The Mathematical Representation of Driven Thermodynamic Systems

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1 Introduction

Abstract

A general framework for the treatment of driven systems in nonequilibrium thermodynamics is discussed for two selected theories and a simple model system. The framework is based upon the of modeling and control of general physical systems proposed by van der Schaft and co-workers. The crucial concept is the notion of a *Dirac structure* representing the dynamical equations of motion as well as the power conserving interconnection structure of the system. We applied the framework to two existing theories and a very simple model system. The two selected theories are the "General Equation for the Non-Equilibrium Reversible-Irreversible Coupling" (GENERIC) formalism of Grmela and Öttinger and the Matrix model of Jongschaap; the model system is a viscous gas in a cylinder and an externally driven piston. It is shown that the new approach provides not only a common framework for both theories, but also useful extensions, in particular an extended GENERIC treatment of driven systems.

Although already significant steps in that direction have been made, a generally accepted consistent formulation of nonequilibrium thermodynamics is still not available. An overwhelming number of theories and a wide variety of approaches are known and the challenge is to combine these various approaches in some kind of common generalized theory and finally to bring nonequilibrium thermodynamics to the same level of clarity and usefulness as equilibrium thermodynamics [13]. In the present paper we want to focus the attention on a method that has not yet received much attention in nonequilibrium thermo-

dynamics, but with promising prospects for this purpose. This method, based upon geometrical objects called *Dirac structures*, was developed by in particular Maschke, van der Schaft and co-workers [16], [20], [4], [21], [1] in the context of modeling and control of general physical systems and is still an important research topic in that field.

Dirac structures, based upon the *Dirac brackets*, originally introduced by Dirac [5], were proposed by Courant and Weinstein [3], [2] to provide a framework for constrained mechanical systems. The algebraic counterpart was given by Dorfman [6] in the context of the study of integrability of systems of partial differential equations. Van der Schaft and Maschke [20] used Dirac structures in physical control system theory to determine the algebraic constraints as well as the dynamical equations of motion and the power conserving interconnection structure of a system.

In the present paper we will discuss a similar approach in nonequilibrium thermodynamics. Our aim is not to develop a complete treatment, but merely to indicate some of its features and prospects. For that purpose we use two specific theories and a single model-system. The two selected theories are the "General Equation for the Non-Equilibrium Reversible-Irreversible Coupling" (GENERIC) formalism of Grmela and Öttinger [8], [18] and the Matrix model of Jongschaap [10], [14], [12], and as model system we choose a driven system consisting of a viscous gas in a cylinder and a piston moving under external pressure and gravitation. The same two frameworks and (almost) the same system was used in an earlier study [7] where the connection between the GENERIC

formalism and the Matrix model was examined. Our present investigation is complementary in the sense that our intention now is not a comparison of the two approaches, but to provide a common framework for both of them.

The new framework provides like the Matrix model as well as GENERIC dynamic equations in the form of matrix expressions with particular symmetry properties and separate reversible and dissipative contributions. With the Matrix model it shares two specific properties: the ability to handle driven systems and an the explicit partition into sub-systems. With GENERIC it has in common the Hamiltonian formulation and the inclusion of the macroscopic conservation laws. In addition Dirac structures provide some nice mathematical features [4] like many algebraic representations, a systematic treatment of constraints, closedness (or integrability) conditions and possible extensions to systems on spatial domains with varying boundary conditions [21].

2 A brief summary of GENERIC and the Matrix model

In GENERIC the time evolution of a set of state variables x, which typically contains position-dependent fields, is represented as

$$\frac{dx}{dt} = L(x)\frac{\delta E(x)}{\delta x} + M(x)\frac{\delta S(x)}{\delta x} \tag{1}$$

with the Poisson and friction matrices $L(x)$ and $M(x)$ operating on the functional derivatives of $E(x)$ and $S(x)$, the total energy and entropy of the system, expressed in terms of x. The matrix $L(x)$ must be skew-symmetric and satisfy the Jacobi identity and $M(x)$ must be Onsager-Casimir symmetric and positive semi-definite.

Equation (1) is supplemented by complementary degeneracy requirements

$$L(x)\frac{\delta S(x)}{\delta x} = 0 \tag{2}$$

and

$$M(x)\frac{\delta E(x)}{\delta x} = 0 \tag{3}$$

Equation (2) expresses the reversible nature of the L-contribution to the dynamics and (3) the conservation of energy by the M-contribution.

Essential for the GENERIC formulation is that the information of the processes is contained in generating functionals of the *total* system. The dynamics of driven, *i.e.* open, systems which exchange energy, linear momentum, *etc.* with their environment cannot be described consistently in this manner. As a consequence the material specific constitutive equations and the universal balance laws of matter are treated simultaneously.

A treatment based upon just the constitutive equations, leaving the balance laws aside is the Matrix model [10], [11]. In comparison with the GENERIC formulation the Matrix model is simpler, but extra variables are needed for the coupling of part of the system described by the model with external variables.

This situation is like fluid mechanics where, in global flow problems, it is sufficient to consider the Navier Stokes equation, *i.e.* a differential equation in the mass density ρ and the velocity field $\mathbf{v}$. An alternative is to consider the balance of momentum and constitutive equations for the shear stress and the pressure. The former case is similar to GENERIC and the latter to the Matrix model. The extra variables needed in the Matrix model are the pressure and the shear stress.

The Matrix model is based upon the identification of a reversible thermodynamic sub-system. This allows the definition of thermodynamic efforts $e^t = (\partial u/\partial x^t)_s$ and flows $f^t = \dot{x}^t$ as variables based upon the fundamental equation $u = u(s, x^t)$ of the internal energy u of that sub-system, with s the entropy and x^t the thermodynamic variables of state. On the other hand, in a driven system u is also determined by an external balance of power. If e^e and f^e are the external effort and flow variables in that balance equation, the dynamic equations for these variables are

$$\begin{bmatrix} e^e \\ f^t \end{bmatrix} = \begin{bmatrix} \eta & -\Lambda^T \\ \Lambda & \beta \end{bmatrix} \begin{bmatrix} f^e \\ -e^t \end{bmatrix} \tag{4}$$

This expression, complemented with the thermodynamic equations of state

$$e^t = e^t(s, x^t) \tag{5}$$

are the main equations of the Matrix model. Depending upon the tensorial

of functional character of the e and f variables the matrix elements in (4) are scalars, tensors or operators and Λ^T is the transposed or adjoint of Λ.

3 Dirac structures

We now briefly review the definition and some elementary properties of Dirac structures in relation with our thermodynamic treatment. For a more extensive treatment of many subjects, including different representations and integrability conditions, we refer in particular to the paper [4] by Dalsmo and van der Schaft. In view of the close connections with general system theory we adopted some notations and terminology of that discipline, in particular, the notion of flow and effort variables.

We start with n-dimensional linear spaces $\mathcal{F}$ of *flow* variables $f \in \mathcal{F}$ and $\mathcal{E}$ of *effort* variables $e \in \mathcal{E}$. With power, defined as the non-degenerate bilinear form

$$\mathcal{P} =< e, f > \tag{6}$$

these spaces become dual, so $\mathcal{E} = \mathcal{F}^*$. A *Dirac structure* $\mathcal{D}$ on the linear space $\mathcal{F}$ is defined then as a subspace of $\mathcal{F} \times \mathcal{E}$ such that

$$< e, f >= 0, \quad \forall (f, e) \in \mathcal{D} \tag{7}$$

and

$$dim(\mathcal{D}) = dim(\mathcal{F}) = n \tag{8}$$

Physically, (7) expresses *conservation of power*. So the Dirac structure can be seen as a subspace of $\mathcal{F} \times \mathcal{E}$ accessible under this constraint. The condition (8) is related to the fact that for a physical system it is not possible to specify flow and and effort variables simultaneously.

The use of Dirac structures has so far been restricted mainly to complex network structures, like electrical circuits and electro mechanical systems. For simple thermodynamic systems their use might seem superfluous. We claim, however, that for more complex systems it has notable advantages since it provides an explicit transparent and flexible representation of important physical characteristics of the system, like its interconnection structure, external couplings and constraints. This becomes also clear by noting that, as will be explained below, parts of the Matrix model as well as GENERIC can be interpreted as representations of Dirac structures. From existing applications of these theories to complex fluids we know that these representations are useful and far from trivial.

Once a base for the space of flows is specified and its dual is assumed on the space of efforts it is possible the give several matrix representations of Dirac structures, each with its own advantages. For our purpose we mainly need two of them.

In the **kernel representation** a Dirac structure $\mathcal{D}$ is represented as

$$\mathcal{D} = \{(f, e) \in \mathcal{F} \times \mathcal{E} \mid Ff + Ee = 0\} \tag{9}$$

for $n \times n$ matrices F and E satisfying

$$EF^T + FE^T = 0, \tag{10}$$

$$rank([F\ E]) = n \tag{11}$$

Particularly useful for our purposes is the kernel representation with $F = 1$ and an antisymmetric matrix E.

In the **hybrid input-output representation**, for a partition $\mathcal{F} = \mathcal{F}_1 \times \mathcal{F}_2$ of the space $\mathcal{F}$ and a corresponding partition $\mathcal{E} = \mathcal{E}_1 \times \mathcal{E}_2$ of the space $\mathcal{E}$, a Dirac structure $\mathcal{D}$ is represented by a *skew-symmetric* matrix J as

$$\begin{bmatrix} e_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} J_{11} & -J_{21}^T \\ J_{21} & J_{22} \end{bmatrix} \begin{bmatrix} f_1 \\ e_2 \end{bmatrix} \tag{12}$$

where $(e_1, e_2) \in \mathcal{E}_1 \times \mathcal{E}_2$, $(f_1, f_2) \in \mathcal{F}_1 \times \mathcal{F}_2$ and $J_{11} = -J_{11}^T$, $J_{22} = -J_{22}^T$.

For nonlinear systems the framework of Dirac structures on linear spaces is not sufficient. Fortunately the above definitions can be extended to the notion of *generalized Dirac structures on manifolds*. Let $\mathcal{X}$ be a n-dimensional manifold with $T_x\mathcal{X}$ the tangent space and $T_x^*\mathcal{X}$ the cotangent space at a point $x \in \mathcal{X}$. A generalized Dirac structure $\mathcal{D}$ on an $\mathcal{X}$ is given then by specifying for every $x \in \mathcal{X}$ an n-dimensional subspace $\mathcal{D}(x) \subset T_x\mathcal{X} \times T_x^*\mathcal{X}$ depending smoothly on x and such that $\mathcal{D}(x)$ is a Dirac structure on $T_x\mathcal{X}$. The adjective "generalized" means in this context "not necessarily integrable". If $\mathcal{D}$ satisfies an additional closedness or integrability condition then $\mathcal{D}$ defines a (true) Dirac structure on

$\mathcal{X}$.

Often a Dirac structure is treated in connection with a Hamiltonian (energy) function. Then an *implicit generalized Hamiltonian system* on $\mathcal{X}$ corresponding to $\mathcal{D}$ and $\mathcal{H}$ with flow variables $\dot{x} \in T_x\mathcal{X}$ and effort variables $\frac{\partial H}{\partial x}(x) \in T_x\mathcal{X}^*$ is given by [19]

$$\left(\dot{x}, \frac{\partial H}{\partial x}(x)\right) \in \mathcal{D}(x), \quad x \in \mathcal{X} \tag{13}$$

If the subspace $\mathcal{D}$ for every x can be parametrized by the cotangent vectors α such that $\mathcal{D}(x) = \{(X, \alpha) | X = J(x)\alpha\}$ then $J(x) = J(x)^T$ and (13) reduces to the *explicit generalized Hamiltonian system*

$$\dot{x} = J(x)\frac{\partial H}{\partial x}(x) \tag{14}$$

which is the classic Hamiltonian dynamics given by the Poisson bracket $\dot{x} = \{x, H\}$. The representation (14) is a special case of the kernel representation (9) with $F = 1$ and $E = -J$. $\mathcal{D}$ is closed (integrable) [4], that is, the Poisson bracket satisfies the Jacobi identity

$$\{F, \{G, K\}\} + \{G, \{K, F\}\} + \{K, \{F, G\}\} = 0 \tag{15}$$

if and only if there exist local coordinates (p, q, r) for which (14) takes the form

$$\dot{q} = \frac{\partial H}{\partial p}, \ \dot{p} = -\frac{\partial H}{\partial q}, \ \dot{r} = 0 \tag{16}$$

A driven Hamiltonian system with $\dot{x} \in T_x\mathcal{X}$, $\frac{\partial H}{\partial x}(x) \in T_x\mathcal{X}^*$ external flows

$f \in \mathcal{F}$ and external efforts $e \in \mathcal{E} = \mathcal{F}^*$ may be represented by a Dirac structure $\mathcal{D} \subset T_x\mathcal{X} \times \mathcal{F} \times T_x\mathcal{X}^* \times \mathcal{E}$, defined by $< \alpha, X > - < e, f >= 0$ for all $(X, f, \alpha, -e) \in \mathcal{D}$, similar to (13) as

$$\left(\dot{x}, f, \frac{\partial H}{\partial x}(x), -e\right) \in \mathcal{D}(x), \quad x \in \mathcal{X} \tag{17}$$

Van der Schaft and Maschke [19] call this an *implicit port-controlled generalized Hamiltonian system*. Under certain conditions (17) can be represented by an explicit expression, similar to (14):

$$\begin{aligned} \dot{x} &= J(x)\frac{\partial H}{\partial x}(x) + g(x)f \\ e &= g^T(x)\frac{\partial H}{\partial x}(x) \end{aligned} \tag{18}$$

This result is also readily expressed as a hybrid input-output representation (12). In control system theory, *port-controlled Hamiltonian systems* are basic building blocks for design, simulation and control of complex dynamical systems.

4 A driven thermodynamic system

We now discuss, in particular in connection with GENERIC and the Matrix model, some features of our approach for a very simple system. The system is a gas in a vertical adiabatic cylinder under a piston of mass m (see Figure 6). This system can be treated either as closed, or by applying an external force to the piston, as a driven system. In both cases it becomes dissipative by giving

the gas a finite bulk viscosity.

First we consider the case of a driven system with a non-viscous gas. The total energy then becomes

$$E = K + \Phi + U = E(p, z, S, V^t) \tag{19}$$

where $K = \frac{p^2}{2m}$ is the kinetic energy, p the momentum, $\Phi = mgz$ the potential energy of the piston and $U = U(S, V^t)$ the internal energy of the gas, expressed as function of the entropy S and the gas volume V^t. An external force F^e, also expressed as an external pressure $P^e = -F^e/A$, is applied to the piston. A is the surface area of the piston. Conservation of energy implies

$$\dot{E} = F^e \dot{z} = -P^e \dot{V}^e \tag{20}$$

with $\dot{V}^e$ an external flow variable equal to the rate of change change $\dot{V}^t$ of the gas volume and also to $A\dot{z}$.

By (19) the rate of change of internal energy is

$$\dot{U} = \dot{E} - \dot{K} - \dot{\Phi} \tag{21}$$

or, using (20) for $\dot{E}$ and expressing the rate of change of kinetic energy as $\dot{K} = v\dot{p}$, the rate of change of potential energy as $\dot{\Phi} = mg\dot{z}$ and the momentum as $p = mv$

$$\dot{U} = -P^{e,gas}\dot{V}^{e,gas} \tag{22}$$

with

$$P^{e,gas} = P^e + \frac{\dot{p}}{A} + \frac{mg}{A} \tag{23}$$

and

$$\dot{V}^{e,gas} = \dot{V}^e \tag{24}$$

expressing an internal energy balance of just the gas. The total force $F^e = -AP^e$, acting upon the system is also split into a part $\dot{p} + mg$, contributing to the kinetic and potential energy of the piston and a part $-AP^{e,gas}$, contributing to the internal energy of the gas.

Apart from (22) U can also be expressed as

$$\dot{U} = T\dot{S} - P^t\dot{V}^t \tag{25}$$

where $T = \left(\frac{\partial U}{\partial S}\right)_{V^t}$ is the temperature and $P^t = -\left(\frac{\partial U}{\partial V^t}\right)_S$ is the thermodynamic pressure. This implies for the dissipation $\Delta \equiv T\dot{S}$

$$\Delta \quad = \quad -P^{e,gas}\dot{V}^{e,gas} + P^t\dot{V}^t \tag{26}$$

This expression is valid is the reversible as well as the dissipative case. In general $\Delta = -P^e\dot{V}^e + P^t\dot{V}^t - v\dot{p} - mg\dot{z}$, so in the non-dissipative case where by the balance of momentum $\dot{p} = -AP^e + AP^t - mg$ one obtains, as expected, $\Delta = 0$; for the dissipative case a dissipative pressure term due to the bulk viscosity of the gas enters the momentum balance: $\dot{p} = -AP^e - AP^d + AP^t - mg$; this implies a nonzero dissipation $\Delta > 0$.

4.1 Dirac structure

To define a useful Dirac structure we rewrite (26) as

$$-P^e\dot{V}^e + P^t\dot{V}^t - v\dot{p} - mg\dot{z} - T\dot{S} = 0 \tag{27}$$

and, using spaces as listed in table 1, express this result as a scalar product $<,>$ of the spaces $\mathcal{F} = \mathcal{F}^e \times \mathcal{F}^t \times \mathcal{F}^p \times \mathcal{F}^\Phi \times \mathcal{F}^s$ and $\mathcal{E} = \mathcal{E}^e \times \mathcal{E}^t \times \mathcal{E}^p \times \mathcal{E}^\Phi \times \mathcal{E}^s$ as

$$< e, f >= 0 \tag{28}$$

with

$$f = \begin{bmatrix} \dot{V}^e \\ \dot{V}^t \\ \dot{p} \\ \dot{z} \\ \dot{S} \end{bmatrix} \qquad e = \begin{bmatrix} P^e \\ -P^t \\ v \\ mg \\ T \end{bmatrix} \tag{29}$$

The spaces $\mathcal{F}$ and $\mathcal{E}$ are dual: $\mathcal{E} = \mathcal{F}^*$ with respect to the scalar product (28) and the orthogonality of the vectors in (29) implies a Dirac structure $\mathcal{D}$

$$(f, e) \in \mathcal{D} \subset \mathcal{F} \times \mathcal{E} \tag{30}$$

A *kernel representation*, of $\mathcal{D}$ is the matrix expression

$$\begin{bmatrix} \dot{V}^e \\ \dot{V}^t \\ \dot{p} \\ \dot{z} \\ \dot{S} \end{bmatrix} = \begin{bmatrix} 0 & 0 & A & 0 & 0 \\ 0 & 0 & A & 0 & 0 \\ -A & -A & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} P^e \\ -P^t \\ v \\ mg \\ T \end{bmatrix} \tag{31}$$

This equation is of the form (9) with $F = 1$ and has the required antisymmetry implied by (10). It represents the interconnection structure, the momentum balance and the reversibility condition $\dot{S} = 0$ of the system.

Note that in (28) the term $-T\dot{S}$ could have been omitted, since for a reversible system this term vanishes identically. We keep this term, however, for compatibility with the GENERIC formalism (see below). Note also that all variables were treated as independent a priori; constraints like $\dot{V}^e = \dot{V}^t = Av = A\dot{z}$ are taken into account by the Dirac structure.

4.2 GENERIC

For a treatment of the present system with GENERIC we refer to the paper [7] by Edwards *et al.* on the relationship between GENERIC and the Matrix model and also to the paper [17] by Muschik *et al.* The result for the fundamental GENERIC expression (1) in the non-dissipative case is [7]

$$\frac{dx}{dt} = L\frac{\delta E}{\delta x} \tag{32}$$

with

$$x = \begin{bmatrix} p \\ z \\ S \end{bmatrix}, \quad L = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \frac{\delta E}{\delta x} = \begin{bmatrix} v \\ mg + \frac{\partial U}{\partial z} \\ T \end{bmatrix} \tag{33}$$

This expression is consistent with our result (31) if one takes into account that GENERIC can only handle isolated systems, so $P^e = 0$, and independent variables, so $\dot{V}^t$ and $AP^t = -\partial U/\partial z$ must be eliminated from (31) before comparison with (32) Having established the link of (31) with GENERIC for the reversible case, we now add a dissipative contribution and use (31) to obtain a representation of the driven system.

The dissipative term in the GENERIC structure is obtained by using the complementary degeneracy requirements (2) and (3). We let the gas be viscous, with a bulk viscosity η_b. The dissipative pressure on the piston then becomes $P^{e,gas}_{diss} = \eta \dot{V}^{e,gas}$ where $\eta = \eta_b / V^{e,gas}$ This pressure causes an extra contribution $-A^2\eta v$ to $\dot{p}$ and an extra contribution $-A^2\eta v^2/T$ to $\dot{S}$ in (31). As a result we obtain

$$\frac{dx}{dt} = L\frac{\delta E}{\delta x} + M\frac{\delta S}{\delta x} \tag{34}$$

with x, L, $\frac{\delta E}{\delta x}$, given by (35) and

$$M = A^2\eta \begin{bmatrix} T & 0 & -v \\ 0 & 0 & 0 \\ -v & 0 & \frac{1}{T}v^2 \end{bmatrix}, \quad \frac{\delta S}{\delta x} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \tag{35}$$

A representation of the driven system is obtained by adding like in (31) a row with and column associated with the external variables $\dot{V}^e$ and P^e. This *extended GENERIC* representation becomes:

$$\begin{bmatrix} \dot{V}^e \\ \frac{dx}{dt} \end{bmatrix} = \begin{bmatrix} 0 & \Gamma \\ -\Gamma^T & L \end{bmatrix} \begin{bmatrix} P^e \\ \frac{\delta E}{\delta x} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} 0 \\ \frac{\delta S}{\delta x} \end{bmatrix} \tag{36}$$

with L and M as above, and (in this case) $\Gamma = [A\ 0\ 0\ ]$ Like in the original GENERIC treatment, the state of the system is described by a set of system variables x and the matrices L and M operate on the derivatives of E and S to produce reversible and dissipative contributions to $\dot{x}$. But now, in addition, the matrix $-\Gamma^T$ produces an extra contribution to $\dot{x}$ due to the external pressure P^e and the conjugate external rate variable $\dot{V}^e$ is determined by Γ, operating on $\delta E/\delta x$. It is important to note that P^e and $\dot{V}^e$ are *external* controllable and observable variables. P^e is not a derivative of an energy neither is V^e part the system variable x. In that sense the extended GENERIC system (36) compares with GENERIC (1) as the port controlled (18) with the autonomous Hamiltonian system (14).

4.3 Matrix model

In the Matrix model the present system is represented as

$$\begin{bmatrix} -P^{e,gas} \\ \dot{V}^t \end{bmatrix} = \begin{bmatrix} \eta & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \dot{V}^{e,gas} \\ P^t \end{bmatrix} \tag{37}$$

with $P^{e,gas}$ and $\dot{V}^{e,gas}$ defined by (23) and (24). This model does not describe the whole system; inertial and gravitational contributions are explicitly excluded. As a result the equation (37) is much simpler than the previous results.

Also for the Matrix model an associated Dirac structure can be defined. This is based upon the bilinear form

$$T\dot{S} =< e^{gas}, f^{gas} >= -P^{e,gas}\,\dot{V}^{e,gas} + P^t\dot{V}^t$$

which vanishes for the non-dissipative case where $P^{e,gas} = P^{e,gas}_{rev}$ and $\dot{V}^t = \dot{V}^t_{rev}$. The associated Dirac structure

$$\mathcal{D}' \subset \mathcal{F}^{e,gas} \times \mathcal{F}^t \times \mathcal{E}^{e,gas} \times \mathcal{E}^t \tag{38}$$

has a hybrid input-output representation (12)

$$\begin{bmatrix} -P^{e,gas}_{rev} \\ \dot{V}^t_{rev} \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \dot{V}^{e,gas} \\ P^t \end{bmatrix} \tag{39}$$

The Matrix model (37) consists also of this representation plus a dissipative contribution

$$\begin{bmatrix} -P^{e,gas}_{diss} \\ \dot{V}^t_{diss} \end{bmatrix} = \begin{bmatrix} \eta & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{V}^{e,gas} \\ P^t \end{bmatrix} \tag{40}$$

Like the previous case the analysis here proceeds in two steps: first a Dirac structures is defined by a suitable representation and next a dissipative contri-

bution is added. The construction of this dissipative contribution is as usual in the Matrix model.

5 General approach

Although this paper is intended to provide just an indication of our new approach and we are still far from a complete understanding, the contours of its basic structure are already emerging. Its treatment of a driven thermodynamic system proceeds along the following steps

1. An analysis of the equilibrium thermodynamic and mechanical properties of the system and its interconnection structure.

2. The determination of a bilinear form based upon the the entropy production that can serve as scalar product for a Dirac structure.

3. The construction of a suitable representation of the Dirac structure.

4. The addition of a dissipative contributions.

This procedure results in a set differential and algebraic equations for the dynamic behavior of the system.

The crucial step in the procedure is point 2. Here the spaces of flow and effort variables are selected. In our example we have seen that for GENERIC this set is different from the one used in the Matrix model. In the former, all mechanical and thermodynamical variables were included, in the latter only the thermodynamic ones and a customized set of external variables. In the case of

GENERIC-like formulations we have seen that in some cases omitting of the $T\dot{S}$ from the bilinear form is possible.

Once the bilinear form with proper variables is available, a representation of the Dirac structure is needed. Here several representations, some of which have been discussed in our example, are available. One should keep in mind that not the representation, but the Dirac form itself, which is an abstract geometrical object, has a physical meaning. The construction of a representation proceeds by inspection. It contains all structural information, like constraints on flow and effort variables, the momentum balance, dependencies by interconnections and a specification of the in and output connections. The symmetry requirements of the Dirac structure representation should be obeyed.

For the addition of the dissipative contributions two procedures have been discussed, so far: the one based upon the GENERIC complementary degeneracy requirement and the one used in the Matrix model, expressed in an hybrid in and output representation. In principle these constructions consists of the definition of coordinates outside the Dirac structure in the $\mathcal{F} \times \mathcal{E}$ space by selection of an appropriate complementary subspace.

For simple homogeneous systems, like the one in our example, this procedure is sufficient. For non homogeneous systems driven at their boundaries in which conductive and convective transport transport processes take place, a general procedure is not yet available. Further development in that direction is guided by GENERIC, which provides a framework for the case of closed systems, in combination with a recent development [15], based upon so called *Stokes-Dirac*

structures which allow to represent continuous systems interacting through their boundary.

6 Discussion

For a simple model system we have shown that both the GENERIC formalism and the Matrix model fit well into a general framework based upon Dirac structures. This not only clarifies the interconnection between these approaches but also provides an extended treatment of driven systems.

The case of the Matrix model where the treatment is concentrated around a sub-system where mechanical and field contributions have been eliminated is similar to the common approach in classical non-equilibrium thermodynamics [9], based upon a local equilibrium hypothesis. Our example indicates that such a treatment can also be based upon Dirac structures.

Contrary to the common GENERIC treatment, where the skew symmetry and the Jacobi identity both follow from properties of the Poisson bracket, these items can be studied separately in Dirac structures. Poisson brackets associated with (generalized) Dirac structures may or may not satisfy the Jacobi identity; (if and) only if the structures are closed (integrable) this is the case. For Dirac structures, the skew symmetry of the matrix in equations like (31) is only partially based upon the underlying Hamiltonian dynamics, and further just a consequence conservation of power. Moreover even in mechanical systems, for example in the case of non-holonomic constraints, violation of the Jacobi identity

may occur. An exploration of this in a treatment based upon generalized Dirac structures may also be relevant for complex fluids.

References

[1] J. Cervera, A. J. van der Schaft, and A. Banos. On composition of dirac structures and its implications for control by interconnection. 281:55–63, 2003.

[2] T.J. Courant. Dirac manifolds. *Trans. American Math. Soc.*, 319:631–661, 1990.

[3] T.J. Courant and A. Weinstein. *Beyond Poisson Structures.* Hermann, Paris, 1988.

[4] M. Dalsmo and A. J. Van der Schaft. On representations and integrability of mathematical structures in energy-conserving physical systems. *Siam J. Control Optim.*, 37(1):54–91, 1998.

[5] P.A.M. Dirac. Generalized hamiltonian dynamics. *Canad. J. Math.*, 2:129–148, 1950.

[6] I. Dorfman. *Dirac Structures and Integrability of Nonlinear Evolution Equations.* John Wiley, Chichester, 1993.

[7] B. J. Edwards, H. C. Öttinger, and R. J. J. Jongschaap. On the relationships between thermodynamic formalisms for complex fluids. *J. Non-Equilib. Thermodyn.*, 22(4):356–373, 1997.

[8] M. Grmela and H. C. Öttinger. Dynamics and thermodynamics of complex fluids. i. development of a general formalism. *Phys. Rev. E*, 56(6):6620–6632, 1997.

[9] S.R. Groot and P. Mazur. *Non-equilibrium Thermodynamics*. North-Holland, Amsterdam, 1969.

[10] R. J. J. Jongschaap. Microscopic modeling of the flow properties of polymers. *Rep. Prog. Phys.*, 53(1):1–55, 1990.

[11] R. J. J. Jongschaap. A generalized thermodynamic approach to microrheological modeling. *Appl. Sci. Res.*, 48(2):117–128, 1991.

[12] R. J. J. Jongschaap, K. H. Dehaas, and C. A. J. Damen. A generic matrix representation of configuration tensor rheological models. *J. Rheol.*, 38(4):769–796, 1994.

[13] R. J. J. Jongschaap and H. C. Öttinger. Nonequilibrium thermodynamics and complex fluids. *J. Non-Newton. Fluid Mech.*, 96(1-2):1–3, 2001.

[14] R.J.J. Jongschaap. Towards a unified formulation of microrheological models. *Springer Lecture Notes in Physics*, 381:215–247, 1991.

[15] B. M. Maschke and A. J. van der Schaft. Hamiltonian representation of distributed parameter systems with boundary energy flow. 259:137–142, 2001.

[16] B. M. Maschke, A.J. van der Schaft, and P. C. Breedveld. An intrinsic hamiltonian-formulation of network dynamics - nonstandard poisson structures and gyrators. *J. Frankl. Inst.-Eng. Appl. Math.*, 329(5):923–966, 1992.

[17] W. Muschik, S. Gümbel, M. Kröger, and H.C. Öttinger. A simple example for comparing generic with rational non-equilibrium thermodynamics. *Physica A*, 285:448–466, 2000.

[18] H. C. Öttinger and M. Grmela. Dynamics and thermodynamics of complex fluids. ii. illustrations of a general formalism. *Phys. Rev. E*, 56(6):6633–6655, 1997.

[19] A.J. van der Schaft and B.M. Maschke. The hamiltonian formulation of energy conserving physical systems with external ports. *Archive für Elektronik und Übertragungstechnik*, 49:362–371, 1995.

[20] A. van der Schaft and B. Maschke. The hamiltonian-formulation of energy conserving physical systems with external ports. *Aeu- Arch. Elektron. Ubertrag.tech.-Int. J. Electron. Commun.*, 49(5-6):362–371, 1995.

[21] A. J. van der Schaft and B. M. Maschke. Hamiltonian formulation of distributed-parameter systems with boundary energy flow. *J. Geom. Phys.*, 42(1-2):166–194, 2002.

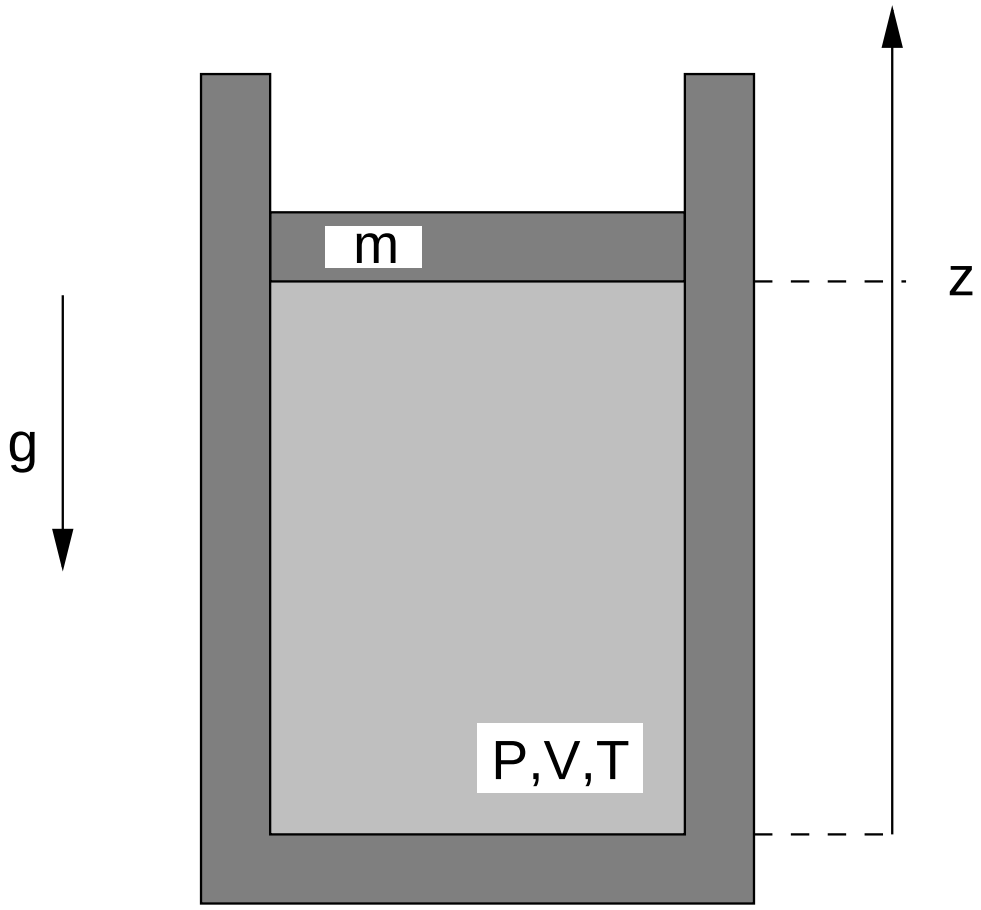

Figure 1: example system: a gas in adiabatic cylinder under a piston with mass m

	Flows		Efforts	
Type	Space	Variable	Space	Variable
External	$\mathcal{F}^e$	$\dot{V}^e$	$\mathcal{E}^e$	P^e
Thermodynamic	$\mathcal{F}^t$	$\dot{V}^t$	$\mathcal{E}^t$	$-P^t$
Momentum	$\mathcal{F}^p$	$\dot{p}$	$\mathcal{E}^p$	$v = \frac{p}{m}$
Potential	$\mathcal{F}^\Phi$	$\dot{z}$	$\mathcal{E}^\Phi$	mg
Entropic	$\mathcal{F}^s$	$\dot{S}$	$\mathcal{E}^s$	T

Table 1: Spaces, flow and effort variables for the various types of contributions in the balance of power