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Vincent Giovangigli

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Erratum for *A Diffuse Interface Lox/Hydrogen Transcritical Flame Model*

Vincent Giovangigli *

CMAP-CNRS, Ecole polytechnique, Palaiseau, France

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ABSTRACT

A few errors and typos have been identified in P. Gaillard, V. Giovangigli and L. Matuszewski, *A Diffuse Interface Lox/Hydrogen Transcritical Flame Model*, Comb. Theor. Mod., 20 486-520 (2016), doi.org/10.1080/13647830.2016.1150518 and are listed here.

1. Entropy production and related fluxes

Thermodynamic methods using entropy production rates have been found to be ambiguous for diffuse interface fluid models [2, 3]. There are indeed various terms in the entropy production rate that involve products of several gradients. The complete Korteweg or Cahn-Hilliard fluid models *can only be derived unambiguously from the kinetic theory of gases or that of dense gas mixtures* [2, 3]. The useful form of entropy production that yields the proper fluxes is presented in this Erratum as well as the corresponding fluxes. The equation numbers used in the following are identical to those of the original publication [1].

The transport fluxes are derived by expressing the entropy production rate in terms of the fluxes and the variable gradients and proceeding as in the thermodynamics of irreversible processes [2, 3]. By using Gibbs relation it may be obtained after some algebra that [3]

$$\begin{aligned} \partial_t \mathcal{S} + \nabla \cdot (\mathbf{v} \mathcal{S}) + \nabla \cdot \left(\frac{\mathcal{Q}}{T} - \sum_{i \in \mathfrak{S}} \frac{\phi_i}{T} (\rho_i \nabla \cdot \mathbf{v} + \nabla \cdot \mathcal{J}_i) - \sum_{i \in \mathfrak{S}} \left(\frac{g_i}{T} - \frac{\nabla \cdot \phi_i}{T} \right) \mathcal{J}_i \right) \\ = - \frac{1}{T} \left(\mathcal{P} - p \mathbf{I} - \sum_{i \in \mathfrak{S}} (\nabla \rho_i \otimes \phi_i - \rho_i \nabla \cdot \phi_i \mathbf{I}) \right) : \nabla \mathbf{v} \\ - \left(\mathcal{Q} - \sum_{i \in \mathfrak{S}} \phi_i (\rho_i \nabla \cdot \mathbf{v} + \nabla \cdot \mathcal{J}_i) + \sum_{i \in \mathfrak{S}} \nabla \cdot \phi_i \mathcal{J}_i \right) \cdot \nabla \left(\frac{-1}{T} \right) \\ - \sum_{i \in \mathfrak{S}} \mathcal{J}_i \cdot \left(\nabla \left(\frac{g_i}{T} \right) - \frac{\nabla (\nabla \cdot \phi_i)}{T} \right) - \sum_{i \in \mathfrak{S}} (g_i - \nabla \cdot \phi_i) \frac{m_i \omega_i}{T}, \quad (11) \end{aligned}$$

where t denotes time, ∇ the usual differential operator, \mathbf{v} the fluid velocity, \mathcal{S} is the entropy per unit volume, \mathcal{Q} denotes the total heat flux, T the absolute temperature,

*Corresponding author. Email: vincent.giovangigli@polytechnique.fr

$\mathfrak{S} = \{1, \dots, n\}$ the species indexing set, n the number of species, ρ_i the partial density of the i th species, \mathcal{J}_i the mass flux of the i th species, g_i the Gibbs function per unit mass of the i th species, \mathcal{P} the total pressure tensor, p the pressure, and \mathbf{I} the unit tensor. The—mass based—vectors ϕ_i , $i \in \mathfrak{S}$, are given by $\phi_i = \sum_{j \in \mathfrak{S}} \varkappa_{ij} \nabla \rho_j$, $i \in \mathfrak{S}$, and \varkappa_{ij} , $i, j \in \mathfrak{S}$, denote the mass based capillary coefficients. Proceeding as in the thermodynamics of irreversible processes, and using the Curie principle, one may deduce from the expression of entropy production (11), that the pressure tensor is given by (12) from [1] and that the total heat flux is in the form

$$\mathcal{Q} = \sum_{i \in \mathfrak{S}} \phi_i (\rho_i \nabla \cdot \mathbf{v} + \nabla \cdot \mathcal{J}_i - m_i \omega_i) - \sum_{i \in \mathfrak{S}} \nabla \cdot \phi_i \mathcal{J}_i + \mathbf{q}, \quad (13)$$

where $\mathbf{\Pi}$ is the viscous tensor and \mathbf{q} the dissipative heat flux. The viscous tensor $\mathbf{\Pi}$ is given by (14) from [1] whereas the the dissipative transport fluxes \mathcal{J}_i , $i \in \mathfrak{S}$, and \mathbf{q} are given by

$$\mathcal{J}_i = - \sum_{j \in \mathfrak{S}} L_{ij} \left(\nabla \left(\frac{g_j}{T} \right) - \frac{\nabla (\nabla \cdot \phi_j)}{T} \right) - L_{ie} \nabla \left(\frac{-1}{T} \right), \quad (15)$$

$$\mathbf{q} = - \sum_{i \in \mathfrak{S}} L_{ei} \left(\nabla \left(\frac{g_i}{T} \right) - \frac{\nabla (\nabla \cdot \phi_i)}{T} \right) - L_{ee} \nabla \left(\frac{-1}{T} \right), \quad (16)$$

where \mathbf{v} denotes the volume viscosity, η the shear viscosity and L_{ij} , $i, j \in \mathfrak{S} \cup \{e\}$, the mass and heat transport coefficients. The matrix of mass and heat transport coefficients L defined by $L = (L_{ij})_{i, j \in \mathfrak{S} \cup \{e\}}$ is symmetric positive semi-definite with nullspace spanned by the vector $(1, \dots, 1, 0)^t$ as for ordinary fluids. The fluxes \mathcal{J}_i , $i \in \mathfrak{S}$, and \mathbf{q} are obtained here in their *thermodynamic form*.

The pressure tensor, the $\mathbf{\Pi}$, the total heat flux (13) and the dissipative fluxes \mathcal{J}_i , $i \in \mathfrak{S}$, and \mathbf{q} given by (15) and (16) are the fluxes obtained from the kinetic theory of dense gases removing the ambiguities associated with thermodynamic methods applied to diffuse interface models [2, 3].

Note that all the ambiguous terms that have been clarified with the help of the kinetic theory of dense gases are zero under the simplifying assumption that all the mass based capillary coefficients are equal $\varkappa_{ij} = \varkappa$, $i, j \in \mathfrak{S}$ that has been used in [1].

2. Nonideal strained diffuse interfaces

2.1. Small Mach number limit for flat interfaces

The zeroth order energy conservation equation in terms of the enthalpy $h = h^0$ takes the simplified form

$$\rho \partial_t h + \rho \mathbf{v} \nabla \cdot h + \nabla \cdot \mathbf{q} = \partial_t \bar{p}^0 + \mathbf{v} \cdot \nabla \bar{p}^0, \quad (29)$$

with a term $\mathbf{v} \cdot \nabla \bar{p}^0$ that is not anymore a priori negligible as for standard fluids. In particular, the correct heat equation involves the dissipative flux is \mathbf{q} and not \mathcal{Q} as was incorrectly written in [1].

2.2. Strained flows

The correct energy equation is

$$\rho\partial_t h + \rho v\partial_\zeta h - v\partial_\zeta \bar{p}^0 + \partial_\zeta q = 0, \quad (33)$$

with naturally q in place of \mathcal{Q} . These typos only appear in the presentation of the model and the proper equations have been used in the simulations.

References

- [1] P. Gaillard, V. Giovangigli and L. Matuszewski, A Diffuse Interface Lox/Hydrogen Transcritical Flame Model, *Combust. Theory Model.* **20**, 486 (2016).
- [2] V. Giovangigli, A kinetic derivation of diffuse interface fluid models, *Phys. Rev. E* **102**, 012110 (2020).
- [3] V. Giovangigli, Kinetic Derivation of Cahn-Hilliard Fluid Models, *Phys. Rev. E*, 104 (2021), 054109.