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One-dimensional turbulence simulations and chemical explosive mode analysis for flame suppression mechanism of hydrogen/air flames

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ABSTRACT

An idealized extinguishing agent with two main inhibition mechanisms was designed to test the chemistry of hydrogen flame extinguishment. The One-Dimensional Turbulence (ODT) model and chemical explosive mode (CEM) analysis (CEMA) were used to perform an in-depth analysis on the role of turbulence-chemistry interaction in diffusion hydrogen/air flame. The function route of the fire extinguishment agent in diffusion flame has been analyzed. The results show that the agent can significantly reduce the CEM. The decrease of CEM will decrease the *Da* number, and lead to flame extinction. The CEMA of ODT results present that the extinction of flame is controlled by the CEM, the mixing rates and the eddy events. The results also illustrated the main inhibition mechanism in which catalytic cycles lead to the destruction of major chain carriers, H. The acting areas of variables and reactions are consistent and clearly visualized with CEMA, which proves that the CEMA is a very efficient method to identify the control variable during the combustion process.

1. Introduction

Safety is critical to the widespread applications of hydrogen due to its ease of leaking, low-energy ignition, wide range of combustible fuel-air mixtures, etc [1–9]. Fire extinguishing agent can be used to control the combustion processes through adding in the hydrogen mixture, or to put off the hydrogen fire [10–13]. The increasing interest in fire safety and environmental protection has heightened the need for development of fire extinguishing agent [14–19]. A research and development program has been sponsored by the Department of Defense in the USA and the National Institute of Standards and Technology (NIST) to improve the understanding of fire suppression and to identify effective replacements [20].

The coupling of detailed chemical kinetics with turbulence is important for combustion simulation of the fire suppression study, because it can provide accurate detailed description of complex turbulence-chemistry interactions which play a key role in the flame extinction and re-ignition phenomena. The direct numerical simulation (DNS) resolves the Navier–Stokes equations fully down to the Kolmogorov length scale, and is a useful tool in fundamental research in turbulence. However, the high computational cost of DNS makes it impossible to apply DNS with detailed chemical kinetic mechanisms in multi-dimensional high Reynolds number reacting flow simulations.

The one-dimensional turbulence (ODT) model can accurately reproduce the DNS data with much less computational cost [21]. The ODT model is an outgrowth of the linear-eddy

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model (LEM), developed by Kerstein [22–25], which is a stochastic mixing model to address the non-linear nature of chemical reactions occurring at molecular mixing scales (fine scales). Compared with LEM, the ODT model solves one or more velocity components to determine the eddy frequency and eddy-size distribution, which can be considered as a mechanism for driving turbulence. As a stand-alone model which can couple turbulence with molecular transport and chemistry, ODT has been successfully applied to a wide range of turbulence problems [21,26–29].

Another problem is how to process the huge datasets that was produced by the turbulence simulation with detailed chemical kinetic mechanisms. For example, the simulation of a laboratory-scale hydrogen jet flame with a 15-species mechanism using ODT model in this paper generated more than 20GB of field data. Scientific method is needed to determine the key acting mechanisms of the fire extinguishing agent in the turbulent reacting flows through such massive datasets. The chemical explosive mode analysis (CEMA) is a systematical method to detect ignition, extinction, premixed flame fronts and the control species and reactions in the flame. The CEMA has developed from the time scale analyses of reacting system based on CSP [30,31]. CEMA is focused on the diagnostics on the chemical properties of the mixtures, and was primarily based on eigen-analysis of the Jacobian for the chemical source term in the governing equations. As such CEMA is simple and efficient to perform while it was found to be advantageous in limit phenomena detection compared with conventional methods based on temperature or a species concentration [31–33].

In this paper, a mechanism for flame inhibition is constructed, and the stand-alone ODT model is applied to simulate hydrogen-air jet diffusion flames with or without fire extinguishing agent. Then the CEMA is used to analyze the fire suppression mechanism in the turbulent reacting flows.

2. Methodology

2.1. ODT model and computation

A description of the detailed configuration of the ODT can be found in Jiang et al. [34]. To summarize, turbulence simulation of a hydrogen jet flame with a co-flow air was performed using the ODT code developed by the author.

ODT can be considered as a method for simulating the evolution of the velocity vector and fluid properties with full spatial and temporal resolution along a one-dimensional line of sight through a three dimensional turbulent flow. The ODT model includes two main components: an evolution representing reactive-diffusion process, and a rule for the implementation of the eddy to represent turbulent advection.

The ODT time-resolved simulation of reaction and of molecular diffusion of momentum, mass, and energy is based on the deterministic solution of the planar boundary layer equations without advection or fluctuating pressure terms.

Momentum

$$\frac{\partial u_i}{\partial t} = \frac{1}{\rho}\frac{\partial}{\partial x}\left(\mu\frac{\partial u_i}{\partial x}\right) \tag{1}$$

Species

$$\frac{\partial Y_k}{\partial t} = -\frac{1}{\rho}\frac{\partial}{\partial x}(\rho Y_k V_k) + \frac{1}{\rho}W_k\dot{\omega}_k \tag{2}$$

Energy

$$\frac{\partial T}{\partial t} = -\frac{1}{\overline{c_p}}\sum_{k=1}^{N} c_{pk}Y_k V_k \frac{\partial T}{\partial x} + \frac{1}{\rho\overline{c_p}}\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right) - \frac{1}{\rho\overline{c_p}}\sum_{k=1}^{N} h_k W_k\dot{\omega}_k \tag{3}$$

where μ is mixture viscosity, V_k is the material diffusivity of species k, λ is the mixture thermal conductivity, $\overline{c_p}$is mixture specific heat, c_{pk} the specific heat of species k, and u_i, Y_k, T, h_k are the velocity, mass species concentration, temperature and enthalpy, respectively. Transport properties and the reaction mechanism are computed using the CHEMKIN library.

In ODT, the turbulent advection is modeled through a series of stochastic rearrangement events. These events are individual turbulent eddies which are referred to as "eddy events" or simply "eddies". Each eddy event interrupts the conserved variables evolution by applying an instantaneous transformation to the fields over some spatial interval (x_0, $x_0 + l$), where y_0 represents the eddy starting location and l is the eddy length.

The triplet map is the essence of any ODT modeling approach, modeling the effects of a three-dimensional eddy with a one-dimensional rearrangement. The functional form chosen for the triplet mapping function, $f(x)$, is the simplest of a class of mappings that satisfy the physical requirements of measure preservation, continuity and scale locality over the eddy interval. It can be represented as

$$f(x;x_0,l) = x_0 + \begin{cases} 3(x-x_0) & \text{for } x_0 \le x \le x_0 + \frac{1}{3}l \\ 2l - 3(x-x_0) & \text{for } x_0 + \frac{1}{3} \le x \le x_0 + \frac{2}{3}l \\ 3(x-x_0) - 2l & \text{for } x_0 + \frac{2}{3} \le x \le x_0 + l \\ x - x_0 & \text{otherwise} \end{cases} \tag{4}$$

The triplet map is augmented by a "kernel transformation" to implement energy transfers while obeying applicable conservation laws [22,23]. The eddy rate distribution and large eddy suppression mechanism were well introduced in references [24,25].

This formulation, consequently, allows for the accurate description of turbulence-chemistry interaction in fine scale, so the ODT model adopted in this work can provide robust information for us to discuss the inhibition effect in turbulent case.

2.2. The concept of CEMA

In the theory of computational singular perturbation (CSP), a reacting system can be formulated as the following ODES:

$$\frac{D\mathbf{y}}{Dt} = \mathbf{g}(\mathbf{y}) \equiv \boldsymbol{\omega}(\mathbf{y}) + \mathbf{s}(\mathbf{y}) \tag{5}$$

where D/Dt is the material derivative, and $\mathbf{y}$ is the vector of the dependent variables such as species concentrations and temperature. $\boldsymbol{\omega}$ is the chemical source term, and $\mathbf{s}$ is the mixing term. If we consider each point in the flame as a