Systems & Control Letters 100 (2017) 51–55

Contents lists available at ScienceDirect

Systems & Control Letters

journal homepage: www.elsevier.com/locate/sysconle

A port-Hamiltonian formulation of the Navier–Stokes equations for reactive flows

R. Altmann, P. Schulze *

Institut für Mathematik, Technische Universität Berlin, Straße des 17. Juni 136, 10623 Berlin, Germany

ARTICLE INFO

Article history:
Received 12 January 2016
Received in revised form 5 December 2016
Accepted 22 December 2016

Keywords:
Reactive flow
Port-Hamiltonian formulation
Navier–Stokes equations
Hamiltonian formulation
Energy-Based modeling

ABSTRACT

We consider the problem of finding an energy-based formulation of the Navier–Stokes equations for reactive flows. These equations occur in various applications, e. g., in combustion engines or chemical reactors. After modeling, discretization, and model reduction, important system properties as the energy conservation are usually lost which may lead to unphysical simulation results. In this paper, we introduce a port-Hamiltonian formulation of the one-dimensional Navier–Stokes equations for reactive flows. The port-Hamiltonian structure is directly associated with an energy balance, which ensures that a temporal change of the total energy is only due to energy flows through the boundary. Furthermore, the boundary ports may be used for control purposes.

1. Introduction

Model-based optimization and control methods are important tools in many application areas. These come with a common need for models which can be evaluated in a short time, but still capture the main features of the considered system. In this context, model reduction techniques have become very popular and have been applied to various fields of application including flow control and robotics, see e. g. [1,2]. All these applications have in common that they are usually modeled based on physical laws, as for instance conservation of energy. One way of preserving energy conservation in all stages from the partial differential equations (PDEs) to the reduced model is a port-Hamiltonian formulation of the system equations.

Port-Hamiltonian systems provide an extension of classical Hamiltonian systems by introducing ports which account for energy exchange with the environment and for energy loss due to dissipation. Their structure implies directly passivity and, under certain conditions for the Hamiltonian, also stability. Moreover, they are invariant under power-preserving interconnection. Therefore, from the control perspective, a port-Hamiltonian formulation is especially helpful, since it allows to apply passivity based control techniques. An introduction to port-Hamiltonian systems theory can be found in [3].

In the case of PDEs, i. e., in the infinite-dimensional setting, there is no general canonical description of port-Hamiltonian systems. Instead, there are various different representations. The most common approaches are the classical evolutionary one, see e.g. [4–7] and the representation by a Stokes–Dirac structure [8,9]. Further concepts from mathematical physicals include polysymplectic [10,11] and multisymplectic [12,13] Hamiltonian systems. The formulation derived in this paper belongs to the classical evolutionary approach.

The general port Hamiltonian setting allows to describe systems from various areas of physics [3]. Here we mainly focus on the applications to fluid dynamics and thermodynamics. For the latter one, a quasi port-Hamiltonian structure has been introduced in [14] to describe irreversible thermodynamics. The introduced structure guarantees conservation of energy as well as a non-decreasing entropy. One of the considered examples was a continuously stirred chemical reactor. However, this approach has not yet been extended to systems with convective flows.

A Hamiltonian formulation for an ideal fluid has been presented in [15]. This has been extended to viscous flows in [16] by using the notion of a metriplectic structure. However, neither the Hamiltonian nor the metriplectic structure accounts for a non-zero energy flow through the boundary. For an ideal fluid, boundary flows have been integrated in [8] leading to an implicit port-Hamiltonian representation by means of a Stokes-Dirac structure. In [17] the dynamics of viscous, isentropic flows with magnetohydrodynamic coupling has been formulated as a port-Hamiltonian system with boundary control. Recently, a Hamiltonian formulation of the full Navier–Stokes equations has been presented in [18].

In this paper, we present a port-Hamiltonian formulation of the full Navier–Stokes equations for reactive flows in a one-dimensional spatial domain accounting for non-zero boundary

* Corresponding author.
E-mail addresses: raltmann@math.tu-berlin.de (R. Altmann), pschulze@math.tu-berlin.de (P. Schulze).

http://dx.doi.org/10.1016/j.sysconle.2016.12.005
0167-6911/

energy flows. The infinite-dimensional formulation is based on the Cartesian coordinate system and on a variational formulation of the governing equations. This appears to be a convenient form for future work about structure-preserving discretizations based on Petrov Galerkin projections to obtain a finite-dimensional port-Hamiltonian system. This will be addressed in another paper. Preceding efforts in the field of structure-preserving discretization methods for port-Hamiltonian systems may be found, for instance, in [19,20], whereas structure-preserving model reduction techniques are discussed, e. g., in [21,22].

This paper is structured as follows. After the derivation of the mathematical model, we present a Hamiltonian formulation of the reactive Navier–Stokes equations with vanishing boundary energy flows. Subsequently, this formulation is extended to a port-Hamiltonian formulation with boundary ports accounting for non-zero boundary energy flows.

2. Mathematical model

We consider the compressible Navier–Stokes equations for reactive flows in a one-dimensional spatial domain $\Omega = (a,\ b)$ and time domain $[0,\ t_{\text{end}})$ with $a, b, t_{\text{end}} \in \mathbb{R}, b > a$, and $t_{\text{end}} > 0$. These may be derived from a generic conservation law, cf. [23], which is reflected by the PDE

$$\partial_t f\,(x,t) + \partial_x \Phi_f\,(x,t) = q_f\,(x,t) + r_f\,(x,t)\,. \tag{1}$$

This equation describes the change of the conserved generic quantity

$$F\,(t) = \int_a^b f\,(x,t)\,\mathrm{d}x$$

by generic fluxes Φ_f, production q_f, and long-range processes r_f. In the following, we neglect the influence of the long-range processes, since their effect is marginal in many applications. From the generic equation (1), one can derive governing equations for the conservation of mass, momentum, energy, and species by replacing the generic quantities by the specific ones stated in Table 1. The resulting governing equations are summarized as

$$\partial_t \rho + \partial_x\,(\rho v) = 0, \tag{2a}$$
$$\partial_t\,(\rho v) + \partial_x\left(\rho v^2 + p + \tau\right) = 0, \tag{2b}$$
$$\partial_t\,(\rho e) + \partial_x\,(\rho e v + (p+\tau)\,v + \phi) = 0, \tag{2c}$$
$$\partial_t\,(\rho y_i) + \partial_x\,(\rho y_i v + j_i) = \tilde{M}_i \omega_i \tag{2d}$$

with density ρ, velocity v, pressure p, shear stress τ, specific total energy e, heat flux density ϕ, mass fraction y_i of the ith species, diffusion flux densities j_i, molar masses $\tilde{M}_i$, and molar rates of formation ω_i. Here, we consider $N \in \mathbb{N}$ different species and, thus, (2d) with $i = 1, \ldots, N$ represents N equations.

Since we neglect the influence of long-range processes, we also assume the change of potential energy to be zero. Thus, we may express the total energy ρe as the sum of internal energy ρu and kinetic energy $\rho v^2/2$. Using this relation and Eq. (2b), we can derive the conservation law for the internal energy from the conservation law of the total energy (2c) as

$$\partial_t\,(\rho u) + \partial_x\,(\rho u v + \phi) + (p+\tau)\,\partial_x v = 0$$

with specific internal energy u, cf. [23]. By applying the product rule, we may write the governing equations as

$$\partial_t \rho + \partial_x\,(\rho v) = 0, \tag{3a}$$
$$\partial_t v + v\partial_x v + \frac{1}{\rho}\partial_x\,(p+\tau) = 0, \tag{3b}$$
$$\partial_t u + v\partial_x u + \frac{1}{\rho}\,(p+\tau)\,\partial_x v + \frac{1}{\rho}\partial_x \phi = 0, \tag{3c}$$

Table 1
Special quantities for conservation of mass, momentum, energy, and species [23].

	F	f	Φ_f	q_f
Mass	m	ρ	ρv	0
Momentum	mv	ρv	$\rho v^2 + p + \tau$	0
Energy	me	ρe	$\rho e v + (p+\tau)\,v + \phi$	0
Species	my_i	ρy_i	$\rho y_i v + j_i$	$\tilde{M}_i \omega_i$

$$\partial_t y_i + v\partial_x y_i + \frac{1}{\rho}\partial_x j_i = \frac{1}{\rho}\tilde{M}_i \omega_i. \tag{3d}$$

Further, u may be expressed as a function of ρ, the specific entropy s, and $y_1, \ldots, y_N$. The Gibbs equation

$$\mathrm{d}u = T\mathrm{d}s - p\mathrm{d}\left(\frac{1}{\rho}\right) + \sum_{i=1}^{N} \mu_i \mathrm{d}y_i \tag{4}$$

describes the change of u with respect to changes of ρ, s, and $y_1, \ldots, y_N$. Here, T denotes the temperature and μ_i the chemical potential of the ith species [24]. With (4) we can express Eq. (3c) in terms of the entropy, namely

$$\partial_t s + v\partial_x s + \frac{\tau}{\rho T}\partial_x v + \frac{1}{\rho T}\partial_x \phi + \sum_{i=1}^{N} \frac{\mu_i}{\rho T}(\tilde{M}_i \omega_i - \partial_x j_i) = 0,$$

where we already have used the relations

$$T = \partial_s u, \qquad p = \rho^2 \partial_\rho u, \qquad \text{and} \quad \mu_i = \partial_{y_i} u. \tag{5}$$

Finally, the governing equations are closed, based on the closure equations of

$$\text{Fourier's law:} \qquad \phi = -\kappa\,\partial_x T, \tag{6}$$
$$\text{Newtonian fluid:} \qquad \tau = -\hat{\mu}\,\partial_x v, \tag{7}$$
$$\text{Fick's law:} \qquad j_i = -\rho D_i \partial_x y_i, \tag{8}$$

where κ denotes the thermal conductivity, $\hat{\mu}$ the dynamic viscosity (scaled by the factor $4/3$ to account for compressible flow, cf. [23]), and D_i the mass diffusivity of the ith species. Fourier's law as stated in (6) is based on the assumptions of a vanishing Dufour effect and negligible heat flux due to diffusion, cf. [23,24]. Furthermore, we assume that the effects of thermal diffusion and pressure diffusion may be neglected which leads to Fick's law as in (8), cf. [23].

Using (5), we can summarize the governing equations as

$$\partial_t \rho + \partial_x\,(\rho v) = 0, \tag{9a}$$
$$\partial_t v + \partial_x\left(\frac{1}{2}v^2 + u + \rho\partial_\rho u\right) + \frac{1}{\rho}\partial_x \tau - T\partial_x s - \sum_{i=1}^{N} \mu_i \partial_x y_i = 0, \tag{9b}$$
$$\partial_t s + v\partial_x s + \frac{\tau}{\rho T}\partial_x v - \frac{1}{\rho T}\partial_x\,(\kappa\,\partial_x T) + \sum_{i=1}^{N} \frac{\mu_i}{\rho T}\left(\tilde{M}_i \omega_i + \partial_x\,(\rho D_i \partial_x y_i)\right) = 0, \tag{9c}$$
$$\partial_t y_i + v\partial_x y_i - \frac{1}{\rho}\partial_x\,(\rho D_i \partial_x y_i) = \frac{1}{\rho}\tilde{M}_i \omega_i \tag{9d}$$

with known constants $\tilde{M}_i$ and known functions $D_i, \omega_i, u, \hat{\mu}, T, \kappa, \mu_i$ which depend on ρ, s, and $y_1, \ldots, y_N$.

For the formulation of the governing equations as Hamiltonian or rather port-Hamiltonian system, we consider the variational formulation (in terms of the space derivatives). For this, we apply a sufficiently smooth test function φ to the equations in (9). Furthermore, we use the integration by parts formula which introduces

boundary terms. These contribute to the boundary ports in Section 4. More precisely, we integrate the term including ρv in (9a) (corresponding to the convective energy flow), the term including τ in (9b) (corresponding to the energy flow due to friction), and the term including $\kappa\partial_x T$ in (9c) (corresponding to the energy flow due to heat conduction). This leads to

$$\langle \partial_t \rho, \varphi\rangle = \langle \rho v, \partial_x\varphi\rangle - \rho v\varphi\big|_a^b, \tag{10a}$$

$$\langle \partial_t v, \varphi\rangle = \Big\langle -\partial_x\Big(\frac{1}{2}v^2 + u + \rho\partial_\rho u\Big) + T\partial_x s, \varphi\Big\rangle + \big\langle \tau, \partial_x(\varphi/\rho)\big\rangle - \frac{\tau\varphi}{\rho}\Big|_a^b + \sum_{i=1}^N \langle \mu_i \partial_x y_i, \varphi\rangle, \tag{10b}$$

$$\langle \partial_t s, \varphi\rangle = -\Big\langle v\partial_x s + \frac{\tau}{\rho T}\partial_x v, \varphi\Big\rangle + \frac{\kappa}{\rho T}\partial_x T\varphi\Big|_a^b - \Big\langle \kappa\partial_x T, \partial_x\Big(\frac{\varphi}{\rho T}\Big)\Big\rangle - \sum_{i=1}^N \Big\langle \frac{\mu_i}{\rho T}\Big(\tilde{M}_i\omega_i + \partial_x(\rho D_i\partial_x y_i)\Big), \varphi\Big\rangle, \tag{10c}$$

$$\langle \partial_t y_i, \varphi\rangle = \Big\langle -v\partial_x y_i + \frac{1}{\rho}\big(\tilde{M}_i\omega_i + \partial_x(\rho D_i\partial_x y_i)\big), \varphi\Big\rangle. \tag{10d}$$

In the following two sections, we show that this variational formulation can be written as Hamiltonian (assuming vanishing boundary terms) or port-Hamiltonian system.

3. Hamiltonian dynamics of reactive flows

For ease of notation, we combine all unknowns within the vector $\boldsymbol{z}$, i. e.,

$$\boldsymbol{z} := [\rho,\ v,\ s,\ y_1,\ \ldots,\ y_N]^T.$$

The total energy or Hamiltonian $\mathcal{H}$ of the reactive flow system described by (9) consists of the kinetic energy and the internal energy, i. e.,

$$\mathcal{H}(\boldsymbol{z}) = \int_a^b \frac{\rho v^2}{2} + \rho u(\rho, s, y_1, \ldots, y_N)\,\mathrm{d}x.$$

Since the Hamiltonian density does not depend on spatial derivatives, the variational derivative $\delta_z\mathcal{H}$ equals the partial derivative of this density and is given by

$$\delta_z\mathcal{H}(\boldsymbol{z}) = \Big[\frac{1}{2}v^2 + u + \rho\partial_\rho u,\ \rho v,\ \rho T,\ \rho\mu_1,\ \ldots,\ \rho\mu_N\Big]^T.$$

The aim of this section is to formulate the system equations (10) as a Hamiltonian system of the form $\partial_t\boldsymbol{z} = \mathcal{J}(\boldsymbol{z})\,\delta_{\boldsymbol{z}}\mathcal{H}(\boldsymbol{z})$ with skew-adjoint operator $\mathcal{J}(\boldsymbol{z})$. For this, we restrict ourselves to the case where the boundary conditions lead to vanishing energy flows through the boundary. Especially, we consider the case where the mass flow ρv, the heat flux $\kappa\partial_x T$, and the shear stress τ are zero at the boundary. This restriction is then dropped in Section 4. In the sequel, $H^1(\Omega)$ denotes the Sobolev space of square integrable functions that also possess a square integrable weak derivative, cf. [25] for an introduction. The dual space of $H^1(\Omega)$, i. e., the space of linear functionals for Sobolev functions, is denoted by $H^1(\Omega)^*$. With this, we define the solution-dependent operator $\mathcal{J} : \mathcal{D}(\mathcal{J}) \to \mathcal{D}(\mathcal{J})^*$ with domain

$$\mathcal{D}(\mathcal{J}) = \big[H^1(\Omega)\big]^{N+3}, \qquad \mathcal{D}(\mathcal{J})^* = \big[H^1(\Omega)^*\big]^{N+3}$$

by

$$\mathcal{J}(\boldsymbol{z}) := \begin{bmatrix} 0 & -\tilde{\partial}_x & 0 & 0 & \ldots & 0 \\ -\partial_x & 0 & \frac{1}{\rho}\partial_x s - \mathcal{J}_{23} & \frac{1}{\rho}\partial_x y_1 & \ldots & \frac{1}{\rho}\partial_x y_N \\ 0 & -\frac{1}{\rho}\partial_x s - \mathcal{J}_{32} & \mathcal{J}_{33} - \hat{\mathcal{J}}_{33} & -\mathcal{M}_1 & \ldots & -\mathcal{M}_N \\ 0 & -\frac{1}{\rho}\partial_x y_1 & \mathcal{M}_1 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & -\frac{1}{\rho}\partial_x y_N & \mathcal{M}_N & 0 & \ldots & 0 \end{bmatrix}. \tag{11}$$

Therein, the operator $\tilde{\partial}_x$ is defined as the partial derivative w. r. t. x applied to the test function or, after an integration by parts, the partial derivative with an additional boundary term,

$$\big\langle \tilde{\partial}_x k, \ell\big\rangle := -\int_a^b k\partial_x\ell\,\mathrm{d}x = \int_a^b \ell\partial_x k\,\mathrm{d}x - k\ell\big|_a^b. \tag{12}$$

Note that we have $\tilde{\partial}_x = \partial_x$ if applied to functions with vanishing boundary conditions. The operator $\mathcal{J}_{23}$ is defined by

$$\big\langle \mathcal{J}_{23}k, \ell\big\rangle := -\int_a^b \frac{\tau}{\rho T}k\partial_x\Big(\frac{1}{\rho}\ell\Big)\,\mathrm{d}x$$

and $\mathcal{J}_{32} := \frac{\tau}{\rho T}\partial_x\big(\frac{1}{\rho}\cdot\big)$, whereas $\mathcal{M}_i$ is given by

$$\mathcal{M}_i := \frac{1}{\rho^2 T}\Big(\tilde{M}_i\omega_i + \partial_x(\rho D_i\partial_x y_i)\Big).$$

The operators $\mathcal{J}_{33}$ and $\hat{\mathcal{J}}_{33}$ are defined by their actions on certain test functions, namely

$$\big\langle \mathcal{J}_{33}k, \ell\big\rangle := -\int_a^b \kappa\partial_x\Big(\frac{1}{\rho}k\Big)\partial_x\Big(\frac{1}{\rho T}\ell\Big)\,\mathrm{d}x,$$

$$\big\langle \hat{\mathcal{J}}_{33}k, \ell\big\rangle := -\int_a^b \kappa\partial_x\Big(\frac{1}{\rho T}k\Big)\partial_x\Big(\frac{1}{\rho}\ell\Big)\,\mathrm{d}x.$$

Note that the operator $\hat{\mathcal{J}}_{33}$ was included artificially in order to obtain the skew-adjointness of the operator $\mathcal{J}$ as we show in the following lemma. The influence of this operator on the solution is discussed afterwards.

Lemma 3.1. *The operator $\mathcal{J} : \mathcal{D}(\mathcal{J}) \to \mathcal{D}(\mathcal{J})^*$ from (11) is skew-adjoint, i. e.,*

$$\langle \boldsymbol{k}, \mathcal{J}\boldsymbol{\ell}\rangle_{H^1(\Omega),\,H^1(\Omega)^*} = -\langle \mathcal{J}\boldsymbol{k}, \boldsymbol{\ell}\rangle_{H^1(\Omega)^*,\,H^1(\Omega)}$$

for all $\boldsymbol{k}, \boldsymbol{\ell} \in \mathcal{D}(\mathcal{J})$.

Proof. Consider test functions $\boldsymbol{k}, \boldsymbol{\ell} \in \mathcal{D}(\mathcal{J})$ with components $\boldsymbol{k} = [k_1, \ldots, k_{N+3}]^T$ and $\boldsymbol{\ell} = [\ell_1, \ldots, \ell_{N+3}]^T$. For the proof we need the relation

$$\big\langle k_1, -\tilde{\partial}_x\ell_2\big\rangle + \big\langle k_2, -\partial_x\ell_1\big\rangle = \big\langle \ell_1, \tilde{\partial}_x k_2\big\rangle + \big\langle \ell_2, \partial_x k_1\big\rangle, \tag{13}$$

which follows directly from the definition of $\tilde{\partial}_x$, see (12). Using (13) and the fact that $\mathcal{M}_i$ is symmetric, we obtain by simple rearrangements $\langle \boldsymbol{k}, \mathcal{J}\boldsymbol{\ell}\rangle = -\langle \mathcal{J}\boldsymbol{k}, \boldsymbol{\ell}\rangle$ which completes the proof. □

For the Hamiltonian formulation of the system equations, we have to apply the operator $\mathcal{J}$ to the variational derivative of the Hamiltonian $\mathcal{H}$. For this, we have to discuss the influence of the operator $\hat{\mathcal{J}}_{33}$ which was included in order to gain the skew-adjointness of the operator $\mathcal{J}$. Here we benefit from the property $\hat{\mathcal{J}}_{33}(\rho T) = 0$.

Theorem 3.2 (*Hamiltonian Structure*)**.** *Under the assumption that $\delta_z\mathcal{H} \in \mathcal{D}(\mathcal{J})$ and that the mass flow ρv, the heat flux $\kappa\partial_x T$, and the*

shear stress τ vanish at the boundary, the variational formulation of the governing equations (10) may be expressed as

$$\partial_t \boldsymbol{z} = \mathcal{J}(\boldsymbol{z})\,\delta_{\boldsymbol{z}}\mathcal{H}(\boldsymbol{z}). \tag{14}$$

Proof. As mentioned in the beginning of this section, the variational derivatives of $\mathcal{H}$ are given by

$$\delta_\rho \mathcal{H} = \frac{v^2}{2} + u + \rho\partial_\rho u, \qquad \delta_v \mathcal{H} = \rho v,$$
$$\delta_s \mathcal{H} = \rho\partial_s u, \qquad \delta_{y_i}\mathcal{H} = \rho\partial_{y_i} u.$$

Using the relations in (5), we can write the variational derivatives $\delta_s\mathcal{H}$ and $\delta_{y_i}\mathcal{H}$ as

$$\delta_s \mathcal{H} = \rho T \quad \text{and} \quad \delta_{y_i}\mathcal{H} = \rho\mu_i.$$

Thus, (14) is equivalent to

$$\langle \partial_t \rho, \varphi\rangle = \langle -\tilde{\partial}_x(\rho v), \varphi\rangle, \tag{15a}$$
$$\langle \partial_t v, \varphi\rangle = \Big\langle -\partial_x\Big(\frac{1}{2}v^2 + u + \rho\partial_\rho u\Big) + T\partial_x s, \varphi\Big\rangle - \big\langle \mathcal{J}_{23}(\rho T), \varphi\big\rangle + \sum_{i=1}^{N}\big\langle \mu_i\partial_x y_i, \varphi\big\rangle, \tag{15b}$$
$$\langle \partial_t s, \varphi\rangle = \big\langle -v\partial_x s + \mathcal{J}_{33}(\rho T) - \hat{\mathcal{J}}_{33}(\rho T), \varphi\big\rangle - \big\langle \mathcal{J}_{32}(\rho v), \varphi\big\rangle - \sum_{i=1}^{N}\big\langle \mathcal{M}_i\rho\mu_i, \varphi\big\rangle, \tag{15c}$$
$$\langle \partial_t y_i, \varphi\rangle = \big\langle -v\partial_x y_i + \mathcal{M}_i\rho T, \varphi\big\rangle \tag{15d}$$

for all smooth test functions φ. Since we assume that ρv, $\kappa\partial_x T$, and τ vanish at the boundary, (15) is nothing else than the variational form of the governing equations as given in (10). □

Remark 3.3. Note that Theorem 3.2 also implies that the Hamiltonian system $\partial_t\boldsymbol{z} = \mathcal{J}(\boldsymbol{z})\delta_{\boldsymbol{z}}\mathcal{H}(\boldsymbol{z})$ is equivalent to the classical formulation of the governing equations (9) if we assume sufficient regularity in order to integrate by parts.

Corollary 3.4. *Under the assumptions of Theorem 3.2, the Hamiltonian $\mathcal{H}$ satisfies the energy balance $\frac{d}{dt}\mathcal{H} = 0$.*

Proof. Since the operator $\mathcal{J}$ is skew-adjoint, cf. Lemma 3.1, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H} = \big\langle \delta_{\boldsymbol{z}}\mathcal{H}, \partial_t\boldsymbol{z}\big\rangle = \big\langle \delta_{\boldsymbol{z}}\mathcal{H}, \mathcal{J}(\boldsymbol{z})\delta_{\boldsymbol{z}}\mathcal{H}\big\rangle = 0. \quad \square$$

In this section we have shown that the variational formulation of the governing equations (10) may be written as a Hamiltonian system if the mass flow ρv, the heat flux $\kappa\partial_x T$, and the shear stress τ vanish at the boundary. In the next section, we drop this restrictive assumption and generalize the Hamiltonian formulation of the system equations (10) to a port-Hamiltonian formulation.

4. Port-Hamiltonian dynamics of reactive flows

In the case of non-vanishing boundary terms, the variational formulation of the system equations (10) is not equivalent to $\partial_t\boldsymbol{z} = \mathcal{J}(\boldsymbol{z})\delta_{\boldsymbol{z}}\mathcal{H}$. To include more realistic boundary conditions, we need to extend the system structure by so-called *ports*. Thus, we aim to formulate the system equations with boundary conditions as a port-Hamiltonian system of the form

$$\partial_t\boldsymbol{z} = \mathcal{J}(\boldsymbol{z})\delta_{\boldsymbol{z}}\mathcal{H} + \mathcal{B}\boldsymbol{u}, \qquad \boldsymbol{y} = \mathcal{B}^*\delta_{\boldsymbol{z}}\mathcal{H}$$

with boundary ports $\boldsymbol{u}$ and $\boldsymbol{y}$. The skew-adjoint operator $\mathcal{J}$ is defined in (11) in Section 3. The following theorem introduces the port-Hamiltonian formulation of the system equations (10) and provides the main result of this paper.

Theorem 4.1 (*Port-Hamiltonian Structure*)**.** *Under the assumption $\delta_{\boldsymbol{z}}\mathcal{H} \in \mathcal{D}(\mathcal{J})$, the governing equations (10) may be expressed as port-Hamiltonian system*

$$\partial_t\boldsymbol{z} = \mathcal{J}(\boldsymbol{z})\delta_{\boldsymbol{z}}\mathcal{H} + \mathcal{B}\boldsymbol{u},$$
$$\boldsymbol{y} = \mathcal{B}^*\delta_{\boldsymbol{z}}\mathcal{H},$$

with $\mathcal{J}$ given in (11), a port $\boldsymbol{y}$, and $\mathcal{B} : [H^1(\Omega)]^3 \to [H^1(\Omega)^*]^{N+3}$ defined by the trace operator, i. e., for $\boldsymbol{u} \in [H^1(\Omega)]^3$ we have

$$\mathcal{B}\boldsymbol{u} = \big[u_1|_a^b, \quad u_2|_a^b, \quad u_3|_a^b, \quad 0, \quad \ldots, \quad 0\big]^T.$$

Proof. We compare the system equations (10) with $\mathcal{J}(\boldsymbol{z})\delta_{\boldsymbol{z}}\mathcal{H}$. For the first component, we obtain

$$\partial_t\rho - \big(\mathcal{J}(\boldsymbol{z})\delta_{\boldsymbol{z}}\mathcal{H}\big)_1 = -\partial_x(\rho v) + \tilde{\partial}_x(\rho v) = -\rho v|_a^b.$$

Recall that the boundary term is well-defined for functions in $H^1(\Omega)$. Moreover, it may be seen as a functional for functions in $H^1(\Omega)$ by $\langle(\rho v)|_a^b, w\rangle_{H^1(\Omega)^*,\,H^1(\Omega)} := (\rho v w)|_a^b$. This requires $w \in H^1(\Omega)$, since we need well-defined boundary values. Similarly, we obtain with the second equation of system (10) that

$$\partial_t v - \big(\mathcal{J}(\boldsymbol{z})\delta_{\boldsymbol{z}}\mathcal{H}\big)_2 = -\left(\frac{\tau}{\rho}\right)\Big|_a^b.$$

For the third component of $\partial_t\boldsymbol{z} - \mathcal{J}(\boldsymbol{z})\delta_{\boldsymbol{z}}\mathcal{H}$, we consider Eq. (10c) and obtain

$$\partial_t s - \big(\mathcal{J}(\boldsymbol{z})\delta_{\boldsymbol{z}}\mathcal{H}\big)_3 = \left(\frac{\kappa}{\rho T}\partial_x T\right)\Big|_a^b.$$

Finally, the last N rows of the difference vanish such that, in summary, the difference of $\partial_t\boldsymbol{z}$ and $\mathcal{J}(\boldsymbol{z})\delta_{\boldsymbol{z}}\mathcal{H}$ defines $\mathcal{B}\boldsymbol{u}$ by

$$(\mathcal{B}\boldsymbol{u})_1 = -\rho v|_a^b, \qquad (\mathcal{B}\boldsymbol{u})_2 = -\left(\frac{\tau}{\rho}\right)\Big|_a^b,$$
$$(\mathcal{B}\boldsymbol{u})_3 = \left(\frac{\kappa}{\rho T}\partial_x T\right)\Big|_a^b, \qquad (\mathcal{B}\boldsymbol{u})_i = 0$$

for $i = 4, \ldots, N+3$. Hence, with the vector

$$\boldsymbol{u} = \big[-\rho v, \quad -\tau/\rho, \quad \kappa\partial_x T/(\rho T)\big]^T$$

and the operator $\mathcal{B} : [H^1(\Omega)]^3 \to [H^1(\Omega)^*]^{N+3}$, defined by

$$\mathcal{B}\boldsymbol{u} = \big[u_1|_a^b, \quad u_2|_a^b, \quad u_3|_a^b, \quad 0, \quad \ldots, \quad 0\big]^T,$$

we get $\partial_t\boldsymbol{z} = \mathcal{J}(\boldsymbol{z})\delta_{\boldsymbol{z}}\mathcal{H} + \mathcal{B}\boldsymbol{u}$. Note that we interpret the evaluation at the boundary again as operator from $H^1(\Omega)$ to its dual as above. Finally, we define

$$\boldsymbol{y} := \mathcal{B}^*\delta_{\boldsymbol{z}}\mathcal{H} = \Big[\big(\frac{1}{2}v^2 + u + \rho\partial_\rho u\big)\big|_a^b, \ (\rho v)|_a^b, \ (\rho T)|_a^b\Big]^T. \quad \square$$

One advantage of the port-Hamiltonian formulation of the system equations is the energy balance which follows from the skew-adjointness of the operator $\mathcal{J}$. Without boundary terms we obtain $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H} = 0$, i. e., the conservation of energy. In the port-Hamiltonian framework, the change of energy only depends on $\boldsymbol{u}$ and $\boldsymbol{y}$ as shown in the following corollary.

Corollary 4.2. *The Hamiltonian $\mathcal{H}$ satisfies the energy balance*

$$\frac{d}{dt}\mathcal{H} = \langle \boldsymbol{y}, \boldsymbol{u}\rangle_{H^1(\Omega)^*,\,H^1(\Omega)} \tag{16}$$

with the boundary ports $\boldsymbol{u}$ and $\boldsymbol{y}$ from Theorem 4.1.

Proof. Since the operator $\mathcal{J}$ is skew-adjoint, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H} = \big\langle \delta_{\boldsymbol{z}}\mathcal{H}, \partial_t\boldsymbol{z}\big\rangle = \big\langle \delta_{\boldsymbol{z}}\mathcal{H}, \mathcal{J}\delta_{\boldsymbol{z}}\mathcal{H} + \mathcal{B}\boldsymbol{u}\big\rangle$$
$$= \big\langle \delta_{\boldsymbol{z}}\mathcal{H}, \mathcal{B}\boldsymbol{u}\big\rangle = \big\langle \mathcal{B}^*\delta_{\boldsymbol{z}}\mathcal{H}, \boldsymbol{u}\big\rangle = \langle \boldsymbol{y}, \boldsymbol{u}\rangle. \quad \square$$

From Eq. (16) we see that the temporal change of the total energy $\mathcal{H}$ is equal to the power product $\langle \boldsymbol{y}, \boldsymbol{u} \rangle$ which is given by

$$\begin{aligned}\langle \boldsymbol{y}, \boldsymbol{u} \rangle &= \left(-\rho v \left(\frac{1}{2} v^2 + u + \rho \partial_\rho u \right) - \tau v + \kappa \partial_x T \right) \Big|_a^b \\ &= \left(-\rho v \left(\frac{1}{2} v^2 + h \right) - \tau v + \kappa \partial_x T \right) \Big|_a^b,\end{aligned}$$

where we have introduced the specific enthalpy $h := u + p/\rho$. Thus, the energy balance (16) can be interpreted as: The total energy $\mathcal{H}$ only changes due to flows of kinetic energy $\rho v v^2/2$, enthalpy flows $\rho v h$, energy flows due to viscous stresses τv, and heat flows $\kappa \partial_x T$ through the boundary. One can easily check that these energy flows correspond naturally to the terms showing up after integrating the divergence term of the total energy balance (2c) over the spatial domain. This comparison may be comprehended by using the relations $e = u + v^2/2$, $h = u + p/\rho$, and Fourier's Law (6).

Remark 4.3. A realistic set of boundary conditions [26] is given by the inflows

$$\rho v(a) = g_1, \quad \tau(a) = 0, \quad \kappa \partial_x T(a) = g_3$$

and outflows

$$\tau(b) = g_2, \quad \kappa \partial_x T(b) = 0.$$

Therein, g_1, g_2, and g_3 denote given functions. In this case, the term $\mathcal{B}\boldsymbol{u}$ from Theorem 4.1 reads $\mathcal{B}\boldsymbol{u} = [g_1 - \rho v(b), -g_2/\rho, -g_3/(\rho T), 0, \ldots, 0]^T$, where the functions g_1, g_2, and g_3 may be used for purposes of boundary control.

5. Conclusion

We have presented a port-Hamiltonian formulation of the Navier–Stokes equations for reactive flows in a one-dimensional spatial domain. We started with introducing a Hamiltonian formulation for the case of vanishing boundary energy flows. To avoid the constraints on the boundary conditions, we have generalized the Hamiltonian formulation to a port-Hamiltonian formulation with boundary ports accounting for the energy flow through the boundary.

The port-Hamiltonian formulation on PDE level is the first step to derive finite-dimensional and reduced-order models which exhibit the port-Hamiltonian structure. For this purpose, structure-preserving discretization and model reduction methods need to be investigated further in order to apply them to the reactive flow setting. Furthermore, the use of boundary ports for passivity-based control will be subject of upcoming research.

Acknowledgments

The first author was supported by the ERC Advanced Grant "Modeling, Simulation and Control of Multi-Physics Systems" MODSIMCONMP. The second author gratefully acknowledges the support by the Deutsche Forschungsgemeinschaft (DFG) as part of the collaborative research center SFB 1029 *Substantial efficiency increase in gas turbines through direct use of coupled unsteady combustion and flow dynamics*.

References

[1] J.T. Borggaard, S. Gugercin, Model reduction for DAEs with an application to flow control, in: Rudibert King (Ed.), Active Flow and Combustion Control 2014, Springer International Publishing, Cham, Switzerland, 2015 pp. 381–396.
[2] U. Nagarajan, K. Yamane, Automatic task-specific model reduction for humanoid robots, in: IEEE/RSJ International Conference on Intelligent Robots and Systems, IROS, Tokyo, Japan, 2013, pp. 2578–2585.
[3] A.J. van der Schaft, D. Jeltsema, Port-Hamiltonian systems theory: An introductory overview, Found. Trends Syst. Control 1 (2–3) (2014) 173–378.
[4] P.J. Olver, Applications of Lie Groups to Differential Equations, second ed., Springer, New York, 1993.
[5] J.E. Marsden, T.S. Ratiu, Introduction to Mechanics and Symmetry, second ed., Springer, New York, 1999.
[6] H. Ennsbrunner, K. Schlacher, On the geometrical representation and interconnection of infinite dimensional port controlled Hamiltonian systems, in: Proceedings of the 44th IEEE Conference on Decision and Control, Seville, Spain, 2005, pp. 5263–5268.
[7] M. Schöberl, H. Ennsbrunner, K. Schlacher, Modelling of piezoelectric structures - a Hamiltonian approach, Math. Comput. Model. Dyn. Syst. 14 (3) (2008) 179–193.
[8] A.J. van der Schaft, B.M. Maschke, Fluid dynamical systems as Hamiltonian boundary control systems, in: Proceedings of the 40th IEEE Conference on Decision and Control, vol. 5, Orlando, USA, 2001, pp. 4497–4502.
[9] A. Macchelli, A.J. van der Schaft, C. Melchiorri, Port Hamiltonian formulation of infinite dimensional systems I. Modeling, in: Proceedings of the 43rd IEEE Conference on Decision and Control, vol. 4, Atlantis Paradise Island, Bahamas, 2004, pp. 3762–3767.
[10] I.V. Kanatchikov, Canonical structure of classical field theory in the polymomentum phase space, Rep. Math. Phys. 41 (1) (1998) 49–90.
[11] G. Sardanashvily, Polysymplectic Hamiltonian Field Theory. Tech. Rep., 2015. ArXiv e-print arXiv:1505.01444v1.
[12] T.J. Bridges, Multi-symplectic structures and wave propagation, Math. Proc. Cambridge Philos. Soc. 121 (1997) 147–190.
[13] G. Nishida, Hamiltonian representation of higher order partial differential equations with boundary energy flows, J. Appl. Math. Phys. 3 (2015) 1472–1490.
[14] H. Ramirez, B. Maschke, D. Sbarbaro, Irreversible port-Hamiltonian systems: A general formulation of irreversible processes with application to the CSTR, Chem. Eng. Sci. 89 (2013) 223–234.
[15] P.J. Morrison, J.M. Greene, Noncanonical Hamiltonian density formulation of hydrodynamics and ideal magnetohydrodynamics, Phys. Rev. Lett. 45 (1980) 790–794.
[16] P.J. Morrison, Some Observations Regarding Brackets and Dissipation. Tech. Rep. PAM228, Center for Pure and Applied Mathematics, University of California, Berkeley, USA, 1984.
[17] A. Siuka, Geometry, Modelling and Control of Infinite Dimensional Port-Hamiltonian Systems, Johannes Kepler University, Linz, Austria, 2011.
[18] B.D. Jones, Navier-Stokes Hamiltonian for the similarity renormalization group, Tech. Rep., 2014. ArXiv e-print arXiv:1407.1035v4.
[19] G. Golo, V. Talasila, A.J. van der Schaft, B.M. Maschke, Hamiltonian discretization of boundary control systems, Automatica 40 (5) (2004) 757–771.
[20] M. Seslija, J.M.A. Scherpen, A.J. van der Schaft, Explicit simplicial discretization of distributed-parameter port-Hamiltonian systems, Automatica 50 (2) (2014) 369–377.
[21] C. Beattie, S. Gugercin, Structure-preserving model reduction for nonlinear port-Hamiltonian systems, in: 50th IEEE Conference on Decision and Control and European Control Conference, Florida, USA, 2011, pp. 6564–6569.
[22] R.V. Polyuga, A.J. van der Schaft, Structure preserving moment matching for port-Hamiltonian systems: Arnoldi and Lanczos, IEEE Trans. Automat. Control 56 (6) (2011) 1458–1462.
[23] J. Warnatz, U. Maas, R.W. Dibble, Combustion, fourth ed., Springer, Berlin, Heidelberg, 2006.
[24] W. Zhou, B. Hamroun, Y. Le Gorrec, F. Couenne, Infinite dimensional port Hamiltonian representation of reaction diffusion processes, IFAC-PapersOnLine 48 (1) (2015) 476–481.
[25] L. Tartar, An Introduction to Sobolev Spaces and Interpolation Spaces, Springer, Berlin, 2007.
[26] J.C. Sutherland, C.A. Kennedy, Improved boundary conditions for viscous, reacting, compressible flows, J. Comput. Phys. 191 (2) (2003) 502–524.