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Simulation of a high Reynolds number reactive transverse jet and the formation of a triple flame

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ABSTRACT

This paper briefly describes a hybrid Eulerian–Lagrangian approach for the numerical simulation of turbulent combustion and its application to the study of transverse reactive jets. Because of their interesting mixing properties, transverse jets are important to a variety of industrial applications such as film cooling, primary or dilution jets in gas turbines, and flame stabilization in high speed combustion. To capture the jet complex structure and the associated reaction dynamics, we developed a fast, multiscale and parallel 3D code using a Lagrangian particle method to solve the vorticity transport equation and an Eulerian adaptive grid-based method to solve the reactive transport equations.

Flame anchoring computations were done for a pure methane jet in a crossflow of air at a Reynolds number Re = 1000 and at a velocity ratio of 5 between the jet and the crossflow velocity. The results show that the reactive jet structure strongly resembles that of the non-reactive case, although the reactive jet is slower to bend into the cross flow and it is wider in the spanwise direction. The flame is anchored downstream of the nozzle in a relatively low velocity region and shows a triple flame structure. This triple flame seats in a region of relatively low scalar dissipation rate. We describe the three dimensional topology of the triple flame, as well as the impact of the jet counter-rotating vortex pair (CVP) on the flame front.

1. Introduction

Accurate and efficient simulation of high Reynolds number turbulent reacting jet flows with fast chemical reactions are important for the study of turbulence–combustion interactions in engineering systems utilized in the automotive, aerospace and utility industries, as well as in problems related to safety and environmental concerns. The reactive jet-in-cross flow, used to stabilize combustion in high-speed flows, is one such problem. Examining combustion dynamics using numerical simulations presents several challenges given the multiscale and multiphysics nature of the underlying flows. In most practical combustion simulations, the range between the geometric length scale of the domain and those of diffusion can extend over several orders of magnitude. In order to resolve the jet structure as it interacts with the primary flow, one must apply a high-resolution multiscale method capable of capturing the evolution of small-scale perturbations within the jet all the way to the large-scale energetic structure in the primary flow. The same disparity is present for the time scales.

In this work, the vortex particle method provides the solution for the momentum equation. Because of their natural adaptivity, Lagrangian vortex methods are powerful tools for computing complex unsteady turbulent flows at high Reynolds numbers [1,2]. Lagrangian methods have been gaining popularity in the last decades but are still not too familiar to most readers in the community. The same holds true for AMR methods. These methods do provide an economical alternative for combustion simulations, especially in open domains. In unconfined and semi-confined flows, in Eulerian based methods, a typical computational domain must extend to a size that incorporates regions where the primary variables, i.e., velocity and pressure, deviate very slightly from their uniform distribution. This can result in an unmanageable computational effort in 3D. Vorticity, on the other hand, can typically be described by computational elements contained in a smaller fraction of the total volume of the flow field. As the result, the computational elements are utilized more efficiently. Lagrangian transport of vorticity guarantees that its evolution in space and time is adaptively well resolved, minimizes numerical diffusion and often relaxes time step constraints. The compact support and larger time step drastically reduce both the CPU and memory load. To avoid the difficulties of extracting spatial derivatives when using particle methods, the chemical species transport equations and the energy conservation equation are solved using an Eulerian formulation. The Eulerian solution uses Adaptive Mesh Refinement (AMR) to account for the need for spatial and temporal adaptivity in reacting flow simulations.

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The relaxed time constraints and compact support of computational elements of the vortex method, together with the high temporal and spatial adaptivity of this Eulerian method drastically reduce the CPU and memory load. The main purpose of speeding up the simulation is not only to present a new simulation strategy, but also to allow for parametric studies. Future studies will analyze the jet and the flame stability for different perturbations (forcing of the jet velocity or nozzle edge perturbations). A study for different *Re* numbers and different velocity ratio (between the jet velocity and the crossflow) would also be very interesting. This work will require numerous simulations which would not be computationally manageable using a more CPU intensive code.

Lagrangian combustion simulations have been performed over the past 20 years. Ghoniem and Knio [3] used the three dimensional vortex-particle core-spreading Transport Element Method (TEM) with single-step Arrhenius kinetics to simulate reacting shear layers. Chang et al. [4] employed locally 1D self-similar shape functions. Soteriou and Ghoniem [5] applied the TEM to simulate combustion in spatially evolving shear flows at finite and infinite-rate kinetics. Lakkis and Ghoniem presented an axisymmetric Lagrangian vortex combustion method for reactive flows [6]. Najm et al. [7] combined Eulerian and Lagrangian methods for 2D reacting flow simulations. Thirifay and Winckelmans [8] employed Lagrangian particles to simulate a planar methane jet with coflowing air in an open domain at low Mach number with infinite and finite rate chemistry. They used temperature-independent finite rate chemistry.

Karagozian [9] provides a detailed literature review of 50 years of experimental, theoretical and numerical studies of the transverse jet. This review discusses the transverse jet flow field and its mixing properties for both reactive jets and non-reactive cases, as well as mechanisms for its control via active means. The problem of a reactive jet in cross flow has also been studied recently using direct numerical simulations (DNS). Grout et al. [10] computed the flame stabilization downstream of a nitrogen-diluted hydrogen square transverse jet for a velocity ratio of $r = U_j/U_{cross\text{-}flow} = 4.5$ and a Reynolds number $Re = 4000$. Later, Grout et al. developed a new parameterization technique to describe jet trajectories and discusses the conditions that are necessary to achieve flame anchoring using these new jet-trajectory based coordinates [11]. The flame stabilization mechanism in a round nitrogen-diluted hydrogen transverse jet has also been investigated by Kolla et al. [12]. The high spatial and temporal accuracy and the modeling of detailed chemistry in their simulations required significant computational time. As discussed earlier, the high spatial and temporal adaptivity of our hybrid approach reduces the CPU and memory load. In this work, we use a rounded jet at a lower Reynolds number and a single step reaction, and focus on the jet structure and the associated flame structure. Because our previous studies focused on the jet vortical structure in a non-reacting flow, especially the CVP, we decided to look closely into the flame anchoring mechanism and the interaction of the CVP and the flame front at the anchoring point. According to [13] "flame/flow interaction is strong near the lifted flame base, but increasingly weaker further downstream" which makes this region particularly interesting. We focused our simulations on lower *Re* numbers to allow us to take a much closer look at the flame anchoring location.

This reactive jet simulation is a continuation of our effort on providing efficient simulation techniques and a mechanistic understanding of the transverse jet vortical structure formation and evolution. This effort started when Marzouk and Ghoniem [14] provided a detailed, mechanistic description of inviscid vorticity dynamics in transverse jets while ignoring the possible separation of the wall boundary layer. This first investigation has then been extended by including viscous diffusion of momentum and by allowing the wall boundary layer to grow and separate according to the dynamics imposed by the flow [15,16]. We have developed a rigorous vorticity-flux boundary condition, which includes full interaction between the wall boundary layer and the jet, by generalizing the vorticity flux boundary condition proposed by Marzouk and Ghoniem [14] and characterized the impact of wall boundary layer separation on the evolution of the jet. When the wall boundary layer is allowed to separate, many additional near-wall vortical structures, whose existence was qualitatively predicted on the basis of experimental measurements [17,18], emerge. Among these structures, tornado-like wall-normal structures on the lee side of the jet, close to the nozzle, contribute significantly to the counter-rotating vortex pair. Indeed, counter-rotating vorticity in the first few diameters above the jet exit results primarily from the entrainment of wall boundary layer vorticity via these structures. Our previous paper [15] and this paper share the same Lagrangian scheme. The validation of the Lagrangian algorithm, obtained by comparing the three dimensional vortical structures and the jet trajectory to experimental results from Kelso et al. [17], and the description of the non-reactive jet flow features can be found in [15] and are not repeated here.

This paper has two main objectives, (i) the description of an alternative simulation technique, where a Lagrangian particle based vortex transport method is used to compute the flow field while an adaptive Eulerian grid-based method is used to compute the chemical reaction and species transport and (ii) the presentation of an example that benefits from this method. We should emphasize however, that the primary objective of this particular paper is to present the results and discuss the physics revealed by the results. Given that the scheme is unconventional, the paper also summarizes the numerical approach.

This paper is organized as follows. The governing equations are given in Section 2 and the numerical formulation is presented in Section 3. Section 4 presents the reactive transverse jet results and analysis. Conclusions are given in Section 5.

2. Governing equations

We use the following approximations:

1. Low Mach number.
2. Constant stagnation pressure, since this is an open domain problem.
3. Ideal gas law.
4. No radiation and no Soret/Dufour effect.

By taking the curl of the non-dimensionalized Navier–Stokes equations, we obtain the vorticity transport equation, written for variable density and viscosity:

$$\frac{\partial \omega}{\partial t} + \mathbf{u}\cdot\nabla\omega = \omega\cdot\nabla\mathbf{u} + \left(\frac{D\mathbf{u}}{Dt} - \frac{1}{Fr}\mathbf{g}\right)\times\frac{\nabla\rho}{\rho} + \frac{1}{Re}\frac{1}{\rho}(\mu\Delta\omega - \nabla\mu\times(\nabla\times\omega) + \frac{4}{3}(\nabla_\mu\times\nabla_\varepsilon)), \quad (1)$$

where $\mathbf{u}$ is the velocity, $\boldsymbol{\omega} = \nabla\times\mathbf{u}$ is the vorticity, $\mathbf{g}$ is the gravitational acceleration, and ε is the divergence of the velocity field. The Froude and the Reynolds number are defined as $Re = \frac{\rho_{ref}U_{jet}D}{\mu_{ref}}$ and $\mathrm{Fr} = \frac{U_{jet}^2}{gD}$, where U_{jet} is the jet velocity and D is its diameter. The subscript "ref" refers to reference. The reference conditions are discussed in Section 4.1. The conservative derivative is defined as $\frac{D\alpha}{Dt} = \frac{\partial\alpha}{\partial t} + \nabla\cdot(\alpha\mathbf{u})$. The species conservation equation is written as

$$\rho\left(\frac{\partial Y_k}{\partial t} + \mathbf{u}\cdot\nabla Y_k\right) = \frac{1}{ReSc}\nabla\cdot(\rho D_k\nabla Y_k) + Da\dot{\omega}_k, \quad (2)$$