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An efficient multi-fluid-mixing model for real gas reacting flows in liquid propellant rocket engines

Daniel T. Banuti[a,1,*], Volker Hannemann[a], Klaus Hannemann[a], Bernhard Weigand[b]

[a] German Aerospace Center (DLR), Institute of Aerodynamics and Flow Technology, Spacecraft Department, Bunsenstr. 10, Göttingen 37073, Germany
[b] Institute of Aerospace Thermodynamics, University of Stuttgart, Pfaffenwaldring 31, Stuttgart 70569, Germany

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ABSTRACT

This paper introduces a new model for real gas thermodynamics, with improved accuracy, performance, and robustness compared to state-of-the-art models. It is motivated by the physical insight that in non-premixed flames, as encountered in high pressure liquid propellant rocket engines, mixing takes place chiefly in the hot reaction zone among ideal gases. We developed a new model taking advantage of this: When real fluid behavior only occurs in the cryogenic oxygen stream, this is the only place where a real gas equation of state (EOS) is required. All other species and the thermodynamic mixing can be treated as ideal. Real fluid properties of oxygen are stored in a library; the evaluation of the EOS is moved to a preprocessing step. Thus decoupling the EOS from the runtime performance, the method allows the application of accurate high quality EOS or tabulated data without runtime penalty. It provides fast and robust iteration even near the critical point and in the multiphase coexistence region. The model has been validated and successfully applied to the computation of 0D phase change with heat addition, and a supercritical reactive coaxial LOX/GH_2 single injector.

1. Introduction

The physical process of supercritical injection, as encountered in liquid propellant rocket engines, is still considered essentially not well understood (Oefelein [1]).

Nonetheless, significant progress has been made in identifying the differences between injection at sub- and at supercritical pressures. Newman and Brzustowski [2] were the first to carry out systematic studies of supercritical injection, looking at the influence of chamber fluid temperature and composition on break-up phenomenology. They were the first to realize that supercritical injection resembles turbulent mixing rather than classical liquid atomization. Mayer and Tamura [3] later demonstrated this in experiments representative for liquid rocket engines, establishing what is today's standard view (e.g., Oschwald et al. [4], Candel et al. [5]). Recently, Dahms et al. [6] suggested that Diesel injection essentially can be classified in the same manner, namely as an Eulerian continuum instead of a Lagrangian droplet cloud.

The first computational fluid dynamics (CFD) model reflecting the Eulerian character of supercritical injection has been introduced by Oefelein and Yang [7]. Thermodynamic properties for dense multicomponent mixtures are evaluated using the extended corresponding states principle: by determining the pseudocritical parameters of the local mixture using appropriate rules (see e.g., Reid et al. [8]), thermodynamic properties of a well known reference fluid may be mapped to the mixture. Transport coefficients are obtained in likewise manner. The injected stream is treated as an Eulerian continuum instead of a discrete Lagrangian droplet cloud. No separate model for primary or secondary atomization is necessary, jet break-up is computed as a turbulent mixing process. The steep but finite property gradients of supercritical fluids are inherently included in the model, no jump conditions across state transitions are required.

This Eulerian approach has become the state-of-the-art. Table 1 compiles an overview of codes using real gas models. It contains work of the pioneering groups, e.g., Bellan and Okong'o [9–12], Oefelein and Yang [7,13,14], Yang et al. [15–17], and more recent work. On a first glance, the diversity seems overwhelming. The fidelity of the methods ranges from DNS, over LES to URANS and RANS. Chemistry is treated using everything from finite rate models, flamelet, eddy dissipation, to equilibrium models. Concerning thermodynamics, however, especially the recent codes follow the same proven approach (e.g., Hickey et al. [18], Masquelet et al.

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* Corresponding author.
E-mail address: dbanuti@stanford.edu, daniel.banuti@dlr.de, daniel@banuti.de (D.T. Banuti).

[1] Present address: Stanford University, Department of Mechanical Engineering, Center for Turbulence Research, Stanford, CA 94305, USA.

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Table 1
Overview of CFD codes for real gas injection. Abbreviations: axi: 2D axisymmetric, 2D: 2D planar, 3D: full 3D, k–ε: Reynolds averaged Navier–Stokes equations using a k–ε turbulence model, LES: large eddy simulation, DNS: direct numerical simulation, SEE: statistical Eulerian–Eulerian continuous spray, SEL: statistical Eulerian–Lagrangian particle tracking, SEL*: statistical Eulerian-Lagrangian where particles are converted to continuum immediately after injection, IATE: interfacial area transport equation, BWR (t): Benedict–Webb–Rubin EOS used for transport coefficients, HBMS: Hirschfelder–Buehler–McGee–Sutton EOS, (m)PR: (modified) Peng–Robinson EOS, (m)SRK: (modified) Soave–Redlich–Kwong EOS, RK: Redlich Kwong EOS, iG: ideal gas EOS, ECS: extended corresponding states principle, vdW: van der Waals mixing rules, ideal: ideal mixing rules.

Source	Dims	Turbulence	Spray	EOS	Mixing
[7,13,14]	2D/axi	DNS/LES	SEE/SEL	BWR/SRK	ECS
[15–17]	2D/axi	LES	SEE/SEL	BWR(t)/SRK	ECS
[30,31]	axi	k–ε	SEE/SEL	HBMS	Ideal
[10–12]	3D	DNS	SEE	mPR	vdW
[32]	axi	k–ε	SEL/IATE	iG	Ideal
[33–36]	axi	k–ε	SEL*	NIST/CEA	Tabulated
[37,38]	axi	k–ε	SEE	PR/iG	vdW
[24,25]	axi	k–ε	SEE	RK/PR	Ideal/vdW
[20–22]	3D	LES	SEE	PR	vdW
[19]	axi	LES	SEE	PR	vdW
[39]	axi	k–ε	SEE	mSRK. PR	vdW
[18]	2D	LES	SEE	PR	vdW
[23,40]	3D	LES	SEE	PR	vdW
[41]	3D	LES	SEE	Tabulated cubic	vdW

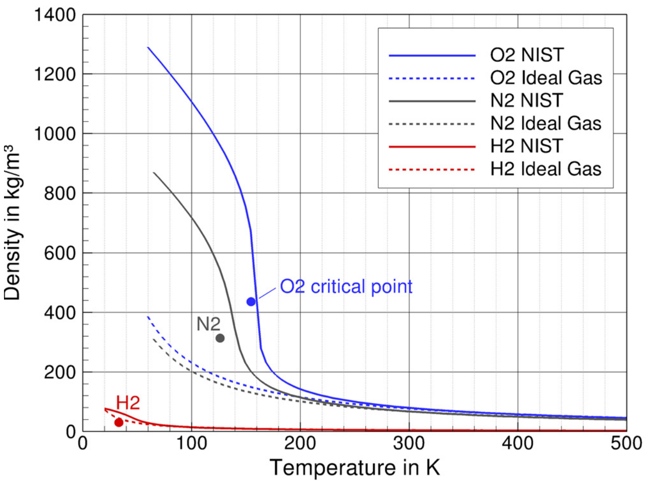

Fig. 1. Ideal and real gas behavior at 6 MPa. Real gas data have been taken from the NIST database [42].

[19], Schmitt et al. [20–22], Niedermayer et al. [23], Poschner and Pfitzner [24,25]): they typically employ a Peng–Robinson [26] or Soave–Redlich–Kwong [27] equation of state, which is evaluated during runtime using single fluid mixture rules (Ely and Hanley [28,29]).

At the core of real fluid modeling lies an appropriate real gas equation of state. Figure 1 shows the differences between real and ideal gas density at low temperatures and high pressure (6 MPa) for oxygen, nitrogen and hydrogen. A measure to distinguish real from ideal gas behavior is the compressibility or real gas factor Z, which may be interpreted as a nondimensional parameter relating the acting pressure to the pressure an ideal gas would exert at the given specific volume v (the reciprocal density ρ) and temperature T:

$$Z = \frac{pv}{RT} \tag{1}$$

For ideal gases, $Z \equiv 1$. In order to capture these real fluid effects, van der Waals [43] extended the ideal gas equation of state (EOS) by two new parameters a and b, accounting for intermolecular attractive forces and a finite molecular volume, respectively. The first simple yet accurate EOS was developed by Redlich and Kwong (RK) [44]. The main improvement over the van der Waals (vdW) equation was to turn the constant parameter a into a temperature dependent function $a(T)$. Its successor, the Soave–Redlich–Kwong [27] EOS (SRK), is still widely used today. It additionally includes Pitzer's acentric factor ω to account for nonspherical molecules. The Peng–Robinson (PR) EOS is similar in structure to the SRK equation but has been fitted particularly to match the compressibility factor Z at the critical point better [26]. It is shown here exemplarily because of its wide use, compare Table 1.

$$p = \frac{RT}{v-b} - \frac{a}{v^2 + 2bv - b^2} \tag{2}$$

with

$$a = 0.457236\frac{(RT_{\mathrm{cr}})^2}{p_{\mathrm{cr}}}\left[1 + m(1 - \sqrt{T_{\mathrm{r}}})\right]^2 \tag{3}$$

$$m = 0.3746 + 1.54226\omega - 0.26992\omega^2 \tag{4}$$

$$b = 0.077796\frac{RT_{\mathrm{cr}}}{p_{\mathrm{cr}}}. \tag{5}$$

Oefelein [14] summarizes that Peng–Robinson and the Soave–Redlich–Kwong equations of state are similarly accurate; PR is to be preferred at supercritical pressures, SRK is better suited for subcritical pressures. Walas [45, p. 71] finds the same for the simple fluid methane, but shows how both fail to predict water isotherms in a $\rho - p$ diagram, except for densities less than half the critical value. While being more accurate than either EOS over a wide range of pressures and temperatures and in near critical conditions, modifications of the Benedict–Webb–Rubin (BWR) [46] EOS have not found widespread use because of their high computational cost (Oefelein et al. [14]). Younglove [47] notes that the critical region of a fluid is generally not describable using analytical functions.

The thermal equation of state does not only determine fluid pvT properties, but also the deviation from ideal gas behavior of the caloric variables specific enthalpy h, specific internal energy e, specific heat capacities c_p and c_v, specific entropy s, and speed of sound a. These departure functions follow from fundamental thermodynamic relations, see e.g. Reid et al. [8].[2] These caloric properties are much more sensitive to EOS quality than pvT behavior (Span and Wagner [48]). Thus, accurately capturing c_p is a very demanding problem for an EOS.

However, this is no reason in itself: Repeatedly, researchers have stressed the importance of a peak in c_p for injection phenomena. Oschwald and Micci [49] and Mayer et al. [50] suggest that a longer liquid core length should be observed if the injected fluid has to pass through the peak to reach the chamber state. Zong and Yang [16] emphasize the "*importance of thermophysical properties in dictating the behavior of a supercritical fluid jet*". They point out that cases which need to pass through the c_p peak are slower to gain temperature along the centerline, while the density is extremely sensitive to temperature at the same state. Oschwald et al. [4] and later Terashima and Koshi [51] found that the c_p peak may explain wide constant temperature regions in cryogenic injection. Oschwald et al. call this process 'pseudo boiling'. Lacaze and Oefelein [52] emphasized that heat capacity must be accurately accounted for when modeling real fluid flames: Performing studies of counterflow diffusion flames, they attribute a significant shift in flame temperature structure to the combined effect of peak heat capacity and a minimum in the thermal diffusion coefficient which they dub 'thermal barrier'. Lacaze and Oefelein suggest that this

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[2] They are shown in Eqs. (25)–(30).