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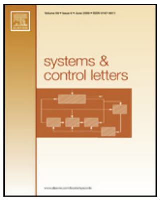

A port-Hamiltonian formulation of the Navier–Stokes equations for reactive flows

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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. 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

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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

$$\partial_t \rho + \partial_x\,(\rho v) = 0, \tag{3a}$$

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

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

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

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

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

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

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