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On the Port-Hamiltonian Structure of the Navier-Stokes Equations for Reactive Flows*

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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.

Keywords: Reactive Flow, Port-Hamiltonian Formulation, Navier-Stokes Equations, Hamiltonian Formulation, Energy-Based Modeling

AMS(MOS) subject classification: 37K05, 76V05, 80A32

1 Introduction

Model-based optimization and control methods are important tools in many application areas. These come with a common need for low-dimensional models which can be evaluated in a short time, but still capture the main features of the dynamical behavior of the considered system. In this context, model reduction techniques have become very popular and have been applied to various fields of application including fluid dynamics, electromagnetic dynamics, structural mechanics, and chemical reactions, see for example [1, 3, 4, 12]. All these systems have in common that they are based on physical laws, as for instance conservation of energy. However, when applying standard model reduction methods, this conservation property is lost in general, leading to reduced-order models which do not reflect this physically meaningful property. One way of preserving energy conversation in all stages from the governing partial differential equations (PDEs) to the reduced order model is the port-Hamiltonian formulation of the system equations. The corresponding structure guarantees important properties such as passivity and stability. Consequently, preservation of this structure automatically leads to

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preservation of these properties. Thus, by making use of the port-Hamiltonian structure, we may obtain a reduced-order model which is stable and passive.

The contribution of this paper is the port-Hamiltonian formulation of the one-dimensional, compressible Navier-Stokes equations for reactive flows. First, we present the Hamiltonian structure of the governing equations with vanishing boundary energy flows. Subsequently, by allowing energy flow through the boundary, we obtain a port-Hamiltonian system, which extends the Hamiltonian formulation by boundary ports.

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 [27]. The port-Hamiltonian structure guarantees stability and passivity and, furthermore, it is invariant under interconnection. This means that the interconnection of two or more port-Hamiltonian systems (by their ports) leads to an overall system which is again port-Hamiltonian and, thus, exhibits the related properties. More details about the analysis and properties of port-Hamiltonian systems may be found in [10, 27]. The port-Hamiltonian formulation provides a generic modeling approach, which has already been applied to various fields of application such as acoustics [26], electrical circuits [5], electro-mechanical systems [6], hydraulic systems [13], robotic systems [29], or plasma dynamics [30]. Also, the thermodynamical behavior of chemical reactions has been formulated as port-Hamiltonian system, see for instance [8, 22, 32]. However, these efforts have in common that they do not account for the fluid dynamics.

A Hamiltonian formulation for an ideal, compressible fluid has been presented in [15, 16]. This has also been extended to the dissipative case in [14] by using the notion of a metriplectic structure, which corresponds to a Hamiltonian system with an additional negative semi-definite part accounting for the dissipation. In this context, the metriplectic structure may be seen as a first step towards port-Hamiltonian systems. However, neither the Hamiltonian nor the metriplectic structure accounts for a non-zero energy flow through the boundary. For the ideal fluid, boundary flows have been integrated in [28] leading to an implicit port-Hamiltonian representation by means of a Dirac structure. In [23] the dynamics of viscous, isentropic flow 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 [11]. Nevertheless, an energy-based formulation of the full compressible Navier-Stokes equations with non-vanishing boundary conditions is still missing.

In this paper, we present a port-Hamiltonian formulation for the full Navier Stokes equations for reactive flows accounting for non-zero boundary energy flows by corresponding boundary ports. This formulation is on the level of the PDEs and, thus, infinite-dimensional. To obtain a corresponding finite-dimensional approximation, structure-preserving discretization methods have to be considered. However, this is not within the scope of this paper. Preceding efforts in this topic may be found in [7, 17, 21]. Furthermore, there have been some efforts for structure-preserving model reduction techniques of linear and nonlinear port-Hamiltonian systems, see for instance [2, 9, 18, 19, 20].

This paper is structured as follows. We begin with the derivation of the mathematical model (Section 2), before we present a Hamiltonian formulation of the governing equations where vanishing boundary energy flows are assumed (Section 3). The main contribution is presented in Section 4 where we extend the Hamiltonian formulation to the case of non-zero boundary flows resulting in a port-Hamiltonian formulation of the governing equations. The energy balance induced by the port-Hamiltonian formulation reveals that the energy of the system only changes due to energy flows through the boundary ports. Finally, we summarize

Table 2.1: Special quantities for conservation of mass, momentum, energy, and species [31].

conservation of	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	$\rho y_i v + j_i$	$\tilde{M}_i \omega_i$

the results and give an outlook to future challenges and possible research directions.

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. [31], which is reflected by the PDE

$$\partial_t f\,(x,t) + \partial_x \Phi_f\,(x,t) = q_f\,(x,t) + r_f\,(x,t)\,. \tag{2.1}$$

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 (2.1), 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 2.1. The resulting governing equations are summarized as

$$\partial_t \rho + \partial_x\,(\rho v) = 0, \tag{2.2a}$$
$$\partial_t\,(\rho v) + \partial_x\left(\rho v^2 + p + \tau\right) = 0, \tag{2.2b}$$
$$\partial_t\,(\rho e) + \partial_x\,(\rho e v + (p+\tau)\,v + \phi) = 0, \tag{2.2c}$$
$$\partial_t\,(\rho y_i) + \partial_x\,(\rho y_i v + j_i) = \tilde{M}_i \omega_i \tag{2.2d}$$

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 density j, molar masses $\tilde{M}_i$, and molar rates of formation ω_i. Here, we consider $N \in \mathbb{N}$ different species and, thus, (2.2d) 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 equation (2.2b), we can derive the following conservation law for the internal energy from the conservation law of the total energy (2.2c) as

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

with specific internal energy u [31]. By applying the product rule, we may write the governing equations as

$$\partial_t \rho + \partial_x (\rho v) = 0, \tag{2.3a}$$

$$\partial_t v + v\partial_x v + \frac{1}{\rho}\partial_x (p + \tau) = 0, \tag{2.3b}$$

$$\partial_t u + v\partial_x u + \frac{1}{\rho}(p + \tau)\partial_x v + \frac{1}{\rho}\partial_x \phi = 0, \tag{2.3c}$$

$$\partial_t y_i + v\partial_x y_i + \frac{1}{\rho}\partial_x j_i = \frac{1}{\rho}\tilde{M}_i \omega_i. \tag{2.3d}$$

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

$$\mathrm{d}u = T\mathrm{d}s - p\mathrm{d}\left(\frac{1}{\rho}\right) + \sum_{i=1}^{N} \mu_i \mathrm{d}y_i \tag{2.4}$$

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 i-th species [32]. With (2.4) we can express equation (2.3c) in terms of the entropy, namely

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

where we already have used the relations

$$T = \partial_s u, \qquad p = \rho^2 \partial_\rho u, \qquad \text{and} \quad \mu_i = \partial_{y_i} u, \tag{2.5}$$

which follow from (2.4). Finally, the governing equations are closed based on the closure equations of

Fourier's law:	$\phi = -\kappa \partial_x T,$	(2.6)
Newtonian fluid:	$\tau = -\hat{\mu}\partial_x v,$	(2.7)
Fick's law:	$j_i = -\rho D_i \partial_x y_i,$	(2.8)

where κ denotes the thermal conductivity, $\hat{\mu}$ the dynamic viscosity (scaled by the factor 4/3 to account for compressible flow, cf. [31]), and D_i the mass diffusivity of the ith species. Fourier's law as stated in (2.6) is based on the assumptions of a vanishing Dufour effect and negligible heat flux due to diffusion, cf. [31, 32]. Furthermore, we assume that the effects of thermal diffusion and pressure diffusion may be neglected which leads to Fick's law as in (2.8) [31].

Using (2.5) we can summarize the governing equations as

$$\partial_t \rho + \partial_x (\rho v) = 0, \tag{2.9a}$$

$$\partial_t v + \partial_x \left(\frac{v^2}{2} + \rho \partial_\rho u + u\right) + \frac{1}{\rho}\partial_x \tau - T\partial_x s - \sum_{i=1}^{N} \mu_i \partial_x y_i = 0, \tag{2.9b}$$

$$\partial_t s + v\partial_x s + \frac{\tau}{\rho T}\partial_x v - \frac{1}{\rho T}\partial_x\left(\kappa\partial_x T\right) + \sum_{i=1}^{N}\frac{\mu_i}{\rho T}\left(\tilde{M}_i\omega_i + \partial_x\left(\rho D_i\partial_x y_i\right)\right) = 0, \tag{2.9c}$$

$$\partial_t y_i + v\partial_x y_i - \frac{1}{\rho}\partial_x\left(\rho D_i\partial_x y_i\right) = \frac{1}{\rho}\tilde{M}_i\omega_i \tag{2.9d}$$

with known constants $\tilde{M}_i$ and known functions D_i, ω_i, u, $\hat{\mu}$, T, κ, μ_i which are dependent on ρ, s, and $y_1, \ldots, y_N$.

For the formulation of the governing equations as Hamiltonian or rather port-Hamiltonian system, we also need the weak formulation (in terms of the space derivatives). For this, we multiply the equations in (2.9) by a sufficiently smooth test function φ and integrate by parts in order to remove the second derivatives of T, v, and $y_1, \ldots, y_N$. However, this introduces additional boundary terms and leads to

$$\begin{aligned}
\langle\partial_t\rho, \varphi\rangle &= \langle-\partial_x\left(\rho v\right), \varphi\rangle, && (2.10a)\\
\langle\partial_t v, \varphi\rangle &= \big\langle -\partial_x\big(v^2/2 + \rho\partial_\rho u + u\big) + T\partial_x s, \varphi\big\rangle + \big\langle\tau, \partial_x(\varphi/\rho)\big\rangle && (2.10b)\\
&\qquad - \frac{\tau\varphi}{\rho}\Big|_a^b + \sum_{i=1}^{N}\big\langle\mu_i\partial_x y_i, \varphi\big\rangle, &&\\
\langle\partial_t s, \varphi\rangle &= \big\langle -v\partial_x s - \frac{\tau}{\rho T}\partial_x v, \varphi\big\rangle - \big\langle\kappa\partial_x T, \partial_x(\frac{1}{\rho T}\varphi)\big\rangle + \frac{\kappa}{\rho T}\partial_x T\varphi\Big|_a^b && (2.10c)\\
&\qquad - \sum_{i=1}^{N}\big\langle\frac{\mu_i\tilde{M}_i\omega_i}{\rho T}, \varphi\big\rangle + \sum_{i=1}^{N}\big\langle\rho D_i\partial_x y_i, \partial_x(\frac{\mu_i\varphi}{\rho T})\big\rangle - \sum_{i=1}^{N} D_i\partial_x y_i\frac{\mu_i\varphi}{T}\Big|_a^b, &&\\
\langle\partial_t y_i, \varphi\rangle &= \langle-v\partial_x y_i, \varphi\rangle - \langle\rho D_i\partial_x y_i, \partial_x(\varphi/\rho)\rangle + D_i\partial_x y_i\varphi\Big|_a^b + \langle\tilde{M}_i\omega_i/\rho, \varphi\rangle. && (2.10d)
\end{aligned}$$

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

3 Hamiltonian Dynamics of Reactive Flows

The total energy or Hamiltonian $\mathcal{H}$ of the reactive flow system described by (2.9) consists of the kinetic energy and the internal energy, i. e.,

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

The aim of this section is to reformulate the weak formulation of the system equations (2.10) as a Hamiltonian system. 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.

We combine all unknowns within the vector z, i. e., $z := [\rho,\ v,\ s,\ y_1,\ \ldots,\ y_N]^T$. 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. Its subspace $H_0^1(\Omega)$ contains the functions which vanish at the boundary of Ω. 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 $\mathcal{J}\colon [H^1(\Omega)]^{N+3} \to [H^1(\Omega)^*]^{N+3}$ by

$$\mathcal{J}(z) := \begin{bmatrix} 0 & -\partial_x & 0 & 0 & \dots & 0 \\ -\partial_x & 0 & \frac{1}{\rho}\partial_x s - \mathcal{J}_{23} & \frac{1}{\rho}\partial_x y_1 & \dots & \frac{1}{\rho}\partial_x y_N \\ 0 & -\frac{1}{\rho}\partial_x s - \mathcal{J}_{32} & \mathcal{J}_{33} - \hat{\mathcal{J}}_{33} & -\mathcal{M}_1 & \dots & -\mathcal{M}_N \\ 0 & -\frac{1}{\rho}\partial_x y_1 & \mathcal{M}_1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & -\frac{1}{\rho}\partial_x y_N & \mathcal{M}_N & 0 & \dots & 0 \end{bmatrix}. \tag{3.1}$$

Therein, the operator $\mathcal{J}_{23}$ equals $\frac{1}{\rho}\partial_x\big(\frac{\tau}{\rho T}\ \cdot\big)$ in the weak form, i. e., for $k, \ell \in H^1(\Omega)$ we have

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

Note that since we assume vanishing boundary energy flows, which implies $\tau(a) = \tau(b) = 0$, we do not include the boundary term $\tau k \ell / (\rho^2 T)|_a^b$ here which appears due to the integration by parts formula. Furthermore, we define $\mathcal{J}_{32} := \frac{\tau}{\rho T}\partial_x\left(\frac{1}{\rho}\ \cdot\right)$. The operator $\mathcal{M}_i$ is again given in the weak form,

$$\langle \mathcal{M}_i k, \ell \rangle := \int_a^b \frac{\tilde{M}_i \omega_i}{\rho^2 T} k \ell \,\mathrm{d}x - \int_a^b \rho D_i \partial_x y_i \partial_x \left(\frac{1}{\rho^2 T} k \ell\right) \mathrm{d}x + \frac{1}{\rho T} D_i \partial_x y_i k \ell \Big|_a^b.$$

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

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

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 $\mathcal{J}\colon \mathcal{D}(\mathcal{J}) \to \mathcal{D}(\mathcal{J})^*$ from (3.1) with domain*

$$\mathcal{D}(\mathcal{J}) := H^1(\Omega) \times H_0^1(\Omega) \times \left[H^1(\Omega)\right]^{N+1}$$

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. Let $\boldsymbol{k} = [k_1, k_2, \dots, k_{N+3}]^T$ and $\boldsymbol{\ell} = [\ell_1, \ell_2, \dots, \ell_{N+3}]^T$ be in the domain of $\mathcal{J}$, i. e., $\boldsymbol{k}, \boldsymbol{\ell} \in \mathcal{D}(\mathcal{J})$. Simple rearrangements then yield

$$\begin{aligned} \big\langle \boldsymbol{k}, \mathcal{J}\boldsymbol{\ell} \big\rangle = \int_a^b \Bigg[& -k_1 \partial_x \ell_2 - k_2 \partial_x \ell_1 + \frac{\partial_x s k_2 \ell_3}{\rho} + \frac{\tau \ell_3}{\rho T}\partial_x\left(\frac{k_2}{\rho}\right) + \frac{k_2}{\rho}\sum_{i=1}^N \partial_x y_i \ell_{i+3} - \frac{\partial_x s k_3 \ell_2}{\rho} \\ & - \frac{\tau k_3}{\rho T}\partial_x\left(\frac{\ell_2}{\rho}\right) - \kappa \partial_x\left(\frac{\ell_3}{\rho}\right)\partial_x\left(\frac{k_3}{\rho T}\right) + \kappa \partial_x\left(\frac{k_3}{\rho}\right)\partial_x\left(\frac{\ell_3}{\rho T}\right) \\ & - \frac{\ell_2}{\rho}\sum_{i=1}^N \partial_x y_i k_{i+3} \Bigg] \mathrm{d}x + \sum_{i=1}^N \big\langle \mathcal{M}_i \ell_3, k_{i+3}\big\rangle - \sum_{i=1}^N \big\langle \mathcal{M}_i \ell_{i+3}, k_3 \big\rangle \end{aligned}$$

$$
\begin{aligned}
&= \int_a^b \Bigg[\ell_2 \partial_x k_1 - k_2 \partial_x \ell_1 + \frac{\partial_x s k_2 \ell_3}{\rho} - \frac{\partial_x s k_3 \ell_2}{\rho} + \frac{\tau \ell_3}{\rho T} \partial_x \left(\frac{k_2}{\rho}\right) - \frac{\tau k_3}{\rho T} \partial_x \left(\frac{\ell_2}{\rho}\right) \\
&\qquad + \frac{k_2}{\rho} \sum_{i=1}^N \partial_x y_i \ell_{i+3} - \frac{\ell_2}{\rho} \sum_{i=1}^N \partial_x y_i k_{i+3} - \kappa \partial_x \left(\frac{\ell_3}{\rho}\right) \partial_x \left(\frac{k_3}{\rho T}\right) \\
&\qquad + \kappa \partial_x \left(\frac{k_3}{\rho}\right) \partial_x \left(\frac{\ell_3}{\rho T}\right)\Bigg] \,\mathrm{d}x + \sum_{i=1}^N \big\langle \mathcal{M}_i \ell_3, k_{i+3} \big\rangle - \sum_{i=1}^N \big\langle \mathcal{M}_i \ell_{i+3}, k_3 \big\rangle \\
&= -\big\langle \mathcal{J} \boldsymbol{k}, \boldsymbol{\ell} \big\rangle .
\end{aligned}
$$

Note that the boundary term $-k_1 \ell_2|_a^b$, which appears as a result of the integration by parts, vanishes due to the assumed zero Dirichlet boundary condition of ℓ_2. □

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 the heat flux $\kappa \partial_x T$ and the shear stress τ vanish at the boundary, the weak formulation of the governing equations* (2.10) *may be expressed as*

$$
\partial_t z = \mathcal{J}(z)\, \delta_z \mathcal{H}(z) , \tag{3.2}
$$

where $\delta_z \mathcal{H}(z)$ denotes the variational derivative

$$
\delta_z \mathcal{H}(z) = \begin{bmatrix} \frac{v^2}{2} + u + \rho \partial_\rho u \\ \rho v \\ \rho T \\ \rho \mu_1 \\ \vdots \\ \rho \mu_N \end{bmatrix} .
$$

Proof. The variational derivatives of $\mathcal{H}$ are given by

$$
\begin{aligned}
&\delta_\rho \mathcal{H} = \frac{v^2}{2} + u(\rho, s, y_1, \ldots, y_N) + \rho \partial_\rho u(\rho, s, y_1, \ldots, y_N), \qquad \delta_v \mathcal{H} = \rho v, \\
&\delta_s \mathcal{H} = \rho \partial_s u(\rho, s, y_1, \ldots, y_N), \qquad \delta_{y_i} \mathcal{H} = \rho \partial_{y_i} u(\rho, s, y_1, \ldots, y_N)
\end{aligned}
$$

Using the relations (2.5), we can write the variational derivatives $\delta_s \mathcal{H}$ and $\delta_{y_i} \mathcal{H}$ as

$$
\delta_s \mathcal{H} = \rho T(\rho, s, y_1, \ldots, y_N) \quad \text{and} \quad \delta_{y_i} \mathcal{H} = \rho \mu_i(\rho, s, y_1, \ldots, y_N) .
$$

Thus, (3.2) is equivalent to the system

$$
\partial_t \rho = -\partial_x (\rho v) , \tag{3.3a}
$$

$$
\partial_t v = -\partial_x \left(\frac{v^2}{2} + u + \rho \partial_\rho u\right) + T \partial_x s - \mathcal{J}_{23}(\rho T) + \sum_{i=1}^N \mu_i \partial_x y_i , \tag{3.3b}
$$

$$\partial_t s = -v\partial_x s - \frac{\tau\partial_x v}{\rho T} + \mathcal{J}_{33}(\rho T) - \hat{\mathcal{J}}_{33}(\rho T) - \sum_{i=1}^{N} \mathcal{M}_i(\rho\mu_i), \tag{3.3c}$$

$$\partial_t y_i = -v\partial_x y_i + \mathcal{M}_i(\rho T). \tag{3.3d}$$

Since we assume that $\kappa\partial_x T(a) = \kappa\partial_x T(b) = 0$ and $\tau(a) = \tau(b) = 0$, (3.3) is nothing else than the weak form of the governing equations as given in (2.10). □

Remark 3.3 Note that Theorem 3.2 also implies that the Hamiltonian system $\partial_t z = \mathcal{J}(z)\delta_z\mathcal{H}(z)$ is equivalent to the classical formulation of the governing equations (2.9) if we assume sufficient regularity in order to integrate by parts.

Corollary 3.4 *Assume $\delta_z\mathcal{H} \in \mathcal{D}(\mathcal{J})$ with $D(\mathcal{J})$ as in Lemma 3.1 which implies that $\rho v(a) = \rho v(b) = 0$. Then, 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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H} = \langle \delta_z\mathcal{H}, \partial_t z\rangle = \langle \delta_z\mathcal{H}, \mathcal{J}(z)\delta_z\mathcal{H}\rangle = 0. \qquad \square$$

In this section we have shown that the weak formulation of the governing equations (2.10) 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 boundaries. In the next section, we drop this restrictive assumption and generalize the Hamiltonian formulation of the system equations (2.10) to a port-Hamiltonian formulation.

4 Port-Hamiltonian Dynamics of Reactive Flows

In the previous section, we have shown that we can express the Navier-Stokes equations for reactive flows in form of a Hamiltonian system, if we assume vanishing boundary energy flows. In order to include more realistic boundary conditions, we need to extend the system structure with so-called *ports*. Thus, we aim to formulate the system equations with boundary conditions as a port-Hamiltonian system of the form

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

with boundary ports u and y. For this, we need to modify the operator $\mathcal{J}$, which we denote by $\tilde{\mathcal{J}}$, in order to maintain the skew-adjointness. We define the solution-dependent operator $\tilde{\mathcal{J}} \colon \mathcal{D}(\tilde{\mathcal{J}}) \to D(\tilde{\mathcal{J}})^*$ with domain

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

by

$$\tilde{\mathcal{J}}(z) := \begin{bmatrix} 0 & -\tilde{\partial}_x & 0 & 0 & \dots & 0 \\ -\partial_x & 0 & \frac{1}{\rho}\partial_x s - \mathcal{J}_{23} & \frac{1}{\rho}\partial_x y_1 & \dots & \frac{1}{\rho}\partial_x y_N \\ 0 & -\frac{1}{\rho}\partial_x s - \mathcal{J}_{32} & \mathcal{J}_{33} - \hat{\mathcal{J}}_{33} & -\mathcal{M}_1 & \dots & -\mathcal{M}_N \\ 0 & -\frac{1}{\rho}\partial_x y_1 & \mathcal{M}_1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & -\frac{1}{\rho}\partial_x y_N & \mathcal{M}_N & 0 & \dots & 0 \end{bmatrix}. \tag{4.1}$$

Therein, $\mathcal{J}_{23}$, $\mathcal{J}_{32}$, $\mathcal{J}_{33}$, $\hat{\mathcal{J}}_{33}$, and $\mathcal{M}_i$ are defined as in Section 3 and the operator $\tilde{\partial}_x$ is defined as the partial derivative w. r. t. x with an additional boundary term, i. e.,

$$\langle \tilde{\partial}_x v, w\rangle := \int_a^b w\partial_x v \,\mathrm{d}x - wv|_a^b .$$

With this, we can show that the operator $\tilde{\mathcal{J}}$ is again skew-adjoint.

Lemma 4.1 *The operator* $\tilde{\mathcal{J}}\colon \mathcal{D}(\tilde{\mathcal{J}}) \to D(\tilde{\mathcal{J}})^*$ *defined in* (4.1) *is skew-adjoint, i. e.,* $\langle \boldsymbol{k}, \tilde{\mathcal{J}}\boldsymbol{\ell}\rangle_{H^1(\Omega),\, H^1(\Omega)^*} = -\langle \tilde{\mathcal{J}}\boldsymbol{k}, \boldsymbol{\ell}\rangle_{H^1(\Omega)^*,\, H^1(\Omega)}$ *for all* $\boldsymbol{k}, \boldsymbol{\ell} \in \mathcal{D}(\tilde{\mathcal{J}})$*.*

Proof. Consider $\boldsymbol{k}, \boldsymbol{\ell} \in \mathcal{D}(\tilde{\mathcal{J}})$. Since the components corresponding to the chemical species require no integration by parts, it is sufficient to consider the left-upper 3×3 block of the operator $\tilde{\mathcal{J}}$ which we denote by $\tilde{\mathcal{J}}^{3\times 3}$. The remaining terms act as in Lemma 3.1. With $\boldsymbol{k}^3 = [k_1,\, k_2,\, k_3]^T$ and $\boldsymbol{\ell}^3 = [\ell_1,\, \ell_2,\, \ell_3]^T$ denoting the first three components of $\boldsymbol{k}$ and $\boldsymbol{\ell}$, respectively, we obtain due to the integration by parts formula

$$\begin{aligned}
&\big\langle \boldsymbol{k}^3, \tilde{\mathcal{J}}^{3\times 3}\boldsymbol{\ell}^3\big\rangle \\
&\quad= \big\langle k_1, -\tilde{\partial}_x \ell_2\big\rangle + \Big\langle k_2, -\partial_x \ell_1 + \frac{\partial_x s}{\rho}\ell_3 - \mathcal{J}_{23}\ell_3\Big\rangle + \Big\langle k_3, -\frac{\partial_x s}{\rho}\ell_2 - \mathcal{J}_{32}\ell_2 + \mathcal{J}_{33}\ell_3 - \hat{\mathcal{J}}_{33}\ell_3\Big\rangle \\
&\quad= \int_a^b \left[-k_1\partial_x\ell_2 + k_2\left(-\partial_x\ell_1 + \frac{\partial_x s}{\rho}\ell_3\right) + \frac{\tau}{\rho T}\ell_3\partial_x\left(\frac{k_2}{\rho}\right) - k_3\left(\frac{\partial_x s}{\rho}\ell_2 + \frac{\tau}{\rho T}\partial_x\Big(\frac{\ell_2}{\rho}\Big)\right)\right] \mathrm{d}x \\
&\qquad\quad - \int_a^b \left[\kappa\partial_x\Big(\frac{1}{\rho}\ell_3\Big)\partial_x\Big(\frac{1}{\rho T}k_3\Big) - \kappa\partial_x\Big(\frac{1}{\rho T}\ell_3\Big)\partial_x\Big(\frac{1}{\rho}k_3\Big)\right] \mathrm{d}x + k_1\ell_2\Big|_a^b \\
&\quad= \int_a^b \left[\ell_2\partial_x k_1 + \ell_1\partial_x k_2 + \frac{\partial_x s}{\rho}k_2\ell_3 + \frac{\tau}{\rho T}\ell_3\partial_x\left(\frac{k_2}{\rho}\right) - \frac{\partial_x s}{\rho}k_3\ell_2 - \frac{\tau}{\rho T}k_3\partial_x\left(\frac{\ell_2}{\rho}\right)\right] \mathrm{d}x \\
&\qquad\quad + \int_a^b \left[\kappa\partial_x\Big(\frac{1}{\rho}k_3\Big)\partial_x\Big(\frac{1}{\rho T}\ell_3\Big) - \kappa\partial_x\Big(\frac{1}{\rho T}k_3\Big)\partial_x\Big(\frac{1}{\rho}\ell_3\Big)\right] \mathrm{d}x - \ell_1 k_2\Big|_a^b \\
&\quad= \big\langle \ell_1, \tilde{\partial}_x k_2\big\rangle + \Big\langle \ell_2, \partial_x k_1 - \frac{\partial_x s}{\rho}k_3 + \mathcal{J}_{23}k_3\Big\rangle + \Big\langle \ell_3, \frac{\partial_x s}{\rho}k_2 + \mathcal{J}_{32}k_2 - \mathcal{J}_{33}k_3 + \hat{\mathcal{J}}_{33}k_3\Big\rangle \\
&\quad= \big\langle \boldsymbol{\ell}^3, -\tilde{\mathcal{J}}^{3\times 3}\boldsymbol{k}^3\big\rangle.
\end{aligned}$$

Thus, we have in total $\big\langle \boldsymbol{k}, \tilde{\mathcal{J}}\boldsymbol{\ell}\big\rangle = -\big\langle \tilde{\mathcal{J}}\boldsymbol{k}, \boldsymbol{\ell}\big\rangle$ which completes the proof. □

In the case of non-vanishing boundary terms, the weak formulation of the system equations (2.10) is not equivalent to $\partial_t z = \tilde{\mathcal{J}}(z)\delta_z\mathcal{H}$. However, in the sequel we show that (2.10) may be written as a Hamiltonian system with additional boundary ports, i. e., a port-Hamiltonian system. The following theorem provides the main result of this paper.

Theorem 4.2 (Port-Hamiltonian structure) *The weak form of the governing equations* (2.10) *may be expressed as port-Hamiltonian system*

$$\begin{aligned}
\partial_t z &= \tilde{\mathcal{J}}(z)\delta_z\mathcal{H} + \mathcal{B}u, \\
y &= \mathcal{B}^*\delta_z\mathcal{H},
\end{aligned}$$

where $\tilde{\mathcal{J}}$ *is given in* (4.1) *and* $\mathcal{B}\colon [H^1(\Omega)]^3 \to [H^1(\Omega)^*]^{N+3}$ *is defined by the trace operator, i. e., for* $u \in [H^1(\Omega)]^3$ *we have*

$$\mathcal{B}u = \begin{bmatrix} u_1|_a^b, & u_2|_a^b, & u_3|_a^b, & 0, & \ldots, & 0\end{bmatrix}^T.$$

Proof. We compare the system equations (2.10) with the equations given by $\tilde{\mathcal{J}}(z)\delta_z\mathcal{H}$. For the first component, we obtain

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

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 (2.10) that

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

For the third component of $\partial_t z - \tilde{\mathcal{J}}(z)\delta_z\mathcal{H}$, we consider equation (2.10c) and obtain

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

Finally, the last N rows of the difference are given by

$$\partial_t y_j - \big(\tilde{\mathcal{J}}(z)\delta_z\mathcal{H}\big)_{3+i} = 0, \qquad i = 1, \dots N.$$

In summary, the difference of $\partial_t z$ and $\tilde{\mathcal{J}}(z)\delta_z\mathcal{H}$ vanishes in the last N components and defines $\mathcal{B}u$ by

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

for $i = 4, \dots, N+3$. Hence, with $u = [-\rho v,\ -\tau/\rho,\ \kappa\partial_x T/(\rho T)]^T$ and the operator $\mathcal{B}\colon [H^1(\Omega)]^3 \to [H^1(\Omega)^*]^{N+3}$ defined by

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

we get $\partial_t z = \tilde{\mathcal{J}}(z)\delta_z\mathcal{H} + \mathcal{B}u$. Note that we interpret the evaluation at the boundary again as operator from $H^1(\Omega)$ to its dual as above. For the second equation we define y by

$$y := \mathcal{B}^*\delta_z\mathcal{H} = \begin{bmatrix} \big(\frac{v^2}{2} + u + \rho\partial_\rho u\big)|_a^b \\ (\rho v)|_a^b \\ (\rho T)|_a^b \end{bmatrix}. \qquad \square$$

One advantage of the port-Hamiltonian formulation of the system equations is the energy balance which follows from the skew-adjointness of the operator $\tilde{\mathcal{J}}$. 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 u and y as shown in the following corollary.

Corollary 4.3 *The Hamiltonian $\mathcal{H}$ satisfies the energy balance*

$$\frac{d}{dt}\mathcal{H} = \langle y, u\rangle_{H^1(\Omega)^*, H^1(\Omega)} \tag{4.2}$$

with boundary ports u and y from Theorem 4.2.

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

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

It is noteworthy that the energy balance (4.2) allows for a physical interpretation. The temporal change of the total energy $\mathcal{H}$ is equal to the power product $\langle y, u\rangle$, which is given by

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

where we have introduced the specific enthalpy $h := u + p/\rho$. Thus, the energy balance (4.2) can be interpreted as: The total energy $\mathcal{H}$ only changes due to flows of kinetic energy ($\rho v \frac{v^2}{2}$), enthalpy flows ($\rho v h$), friction (τv), and heat flows ($\kappa \partial_x T$) through the boundaries.

Remark 4.4 A realistic set of boundary conditions [24] 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 $\mathcal{B}u$ from Theorem 4.2 reads $\mathcal{B}u = [g_1 - \rho v(b),\ -g_2/\rho,\ -g_3/(\rho T),\ 0,\ \dots,\ 0]^T$ and thus, may be seen as an input of the system.

5 Conclusions

We have presented a port-Hamiltonian formulation of the Navier-Stokes equations for reactive flows in a one-dimensional spatial domain. The model assumptions include a negligence of long-range processes, as gravity or radiation, which is why the change in potential energy is also neglected. We started with introducing a Hamiltonian formulation of the governing equations for the case of vanishing boundary energy flows. However, this setting imposes strong restrictions on the boundary conditions. To avoid these constraints, we generalized the Hamiltonian formulation to the case of arbitrary boundary conditions and derived a port-Hamiltonian formulation with boundary ports accounting for the energy flow through the system boundaries. The corresponding energy balance (4.2), which follows directly from the port-Hamiltonian structure, allows for a physically meaningful interpretation. The total energy of the system only changes due to energy flows through the boundary.

An extension of the port-Hamiltonian formulation to three-dimensional spatial domains is one of the next steps to apply to more practical settings. Furthermore, the port-Hamiltonian formulation includes one evolution equation for the specific entropy. However, in practical applications, initial and boundary conditions are usually expressed in terms of the temperature or the pressure. Thus, a port-Hamiltonian formulation based on the temperature or the pressure formulation of the energy equation is desirable.

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 along with the connected energy balance and other properties. 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.

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