TOWARD LARGE-EDDY/REYNOLDS-AVERAGED SIMULATION OF SUPersonic
COMbustion

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While flamelet-based progress variable models have matured to production-level in recent
years for incompressible flows, little development toward compressible formulations of the flamelet
model has ensued. For supersonic and hypersonic flows exhibiting combustion, an applicable
flamelet-based combustion model must reflect the compressible nature of the flow, the tight
coupling of the flow and flamelet equations, and the problem of multiple flamelet boundary
conditions. This paper describes recent work toward developing a compressible formulation for use
with large-eddy/Reynolds-averaged simulations and implementing flamelet-based progress variable
models in a production-level research code frequently used to simulate high-speed reacting flows.
The proposed model relies on first solving transport equations for momentum, species mass
fraction, and temperature for an axisymmetric opposed-flow diffusion flame for a range of strains
and pressures. The solution space is tabulated and subsequently parameterized by mixture
fraction, progress variable, and pressure. At runtime, transport equations for mass, momentum,
energy, mixture fraction, and progress variable are solved, and at each time step, relevant chemical
properties are retrieved from the flamelet table. By mapping the chemistry to a small set of
tracking scalars, finite-rate simulations of high-speed reacting flows are made comparable in
computational cost to a frozen-chemistry simulation.

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>(Y_{\alpha})</td>
<td>mass fraction of species (\alpha)</td>
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<tr>
<td>(X)</td>
<td>scalar dissipation rate</td>
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<tr>
<td>(Z)</td>
<td>mixture fraction</td>
</tr>
<tr>
<td>(h_{\alpha})</td>
<td>enthalpy of species (\alpha)</td>
</tr>
<tr>
<td>(D_{\alpha})</td>
<td>diffusivity coefficient of species (\alpha)</td>
</tr>
<tr>
<td>(\dot{\omega}_{\alpha})</td>
<td>production rate of species (\alpha)</td>
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<tr>
<td>(R)</td>
<td>gas constant</td>
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<tr>
<td>(p)</td>
<td>pressure</td>
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<tr>
<td>(t)</td>
<td>time</td>
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<tr>
<td>(T)</td>
<td>temperature</td>
</tr>
<tr>
<td>(u_i)</td>
<td>tensor notation velocity</td>
</tr>
<tr>
<td>(x_i)</td>
<td>tensor notation coordinates</td>
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<tr>
<td>(E)</td>
<td>total energy</td>
</tr>
<tr>
<td>(\kappa)</td>
<td>thermal conductivity</td>
</tr>
<tr>
<td>(\delta_{ij})</td>
<td>Kronecker delta</td>
</tr>
<tr>
<td>(C)</td>
<td>progress variable</td>
</tr>
<tr>
<td>(k)</td>
<td>kinetic energy</td>
</tr>
<tr>
<td>(\rho)</td>
<td>density</td>
</tr>
<tr>
<td>(c_p)</td>
<td>specific heat at constant pressure</td>
</tr>
<tr>
<td>(A)</td>
<td>constant eigenvalue of axisymmetric momentum equation for opposed-flow diffusion flame</td>
</tr>
<tr>
<td>(\mu)</td>
<td>molecular viscosity</td>
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</table>
Introduction

Large-eddy/Reynolds-averaged simulation (LES/RAS) of turbulent combusting flows generally requires significantly greater modeling considerations and computational resources than cases without chemical reactions. In the case of high-speed flows, such as those within ramjet and scramjet engines, the difference in computational cost required to simulate a combusting flow versus a chemically frozen flow can be orders of magnitude. Much of this difference can be attributed to the complexity of the mechanism used to model the finite rate chemical kinetics of the system. In the case of a hydrocarbon fuel, a detailed reaction mechanism may require the solution of hundreds, or even thousands, of chemical species [1-3].

The most direct simulation of a reacting flow entails solving a transport equation for each chemical species independently; however, this approach is extraordinarily expensive for complex chemical systems. Due to the wide range of time scales present in such a system, the governing transport equations are highly-stiff and require limited time steps [4]. Further, evaluations of the species source terms are costly due to the numerous exponential calculations required. On account of this expense, researchers generally do not use detailed mechanisms. Instead, reduced mechanisms are often used, such as skeletal mechanisms [5], or expensive chemical terms are tabulated, such as with in-situ adaptive tabulation (ISAT) [6]. In some cases, the chemical composition is parameterized by a small set of tracking variables, like with flamelet-generated manifolds (FGM) [7], eddy-dissipation concept (EDC) models [8], and progress variable (PV) methods [9]. Current computational resources generally permit design-purposed simulations of scramjet combustors using RAS with either reduced mechanisms (no more than about ten species) or with parameterized chemistry models. In nearly all cases, turbulence-chemistry interactions are neglected by assuming laminar chemistry or are modeled using an assumed PDF method [10, 11].

The current research aims to develop a flamelet-based combustion model applicable to high-speed compressible reacting flows of the nature typically encountered in scramjet engines. The model will be implemented in the Viscous Upwind aLgorithm for Complex flow ANalysis (VULCAN) computational fluid dynamics (CFD) code [12]. The current paper describes work toward developing a flamelet-based progress-variable model incorporating compressibility effects and summarizes the status of ongoing efforts toward implementation of flamelet-based combustion models in the VULCAN CFD solver. The combustion models developed as part of this work will be validated using experimental data for the HiFIRE Direct Connect Rig (HDCR) [13].

Background

Methods of reducing the cost and complexity of chemically-reacting flow simulations have been pursued for many decades in varied capacities. Flamelet-based methods for modeling turbulent combustion have become particularly useful on account of their amenability to detailed reaction mechanisms and decoupling of the chemical kinetics from the governing flow equations. While the notion of a laminar flamelet has existed for many decades, the proposition of using laminar flamelets as a means of modeling turbulent flames was not widely-realized until the early 1980s when Peters published a detailed review of laminar flamelets and their potential application to modeling turbulent combustion [14]. Significant work toward flamelet-based combustion models ensued, and in the early 2000s, Oijen [7] and Pierce [9] independently developed what constitutes the foundation of
modern incompressible flamelet-based models for turbulent combustion in the form of flamelet-generated manifolds and progress-variable models, respectively. In the years since inception, these models have been implemented in numerous solvers and have been used successfully to perform RAS and LES of incompressible reacting flows of varying geometric complexity [15, 16].

Classically, the laminar flamelet governing equations for non-premixed flames are derived from the general low-Mach number transport equations for chemical species and energy by assuming constant pressure, no viscous heating, no radiative transport, unity Lewis number, and a linear mapping of physical space to mixture fraction space. These assumptions allow one to recast the transport equations for species mass fractions and enthalpy in the forms presented in Eq. 1-3, subject to species mass fraction and temperature conditions imposed at the flamelet boundaries. An order-of-magnitude analysis of temperature-dependent terms yields Eq. 2 [14].

\[ \rho \frac{\partial y_a}{\partial t} - \rho \frac{\chi}{2} \frac{\partial^2 y_a}{\partial z^2} - \dot{\omega}_a = 0 \]  

(1)

\[ \rho \frac{\partial \tau}{\partial t} - \rho \frac{\chi}{2} \frac{\partial^2 \tau}{\partial z^2} + \sum_a \alpha_a \dot{\omega}_a = 0 \]  

(2)

\[ \chi = 2D \frac{\partial z_i}{\partial x_j} \frac{\partial z_j}{\partial x_i} \]  

(3)

Within this system, the flamelet structure is completely defined by mixture fraction and temperature. The effect of a convective flow field may be imparted on a flamelet solution by the scalar dissipation rate as defined in Eq. 3. Due to the general nature of the equations, any chemical kinetics reaction mechanism can be used to simulate the flamelet chemistry, and though the classical flamelet equations neglect differential diffusion, its effects can easily be included. The utility of these equations resides in their generality and amenability.

Conventionally, modeling of turbulent combustion using laminar flamelets relies on the assumption of Damköhler number greater than one, for which the characteristic chemical time scale is significantly lower than that of the characteristic convective time scale. In this limit, convective processes have little influence on the chemical reactions. Further, one can imagine a turbulent flame as being a wrinkled sheet of one-dimensional laminar flames. Under these assumptions, the chemistry can be effectively decoupled from the flow field by mapping chemical properties to a small set of tracking scalars. In this case, one may pre-tabulate and parameterize all the necessary chemical information by solving the set of flamelet equations for a range of relevant boundary conditions prior to a simulation. At runtime, instead of solving transport equations for each chemical species, one would instead solve an additional transport equation for each tracked scalar.

In most flamelet-based models, these tracking scalars include mixture fraction and a progress variable, which is commonly a linear combination of reactive scalars. At each simulation time step, a call is made using the tracking scalars to the flamelet table, and all chemical information necessary for integration of the governing equations is retrieved, including species mass fractions, production rates, temperature, etc. This approach is common to current flamelet-based combustion models, and the great power of the approach lies in the effective decoupling of the chemical kinetics from the flow simulation.

Combustion Model
While effective, current flamelet-based combustion models are restricted to
incompressible flows, since the models are not designed for the complexities imposed by high-speed reacting flows. An adequate model must account for wide variations in pressure and energy across the flow field and may not explicitly decouple the energy calculation from the flow equations, as the energy is intricately linked to the convective flow field. The model developed and implemented in the current work modifies the standard flamelet-based model such that the flamelet table is further parameterized by pressure and such that a transport equation is solved at runtime for energy, rather than tabulating energy or temperature in the table based on the flamelet solutions.

By default, VULCAN solves a system of governing equations that includes conservation of mass, momentum, energy, and chemical species. The system is closed by solving for pressure using the ideal gas law. In total, the number of partial differential equations (PDEs) solved is equivalent to $5 + N - 1$, where $N$ is the number of chemical species present in the flow field. Without a combustion model, a simulation utilizing the GRI3.0 reaction mechanism would require solution of 57 PDEs ($5 + 53 - 1$). The computational requirements required by such a large stiff system of PDEs is insurmountable for a high-speed flow of engineering interest.

With the recently-implemented flamelet-based approach, the number of PDEs solved by VULCAN is reduced to seven, which includes mass, momentum, energy, mixture fraction, and a single reactive scalar, and the system is closed using the ideal gas law. These transport equations are included in Eqs. 4-8; the equation of state is included in Eq. 9. At each integration time step, a call is made to the flamelet table using mixture fraction, the progress variable, and pressure in order to retrieve mass fractions, production rates, and transport properties. The temperature is calculated at each time step by performing Newton-Rhapson iteration on the expression given in Eq. 10.

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} &= 0 \\
\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} &= -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] \\
\frac{2}{3} \mu \delta_{ij} \frac{\partial u_k}{\partial x_k} &= 0 \\
\frac{\partial \rho E}{\partial t} + \frac{\partial \rho u_j E}{\partial x_j} &= -\frac{\partial \rho u_i}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \kappa \frac{\partial T}{\partial x_j} + \sum_\alpha \rho D_\alpha h_\alpha \frac{\partial \gamma_\alpha}{\partial x_j} \right] \\
\frac{\partial \rho z}{\partial t} + \frac{\partial \rho u_j z}{\partial x_j} &= \frac{\partial}{\partial x_j} \left( \rho D_z \frac{\partial z}{\partial x_j} \right) \\
\frac{\partial \rho c}{\partial t} + \frac{\partial \rho u_j c}{\partial x_j} &= \frac{\partial}{\partial x_j} \left( \rho D_c \frac{\partial c}{\partial x_j} \right) + \rho \dot{\omega}_c \\
p &= \rho RT \\
0 &= E(T) - h(T) + RT - k
\end{align*}
\]

While conventional flamelet-based models use Eqs. 1 and 2 to build the necessary flamelet tables, the proposed model uses an alternative approach. Instead of solving Eq. 1 and 2 over a range of specifications for flame strain rate and temperature (or energy) and subsequently parameterizing the solution space by mixture fraction and a reactive scalar, the current approach solves the set of axisymmetric low Mach number flamelet equations, given below in Eqs. 11 – 13, for a range of strain rates, temperatures (or enthalpies), and pressures. This system of equations is derived for an opposed-flow diffusion flame configuration whose dimension is reduced using a similarity transformation; an illustration of the flow system is included in Fig. 1.
The solution space is then parameterized by mixture fraction, a reactive scalar, and pressure, and is tabulated for interfacing with VULCAN.

Unlike the conventional flamelet equations, this system includes an equation for transport of momentum [17]. An illustration of the linking of the flamelet model with the VULCAN solver is included in Fig. 2.

The implementation of the current model in VULCAN required the development of two independent sets of software—the first being a Python script utilizing Cantera libraries [18] to build the flamelet table and the second being a FORTRAN module for VULCAN to interface with the table. Upon defining the range of pressures required by the simulation, the Python...
script utilizes Cantera’s opposed-flow diffusion flame solver to construct flamelet solutions for a given strain and pressure. The strain is increased until extinction is reached, and the pressure is increased across the user-defined range. Once the table is built, LES/RAS may be performed using VULCAN with the appropriate flags included in the input deck.

Conclusions and Future Work
While conventional flamelet-based combustion models are limited to incompressible flows, work toward the development of a formulation tailored to high-speed compressible flows is presented. A flamelet-based progress variable model is introduced that uses pressure as a parameterizing variable. This model is implemented in the VULCAN CFD code, which has been modified to solve transport equations for continuity, momentum, energy, mixture fraction, and a progress variable.Contrary to classical flamelet approaches, the current implementation does not decouple the energy from the flow equations. Rather, at each integration time step, the temperature is calculated using the total transported energy. The model is implemented in the form of a pre-processing flamelet table generation script written primarily in Python and a FORTRAN module compiled with VULCAN for interfacing with the flamelet table. Future work includes validating the model for unit flows using RAS and LES/RAS and for the HDCR flow path using LES/RAS.

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