ARTICLE IN PRESS

Nonlinear Analysis ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Nonlinear Analysis

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Asymptotic stability and relaxation for fast chemistry fluids

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ARTICLE INFO

Article history:
Received 31 March 2016
Accepted 23 February 2017
Communicated by S. Carl

Keywords:
Fast-chemistry
Multicomponent
Hyperbolic–parabolic

ABSTRACT

Global existence for multicomponent reactive fluids with fast chemistry is investigated. The system of partial differential equations derived from the kinetic theory is symmetrizable hyperbolic–parabolic with stiff chemical sources. New a priori estimates are obtained uniformly with respect to chemistry relaxation times and lead to asymptotic stability results for well prepared initial conditions. Convergence towards the chemical equilibrium fluid model when chemistry times go to zero is established as well as error estimates.

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1. Introduction

Chemical equilibrium fluids are reduced models which are of interest in various scientific and engineering applications such as reentry of space vehicles into Earth's atmosphere [1,42], engine rocket nozzle flows [52], or chemical reactors [31]. These equilibrium models are valid when the chemical characteristic times are smaller than the flow characteristic times and lead to an important reduction of the number of unknown variables with species densities replaced by atom densities. This is a strong motivation for investigating the fast chemistry limit of multicomponent flow models. In this work, global existence results for fast chemistry fluids are established as well as convergence towards the chemical equilibrium fluid model as chemical characteristic times go to zero.

The system of partial differential equations modeling fluids out of chemical equilibrium as derived from the kinetic theory of gases is first presented [17]. The balance equations express the conservation of species mass, momentum and energy and involve convective, dissipative as well as chemical source terms. The dissipative transport fluxes have a complex structure derived from the kinetic theory and couple all species equations as well as the energy equation through the Soret and Dufour cross effects. The chemistry terms are written

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http://dx.doi.org/10.1016/j.na.2017.02.025
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Please cite this article in press as: V. Giovangigli, W.A. Yong, Asymptotic stability and relaxation for fast chemistry fluids, Nonlinear Analysis (2017), http://dx.doi.org/10.1016/j.na.2017.02.025

for an arbitrary complex chemical reaction mechanism with rates deduced from the kinetic theory as well as from statistical thermodynamics. Thermodynamic properties obtained from the kinetic theory of dilute gases coincide with that of ideal gas mixtures and chemical equilibrium states are characterized in terms of Gibbs potentials. The reaction mechanism is assumed to be sufficiently detailed in such a way that its chemical equilibrium states coincide with natural equilibrium states obtained when all possible reactions are considered. The slow variables of the out of equilibrium system – that are the relevant variables of the limiting chemical equilibrium fluid – are then associated with atomic mass densities, momentum and energy. The governing equations finally form a second order quasilinear system of partial differential equations in terms of the conservative variable $\mathsf{u} \in \mathbb{R}^{\mathsf{n}}$ that is of dimension $\mathsf{n} = n + d + 1$ where n denotes the number of reactive species and d the space dimension.

Symmetrized forms for the system of partial differential equations are then discussed [30,16,48,34,36,7,21,22,17,10,58,13,54,37,4]. Existence of symmetrized forms is related to the existence of a mathematical entropy σ compatible with convective terms, dissipative terms and chemistry. The natural entropic symmetrized form for fluids out of chemical equilibrium is evaluated and appears as a symmetric second order system in terms of the entropic variable $\mathsf{v} = (\partial_{\mathsf{u}}\sigma)^t$. These entropic forms or entropic variables have been a key tool in the study of cross diffusion effects [21,22,17,33,6]. The source term is shown to be of quasilinear form as is typical in a relaxation framework and often encountered in mathematical physics [55]. Normal forms, that is, symmetric hyperbolic–parabolic composite forms of the system of partial differential equations [34,36] are further investigated using normal variables w and the mathematical framework needed to investigate the fast chemistry limit is completed by introducing the small parameter ϵ associated with fast chemistry relaxation. Strict dissipativity of the system in normal form is investigated and it is established that there exists a compensating matrix K compatible with the fast manifold. More specifically, denoting by $\overline{\mathcal{E}}$ the slow equilibrium manifold with respect to the normal variable and by π the orthogonal projector onto the fast manifold $\overline{\mathcal{E}}^{\perp}$, it is established that there exist a compensating matrix such that $K\pi = 0$. This is a natural assumption since, on the one hand, hyperbolic–parabolic coupling aspects are associated with total mass, momentum and energy conservation equations, and, on the other hand, chemical reactions neither create mass, momentum nor energy. The governing equations at chemical equilibrium, the thermodynamics of chemical equilibrium, the corresponding symmetrized forms as well as strict dissipativity at equilibrium are also investigated.

The system of partial differential equations in the normal variable $\mathsf{w} \in \mathbb{R}^{\mathsf{n}}$ out of chemical equilibrium is found in the form

$$\overline{\mathsf{A}}_0(\mathsf{w})\partial_t \mathsf{w} \ + \sum_{i\in\mathcal{D}} \overline{\mathsf{A}}_i(\mathsf{w})\partial_i \mathsf{w} - \sum_{i,j\in\mathcal{D}} \partial_i\big(\overline{\mathsf{B}}_{ij}(\mathsf{w})\partial_j \mathsf{w}\big) + \frac{1}{\epsilon}\overline{\mathsf{L}}(\mathsf{w})\mathsf{w} = \sum_{i,j\in\mathcal{D}} \overline{\mathsf{M}}_{ij}(\mathsf{w})\,\partial_i \mathsf{w}\,\partial_j \mathsf{w}, \tag{1.1}$$

where ∂_t denotes the time derivative operator, ∂_i the space derivative operator in the ith direction, $\mathcal{D} = \{1, \dots, d\}$ the spatial directions, $\mathsf{w} \in \mathbb{R}^{\mathsf{n}}$ the normal variable decomposed into $\mathsf{w} = (\mathsf{w}_{\mathrm{I}}, \mathsf{w}_{\mathrm{II}})^t$, $\mathsf{w}_{\mathrm{I}} \in \mathbb{R}^{\mathsf{n}_{\mathrm{I}}}$ the hyperbolic components with $\mathsf{n}_{\mathrm{I}} = 1$, $\mathsf{w}_{\mathrm{II}} \in \mathbb{R}^{\mathsf{n}_{\mathrm{II}}}$ the parabolic components with $\mathsf{n}_{\mathrm{II}} = n + d$, and $\epsilon \in (0, 1]$ the positive relaxation parameter. The matrix $\overline{\mathsf{A}}_0 \in \mathbb{R}^{\mathsf{n},\mathsf{n}}$ is symmetric positive definite and block-diagonal, $\overline{\mathsf{A}}_i \in \mathbb{R}^{\mathsf{n},\mathsf{n}}$, $i \in \mathcal{D}$ are symmetric, $\overline{\mathsf{B}}_{ij} \in \mathbb{R}^{\mathsf{n},\mathsf{n}}$ and $\overline{\mathsf{B}}_{ij}^t = \overline{\mathsf{B}}_{ji}$, $i, j \in \mathcal{D}$, $\overline{\mathsf{B}}_{ij}$ has nonzero components only into the right lower $\overline{\mathsf{B}}_{ij}^{\mathrm{II},\mathrm{II}} \in \mathbb{R}^{\mathsf{n}_{\mathrm{II}},\mathsf{n}_{\mathrm{II}}}$ blocks, $\overline{\mathsf{B}}^{\mathrm{II},\mathrm{II}} = \sum_{i,j\in\mathcal{D}} \overline{\mathsf{B}}_{ij}^{\mathrm{II},\mathrm{II}}(\mathsf{w})\xi_i\xi_j$ is positive definite for $\boldsymbol{\xi} \in \Sigma^{d-1}$ where Σ^{d-1} is the sphere in d dimension, $\overline{\mathsf{L}} \in \mathbb{R}^{\mathsf{n},\mathsf{n}}$ is positive semi-definite with a fixed nullspace $\overline{\mathcal{E}}$, and $\overline{\mathsf{M}}_{ij} \in \mathbb{R}^{\mathsf{n},\mathsf{n},\mathsf{n}}$, $i, j \in \mathcal{D}$, are third order tensors. The nullspace $\overline{\mathcal{E}} \subset \mathbb{R}^{\mathsf{n}}$ of the linearized source term $\overline{\mathsf{L}}$ represents the slow manifold and is of dimension $\mathsf{n}_{\mathrm{e}} = n_{\mathrm{a}} + d + 1$ where n_{a} denotes the number of atoms. The orthogonal complement $\overline{\mathcal{E}}^{\perp} \subset \mathbb{R}^{\mathsf{n}}$ of dimension $n - n_{\mathrm{a}}$ is the fast manifold and $\pi\mathsf{w} \in \mathbb{R}^{\mathsf{n}}$ the fast variable. The quadratic residual $\overline{\mathsf{Q}} = \sum_{i,j\in\mathcal{D}} \overline{\mathsf{M}}_{ij}(\mathsf{w})\,\partial_i \mathsf{w}\,\partial_j \mathsf{w}$ may also be written $\overline{\mathsf{Q}} = -\sum_{i,j\in\mathcal{D}} \partial_i(\partial_{\mathsf{w}}\mathsf{v})^t\,(\partial_{\mathsf{v}}\mathsf{w})^t\,\overline{\mathsf{B}}_{ij}\partial_j \mathsf{w}$ where v denotes the entropic variable and only involves the parabolic components $\overline{\mathsf{M}}_{ij}(\mathsf{w})\partial_i \mathsf{w}\partial_j \mathsf{w} = \big(0,\, \overline{\mathsf{M}}_{ij}^{\mathrm{II},\mathrm{II},\mathrm{II}}(\mathsf{w})\partial_i \mathsf{w}_{\mathrm{II}}\partial_j \mathsf{w}_{\mathrm{II}}\big)^t$.

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