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Rule-Based Compressible Solver for Supercritical and Subcritical Combustion in Rocket Injectors Using Flamelet Models

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Abstract: The goal of the present work is to develop a computational tool capable of unsteady turbulent combustion using state-of-the-art flamelet methodology coupled with efficient Lagrangian particle (droplet) tracking capability. This work seeks to develop a high performance, high fidelity simulation capability to enable accurate, fast and robust simulation of unsteady turbulent, reacting flows involving cryogenic propellants (such as LOX/LH2 and LOX/LCH4). The key features of this capability are: (a) flamelet modeling for turbulent combustion and (b) LES and Hybrid RANS-LES (HRLES) methodologies, incorporated in a proven existing solver called Loci-STREAM. The enhancements in Loci-STREAM are anticipated to yield higher fidelity and more reliable analytical/design capability relative to existing capability for turbulent reacting flows in liquid rocket engines.

Keywords: Multiphase combustion, Flamelet model, Evaporation model, Lagrangian particle tracking

1 Introduction

Computational methods have become an important design tool in the product development cycle of rocket engines as one way to alleviate testing costs and to develop these devices better, faster and cheaper. In the design of advanced propulsion systems, computational fluid dynamics (CFD) plays a major role in defining the required performance over the entire flight regime, as well as in testing the sensitivity of the design to the different modes of operation. This necessitates continuing improvement of computational tools which can be used effectively and reliably in a design environment. The goal of the present work is to develop a computational tool capable of unsteady turbulent combustion using state-of-the-art flamelet methodology coupled with efficient Lagrangian particle (droplet) tracking capability.

The computational tool used as the basis for the present work is called Loci-STREAM [1]. It integrates proven numerical methods for generalized grids and state-of-the-art physical models in a novel rule-based programming framework called *Loci* [2] which allows: (a) seamless integration of multidisciplinary physics in a unified manner, and (b) automatic handling of massively parallel computing. An immediate application of interest is simulation of unsteady reacting flows in liquid rocket combustion systems.

The framework for application development called *Loci* [2] is designed to reduce the complexity of assembling large-scale finite-volume applications as well as the integration of multiple applications in a multidisciplinary environment. Unlike traditional procedural programming systems (C, FORTRAN) in which one writes code with subroutines, or object-oriented systems (C++, Java) in which objects are the major program components, *Loci* uses a rule-based framework for application design. Users of *Loci* write applications using a collection of "rules" and provide an implementation for each of the rules in the form of a C++ class. In addition, the user must create a database of "facts" which describe the

particular knowns of the problem, such as boundary conditions. Once the rules and facts are provided, a query is made to have the system construct a solution. One of the interesting features of *Loci* is its ability to automatically determine the scheduling of events of the program to produce the answer to the desired query, as well as to test the consistency of the input to determine whether a solution is possible given the specified information. The other major advantage of *Loci* to the application developer is its automatic handling of domain decomposition and distribution of the problem to multiple processors.

2 Methodology

The Loci-STREAM CFD code is an Eulerian-Lagrangian all-speed flow solver. The algorithm for solving the fluid dynamics equations in Loci-STREAM is based on the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm [3]. It uses a control volume approach with a collocated arrangement for the velocity components and the scalar variables like pressure. Pressure-velocity decoupling is prevented by employing the momentum interpolation approach [4]; this involves adding a fourth-order pressure dissipation term while estimating the mass flux at the control volume interfaces. The velocity components are computed from the respective momentum equations. The velocity and the pressure fields are corrected using a pressure correction (p') equation. The correction procedure leads to a continuity-satisfying velocity field. The whole process is repeated until the desired convergence is reached. Detached-Eddy Simulation (DES) [5] and Large Eddy Simulation (LES) [6] models are available in Loci-STREAM for turbulent flow simulations. A Lagrangian particle tracking (LPT) algorithm is implemented in Loci-STREAM to handle liquid droplets. Turbulent combustion is handled by employing flamelet model-based methodology.

2.1 Eulerian-Lagrangian Formulation

For liquid rocket injector applications, tracking every particle (droplet) is prohibitively expensive and as a result, in the Lagrangian droplet tracking approach employed in Loci-STREAM, the liquid spray is represented by a number of discrete computational "particles". Individual particles are tracked through the flow domain from their injection point until they escape the domain or until some integration limit criterion is met. Each fluid particle typically represents a large number of droplets with a given size distribution and transport properties. The larger number of particles or trajectories gives a reasonable representation of the liquid behavior. One of the advantages of the Lagrangian approach is that an accurate representation of the droplet distribution can be obtained at a lower cost than the Eulerian approach for the liquid phase, where tracking the interface between all the droplets and the gas phase can be a prohibitive task in terms of computing costs.

For spray flows described in the Lagrangian approach, the particle motion is simulated using the Basset-Boussinesq-Oseen (BBO) equations. It is assumed that: (a) the density of the particle (liquid drop) is much larger than that of the background fluid, (b) particle size is small compared to the turbulence integral length scale, and (c) that the effect of shear on particle motion is negligible. The high value of density ratio implies that the Basset force and the added mass term are small and are therefore neglected. The basic conservation equations of mass, momentum, and energy for the gas phase are modified to include additional terms, which account for two-phase effects. The continuity equation for gas-phase species includes a source term due to vaporization of droplets. The momentum equation includes a term for the rate of momentum gain per unit volume due to the spray. The energy conservation equations includes a source term for the energy exchange involved in droplet vaporization. In most commonly used approaches, the current status of turbulence modeling uses ensemble-averaged equations in which turbulence transport properties are computed from a turbulence model. For sprays, the turbulent kinetic energy and dissipation rate equations each contain an additional term due to spray interactions.

In the Lagrangian particle/droplet tracking approach, particles (droplets) are explicitly tracked in the fluid by solving ordinary differential equations (ODEs) that describe the Newtonian motion of dispersed particles under the influence of empirically derived fluid drag forces. The fluid motion is governed by

the Navier-Stokes equations along with particle forcing functions in the momentum equations. A laminar flamelet model has already been incorporated into Loci-STREAM [1] for turbulent combustion simulations – it has been extended to include spray combustion in conjunction with Lagrangian particle (droplet) tracking and evaporation models.

2.2 Gas Phase

The turbulent combustion occurring in the gaseous phase is modeled with the fluid dynamic equations augmented with a laminar flamelet model [7]. Flamelet models are based on the view of a turbulent diffusion flame as an ensemble of stretched laminar flamelets. Inherent to this view is the assumption of a thin reaction zone which is thinner than the scale of a Kolmogorov eddy. The effect of turbulence is therefore limited to the deformation and stretching of the flame sheet but does not penetrate the reaction zone. Flamelets are then thin laminar reactive diffusive layers embedded in an otherwise non-reacting turbulent flow field. In this work, a flamelet/progress variable (FPV) formulation is employed. In this model, a reaction progress variable C along with the mixture fraction Z is used. The progress variable is defined using a linear combination of reaction product species, which allows a unique identification of each single flamelet along the entire classical S-shape curve. C usually represents a reaction-controlling parameter. For example, for methane/air chemistry the following definition is used:

$$C = Y_{CO_2} + Y_{H_2O} + Y_{H_2} + Y_{CO}$$
(1)

Transport equations for the mixture faction (Z) and the progress variable (C) are solved. Then, in the FPV model, all thermochemical quantities are parameterized in terms of mixture fraction Z and progress variable C, and the turbulence/chemistry interaction is modeled through a presumed PDF closure model. The parameterization can be represented as:

$$\tilde{Z}, \tilde{Z}^{"2}, \tilde{C} \xrightarrow{\text{flamelet lookup table}} \tilde{Y}_i, \tilde{T}$$
 (2)

The governing equations used in this approach are the Favre-averaged Navier-Stokes equations, in addition to the transport equations for flamelet manifold variables *Z* and *C*, as given below:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho} u_j}{\partial x_j} = 0$$
(3)

$$\frac{\partial \overline{\rho} u_i}{\partial t} + \frac{\partial \overline{\rho} u_j u_i}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\tilde{\tau}_{ij} - \overline{\rho u_i^{"} u_j^{"}} \right)$$
(4)

$$\frac{\partial \overline{\rho} E}{\partial t} + \frac{\partial}{\partial x_{j}} \left(\overline{\rho} u_{j} E \right) = \frac{\partial}{\partial x_{j}} \left[\left(\frac{\lambda}{c_{p}} + \frac{\mu_{r}}{Pr_{r}} \right) \frac{\partial h}{\partial x_{j}} \right] + \frac{\partial}{\partial x_{j}} \left(\sum_{k=1}^{NS} \left(\overline{\rho} D_{k} - \frac{\lambda}{c_{p}} \right) h_{k} \frac{\partial Y_{k}}{\partial x_{j}} \right) + \frac{\partial}{\partial x_{i}} \left[u_{j} \left(\tilde{\tau}_{ij} - \overline{\rho u_{i} u_{j}} \right) - u_{j} p \right]$$
(5)

$$\frac{\partial \overline{\rho} Z}{\partial t} + \frac{\partial \overline{\rho} u_j Z}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\overline{\rho} D + \frac{\mu_t}{Sc_t} \right) \frac{\partial Z}{\partial x_j} \right]$$
(6)

$$\frac{\partial \overline{\rho} Z^{\prime\prime 2}}{\partial t} + \frac{\partial \overline{\rho} u_j Z^{\prime\prime 2}}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{Sc_t} \frac{\partial Z^{\prime\prime 2}}{\partial x_j} \right) + 2 \frac{\mu_t}{Sc_t} \frac{\partial Z}{\partial x_j} \frac{\partial Z}{\partial x_j} - \overline{\rho} \chi$$
(7)

$$\frac{\partial \rho C}{\partial t} + \frac{\partial \rho u_j C}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho \alpha \frac{\partial C}{\partial x_j} \right) + \rho \dot{\omega}_C \tag{8}$$

Where

$$\tilde{\tau}_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij}$$
(9)

$$-\overline{\rho u_{i}u_{j}}^{*} = \mu_{t}\left(\frac{\partial u_{i}}{\partial x_{j}} + \frac{\partial u_{j}}{\partial x_{i}}\right) - \frac{2}{3}\mu_{t}\frac{\partial u_{k}}{\partial x_{k}}\delta_{ij} - \frac{2}{3}\overline{\rho}k\delta_{ij}$$
$$\chi(Z) = c_{\chi}c_{\mu}\omega Z''^{2}, \quad \text{where } c_{\chi} = 2, \ c_{\mu} = 0.09$$
(10)

For DES/LES, Eq. (7) is replaced by

$$Z''^{2} = C_{s} \Delta^{2} \left| \nabla \tilde{Z} \right|^{2} \tag{11}$$

The effect of the liquid droplet phase on the gas-phase is represented by the source terms \dot{S}_m , \dot{S}_u , \dot{S}_z and \dot{S}_{zz^2} . These terms are formulated as follows:

$$\dot{S}_m = -\frac{1}{\Delta V} \sum_i N_d^i \dot{m}_d^i \tag{12}$$

$$\dot{S}_{u} = -\frac{1}{\Delta V} \sum_{i} N_{d}^{i} \frac{d\left(m_{d}^{i} u_{d}^{i}\right)}{dt}$$
(13)

$$\dot{S}_Z = -\frac{1}{\Delta V} \sum_i N_d^i \dot{m}_d^i \tag{14}$$

$$\dot{S}_{Z^{*2}} = -\frac{1}{\Delta V} \sum_{i} N_d^i \left[2Z^s \left(1 - Z^s \right) - \tilde{Z} \left(2 - \tilde{Z} \right) \right] \dot{m}_d^i \tag{15}$$

where the index *i* refers to the i^{th} parcel, containing N_d particles, and Z^s is the mixture fraction at the droplet interface.

2.3 Liquid (Droplets) Phase

To describe the liquid phase beyond the primary atomization stage, the individual spray particles are represented by parcels consisting of a finite N_d number of individual droplets, which have identical properties. This representation is justified on the basis that we are here concerned with secondary breakup and spray combustion, in which the size of individual spray-particles is small (typically less than 50 µm). Each individual droplet in this parcel is then represented by the droplet location \mathbf{x}_d , droplet velocity \mathbf{u}_d , droplet diameter d_d , and all droplets have identical properties.

The governing equations for the particle movements are derived using the Basset-Boussinesq-Oseen (BBO) assumption that the density of the particle is much larger than that of the fluid and particle size is small compared to turbulence integral length scale, and that the effect of shear on particle motion is negligible. The Lagrangian equations, describing the evolution of the liquid spray phase can then be written as:

$$\frac{d\mathbf{x}_d}{dt} = \mathbf{u}_d \tag{16}$$

$$\frac{d\boldsymbol{u}_d}{dt} = \frac{f_1}{\tau_d} \left[\boldsymbol{u}(\boldsymbol{x}_d) - \boldsymbol{u}_d \right] + g \tag{17}$$

$$\frac{dh_d}{dt} = \frac{Nu}{3\Pr} \frac{f_2}{\tau_d} C_p \left(T(\boldsymbol{x}_d) - T_d \right) + h_{vap} \frac{\dot{m}_d}{m_d}$$
(18)

where u_d , h_d , and T_d are the droplet velocity, enthalpy per unit mass, and temperature, respectively, and u, T, Pr, and C_p are the gas-phase velocity, temperature, Prandtl number, and heat capacity interpolated to the droplet location x_d . The force of gravity is represented by the acceleration vector, g. The correlation function f_1 is a drag correction for departure from Stokes flow, while the correlation f_2 provides a correction for evaporating droplets. The particle response time, τ_d is defined as

$$\tau_d = \frac{\rho_d d_d^2}{18\mu} \tag{19}$$

where ρ_d is the droplet material density, d_d is the droplet diameter, and μ is the fluid (gas) velocity. The Nusselt number, Nu, is typically modeled using the correlation

$$V_u = 2 + 0.6 \operatorname{Re}_d^{1/2} \operatorname{Pr}^{1/3}$$
(20)

where $Pr = \mu C_p / \kappa$ is the vapor phase Prandtl number. In above equations, κ , c_{p_p} and c_p are the gas phase thermal conductivity, the specific heat of particle material, and the specific heat of the gas phase at constant pressure, respectively.

2.4 Phase Transition: Evaporation Modeling

The particle evaporation model employed is the Langmuir-Knudsen II model detailed in Miller et al [8]. This is considered to be a robust evaporation model for flows with high Reynolds numbers, which is the type of flow that would be encountered in a spray jet.

The mass transfer model is given as follows.

$$\frac{dm_d}{dt} = -\left(\frac{Sh}{3Sc}\right)\left(\frac{m_d}{\tau_d}\right)H_M$$
(21)

The Langmuir-Knudsen mass transfer model uses the following definitions for functions f_1 and f_2 .

$$f_{1} = \frac{1 + 0.545 \operatorname{Re}_{d} + 0.1 \sqrt{\operatorname{Re}_{d} (1 - 0.03 \operatorname{Re}_{d})}}{1 + a |\operatorname{Re}_{b}|^{b}}$$
(22)

where $a = 0.09 + 0.077e^{-0.4Re_p}$, $b = 0.4 + 0.077e^{-0.04Re_p}$. Re_b is the blowing Reynolds number and is defined as $Re_b = \frac{\rho_g u_b D}{\mu_g}$, where u_b is the blowing velocity defined from $\dot{m}_d = -\pi \rho_g D^2 u_b$. The droplet Reynolds number is defined as $Re_d = \frac{\rho_g u_s D}{\mu_g}$, where $u_s = |u_i - v_i|$, i.e., the slip velocity is the difference between the particle velocity and the ambient velocity. The second function used by the Langmuir-Knudsen II model is the following.

$$f_2 = \frac{\beta}{e^\beta - 1} \tag{23}$$

where β is defined as: $\beta = \frac{\Pr Re_b}{2}$.

The mass transfer function, H_M , is defined as

$$T_M = \ln\left(1 + B_{M,neq}\right) \tag{24}$$

The non-equilibrium Spalding transfer number, $B_{M,neq}$, is defined as

$$B_{M,neq} = \frac{Y_{s,neq} - Y_G}{1 - Y_{s,neq}}$$
(25)

The non-equilibrium Spalding transfer number requires $Y_{s,neq}$ which is the non-equilibrium mass fraction of the vapor at the surface of the droplet. The value of Y_G is a background value of the vapor mass fraction in the carrier gas that the droplet is in; this would come from a value of the cell that a droplet is located in, for example. The non-equilibrium mass fraction of the droplet vapor at the surface is given by the following:

$$Y_{s,neq} = \frac{\chi_{s,neq}}{\chi_{s,neq} + (1 - \chi_{s,neq})\theta_2}$$
(26)

The variable $\chi_{s,neq}$ is the value of the non-equilibrium mole fraction at the droplet surface. It is defined as follows:

$$\chi_{s,neq} = \chi_{s,eq} - \frac{L_k}{\left(D_d/2\right)}\beta$$
(27)

where L_k is the Knudsen thickness, β is the non-dimensional evaporation parameter that was defined earlier, and $\chi_{s,eq}$ is the equilibrium mole fraction of vapor at the surface of the droplet. The value of the equilibrium mole fraction at the surface of the droplet is given as the ratio of the saturation pressure of the vapor to the total pressure,

$$\chi_{s,eq} = \frac{P_{sat}}{P_G} \tag{28}$$

The other relations that are critical to closing the system of equations are:

$$L_{k} = \frac{\mu_{G}\sqrt{2\pi T_{d}R_{d}}}{\alpha_{e}\,Sc_{G}\,P_{G}} \tag{29}$$

where T_d is the droplet temperature, R_d is the gas constant associated with the droplet phase, α_e is the molecular accommodation coefficient (which is assumed to be one).



Figure 1. Physical setup of an isolated particle in cross flow experiencing evaporation.

The first validation case involves a water droplet in a quiescent flow with the conditions shown in Table 1.

Table 1. Main simulation parameters for the evaporating water droplet case	
Droplet Diameter, D_0	1.1 mm
Initial Droplet Temperature, $T_{d,0}$	282 K
Ambient Gas Temperature, T_G	298 K
Ambient Fluid Velocity, u_G	0 m/s

The predicted droplet diameter history computed by the Langmuir-Knudsen I model as shown in Figure 2 matches the experimental data as well as the predictions for the Langmuir-Knudsen model [8].

The second validation case chosen involves a decane droplet for which the setup conditions are shown in Table 2.

Table 2: Main simulation parameters for the evaporating decane droplet case	
Droplet Diameter, D_0	2.0 mm
Initial Droplet Temperature, $T_{d,0}$	315 K
Ambient Gas Temperature, T_G	1000 K
Initial Droplet Reynolds Number, $Re_{p,0}$	17
Droplet Boiling Temperature, T_B	447.7 K



Figure 2. The model predictions and experimental data for the water droplet diameter history show close agreement.



Figure 3. The model predictions and experimental data for the decane droplet diameter history show close agreement.

From Figure 3, it can be observed that the prediction of the Langmuir-Knudsen I (LK-I) model follows closely the empirical and earlier predictions by Miller et al [8].

2.3 Turbulent Combustion Model: Compressible Flamelet Model

The approach presented in this section utilizes the flamelet (FPV) methodology extended to account for compressibility involving both ideal and real fluids. The basic ideas of this methodology are derived from the work of Ma et al. [9]. The ideal-gas thermodynamics is modeled by linearizing the specific heat ratio whereas the parameters needed for the cubic Peng Robinson equation of state are pre-tabulated for the evaluation of departure functions and a quadratic expression is used to model the attraction parameter. This compressible model is able to account for temperature and pressure variations from the baseline flamelet table using a computationally tractable pre-tabulated combustion chemistry in a thermodynamically consistent fashion.

2.3.2 Thermodynamics and Transport Properties

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Augmenting the above governing PDEs is a flamelet tabulation, based on the Peng-Robinson equation of state (PR-EoS) that provides both ideal-gas reference state and real-fluid thermodynamic information about the mixture (for a given Z and C) so that the density and temperature of the fluid may be recovered from the solved state variables (p, E, Z and C) using an efficient bracketed secant method iterative process. The Peng-Robinson (PR) equation of state [10] is employed for the evaluation of thermodynamic quantities; it can be written as:

$$p = \frac{RT}{v-b} - \frac{a}{v^2 + 2bv - b^2}$$
(30)

where p is the pressure, R is the gas constant, T is the temperature, v is the specific volume, and the attraction parameter a and effective molecular volume b are dependent on temperature and composition to account for effects of intermolecular forces. For mixtures, the parameters a and b are evaluated as

$$a = \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} X_{\alpha} X_{\beta} a_{\alpha\beta}$$
(31)

$$b = \sum_{\alpha=1}^{N_s} X_{\alpha} b_{\alpha} \tag{32}$$

where X_{α} is the mole fraction of species α . Extended corresponding states principle and single-fluid assumption for mixtures are adopted [11, 12]. The parameters *a* and *b* are evaluated using the recommended mixing rules by Harstad et al. [13]:

$$a_{\alpha\beta} = 0.457236 \frac{\left(RT_{c,\alpha\beta}\right)^2}{p_{c,\alpha\beta}} \left(1 + c_{\alpha\beta} \left(1 - \sqrt{\frac{T}{T_{c,\alpha\beta}}}\right)\right)^2$$
(33)

$$b_{\alpha} = 0.077796 \frac{RT_{c,\alpha}}{p_{c,\alpha}} \tag{34}$$

$$c_{\alpha\beta} = 0.37464 + 1.54226\omega_{\alpha\beta} - 0.26992\omega_{\alpha\beta}^2$$
(35)

where $T_{c,\alpha}$ and $p_{c,\alpha}$ are the critical temperature and pressure of species α , respectively. The critical mixture conditions for temperature $T_{c,\alpha\beta}$, pressure $p_{c,\alpha\beta}$ and acentric factor $\omega_{c,\alpha\beta}$ are determined using the corresponding state principles [14].

Partial derivatives and thermodynamic quantities based on the PR-EoS that are required for evaluating other thermodynamic variables can be derived analytically, as given below:

$$\left(\frac{\partial p}{\partial T}\right)_{v,X_i} = \frac{R}{v-b} - \frac{\left(\partial a/\partial T\right)_{X_i}}{v^2 + 2bv - b^2}$$
(36)

$$\left(\frac{\partial p}{\partial T}\right)_{\mathrm{T},x_{i}} = -\frac{RT}{\left(v-b\right)^{2}} \left\{ 1 - 2a \left[RT\left(v+b\right) \left(\frac{v^{2}+2bv-b^{2}}{v^{2}-b^{2}}\right)^{2} \right]^{-1} \right\}$$
(37)

$$\left(\frac{\partial a}{\partial T}\right)_{X_i} = -\frac{1}{T} \sum_{\alpha=1}^{N_i} \sum_{\beta=1}^{N_i} X_{\alpha} X_{\beta} a_{\alpha\beta} G_{\alpha\beta}$$
(38)

$$\left(\frac{\partial^2 a}{\partial T^2}\right)_{X_i} = 0.457236 \frac{R^2}{2T} \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} X_{\alpha} X_{\beta} c_{\alpha\beta} \left(1 + c_{\alpha\beta}\right) \frac{T_{c,\alpha\beta}}{p_{c,\alpha\beta}} \sqrt{\frac{T_{c,\alpha\beta}}{T}}$$
(39)

$$G_{\alpha\beta} = \frac{c_{\alpha\beta}\sqrt{T/T_{c,\alpha\beta}}}{1 + c_{\alpha\beta}\left(1 - \sqrt{T/T_{c,\alpha\beta}}\right)}$$
(40)

$$K_{1} = \int_{+\infty}^{\nu} \frac{d\nu}{\nu^{2} + 2b\nu - b^{2}} = \frac{1}{\sqrt{8b}} \ln\left(\frac{\nu + (1 - \sqrt{2})/b}{\nu + (1 + \sqrt{2})/b}\right)$$
(41)

For real fluids, thermodynamic quantities are typically evaluated from the ideal-gas value plus a departure function that accounts for the deviation from the ideal-gas behavior. The ideal-gas enthalpy, entropy and specific heat are evaluated from the NASA polynomials at a reference temperature of 298 K. The specific internal energy can be written as

$$e(T,\rho,X_i) = e^{ig}(T,X_i) + \int_{0}^{\rho} \left[p - T\left(\frac{\partial p}{\partial T}\right)_{\rho,X_i} \right] \frac{d\rho}{\rho^2}$$
(42)

where superscript "ig" indicates the ideal-gas value of the thermodynamic quantity, and Eq. (42) can be integrated analytically for PR-EoS to give

$$e = e^{ig} + K_1 \left[a - T \left(\frac{\partial a}{\partial T} \right)_{X_i} \right]$$
(43)

where K_1 is evaluated using Eq. (41). The specific enthalpy can be expressed as:

$$h = h^{ig} - RT + K_1 \left[a - T \left(\frac{\partial a}{\partial T} \right)_{X_i} \right] + pv$$
(44)

The specific heat capacity at constant volume and constant pressure, respectively, are evaluated as

$$c_{\nu} = \left(\frac{\partial e}{\partial T}\right)_{\nu, X_{i}} = c_{\nu}^{ig} - K_{1}T\left(\frac{\partial^{2}a}{\partial T^{2}}\right)_{X_{i}}$$
(45)

$$c_{p} = \left(\frac{\partial h}{\partial T}\right)_{p,X_{i}} = c_{p}^{ig} - R - K_{i}T\left(\frac{\partial^{2}a}{\partial T^{2}}\right)_{X_{i}} - T\frac{\left(\frac{\partial p}{\partial T}\right)_{v,X_{i}}^{2}}{\left(\frac{\partial p}{\partial v}\right)_{T,X_{i}}}$$
(46)

The speed of sound for a real fluid is given by

$$c^{2} = \left(\frac{\partial p}{\partial \rho}\right)_{s,X_{i}} = \frac{\gamma}{\rho \kappa_{T}}$$

$$\tag{47}$$

where γ is the specific heat ratio and κ_{T} is the isothermal compressibility defined as

$$\kappa_T = -\frac{1}{\nu} \left(\frac{\partial \nu}{\partial p} \right)_{T, X_i} \tag{48}$$

The specific heat ratio is linearized around temperature to eliminate the costly iterative procedure to determine temperature, and also to obtain other thermodynamic quantities which are functions of temperature. The underlying strategy rests on correcting the tabulated values with the transported quantities based on the EoS used. Specifically, since PR-EoS is employed, along with thermodynamic quantities needed for evaluation of the ideal gas thermodynamic quantities, parameters a and b, and the first and second derivatives of the parameter a w.r.t. temperature are needed for the calculations of the partial derivatives in Eqs. (36)-(39) which are required for the evaluation of the departure functions. However, the parameter a, along with its derivatives, is a function of both the species composition and the temperature, and thus may not be consistent with the temperature corresponding to the transported variables. The following procedure is adopted for the evaluation of the parameter a and its derivatives: the dependence of the parameter a on temperature is assumed to be a quadratic function as follows:

$$a = C_1 \tilde{T}^2 + C_2 \tilde{T} + C_3 \tag{49}$$

where the coefficients C_1, C_2, C_3 can be obtained from tabulated quantities:

$$C_1 = \frac{1}{2} \left(\frac{\partial^2 a}{\partial T^2} \right)_0 \tag{50}$$

$$C_2 = \left(\frac{\partial a}{\partial T}\right)_0 - 2C_1 T_0 \tag{51}$$

$$C_3 = a_0 - C_1 T_0^2 - C_2 T_0 \tag{52}$$

where subscript "0" indicates the stored baseline quantities in the table. The real-fluid energy is then evaluated as

$$\tilde{e} = \tilde{e}^{ig} + \tilde{e}^{dep} \tag{53}$$

where \tilde{e}^{ig} and \tilde{e}^{dep} are the ideal-gas and departure function values of the internal energy. The ideal-gas value including the chemical energy of the mixture is calculated with linearized specific heat ratio:

$$\tilde{e}^{ig} = \tilde{e}_{0}^{ig} + \frac{\tilde{R}}{a_{\gamma}^{ig}} \ln \left(1 + \frac{a_{\gamma}^{ig}(\tilde{T} - T_{0})}{\tilde{\gamma}_{0}^{ig} - 1} \right)$$
(54)

where T_0 , \tilde{e}_0^{ig} , \tilde{R} , a_{γ}^{ig} , $\tilde{\gamma}_0^{ig}$ are parametrized with \tilde{Z} , $\tilde{Z}^{\prime\prime 2}$, \tilde{C} and stored in the flamelet table. The departure function is given by

$$\tilde{e}^{dep} = K_1 \left[a - \tilde{T} \left(\frac{\partial a}{\partial T} \right)_{X_i} \right]$$
(55)

where Eqs. (49)-(52) are used to compute the parameters required for PR-EoS. Temperature and density are obtained by a bracketed secant iteration method from the computed pressure and energy, using Eqs. (30) and (43), respectively.

Transport quantities are evaluated based on the method due to Chung et al [15, 16]. A power-law is used to approximate the temperature dependency:

$$\frac{\tilde{\mu}}{\tilde{\mu}_0} = \left(\frac{\tilde{T}}{T_0}\right)^{a_{\mu}} \tag{56}$$

$$\frac{\lambda}{\tilde{\lambda}_0} = \left(\frac{\tilde{T}}{T_0}\right)^{a_\lambda} \tag{57}$$

The new compressible flamelet methodology discussed above is thermodynamically consistent in the entire flow path of a rocket engine (from oxidizer and fuel manifolds to the exit of the nozzle) and completely circumvents the need for ad hoc compressibility corrections of the FPV model in Loci-STREAM.

2.4 Preliminary Results

2.1.1 GOX-GH2 Combustion in Shear Coaxial Rocket Injectors

In this section, we present computational results for a gas-gas (GOX/GH2) uni-element rocket injector. The test case used to test the flamelet models is based on experiments conducted by Pal et al [17]. The experimental setup consists of a single element shear coaxial injector, a main cylindrical combustion chamber and two GOX/GH2 preburners which provide hot, oxidizer-rich and fuel-rich streams. A schematic of their experimental setup is shown in Figure 4. The main chamber wall is instrumented with coaxial heat flux gauges which provide both temperature and heat flux profiles. Details of the experimental conditions are provided in Pal et al [17].

Computational domain and boundary condition types for the injector geometry are shown in Figure 4. Axisymmetric domain is modeled with a 1-degree pie-shaped grid (circumferential dimension is exaggerated in Figure 4 for clarity). An extrapolated boundary condition is used at the supersonic exit, so the chamber pressure is not imposed but extrapolated from the solution.

The simulation was conducted on a grid consisting of 175,000 cells (labelled the coarse grid). Figure 5 shows the temperature field for RANS and DES simulations. For the DES simulations, the second-order backward time-differencing scheme (BDF2) and the second-order upwind spatial scheme (SOU) are employed. A timestep size of 1e-6 is used. Figure 2(c) shows the comparison of wall heat transfer from the FPV simulation with the experimental data.



Figure 4. (Top) Schematic of the experiment40 and (Bottom) schematic of the computational domain used for the simulations.

2.1.1 Acetone-Air Spray Combustion

To test the full integration of Lagrangian particle tracking and evaporation models with the flamelet model, a case from the paper by Gounder et al. [18] is being used for validation. This case includes an acetone spray jet configuration with droplets that are evaporating and combusting.



Figure 5. FPV model results for GOX/GH2 injector: wall heat transfer.



Figure 6. .Instantaneous temperature contour plot for the RCM1 injector (including the nozzle) the new compressible flamelet model in Loci-STREAM.

Two different grids were generated. The first grid has two flat injection boundaries and provides a simplistic matching to the experiment in terms of mass fluxes and flow velocities. The mesh is tetrahedral with no boundary layer elements in the domain. The second grid was selected to capture more of the physical spray burner geometry upstream of the jet outlet. This was done to capture the physics of the boundary layer formation within the spray burner as well as on the exterior of the spray burner. On the second grid, the regions of co-flow, secondary co-flow, and carrier flow are better separated because of the geometry. Boundary-layer meshes were generated on the protruding geometry to capture the effect of the velocity gradients near the jet outlet caused by the boundary layer s. The two grids were used to provide a comparison of the sensitivity of the solution to the boundary layer effects of the upstream spray burner geometry. The grid with the spray jet geometry included was a better choice for the simulation as it produced the characteristic unsteady turbulent jet profile when it was used in a Detached Eddy Simulation (DES) mode.

The setup of the computational domain for the grid with the protruding jet outlet is shown in Figure 7. The relevant boundary conditions are also marked in these figures. The main dimensions of the injector are shown in Fig. 7. The diameter of the carrier air tube is 10.5 mm with a wall thickness of 0.5 mm. The diameter of the co-flow annulus is 25 mm with a wall thickness of 0.2 mm.



Figure 7. (Left) Experimental setup [10]. (Right) Computational setup.

The monodispersed droplets are specified by a particle injection boundary condition on the inner jet boundary. The simulation boundary condition is specified by measuring the particle distribution of droplets just outside of the jet outlet in the experimental case and matching the injection distribution to the experimental measurement. The experimental data of the droplet diameter distributions just outside of the jet outlet was fit to a log-normal distribution to extract the best-fit parameters that were then used as an input to the particle injection boundary condition.

The experiment was run within a wind tunnel that runs at ambient outdoors conditions. Therefore, we have assumed that the pressure is 101.325 kPa within the tunnel. The density of liquid acetone is chosen to be $791 \frac{kg}{m^3}$. The specific heat is selected to be $2440 \frac{kJ}{kgK}$ at a temperature of 25 degrees Celsius. The boiling temperature of acetone at 750 mmHg (101.325kPa) is 56.3 °C. The surface tension is $23.1 \cdot 10^{-3} \frac{N}{m}$ at 25 °C. The molecular weight of acetone is $58.08 \frac{g}{mol}$. The molecular weight was used to convert the heat of vaporization from units of $\frac{kJ}{mol}$ to $\frac{kJ}{kg}$. The thermophysical properties such as specific heat, boiling temperature, boiling pressure, and surface tension were obtained from the Dow Jones chemical data sheet [19]. The data for the heat of vaporization of acetone was obtained from the NIST Webbook [20], and it was computed to be $552.63 \cdot 10^3 \frac{J}{kg}$.

The Lagrangian droplet phase simulation results follow the experimental data closely as can be seen from Figure 3. The simulation under-predicts the smaller droplet sizes as well as some of the larger droplet sizes. The secondary breakup model currently employed may influence the distribution of the droplets as it provides a path for the cascade of the droplet diameters towards smaller values, but does not currently provide a path for the agglomeration of droplets into larger diameter drops. Further work on this aspect is required.



(a) Acetone vapor distribution.



(b) Velocity magnitude field with particles colored by velocity magnitude.



(c) Droplet spray jet at one instant using an unsteady DES for the fluid phase. Particle distribution colored with particle diameters.

(d) The simulation and experimental distributions of the droplet diameters at a location of x/D=10 away from jet outlet plane.

Figure 8. Simulation of unsteady spray combustion of acetone using Loci-STREAM.

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3 Conclusion and Future Work

The overall goal of the present work is to develop a computational tool capable of unsteady turbulent combustion using state-of-the-art flamelet methodology coupled with efficient Lagrangian particle (droplet) tracking capability. This work seeks to develop a high performance, high fidelity simulation capability to enable accurate, fast and robust simulation of unsteady turbulent, reacting flows. Key elements of this methodology such as a compressible flamelet model, evaporation model and an efficient Lagrangian particle tracking capability have been presented in this paper. Computational results are presented for a GOX-GH2 uni-element rocket engine injector and an acetone spray combustor. Further work is required to fully validate the overall methodology. The enhancements in Loci-STREAM are anticipated to yield higher fidelity and more reliable analytical/design capability relative to existing capability for turbulent reacting flows in liquid rocket engines.

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