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Fully explicit implementation of direct numerical simulation for a transient near-field methane/air diffusion jet flame

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ABSTRACT

Direct numerical simulation (DNS) is a kind of ultimate numerical simulation tool for studying fundamental turbulent flows, mixing, chemical reactions and interactions among them. In the present work, a fully explicit method of implementing DNS is presented for investigating transient multi-component methane/air jet flame in the near field. The detailed methodology, enclosing non-dimensional governing equations, inlet velocity disturbance, chemical scheme and fluid property, was discussed. An explicit eighth-order finite-difference scheme was used combined with an explicit tenth-order filter. Conservative variables are temporally advanced in two segmented stages that handle Euler terms and viscous terms respectively. A modified non-reflecting boundary condition was used, which has better performance about the characteristic waves on boundary planes. The developed code was firstly tested with an air jet and evaluated in terms of accuracy and parallel efficiency. Then a methane/air combusting jet was simulated to study the characteristics of the chemical heat-release in turbulence.

1. Introduction

In real industrial applications, such as gas turbine, boiler furnace and internal-combustion engine, etc., combustion is generally processed combining with the effect of turbulence. Turbulence not only affects the combustion efficiency, but also partially determines the features like temperature distribution and pollutant emissions. Therefore, how to predict those effects has been always one of the central topics in combustion and energy utilization fields. In many cases, Reynolds-averaged Navier–Stokes (RANS) method [1–3] with submodels can provide correct predictions in macroscale, which are usually good enough for specific engineering designs and optimization problems [4–7]. However, the RANS models and different submodels are usually case dependent and omnifarious modes have been developed for varied conditions. More precise and universal models are always needed for different problems. But, the model development usually greatly depends on the understanding of microsale flow mechanisms and turbulence-flame interactions. RANS can offer no help for model development, because the flame wrinkle, species mixing and chemical reaction all take place in smaller physical scales beyond the resolution of RANS. As for large-eddy simulation (LES) [8–10], it has just become realistic to simulate more complex flow and combustion phenomenon, but the subgrid model still need validation from experiment or direct numerical simulation (DNS).

In DNS, all the length and time scale are resolved directly without any arbitrary models. DNS has been proven to be one of the best tools for fundamental turbulence and combustion phenomenon research. It has been successfully applied to discover the autoignition phenomenon of non-premixed fuel/air mixture [11–13], the mechanism of vortex-caused strain rate and curve effect on flame propagation [14–16], NO_x [17] and soot formation [18] and also the flame-wall interaction [19,20], etc. Chen et al. [16], Poinsot et al. [20] and Vervish and coworker [10] have done a lot of excellent works in this area. The work reported here is propelled by the curiosity on reactive flow in turbulence. In more practical conditions, combusting mixture may include oil droplets and char particles injected into the combustion chambers at the same time, which will raise many unresolved problems on DNS methodology. However, DNS of multi-phase, multi-component, reactive flow with more detailed chemical kinetics and higher Reynolds number is always the targets for us and all DNS researchers which need continuous efforts. As a rudimentary step, a DNS code that can deal with 3D jet flow with combusting mixture is accordingly developed and tested here.

DNS tends to resolve all the energy containing and dissipation eddies in flow field with very fine grid system which should be in the order of Kolmogrov length and time scale [21]. The huge computational load is still the main obstacle restricting its application. In the early stage, DNS was usually implemented based on 2D turbulence, simple chemistry and periodic flow assumptions. However, with the great development of computer technology, parallel calculation provides a good path for DNS advancement

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with spatial and temporal resolved 3D simulation. Additionally, DNS is quite sensitive to the boundary treatment and the proposed non-reflecting condition [22] that assumes characteristic waves always perpendicularly penetrate computational boundaries may not be well adaptable in 3D flow configuration. Therefore, a modified boundary condition should be initially employed.

The paper was organized in three parts: firstly, a fully explicit method to implement 3D DNS with multi-component and combustion was given in a detailed and comprehensive description; secondly, parallelized DNS code was tested and evaluated in terms of computational efficiency and accuracy; finally, a methane/air jet flame was simulated and some perceptions about chemistry characteristics in turbulence was discussed.

2. DNS implementation

In this section, the governing equations for combusting mixture are firstly presented, followed by the treatment of the relevant fluid properties. Afterwards, numerical methods involved here are specified, including the spatial difference, time advancement and filtering, etc. A modified non-reflecting boundary condition for 3D jet flow is specifically highlighted.

2.1. Fluid dynamics

2.1.1. Governing equation and dimensionless method

The governing equations are compressible, multi-component Navier–Stokes equations, consistent with those used in previous studies [11–20]. In essence they comprise balance equations for mass, momentum, energy and species concentrations, as shown below:

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u_j)}{\partial x_j}=0 \tag{1}$$

$$\frac{\partial(\rho u_i)}{\partial t}+\frac{\partial(\rho u_i u_j)}{\partial x_j}=-\frac{\partial p}{\partial x_j}+\frac{\partial \tau_{ij}}{\partial x_j} \tag{2}$$

$$\frac{\partial(\rho Y_s)}{\partial t}+\frac{\partial(\rho Y_s u_j)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{k}{c_p Le_s}\frac{\partial Y_s}{\partial x_j}\right)+\omega_s \tag{3}$$

$$c_v\frac{\partial \rho T}{\partial t}+c_v\frac{\partial \rho T u_j}{\partial x_j}=-p\frac{\partial u_j}{\partial x_j}+\frac{\partial}{\partial x_j}\left(k\frac{\partial T}{\partial x_j}\right)+\tau_{ij}\frac{\partial u_i}{\partial x_j}-\sum_s h_s\omega_s+\frac{k}{c_p}\frac{\partial T}{\partial x_j}\sum_s\frac{c_{ps}}{Le_s}\frac{\partial Y_s}{\partial x_j} \tag{4}$$

$$\tau_{ij}=\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}-\frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right) \tag{5}$$

There are some assumptions underlying these equations. Because the research aims to evaluate turbulent effect on flame, no gravity and buoyancy are specified and gas phase radiation is also neglected here. Soret and Dufour effect [23], considered to be negligible compared with used heat and mass sources, are precluded as well. The above equations should be solved in non-dimensionalized forms avoiding computational truncation errors. According to Wang et al. [21], non-dimensional variables are defined as:

$$x_j^n=\frac{x_j}{l_r};\quad u_i^n=\frac{u_i}{u_r};\quad \rho^n=\frac{\rho}{\rho_r};\quad t^n=\frac{t\cdot u_r}{l_r};\quad p^n=\frac{p}{\rho_r u_r^2};$$
$$T^n=\frac{T}{T_r},T_r=p_r/(\rho_r R_r);\quad Y_s^n=\frac{Y_s}{Y_r};\quad k^n=\frac{k}{k_r};\quad \mu^n=\frac{\mu}{\mu_r};$$
$$c_p^n=\frac{c_p}{c_{pr}};\quad c_{ps}^n=\frac{c_{ps}}{c_{pr}};\quad c_v^n=\frac{c_v}{c_{vr}},c_{vr}=c_{pr}-R_r$$
$$\mathrm{Re}=\frac{\rho_r u_r l_r}{\mu_r};\quad \mathrm{Pr}=\frac{\mu_r c_{pr}}{k_r};\quad \gamma_r=\frac{c_{pr}}{c_{vr}} \tag{6}$$

Then non-dimensional governing equations are listed as:

$$\frac{\partial \rho^n}{\partial t^n}+\frac{\partial\left(\rho^n u_j^n\right)}{\partial x_j^n}=0 \tag{7}$$

$$\frac{\partial(\rho^n u_i^n)}{\partial t^n}+\frac{\partial\left(\rho^n u_i^n u_j^n\right)}{\partial x_j^n}=-\frac{\partial p^n}{\partial x_j^n}+\frac{1}{\mathrm{Re}}\frac{\partial \tau_{ij}^n}{\partial x_j^n} \tag{8}$$

$$\frac{\partial(\rho^n Y_s^n)}{\partial t^n}+\frac{\partial\left(\rho^n Y_s^n u_j^n\right)}{\partial x_j^n}=\frac{1}{\mathrm{RePr}}\frac{\partial}{\partial x_j^n}\left(\frac{k^n}{c_p^n Le_s}\frac{\partial Y_s^n}{\partial x_j^n}\right)+\frac{l_r}{\rho_r Y_r u_r}\omega_s \tag{9}$$

$$\frac{\partial \rho^n T^n}{\partial t^n}+\frac{\partial \rho^n T^n u_j^n}{\partial x_j^n}=-(\gamma_r-1)\frac{p^n}{c_v^n}\frac{\partial u_j^n}{\partial x_j^n}+\frac{\gamma_r}{\mathrm{RePr}}\frac{1}{c_v^n}\frac{\partial}{\partial x_j^n}\left(k^n\frac{\partial T^n}{\partial x_j^n}\right)+\frac{\gamma_r-1}{\mathrm{Re}}\frac{\tau_{ij}^n}{c_v^n}\frac{\partial u_i^n}{\partial x_j^n}-\frac{(\gamma_r-1)t_r}{p_r}\frac{1}{c_v^n}\sum_s h_s\omega_s+\frac{Y_r\gamma_r}{\mathrm{RePr}}\frac{k^n}{c_p^n c_v^n}\frac{\partial T^n}{\partial x_j^n}\sum_s\frac{c_{ps}^n}{Le_s}\frac{\partial Y_s^n}{\partial x_j^n} \tag{10}$$

Here, superscript "n" denotes the non-dimensional variables and subscript "r" denotes the reference values. Re and Pr are Reynolds number and Prandtl number, respectively, which can be used to characterize the simulated jet flow. The production rate of the sth species ω_s is solved in subroutine in dimensional forms. In light of the practical consideration, energy equation is rewritten in temperature form, rather than in total energy form, so that it has a more clear relationship with other variables and would be much more easily handled.

2.1.2. Fluid property

The enthalpy h_s and specific heat at constant pressure c_{ps} are both temperature T dependent and calculated through temperature fitted polynomials. The coefficients for those polynomial fitting were taken from CHEMKIN thermal data-package [24]. The specific heat c_p of the entire mixture was calculated by weighted-average c_{ps} and mass fraction:

$$c_p=\sum_s Y_s c_{ps} \tag{11}$$

Then the conductivity of the mixture can be deduced though the following equation [25]:

$$\frac{k}{c_p}=2.58\times10^{-5}\left(\frac{T}{298}\right)^{0.7} \tag{12}$$

As for the species viscosity μ_s, they are all determined by the n exponents equations:

$$\frac{\mu_s}{\mu_s^0}\approx\left(\frac{T}{T_0}\right)^n \tag{13}$$

And the mixture viscosity was calculated as:

$$\mu=\sum_s Y_s\mu_s \tag{14}$$

In the present study, Lewis number Le was used to quantify the diffusivity of a certain species. Furthermore, all Lewis numbers are assumed to be unity, because oxygen, methane and nitrogen, together, nearly preserve the entire mass of the mixture and the Lewis numbers of these three species are approximate to unity. Here it should be pointed out that unity approximation do cause somewhat effect on flame predication, but the essence of the flame-turbulent interaction does not change, which is exactly the primary topic of this research [26–29].

2.1.3. Inlet velocity disturbance

The conventional way for generating turbulent inflow profile is to impose random fluctuations on the mean inflow velocity. It has