1}^{n} \mu_i dn_i$$

Here the displacement variables are volume V, entropy S and the molar masses n_i. The corresponding efforts are pressure P, temperature T and chemical potential μ. Note the sign minus in front of the pressure translates as the hydraulic power orientation.

Multiport I

The multiport I corresponds to several inductors or masses in mechanics in interaction as shown on figure A.13.

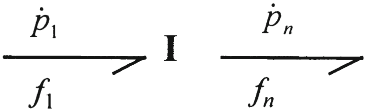


FIGURE A.13. Multiport I

The multiport I is the analogue to the multiport C, only effort and displacement are turned into momentum p_i and flow f_i. Hence we have the equation:

$$\begin{aligned} E &= \int_{t_0}^{t} \sum_{i=1}^{n} (e_i f_i)\, dt = \int_{t_0}^{t} \sum_{i=1}^{n} (f_i \dot{p}_i)\, dt = \int_{p_0}^{p} \sum_{i=1}^{n} f_i(p) dp_i \\ &= \int_{p_0}^{p} \sum_{i=1}^{n} f(p) dp = E(p) \end{aligned} \quad (A.8)$$

where

$$\begin{aligned} p &= \begin{bmatrix} p_1 & \dots & p_n \end{bmatrix}^T \\ f &= \begin{bmatrix} f_1 & \dots & f_n \end{bmatrix}^T \end{aligned}$$

Generally we have a matrix linking all displacements and efforts. The off-diagonal entries of the matrix indicate the coupling of variables.

A.4.1 Mixed Multiport IC

We have also a combination between C and I multiport , having n ports as multiport C and m ports as multiport I, as shown on figure A.14.

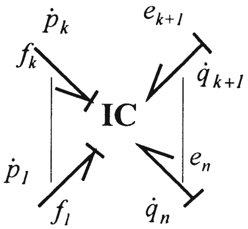


FIGURE A.14. Multiport IC

The stored energy is:

$$E = \int_{t_0}^{t} \sum_{i=1}^{n} (e_i f_i)\, dt = \int_{p_0}^{p} \sum_{i=1}^{k} (f_i)\, dp_i = \int_{p_0}^{p} \sum_{i=1}^{n} f_i(p) dp_i + \int_{q_0}^{q} \sum_{j=k+1}^{n} e_j dq_i \tag{A.9}$$

Here p is the momentum vector and q the displacement vector. The first k ports represent a multiport C and the multiports I, and the port from $k+1$ to n represent the multiports C.

The multiport IC is used mostly for electromagnetic effects with mechanical parts. Here the electric part is a multiport I and the mechanical part a multiport C.

A.4.2 Multiport R

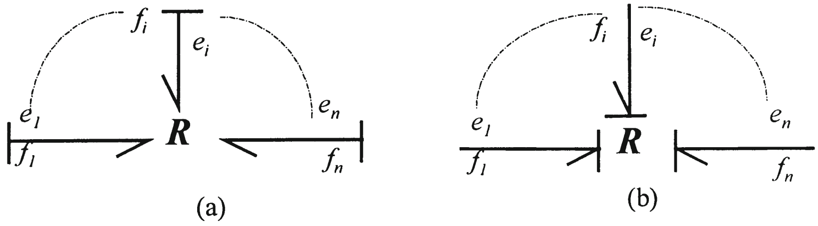
This is essentially coupled resistor network, which links, in a algebraic relation between the n flows and n efforts without storing energy. The constitutive law can be linear, like Ohm's law or non linear, like the hydraulic resistors. In resistance causality (Fig. A.15a), we have:

$$e_i = \Phi_{Ri}\left(f_1, \ldots f_n\right), \; i = 1, 2, \ldots n \tag{A.10}$$

and in conductance causality (Fig. A.15ba),

$$f_i = \Phi_{Ri}^{-1}\left(e_1, \ldots e_n\right) \tag{A.11}$$

The multiport R is generally symmetric in conductance and resistance causality. In thermodynamics, the corollary is the symmetry or reciprocity of Onsager.



(a) (b)

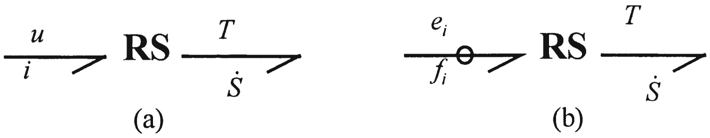
FIGURE A.15. Multiport R

A.4.3 Multiport RS

We know that the R-elements dissipate power and that this power comes out as heat. So including thermal effects, an R-element becomes an irreversible and power conserving structure. It is denoted as multiport RS (Fig. A.16a). So power can flow only as indicated by the half arrows, and not backwards. In other words it cannot become negative. So, when we are not interested in thermal effects, we speak of R-elements and multiport-R, otherwise of multiport-RS.

Regarding the multiport RS, it can have bonds with several strands as shown on figure A.16b.

With multiport RS, irreversibility and energy conservation of multiport R are as follows: with several strands, only the sum of the non thermal bonds must be positive, but in single strands power can become negative as long as it is more positive in others. One can also say that power in the thermal bond must by always positive.



(a) (b)

FIGURE A.16. Element (a) and Multiport (b) RS

A.5 Causality Concept

One important structural propriety of the bond graph is its causality concept. Indeed, the determination of causes and effects in the system is directly deduced from the graphical representation and shows at the time the transition to the block diagram. The idea of bond graphs is to write it at first without causality, perhaps without power directions, and to worry about these later.

The relation between cause and effect on a bond graph are indicated by a vertical stroke. By convention, the side of the stroke indicates where the effort is acting, and the flow acts then in the reverse. In this sense, a causality stroke replaces two connections in opposed sense in a block diagram.

In our example given by the figure A.17a, the element **A** applies an effort on **B**, which replies by a flow acting backwards from **B** to **A**; so the effort from **A** is given from the outside to **B**. In the corresponding block diagram the direction of action is indicated by an arrow on each connection as illustrated by figure A.17b. Independently of the causality, the direction of the positive power is indicated by the half-arrow on the bond.

(a) (b)

FIGURE A.17. Causality

The notion of causality in bond graphs allows to resolve the algorithmic level of modelling. One tries to choose the causalities always integral and not derivative. Indeed, in numerical form, integration is simpler and more accurate than derivation. In other words, with the C-element the effort-out causality is preferred and with I element the effort in causality is preferred.

As shown on the figure A.18, the bond graph symbol gives us four informations:

1. the *existence of physical link* between two systems by the bond,
2. the *type of power* (electric, mechanical...) by the power variables,
3. the *power direction* by the half arrow,
4. the *causality* by the stroke.

A.5.1 Rules of Causality Selection

The choice of causality is free in principle but subject to some limitation : for example sources always impose an effort or a flow to the system.

Briefly they are:

- The sources impose always one causality, imposed effort by effort sources and imposed flow by flow sources.

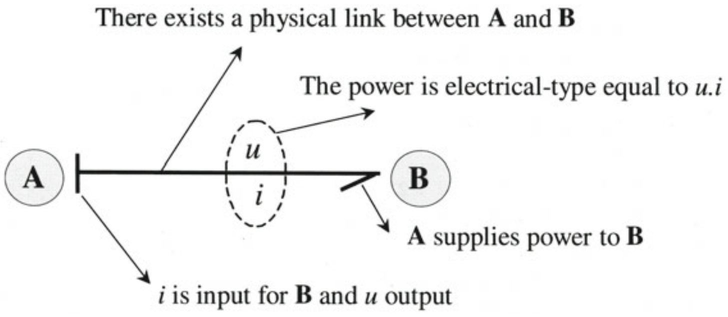


FIGURE A.18. Informations given by bond graph representation

- With the one ports, a C-element has one (or several) flows as an input and gives effort as an output.
- The I-element takes one or several efforts as input and has flow as output. This choice results in integration of inputs to obtain the output. The reverse choice would give the undesirable derivation.
- In linear R-elements, the causality is in principle indifferent, but indicates whether resistance or conductance need to be entered as parameter. In non linear R-elements, equations are more comfortable in one direction, like our mass (or volume) flow and pressure characteristic in equation 2.11. There we have effort as input and flow as output.
- With the two ports, on the transformers TF, effort and flows point through and with gyrators GY, an effort produces a flow; this in both directions.
- With the three ports (junctions), we have on the parallel junction (0-junction) one input of effort, which is common to all bonds. It must be given by one bond, and all the other bonds have flow pointing to the junction and efforts going away.
- The series junction (1-junction), one flow, the common flow points to the junction, and all flows point away. In other word, all but one effort pushes to the series junction, and all other efforts push away.

From these considerations, the practical rules of causality application are [*Karnopp 1975*] [*Thoma 1991*] and [*Borne et al. 1992*]:

1. Apply a fixed causality to the source elements Se and Sf.
2. Apply a preferred causality to C and I elements.
3. Extend the causality through the nearly junction ,0, 1, TF an GY.

4. Assign a causality to R element which have indifferent causality .

5. If these operations give a derivative causality on one element, we have a causal conflict. One can handle derivative causalities (leading to so called DAE = Differential Algebraic Equations). In our experience it is usually better to add small C- or I-elements to avoid causal conflicts; often enough physical reasons can be found for such elements like small dead volumes. Naturally, such small C- or I-elements increase the state space of the system, but with modern computers, that is less a problem. Often they do not modify measurably the dynamics of the system. An can also make the small C-elements larger, say ten times as large do so called "remedy of the bad conscience". Bad conscience because we do not know for sure what the influence on the visible system dynamics will be.

The causalities of bond graph elements are given by the figure A.19 and A.20.

A.6 Bicausal Bond Graphs

As we have seen, causality imposes a certain propagation throughout the bond graph. It implies that if effort acts in one sense, flow acts in the reverse which is true if we know then values of the bond graph elements. If not, other rules are necessary. One generalization of the causality selection proposed by [*Gawthrop, 1985*], the bicausal bond graph. There one divides the causality stroke into two. One half indicates the direction of effort, the other the direction of flow as shown on figure A.21.

On the figure A.21, the causality of R indicates that both effort and flows enter the R-element. This allows to calculate the resistance R. Causality on the effort source indicates, that the effort is imposed, and the flow is known, for example by a flow sensor. If one affects bicausality to a C-element, an effort sensor must be added on the element.

A.7 State Space Equations Associated to a Bond Graph

The state vector, denoted by x, is composed by the variables p and q, the energy variables of C- and I-elements.

$$x = \begin{bmatrix} p_I \\ q_C \end{bmatrix}$$

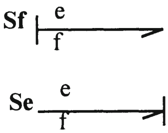
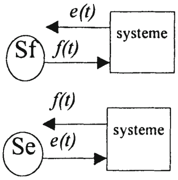
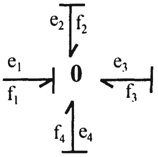
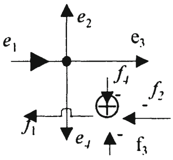
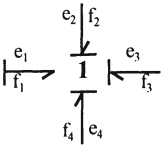
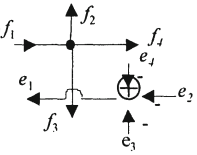
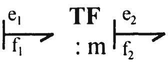
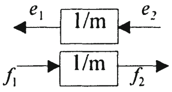
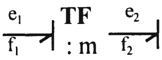
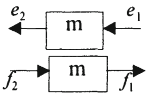
Element	***Causal form***	***Relation***	***Block diagram***	***Rule***
Effort source (Se) and flow source (Sf)		*f given* *e given*		Effort or flow source is given. ***The causality is obligatory (required)***.
0 Junction		$e_2 = e_1$ $e_3 = e_1$ $e_4 = e_1$ $f_1 = -(f_2 + f_3 + f_4)$		Only one effort gives its value to the others, (here e_1). ***Only one causal stroke on 0 junction.***
1 Junction		$f_2 = f_1$ $f_3 = f_1$ $f_4 = f_1$ $e_1 = -(e_2 + e_3 + e_4)$		Only one flow gives its value to the others, (here f_1). ***Only one bon with out causal stroke on***
transfor-mer ***TF***		$e_1 = me_2$ $f_2 = mf_1$		e_2 and f_1 *ar known.* ***Only one causal stroke on TF***
		$f_1 = f_2/m$ $e_2 = e_1/m$		e_1 and f_2 *ar known.* ***Only one causal stroke on TF***

FIGURE A.19. Causalities of bond graph elements (part 1)

Properties of State Variables

- The state vector does not appear on the bond graph, but only its derivative

$$\dot{x} = \begin{bmatrix} e_I \\ f_C \end{bmatrix} = \begin{bmatrix} \dot{p}_I \\ \dot{q}_C \end{bmatrix}$$

- The dimension of the state vector is equal to the number of C- and I-elements in integral causality
- If among the n C and I-elements, n_l are in derivative causality, so the order of the model is $n - n_l$. The sate vector is then split up into the parts x_i and x_d (i for integral and d for derivative).

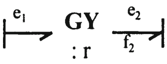
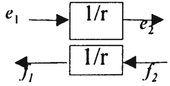
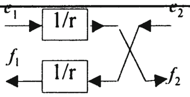
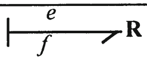
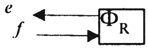
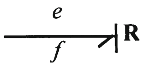
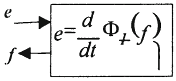
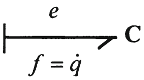
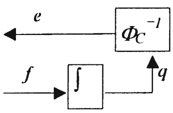
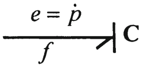
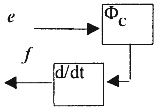
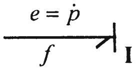
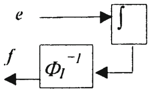
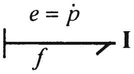
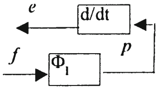
Element	***Causal form***	***Relation***	***Block diagram***	***Rule***
Gyrator		$e_1 = rf_2$ $e_2 = rf_1$		f_2 and f_1 are given for GY ***No causal stroke on GY***
GY		$f_1 = e_2/r$ $f_2 = e_1/r$		e_2 and e_1 are given for GY ***2 causal strokes on GY***
Resistance		$e = \phi_R(f)$		f is given for R ***Indiff. causality***
R		$f = \phi_R^{-1}(e)$		e is given for R. ***Indifferent causality***
Capacity		$e = \phi_C^{-1}\left(\int f dt\right)$		e is given for C ***Derivative causality***
C		$f = \frac{d}{dt}\phi_C(e)$		e is given for C-element. ***Derivative causality***
Inertia		$f = \phi_I^{-1}\left(\int e dt\right)$		e is given for I-element. ***Integral causality***
I		$e = \frac{d}{dt}\phi_I(f)$		f is given for I-element. ***Derivative causality***

FIGURE A.20. Causalities of bond graph elements (part 2)

$e_1 = e_2$, $f_1 = f_2$ $\qquad$ $e_2 = e_1$, $f_2 = f_1$

FIGURE A.21. Bicausal bond graph

A.8 Pseudo Bond Graphs

The true bond graphs, as shown above on the table 4.1 have the physical power as product of effort and flow. Precisely, it is the instant power travelling along a bond or entering a port. Such bond graphs are well suited for mechanical., hydraulic and electric systems.

In the pseudo bond graphs [*Karnopp, 1979*], the product effort-flow has no more the meaning of a power, it has no meaning in general. Such bond graphs are more necessary for fluid lines, as treated in section 2.1, but also in physical chemistry, diffusion and chemical reactions. We have then pseudo bonds, but the rules of causalities and signs remain valid in C, I and R-elements.

One finds the pseudo bond graphs in the following fields:

1. In thermal conduction and engineering, one uses the heat flow and not of entropy flow. This is because heat flow is conserved in such problem and allows to write a simple RC circuit for such problems. Entropy flow is not conserved and increases generally with decreasing temperature.

2. In chemistry, one uses often not a chemical potential (which forms with molar flow a true bond graph) but the concentration. Their relation is explained in section 3.1 and formula 3.49.

3. In compressible fluid mechanics, there are conduction phenomena. So one use as flows the mass flow and the enthalpy flow because they have simple conservation principles. Mass flow is always conserved, except in leakage, which is reticulated be a parallel junction and an R-element. Enthalpy flow can be derived from a power balance.“ The true Bond graphs are a virtue, but the pseudo Bond graphs are a necessity”.

A.9 Conservation of Power and Conservation of Energy

For the junctions, the transformer and the gyrator, there is conservation of power and therefore conservation of energy. There is in bond graph another conservation of energy in the elements C and I. These elements do not conserve power but can absorb it. Then they change their state and in order to return to the initial energy one must take out exactly the same energy. Hence, energy is conserved over one cycle. Therefore, it is of advantage to make a difference between power conservation and energy conservation.

In the multiports C and I, energy conservation is different. It can go out though another bond, but the total energy is always the same to return to the initial state.

The R-element is irreversible and absorbs but give out power. In the multiport R, the condition is weaker: The sum of powers is always positive, but some power may come out from one bond, be negative, as long as the sum over all bonds remains positive. One application is the thermoelectricity and the Peltier effect [*Thoma, 1975*].

Any multiport that has a more complex structure will be represented in this book by four or five letters, the symbols with one to three letters reserved for standard bond graph elements. Examples are the designations $Reco$, $Hexa$ and $Tefma$, which designate resistance for convection, heat exchanger and thermal turbomachine; they are developed in chapter 2.

A.10 Thermal Inertia and Second Law of Thermodynamics

The thermodynamic literature [*Cellier, 1994*] says that a thermal element I can not exist because it would be contrary to the second law of thermodynamics. This not the case as we shall show below.

Figure A.22 shows two pistons in two cylinders, which are in communication, not by a leakage with mass flow, but simply by a thermal conduction with temperature and entropy flow. The pistons serve only to vary pressure and volume and therefore the temperature according to the constitutive equation of the enclosed gas. Each change of the temperature generates a flow of entropy from the higher to the lower temperature and becomes zero when equality of temperatures is obtained. A new position of the pistons introduces a new difference of temperature somewhat similar to the electric circuit of section 3.3.

The figure A.22b shows the corresponding bond graph. Let us note, that here we have a true bond graph with T and $\dot{S}$ and not a pseudo-bond graph, which is better for simulation. Since we are already in the thermal domain, the new entropy of the multiport RS is injected by the switch $SWIT$ in the bond of lower temperature. The second law of thermodynamics says that this dissipation is always positive and that the new entropy can not be destroyed.

One arguments now, that an element I in series on figure A.23 can displace entropy from lower to higher temperature which is not according to the second law. Consequently a thermal I-element can not exist.

It is true that I-element can pump the entropy from the lower to higher temperature but this supposes that the stored energy in this element is consumed and it can work only as long as there is some energy. Therefore the energy for charging the element C- comes from the element I and that

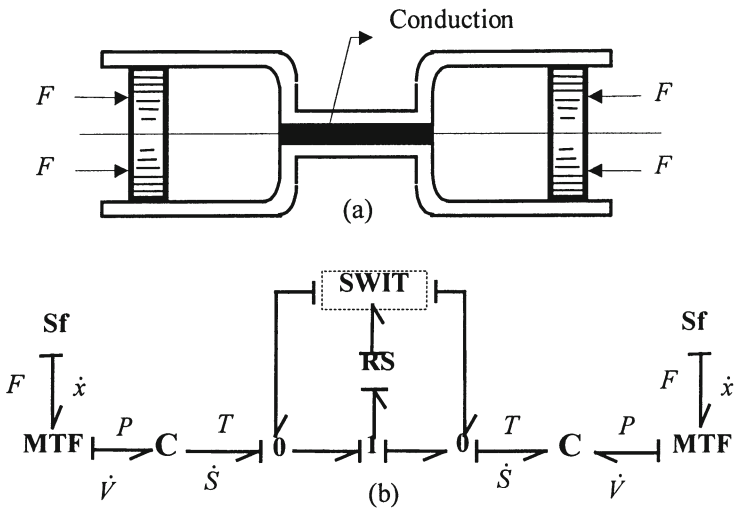


FIGURE A.22. Thermal conduction between two cylinders. a. Schema, b. bond graph model

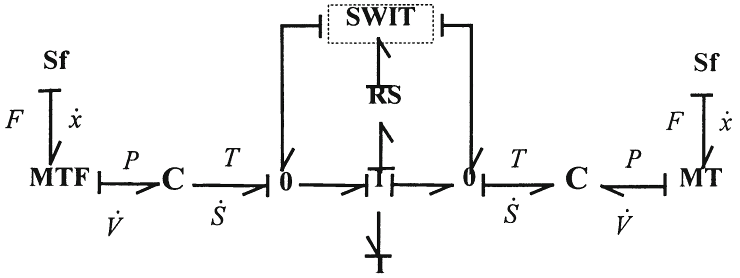


FIGURE A.23. Bond graph model of thermal conduction between two Cylinders with a thermal I-element is perfectly possible. As always the elements I and C are reversible and the only irreversibility is in the multiport RS.

The error comes from the fact, that the second law as the first law is applicable only to the continuous movement or steady state. In discontinuous or unsteady process, the first law is also not obeyed as show all play toys with a spring that produces mechanical energy.

A.11 Inverse Analogy

It should be mentioned for completeness, that there exist also mechanical bond graphs, where the role of effort and flow is interchanged. In other words, velocity is considered an effort and force a flow, or similarly rotation frequency an effort and torque a flow. We call this the inverse analogy. It is not used by practical bond graphers but has some theoretical advantages. It relates to an other graph theoretical method, the linear graphs.

With linear graphs, one divides the variables not in effort or flow, but in across and through variables. An across variable can be measured by applying a voltmeter, in the electrical case, on two bonds adjacent to an element, while a trough variable requires cutting a link, to insert an Ammeter. Writing now a bond graph in the inverse analogy has the effect that all efforts are across variables and all flows are through variables. Then graph theoretical methods can be used and such a bond graph is easily converted to a linear graph.

Author Jean Thoma has discussed the question of analogies with Henry Paynter at several times. Our conclusion was there is no theoretical reason to prefer one analogy or the other, both work and give computable bond graphs. However, the inverse analogy goes against the picture of electricity of Faraday and Maxwell, where one speaks of electromagnetic force and not about electromagnetic flow. Therefore all practical bond graphers including the authors use the normal analogy as expounded here.

A.12 References

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[Ganwtrop, 1995] Gawthrop P.J. "Bicausal Bond Graphs" International confernce on Bond Graph Modeling and Simulation" (IBGM'95), pp. 83-88, Las Vegas, USA, 1995.

[Karnopp, 1975] Karnopp D. C. and R.C. Rosenberg "Systems dynamics. A unified Approach", Wileey Intersciences; New York, 1975.

[Karnopp, 1979] Karnopp, D. K, "State Variables and Pseudo-Bond Graphs for Compressible Thermofluid Systems", Trans. ASME J. DSMC, Vol. 101, pp. 201-204, 1979.

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Appendix B

Listing of Simulation Programs

B.1 Hydro-Pneumatic Accumulator (Tutsim)

```
=Timing: 0.0020000 ,DELTA ; 10.0000 ,RANGE
   =PlotBlocks and Scales:
   =Format:
   = BlockNo, Plot-MINimum, Plot-MAXimum; Comment
   =Horz: 0 , 0.0000 , 10.0000 ; Time
   = Y1: 23 , 0.0000 , 10.0000 ; gas pressure
   = Y2: 31 , 273.0000 , 373.0000 ; tempera gas
   = Y3: 33 , 273.0000 , 373.0000 ; heat capac wall
   = Y4: 35 , 0.0000 , 500.0000 ; ext heat conduc
   12 SF 121 P1= 2.0000 ;Frequency excitation
   14 I -15 19 P1= 300.0000 ;mass of 1/4 car P2= 0.0000
   15 CON P1= 3.000E+03 ;gravity
   19 TF 22 23 P1= 1.000E+03 ;piston press area
   21 TF 12 -14 P1= 1.000E+03 ;pisto area (flow)
   22 R 21 P1= 0.0500000 ;damping resist
   23 DIV 413 212 ;gas pressure
   31 ATT 412 P1= 1.4000 ;tempera gas
   32 R 31 -33 P1= 10.0000 ;int heat conduct
   33 C 32 -35 P1= 10.0000 ;heat capac wall P2= 298.0000
   35 R 33 -36 P1= 2.0000 ;ext heat conduc
   36 CON P1= 298.0000 ;ambient temper
   41 MUL 21 23 ;compression power
   121 FRQ P1= 0.5000000 ;frequency genera P2= 0.0000
   211 INT 21 P1= 0.0000 ;calcul volumen
   212 SUM -211 213 ;effect volu
   213 CON P1= 120.0000 ;init volu
   221 MUL 21 22 ;damping power
   411 INT 221 41 -32 P1= 300.0000 ;calcul intern enrgy
   412 ATT 411 P1= 0.7180000 ;divi by Cv
   413 GAI 411 P1= 0.4000000 ; mult by R/Cv
```

B.2 Refueling Pneumatic Automobiles (Tutsim)

```
=Timing: 0.0040000 ,DELTA ; 100.0000 ,RANGE
   =PlotBlocks and Scales:
```

```
=Format:
= BlockNo, Plot-MINimum, Plot-MAXimum; Comment
=Horz: 0 , 0.0000 , 100.0000 ; Time
= Y1: 13 , 0.0000 , 20.0000 ; pressu right
= Y2: 23 , 0.0000 , 20.0000 ; pressu left
= Y3: 14 , 200.0000 , 400.0000 ; tempera bootle 1
= Y4: 24 , 200.0000 , 400.0000 ; tempera bottle 2
1 CON P1= 0.0000 ;air bottle filling
2 CON P1= 0.0000 ;fully chokd flow by FNC234
3 CON P1= 0.0000 ;scanvening by mdot41
13 ATT 323 P1= 3.000E+03 ;pressu right
14 DIV 322 311 ;tempera bootle 1
23 ATT 623 P1= 300.0000 ;pressu left
24 DIV 622 611 ;tempera bottle 2
31 MUL 131 132 91 234 ; mass flow
32 GAI 325 P1= 1.0050 ;enthalpy flux
41 GAI 46 P1= 1.0000 ;mass flow pump
42 GAI 241 P1= 1.0050 ;enthalpy flow pump
46 FNC 999
X,Y- 1 0.0000 0.0000
X,Y- 2 15.0000 0.0000
X,Y- 3 15.1000 1.0000
X,Y- 4 90.0000 1.0000
X,Y- 5 90.1000 0.0000
X,Y- 6 200.0000 0.0000
91 CON P1= 113.0000 ;window area
131 DIV 13 141 ;divi by root tempera
132 CON P1= 0.0600000 ;flow constant
141 SQT 14 ;root temperature
234 FNC 235
X,Y- 1 0.0000 0.5000000
X,Y- 2 0.5000000 0.5000000
X,Y- 3 0.6000000 0.4900000
X,Y- 4 0.7000000 0.4580000
X,Y- 5 0.8000000 0.4000000
X,Y- 6 0.9000000 0.3000000
X,Y- 7 0.9500000 0.2180000
X,Y- 8 1.0000 0.0000
235 DIV 23 13 ;pressu ratio
241 MUL 24 41 ;part enthalpy flow pump
311 INT -31 41 P1= 770.0000 ;mass left bottle
321 INT -32 42 P1= 150.000E+03 ;inter ebrgy left
322 ATT 321 P1= 0.7180000 ;left int energy divi Cv
323 GAI 321 P1= 0.4000000 ;divi R/Cv right
325 MUL 31 14 ;mult by temperature
```

```
  611 INT 31 -41 P1= 19.3000 ;mass right bottle
  621 INT 32 -42 P1= 3.750E+03 ;inter enrgy right
  622 ATT 621 P1= 0.7180000 ;right int energy divi Cv
  623 GAI 621 P1= 0.4000000 ;divi R/Cv left
```

B.3 Cooling of fuel for Diesel Cars (Tutsim)

```
=Timing: 0.0020000 ,DELTA ; 5.0000 ,RANGE
  =PlotBlocks and Scales:
  = BlockNo, Plot-MINimum, Plot-MAXimum; Comment
  =Horz: 0 , 0.0000 , 5.0000 ; Time
  = Y1: 32 , 0.0000 , 0.0500000 ; mass flow of hexa 2
  = Y2: 13 , 0.0000 , 1.0000 ; pressu before Hexa 3
  = Y3: 14 , 0.0000 , 1.0000 ; pressu before canister 4
  = Y4: 11 , 0.0000 , 1.0000 ; pressu before Hexa 1
  ,Fuel circuit with IP (Injection Pump), 3 hexa, canister and tank ,Multi-BG
with thermal bonds with md and Hd
  11 ATT 311 P1= 5.0000 ;pressu. before Hexa 1
  12 ATT 321 P1= 1.0000 ;pressu. before Hexa 2
  13 ATT 331 P1= 1.0000 ;pressu. before Hexa 3
  14 ATT 341 P1= 5.0000 ;pressu before canister 4
  15 ATT 351 P1= 1.0000 ;pressu. in tank 5
  21 ATT 412 P1= 1.0000 ;temp. in IP 1 input
  22 ATT 422 P1= 1.0000 ;temp in Hexa 2 input
  23 ATT 432 P1= 1.0000 ;temp in Hexa 3 input
  24 ATT 442 P1= 1.0000 ;temp in Canister 4 input
  25 ATT 452 P1= 1.0000 ;temp in tank 5
  28 CON P1= 0.0000 ;enviromental temperature
  31 ATT 11 -12 P1= 5.0000 ;mass flow in IP 1
  32 ATT 12 -13 P1= 0.2000000 ;mass flow of hexa 2
  33 ATT 13 -14 P1= 5.0000 ;mass flow of hexa 3
  34 SF 93 P1= 0.5000000 ;mass flow tank to canister
  36 ATT 14 -11 P1= 0.2000000 ;mass flow hexa 6
  41 CON P1= 0.0000 ;enthalpy inflow IP
  42 GAI 221 P1= 1.0000 ;enthalpy in hexa 2 input
  43 GAI 241 P1= 1.0000 ;enthalpy in Hexa 3 input
  44 GAI 251 P1= 1.0000 ;enthalpy flow tank to canister
  46 GAI 241 P1= 0.0000 ;enthalpy hexa 6
  51 CON P1= 0.0000 ;add mech energy
  82 ATT 22 -28 P1= 5.0000 ;therm conduc hexa 2 w enviro
  83 ATT 23 -28 P1= 5.0000 ;therm conduc hexa 3 w enviro
  84 ATT 24 -25 P1= 5.0000 ;therm conduc tank to can
  85 ATT 24 -28 P1= 5.0000 ;therm condu tank 5 w enviro
```

```
86 ATT 21 -28 P1= 5.0000 ;therm condu hexa 6 w enviro
93 CON P1= 1.0000 ;control signal
211 MUL 31 21 ;mass flow * temp21 of IP
212 GAI 211 P1= 1.0000 ;enthalpy without mech power
221 MUL 22 32 ;prod mass flow*tempera hexa 2
241 MUL 24 34 ;prod mass flow*tempera hexa 6
251 MUL 25 34 ;prod mass flow*tempera canister
311 INT 36 -31 P1= 0.5000000 ;mass in IP input
312 CON P1= 0.5000000 ;torque signal phi
313 CON P1= 1.0000 ;one for 1-phi
314 SUM -312 313 ;parameter 1-phi for spilled flow
319 MUL 314 31 ;mass spill flow
321 INT 319 -32 P1= 1.0000 ;mass in hexa 2
331 INT 32 -33 P1= 1.0000 ;mass in hexa 3
341 INT 33 -34 -36 P1= 1.0000 ;mass in hexa 4
351 INT -34 P1= 10.0000 ;fuel mass in tank
361 INT 33 -84 44 P1= 10.0000 ;mass in hexa 6
411 INT 469 41 P1= 0.0000 ;mass in IP 1
412 DIV 411 311 ;enthalpy mass rat in IP 1
419 MUL 314 41 ;spilled enthalgy flow
421 INT 419 -42 P1= 1.0000 ;stored energy hexa 2
422 DIV 421 321 ;enthal/mas ratio hexa 2
429 SUM 42 -82 ;enthalpy in output hexa 2
431 GAI 241 33 P1= 1.0000 ;stored energy hexa 3
432 DIV 431 331 ;enthal/mass ration hexa 3
439 SUM 43 -83 ;enthalpy in output hexa 3
441 INT 439 -44 -36 P1= 1.0000 ;int,stored energy hexa 4
442 DIV 441 341 ;enthalpy/mass ratio in canister 4
451 INT 44 84 -85 P1= 10.0000 ;stored enthalpy in tank
452 DIV 451 351 ;enth/mass ratio in tank 5
469 SUM 46 -86 ;enthalpy output hexa 6
```

B.4 Ventilation of a building (Twentesim)

- **20-sim Experiment Description**

```
=================================
Model: vent3a1
Experiment: exp1
Date: 08/31/99
Time: 15:34:57
Version: PC Version 2.3
License: Prof. G. Dauphin-Tanguy
 +cole Centrale de Lille, LAIL
```

Parameters:

```
===========
data2d‘filename 1.98855e-307
data2d‘col 1
data2c‘filename 1.98855e-307
data2c‘col 1
data2b‘filename 1.98855e-307
data2b‘col 1
data2a‘filename 1.98855e-307
data2a‘col 1
data1b‘filename 1.98855e-307
data1b‘col 1
data1a‘filename 1.98855e-307
data1a‘col 1
vent_3‘R13 0.01
vent_3‘Tref 273
vent_3‘Cp 0.001005
vent_2‘R13 0.01
vent_2‘Tref 273
vent_2‘Cp 0.001005
vent_1‘R13 0.01
vent_1‘Tref 273
vent_1‘Cp 0.001005
fanx‘R37 0.01
fanx‘Tref 273
fanx‘Cp 0.001005
fanx‘filename 1.98855e-307
fanx‘col 1
r_362‘R 25
r_361‘R 25
r_262‘R 25
r_261‘R 25
r_162‘R 25
r_161‘R 25
r_35‘R 50
r_25‘R 50
r_15‘R 50
c_36‘c1 36
c_26‘c1 36
c_16‘c1 36
C2‘Cv 0.000718
C2‘Tref 0
C2‘R 0.000287
C2‘Pref 0
C2‘V 60
```

```
C1‘Cv 0.000718
C1‘Tref 0
C1‘R 0.000287
C1‘Pref 0
C1‘V 60
Initial Conditions:
====================
c_36‘state 0
c_26‘state 0
c_16‘state 0
C2‘mdot_state 78500
C2‘hdot_state 0
C1‘mdot_state 78500
C1‘hdot_state 0
Run Specifications:
====================
Integration Method Euler
Start Time 0
Finish Time 100
Step Size 0.01
Multiple Run Specifications:
=============================
Multiple Run Type : Plain Multiple Run
Number Of Steps : 2
Plot Specifications:
=====================
X-Axis Time 0 100
A C1‘hdot_in.e -1 1
B C2‘hdot_in.e -1 1
C C2‘mdot_in.e -0.5 0.5
D fanx‘hdot_out.f 0 50
```

- **Two ports C:C2**

```
class 2c version 2
interface
 ports: hdot_in,mdot_in
 orientation restrictions
 fixed in hdot_in,mdot_in
 causality restrictions
 fixed effort hdot_in,mdot_in
parameters
 real Cv # 0.718e-3 [KJ/kgr]
 real Tref # Reference termperature, not mentioned in Tutsim Listing so take:
0 [K]
```

```
 real R # 0.287e-3
 real Pref # Reference Pressure, not mentioned in Tutsim Listing so take: 0 [kPa]
 real V # Room volume 60 [m3]
variables
 real mdot_state # initial value 78.5e3 [gr]
 real hdot_state # initial value 0
equations
 mdot_state = int(mdot_in.f) # int141
 hdot_state = int(hdot_in.f) # int131
 mdot_in.e = (hdot_state*R)/(Cv*V) - Pref
 hdot_in.e = (hdot_state/Cv)/mdot_state - Tref
```

- **Two ports C:C1**

```
class cdouble version 1
interface
 ports: hdot_in,mdot_in
 orientation restrictions
 fixed in hdot_in,mdot_in
 causality restrictions
 fixed effort hdot_in,mdot_in
parameters
 real Cv # 0.718e-3 [KJ/kgr]
 real Tref # Reference termperature, not mentioned in 20sim Listing so take: 0 [K]
 real R # 0.287e-3
 real Pref # Reference Pressure, not mentioned in 20sim Listing so take: 0 [kPa]
 real V # Room volume 60 [m3]
variables
 real mdot_state # initial value 78.5e3 [gr]
 real hdot_state # initial value 0
equations
 mdot_state = int(mdot_in.f) # int141
 hdot_state = int(hdot_in.f) # int131
 mdot_in.e = (hdot_state*R)/(Cv*V) - Pref
 hdot_in.e = (hdot_state/Cv)/mdot_state - Tref
```

- **Fanx1**

```
class fanx version 1
interface
 ports: mdot_in, hdot_in, hdot_out
 causality restrictions
 fixed flow mdot_in
```

```
 fixed flow hdot_in
 fixed flow hdot_out
 orientation restrictions
 fixed in mdot_in
 fixed in hdot_in
 fixed out hdot_out
parameters
 real R37 # Hydraulic resistance for mdot, 0.01 [sec*kPa/gr]
 real Tref # Reference temperature, 273 [K]
 real Cp # Specific heat for hdot, 1.005e-3 [kJ/kgr]
 string filename # parameter for filename table
 real col # columnnumber of data for table
variables
 real data3,var1,var2
equations
 data3 = from_file(filename,col) # Equal to Se_370
 mdot_in.f = (mdot_in.e + data3)/R37
 var1 = if mdot_in.f <= 0 then hdot_in.e else hdot_out.e
 var2 = Cp*mdot_in.f*(Tref + var1)
 hdot_in.f = var2
 hdot_out.f = var2
```

- **Vent1**

```
class vent version 1
interface
 ports: mdot_in, hdot_in, hdot_out
 causality restrictions
 fixed flow mdot_in
 fixed flow hdot_in
 fixed flow hdot_out
 orientation restrictions
 fixed in mdot_in
 fixed in hdot_in
 fixed out hdot_out
parameters
 real R13 # Hydraulic resistance for mdot, 0.01 [sec*kPa/gr]
 real Tref # Reference temperature, 273 [K]
 real Cp # Specific heat for hdot, 1.005e-3 [kJ/kgr]
variables
 real var1,var2
equations
 mdot_in.f = mdot_in.e/R13 # Note that I use the reciprocal equation
 var1 = if mdot_in.f <= 0 then hdot_in.e else hdot_out.e
 var2 = Cp*mdot_in.f*(Tref + var1)
```

```
hdot_in.f = var2
hdot_out.f = var2
```

B.5 Instrumentation of a Steam generator

Sensor	Parameter	Unit	Value
L1	Level in the tank	L	200
T2	Temperature of water	$^\circ C$	37
F3	Flow of feedwater	L/h	950
Q4	Heat power	kW	60
T5	Temperature of water in the boiler	$^\circ C$	168
T6	Temperature of vapour in the boiler	Bar	170
P7	Pressure in the boiler	Bar	8
L8, L9	Level of water	L	150
F10	Flow of Outlet steam expansion	kg/h	83
P11	Pressure depending on F10	Bar	8
P12, P13	Upstream, downstream pressure in branche 1	Bar	8
P14, P15	Upstream, downstream pressure in branche 2	Bar	5
P16	Inlet pressure to condenser	Bar	5
T17	Temperature at entrance of condenser	$^\circ C$	120
VM1, VM2	Control valve	%	-
F23	Flow of Inlet cooling water	kg/h	2600
L18, L19	Level of condensate	%	50
T20	Temperature output of condenser	$^\circ C$	52
T21	Temp. of inlet cooling water	$^\circ C$	40
T22	Temp. of outlet cooling water	$^\circ C$	70
V3-V5	Control valves		
F24	Flow cooling water in aerorefrigerator	kg/h	
T25	Temp. of inlet cooling water	$^\circ C$	70
T26	Temp. of outlet cooling water	$^\circ C$	30
T27	Ambient temp.	$^\circ C$	20

TABLE B.1. Instrumentation of steam generator of figure 5.15

Appendix C

Polynomial thermodynamic Functions

1. Enthalpy of steam function as function of pressure

$$h_v(P) = -0,74P^2 - 17,21P_3 + 2680 \tag{C.1}$$

2 Enthalpy of liquid as function of pressure

$$h_l(P) = -0,0243P^4 + 0,8487P^3 - 11,9P^2 - 99.97P + 347 \tag{C.2}$$

3 Specific volume of steam as function of pressure

$$\begin{gathered} \nu_v(P) = -5,3 * 10^{-5}P^5 + 0,00207P^4 - 0.032P^3 \\ +0,2498P^2 - 1,03P + 2,166 \end{gathered} \tag{C.3}$$

4 Specific volume of liquid as function of pressure

$$\nu_l(P) = -3,59 * 10^{-7}P^3 + 1,2456 * 10^{-5}P^2 + 1,039 * 10^{-3} \tag{C.4}$$

5 Temperature as function of pressure

$$f_T(P) = T = 0,459.P^2 + 12,7243.P + 99,005 \tag{C.5}$$

6 Partial derivative of mass density of steam at saturation as function of temperature

$$\begin{aligned} dRho = \left(\frac{\partial \rho_3}{\partial T}\right)_{T=T_{SAT}} &= 5 * 9,18 * 10^{-12}T^4 \\ &+1,59159 * 10^{-9}T^3 \\ &+3 * 2,6823812 * 10^{-7}T^2 \\ &+2 * 5,672779398 * 10^{-6}T \\ &+1,9036631098 * 10^{-4} \end{aligned} \tag{C.6}$$

7 Latent heat of steam as function of temperature

$$\begin{aligned} L_V(T) = -3,4 * 10^{-11}.T^4 + 4,421 * 10^{-11}.T^3 \\ -1,54503768 * 10^{-6}.T^2 - 2,21405632169 * 10^{-3}.T \\ +2,49715620119075 * 10^6 \end{aligned} \tag{C.7}$$

8 Enthalpy of liquid as function of temperature

$$h_L(T) = 4,337.T - 1,2025 * 10^3 \tag{C.8}$$

9 Enthalpy of steam as function of temperature

$$h_V(T) = 1,1248T + 2267,5 \tag{C.9}$$

Remark 1 *Used units:*

Enthalpy h in kJ/kg, Temperature in $°C$, Pressure P in bar , specific volume in m^3/kg.

Appendix D

Heat Losses and Heat Exchanger Coefficients of Collectors

We shall give here the main empirical relations for the calculation of thermal losses in steam generators. Since the theoretical determination is complex, one uses generally empirical relations for the parameters.

D.1 Not Insulated Steam Conduit

If there is no thermal insulation, such as in conduits for expansion the heat flow lost is [*Positello, 1983*]

$$\dot{Q} = \frac{\pi L(ti - te)}{\frac{1}{K_i D_i} + \frac{1}{2\lambda_t}\ln(\frac{D_{et}}{D_i}) + \frac{1}{K_e D_e}} \tag{D.1}$$

D.2 Insulated Steam Conduit

$$\dot{Q} = \frac{\pi L(T_i - T_e)}{\frac{1}{K_i D_i} + \frac{1}{2\lambda_t}\ln(\frac{D_{et}}{D_i}) + \frac{1}{2\lambda_C}\ln(\frac{D_e}{D_{et}})\frac{1}{K_e D_e}} \tag{D.2}$$

Where:
$\dot{Q}$: heat loss (W)
L. Length of conduit, insulated or not (m)
T_i: internal temperature conduit ($^\circ C$)
T_e: external temperature ($^\circ C$)
π: pi = 3.14159
K_i: heat transfer coefficient between internal fluid and wall of the conduit ($W/(m^{2\circ}C)$)
D_i: interior diameter of tube (m)
D_{et}: external diameter of tube (m)
λ_t: thermal conductivity of tube material ($W/(m.K)$)
K_e: heat transfer coefficient between external wall and the external fluid, here air ($W/(m^{2\circ}C)$)

λ_C: thermal conductivity of the insulating material (determined from curves) ($W/(m.K)$)

D.3 Calculation of Heat Exchange Coefficients

D.3.1 Superficial Heat Exchange Coefficient

The heat exchange coefficient K_i depends on:

- Properties of the fluid (density, conductivity, specific heat, viscosity, and so on)
- Properties of wall surface (rugosity, possible pores, and so on)

K_i is the superficial heat exchange coefficient between fluid and wall; it is the sum of exchange of convection K_{ic} and exchange due to heat radiation K_{ir} :

$$K_i = K_{ic} + K_{ir} \tag{D.3}$$

In practice, K_{ir} is often negligible.
For steam, K_i is calculated by the formula of Mc Adams

$$K_i = 0,024\frac{\lambda_f}{D_i}\left(\frac{\rho V D_i}{\mu}\right)^{0,8} \tag{D.4}$$

with:
λ_f: Heat conduction coefficient of steam given by curves in function of temperature (T) and pressure (P). For example at $T = 180°$ and $P = 10 bars$, $\lambda_f = 67.4 * 10^{-2} W/(mK)$.
ρ : density of steam (kg/m^3) given as function of temperature
V: steam velocity (m/s)
μ: dynamic viscosity of fluid in $Pa.s$
D_i: internal diameter (m).

D.3.2 External Heat Exchange Coefficient

$$K_e = K_{ec} + K_{er} \tag{D.5}$$

$$K_e = \frac{\lambda f}{D_e}\left(0,45 + 0,33(\frac{\rho v D_e}{\mu})\right)^{0,56} + K_{er} \tag{D.6}$$

$$K_{er} = R\frac{(T_{se}^4 - T_e^4)}{T_{se} - T_e} \tag{D.7}$$

Where:
R: heat radiation coefficient of the sheet metal covering the insulation $(W/(m^2.K)$. For a galvanized metal $R = 1.59 * 10^{-8} W/(m^2.K)$.
T_e: exterior or environment temperature,
$T_{se:}$ temperature of exterior surface given approximately by:

$$T_{se} \approx T_e + \frac{T_i - T_e}{10} \tag{D.8}$$

For small diameters and calm air, one takes usually:

$$K_e = 1,15(\frac{T_{se} - T_e}{D_e})^{\frac{1}{4}} + K_{er} \tag{D.9}$$

Remark 2 *If the external temperature T_{se} is known, we can calculate directly the losses by the relation:*

$$\dot{Q} = K_e \pi L \left(T_{se} - T_e\right) \tag{D.10}$$

The coefficient K_e is calculated from equation D.6. This formula allows to verify the value taken for the calculation of K_e.

D.4 REFERENCES

[Positello, 1983] Positello, R., 1983, "La vapeur d'eau industrielle", Technique et documemntatiom, Lavoisier, Paris 1983.

Appendix E

Simulation Programs under Matlab-Simulink

E.1 Block Diagram for the Steam Accumulator

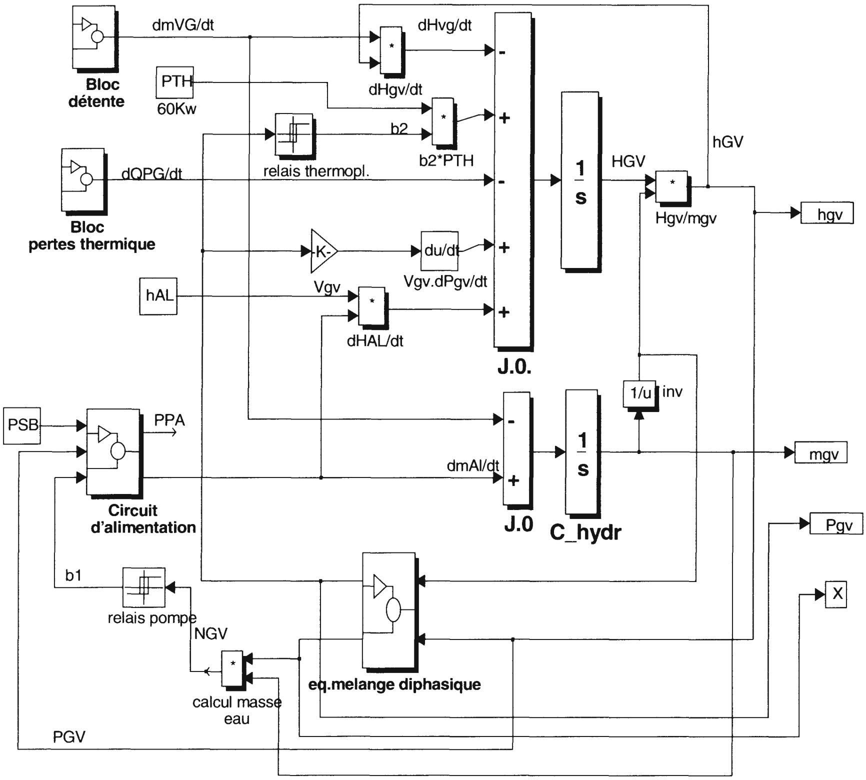

FIGURE E.1. Simulink block diagram of the steam Accumulator

E.2 Resolution of the equation of two phase mixture

```
% calculation of pressure PGV (in bar) and quality of steam X (in %) of
   % the mixture water-vapour. Given data are: specific volume
   % Vmg (Vmg=Vgv/Mgv) in m3/kg and specific enthalpy hgv
   % (hgv=Egv/Mgv) in j/kg of the mixture
   function yXP=XPgv(u)
   % Inputs:
   hgv0=u(2)*1e-3; % enthalpy calculated by the model of the boiler in j/kg;
   VM=0.175*u(1); % 0.175m3 is the geometric volume of the boiler
   Pgvmem=u(3); % pressure value calculated by the step before.
   %Thermodynamic functions
   % VMl, is the specific volume of liquid , VMv, specific volume of steam
   % hl, enthalpy of liquid in kJ/kg et hv, enthalpy of steam in kJ/kg
   VMl=[0 0 0 -3.59e-7 1.2456e-5 1.039e-3];
   VMv=[-5.3e-5 2.07e-3 -3.20e-2 2.498e-1 -1.03 2.166];
   hl=[0 -2.43e-2 8.487e-1 -1.19e1 9.997e1 3.47e2];
   hv=[0 0 0 -7.4e-1 1.721e1 2.68e3];
   % specific enthalpy of the mixture calculated by the model of the boiler
   hgv=[0 0 0 0 0 hgv0];
   % specific volume of the the mixture (VMgv=Vgv/Mgv)
   VMgv=[0 0 0 0 0 VM];
   % Resolution of the mixture equation
   V=conv((VMv-VMl),(hgv-hl))-conv((hv-hl),(VMgv-VMl));
   Pgv1=roots(V) % pressure in the boiler in bars
   % Selection of positive and real roots
   Pgvreel=zeros(size(Pgv1));
   for i=1:length(Pgvreel);
   if imag(Pgv1(i))==0 & 0<real(Pgv1(i)) Pgvreel(i)=Pgv1(i)
   end;end
   %Selection of one roots
   Pgv=0;
   for i=1:length(Pgvreel);
   if abs(Pgvreel(i)-Pgvmem)<abs(Pgv-Pgvmem) Pgv=Pgvreel(i);
   end;end
   X=((hgv(6)-polyval(hl,Pgv)))/((polyval(hv,Pgv)-polyval(hl,Pgv)))
   yXP=[Pgv X 0]
```

Appendix F

Heat Radiation and Solar Energy

F.1 Units and Usual values of Power

A quantitative appreciation of usual power values is very useful to get a picture of our civilization. At the same time allows to estimate solar energy and also the so called glasshouse effect, both used in modern environmental discussions.

The unit of power is the Watt, as used universally for all powers and not only for electric power. This unit is combining with the prefixes milli, kilo, etc. to arrive at some usual powers.

1. A micro watt (μW or $10^{-6} Watt$) is the consumption of an electronic wrist watch.
2. A milliwatt (mW or $10^{-3} W$) is the consumption of pilot lamps of electric appliances and computers.
3. A watt (W) is the power of a flashlight (torch).
4. A kilowatt (kW or $10^{3} watt$) is the power of an electric heater.
5. A megawatt (MW or $10^{6} watt$) is a Diesel locomotive.
6. A gigawatt (GW or $10^{9} watt$) is the power of a nuclear electric power plant.
7. A terawatt (TW or $10^{12} watt$) is the electric consumption of a small country.
8. A petawatt (PW or $10^{15} watt$) has no direct signification, but 175 PW is the solar power that strikes the disc or projection of the earth.

Let us cite some intermediate values: the electric power installed in all power plants is about $360 TW$ for the USA, 70 TW for France and 8 TW for Switzerland. With locomotives, this 1 MW corresponds to relatively small ones, where one puts several in front of a train. Electric locomotives in Europe have more power, about 5 MW, and the French high speed train (TGV) still more, about 12 MW.

F.2 Heat Radiation and Solar Energy

F.2.1 Solar Energy

The solar energy is almost $1.4kW/m$ which is the total solar power, divided by the interception by the earth, according to it's projected surface. The surface of the earth is:

$$S_T = \pi R_T^2 = \pi * 6000m^2 \tag{F.1}$$

This power comes to the surface at high altitude. A part is absorbed right away, so that approximately 1 kW/m^2 touches the earth at sea level on a bright day, much less if the sky is covered or foggy.

The efficiency of photocells is at best 20%, one can draw about $200W$ per m^2 on a clear day and if the cell is oriented towards the sun.

The entropy is calculated from the thermal energy, adding the factor 4/3 (see equation F.12 and F.13 below). It is 38 TW/K for incoming radiation.

F.2.2 Thermal Balance of the Earth

The thermal balance of the earth is shown on figure F.1. The same power as incoming is reradiated in the space in all directions, as shown. Most of this reflection takes place in the upper atmosphere, where the temperature is colder, about 250 K. Hence the entropy current leaving the earth is greater, about $950TW/K.m^2$. Compared to this figure, the entropy generated, by humans or by decomposition in the nature, which is important, remains negligible.

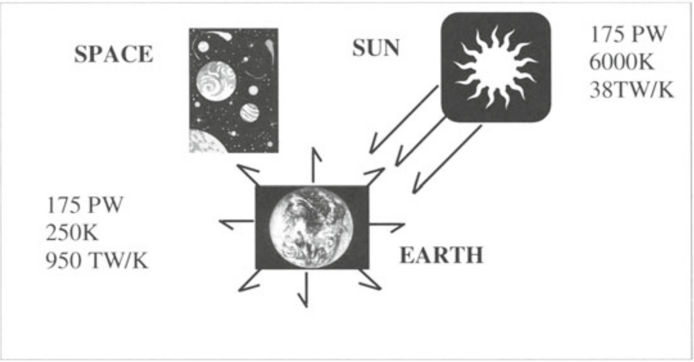

FIGURE F.1. Thermal balance of the earth

F.2.3 Thermal Radiation

After study of thermal radiation by conduction modelled by a simple *R*-Element and by convection, we introduce in this paragraph the thermal radiation. Let us remind that convection is expressed by a enthalpy balance and a coupled power bond.

In the transmission of heat by heat by radiation, the thermal transfer goes by electromagnetic vibrations which travel in a straight line without support of matter, contrary to conduction and convection. It consists of electromagnetic waves of a wave length of about 0.01 to 100 μm, including the visible spectrum 0,38 to 0.76 μm. Thermal radiation is important for solar energy and interesting because the equation of Carnot 3.1 must be modified. Thermal radiation requires both the thermal phenomena and the electric phenomena. They were studied at the end of the last century (1880-1902) by he great physicist Kirchhoff and Max Plank.

Let us consider a black cavity filled with electromagnetic waves and with a relative small hole for the admission and evacuation of radiation. The walls have a certain temperature and we want to find the energy and entropy in its function. Figure F.2 shows this cavity and we must first distinguish between energy and energy divided by volume and also between entropy and entropy per volume.

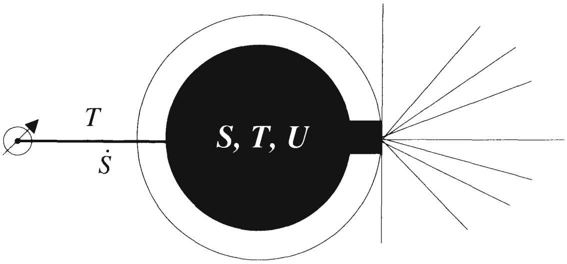

FIGURE F.2. Radiation of a black body

We have therefore:

$$\begin{aligned} U &= uV \\ S &= sV \end{aligned} \tag{F.2}$$

The following derivation comes from [*Pipard 1966*] who has a second formulation in a foot note. Fuchs 1996, gives a longer derivation and speaks of the contents of the cavity as a photon gas which is the right way and it known since about the year 1900.

It follows from the theory of electromagnetic radiation developed by Max Plank [*Plank, 1923*], that the waves send out by a black body exercise a radiation pressure on the walls which is equal to one third of the energy density u.

$$P = \frac{u}{3} \tag{F.3}$$

Let us take now the fundamental (or Gibbs) equation of a multiport C in the usual form dU, but written with a parameter t, which could be the time

$$\frac{dU}{dt} = T\frac{dS}{dt} - P\frac{dV}{dt} \tag{F.4}$$

The variables U, S, and V are the total values, not the quantities per volume, which are designated by small letters. By inserting (F.2) into (F.4) one obtains:

$$V\frac{du}{dt} + u\frac{dV}{dt} = TV\frac{ds}{dt} + TS\frac{dV}{dt} - P\frac{dV}{dt} \tag{F.5}$$

from which one takes

$$\frac{du}{dt} = T\frac{ds}{dt} + \left(Ts - \frac{u}{3} + u\right)\frac{dV}{dt} \tag{F.6}$$

Since the energy per volume must be independent of the volume, the expression inside the parenthesis must zero. This gives:

$$\begin{aligned} u &= \frac{3}{4}Ts \\ s &= \frac{4}{3}\frac{u}{T} \end{aligned} \tag{F.7}$$

Considering the fundamental equation per volume:

$$du = Tds = \frac{4}{3}\frac{u}{s}ds \tag{F.8}$$

as a differential equation of u as function of s, one has the solution

$$u = cste.s^{\frac{4}{3}} \tag{F.9}$$

which gives with equation F.8 the expression

$$s = aT^3 \tag{F.10}$$

where a is a constant not determined by our derivation. We use equation F.8 still to determine the internal energy

$$u = \frac{3}{4}aT^4 \tag{F.11}$$

The equation F.11 is the radiation law of Stephan Boltzmann of the total energy. In order to determine the distribution on the different frequencies there must take the formula of Planck which was at the same time the beginning of the quantum mechanics. The radiation that comes out by the small hole is simply volume density multiplied by the speed of light

$$\begin{aligned} \dot{S} &= acT^3 \\ \dot{Q} &= \frac{3}{4}acT^4 \end{aligned} \tag{F.12}$$

where c is the speed of light. One deducts:

$$\begin{aligned} \dot{Q} &= \frac{3}{4}T\dot{S} \\ \dot{S} &= \frac{4}{3}\frac{\dot{Q}}{T} \end{aligned} \tag{F.13}$$

Equation F.13 gives a relation between the power flux by radiation $\dot{Q}$ and the flux of entropy $\dot{S}$.. We can also say that the thermal radiation contains 133 % of entropy compared to the 100 % of entropy in thermal conduction.

F.2.4 Solar Collector

The figure F.3 shows the principle of transmission and connection of solar energy

The corresponding word bond graph appears on figure F.3b. The cavity has a bond which collects entropy and heat which its purpose. However, it produces a reflection of energy according to its own temperature in all the hemisphere. Since the sun has a temperature T_1 if both temperatures are equal, $T_1 = T_2$, the irradiation in the space is the same and there is nothing to collect. A collector must therefore have a lower temperature. The temperature of the sun is high, about $6000°C$, according to the method of Fuchs [*Fuchs,1996*].

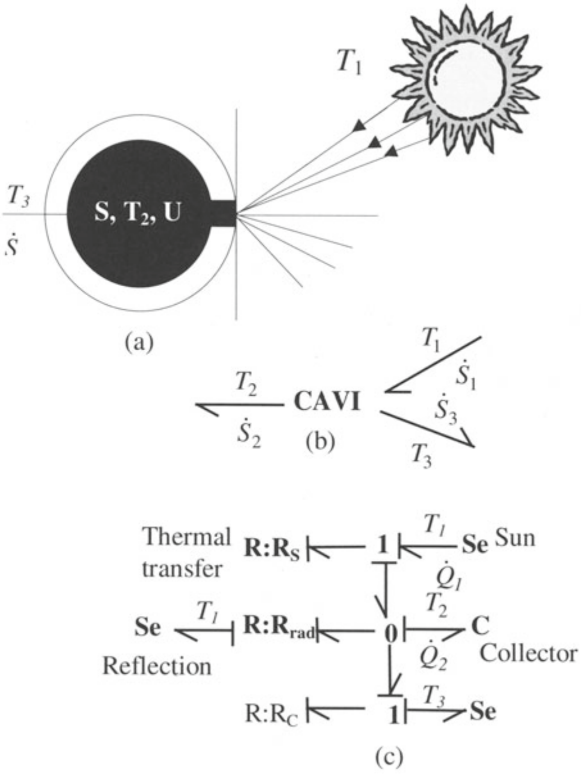

FIGURE F.3. Solar collector. a. Scheme, b. simplified word bond graph, c. pseudo bond graph model

The pseudo bond graph model is given by figure F.3c, where RS, R_{rad} and R_C denote respectively the thermal resistance of solar energy towards the earth, the resistance of reflection and the resistance of conduction. The multiport-C associated gives the storing of energy by the collector.

F.2.5 Glass House Effect and Thermal Death

On speaks much since the time of Clausius, about 1850, about the thermal death of the earth and cites the entropy as responsible. But this is independent of the notion of entropy and Carnot's equation 1.3. Simply, each process has some friction which produces heat (and entropy) and heats the world.

Therefore, according the analysis of thermal death, the earth will be submerged in an excess of heat and entropy. We see that this is not so, because all heat and entropy is sent to the space. Spaces has a temperature of only about 4 K and can absorb all heat all long as this is so. More probably is the cold death of the earth by exhaustion of the sun, but this will not happen in the next two billions of years.

One speaks also much of the glass house effect, which means a heating of the planet because of to much CO_2 in the atmosphere. This also is not worrying, because a slight increase of the temperature of the atmosphere say of 1 °C, would introduce a larger radiation of 2.8 PW into space by Planks radiation law or equation F.12.

What is more to worry, is a return to the ice age, of which the last one has terminated only 20 thousand years ago. By comparison, the dinosaurs have disappeared since about 63 million years.

F.3 Philosophical Questions

We are at the end of our book and would like to think about the method employed. It seems that we have returned to the method of energy used by Ernst Mach (1838 - 1916) and Walter Ostwald (1853 - 1932) mainly until the years 1895 and we use energy as fundamental quantity. Ostwald said himself, that the natural system of units in physics is length, time and energy, instead of length, time and mass used in the SI units. This seems right to us.

This energy method was later eclipsed by the atomic approach of Plank and Einstein. It started with the kinetic gas theory by Maxwell (1831 - 1879) and Boltzmann (1844 - 1906).

We have used the energy method and have introduced, just like in electricity, two factors in the flux of thermal energy: temperature and entropy. This a return to the ideas of Sadi Carnot (1796 - 1832). It is expressed by the equation of Carnot 1.3 which applies exactly to substances without movement. For matter in movement, it remains approximately true and is calculated in convection by the concept of enthalpy.

The entropy as fundamental thermal quantity is a partial return to the theory of "caloricum", fashionable around 1800. It is a substance without mass, like electric charge, which can be indefinitely generated by dissipation. This introduces the notion of time, because each dissipation is irreversible. On the contrary, the mechanics of mass points or celestial mechanics, and also the electrodynamics of Maxwell are reversible. So with the energy method, we do not have the philosophical difficulty to explain irreversibility by reversible process.

Atomic theory is universally accepted to day. The temperature is there explained as proportional to the square of the momentum (or speed) of each DOF (Degree Of Freedom). This formulation goes well with bond graphs with the notion of effort and flow and is one reason why we are so attracted by the bond graph method.

For conclusion on atomic and energetic approaches, we think that both are valid methods of developing knowledge and one must use the one best suited for the problem at hand. Jean Thoma has discussed these questions with Gottlieb Falk (1923 - 1992). He wanted to unify both approaches in his mind, but deceased in 1992 before finishing his work.

F.4 REFERENCES

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7

Liste of Used Symbols

Symbol	Designation	Unit
A	Area	m^2
A_f	Forward affinity	$J/mole$
A_r	Reverse affinity	$J/mole$
c_p	Specific heat per mass at constant pressure	$J/(K.kg)$
C_p	Global Specific heat at constant pressure	J/K
c_v	Specific heat per mass at constant volume	$j/(K.kg)$
C_v	Global Specific heat at constant volume	J/K
D	Diameter	m
$\dot{E}$	Energy flow, power	W
e	Thickness	m
H	Total enthalpy	J
$\dot{H}$	Enthalpy flow	W
h	Specific enthalpy	J/kg
i	Electric current	A
K_C	Thermal conductance	W/K
l	Width	m
L	Length	m
$\dot{m}$	Mass flow	kg/s
m	Mass	kg
n	Molar mass	–
N	Level	m
P	Pressure	Pa
Pu	Power	W
$\dot{Q}$	Thermal power by conduction	W
q	Electric charge	$Coulomb$
$\dot{S}$	Entropy flow	W
S	Entropy	J
s	Entropy density	J/kg

Symbol	**Designation**	**Unit**
T	Temperature	$°C$ or K
$\dot{n}$	Molar flow	$mole/s$
u	Electric voltage	V
v	Volume per mass	m^3/kg
$\dot{V}$	Volume flow	m^3/s
V	Volume	m^3
X	Quality of steam	$[0-1]$
U	Internal energy	J
$\dot{U}$	Internal energy flow	W
x	Displacement	m
ν	Specific volume	m^3/kg
μ	Chemical potential or tension	$J/mole$
ρ	Mass volumic (density)	Kg/m^3
λ	Thermal conductivity	$W/(m.K)$
$\dot{\xi}$	Speed of chemical reaction	$1/s$
ξ	Advancement of reaction	-

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