Combustion and Flame 161 (2014) 2933–2950

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Direct numerical simulations of non-premixed ethylene–air flames: Local flame extinction criterion

Vivien R. Lecoustre [a,*], Paul G. Arias [b,c], Somesh P. Roy [d], Zhaoyu Luo [e], Dan C. Haworth [d], Hong G. Im [b,c], Tianfeng F. Lu [e], Arnaud Trouvé [a]

[a] Fire Protection Engineering, University of Maryland, College Park, MD 20742, USA
[b] Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia
[c] Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI 48109, USA
[d] Department of Mechanical and Nuclear Engineering, Pennsylvania State University, University Park, PA 16802, USA
[e] Department of Mechanical Engineering, University of Connecticut, Storrs, CT 06269, USA

ARTICLE INFO

Article history:
Received 5 November 2013
Received in revised form 21 January 2014
Accepted 20 May 2014
Available online 26 June 2014

Keywords:
Flame extinction
Turbulent diffusion flame
Direct numerical simulation
Chemical Explosive Mode Analysis
Extinction criterion

ABSTRACT

Direct Numerical Simulations (DNS) of ethylene/air diffusion flame extinctions in decaying two-dimensional turbulence were performed. A Damköhler-number-based flame extinction criterion as provided by classical large activation energy asymptotic (AEA) theory is assessed for its validity in predicting flame extinction and compared to one based on Chemical Explosive Mode Analysis (CEMA) of the detailed chemistry. The DNS code solves compressible flow conservation equations using high order finite difference and explicit time integration schemes. The ethylene/air chemistry is simulated with a reduced mechanism that is generated based on the directed relation graph (DRG) based methods along with stiffness removal. The numerical configuration is an ethylene fuel strip embedded in ambient air and exposed to a prescribed decaying turbulent flow field. The emphasis of this study is on the several flame extinction events observed in contrived parametric simulations. A modified viscosity and changing pressure (MVCP) scheme was adopted in order to artificially manipulate the probability of flame extinction. Using MVCP, pressure was changed from the baseline case of 1 atm to 0.1 and 10 atm. In the high pressure MVCP case, the simulated flame is extinction-free, whereas in the low pressure MVCP case, the simulated flame features frequent extinction events and is close to global extinction. Results show that, despite its relative simplicity and provided that the global flame activation temperature is correctly calibrated, the AEA-based flame extinction criterion can accurately predict the simulated flame extinction events. It is also found that the AEA-based criterion provides predictions of flame extinction that are consistent with those provided by a CEMA-based criterion. This study supports the validity of a simple Damköhler-number-based criterion to predict flame extinction in engineering-level CFD models.

1. Introduction

Flame extinction in non-premixed flames is a central subject of research in combustion science that has important ramifications for engineering applications; whether the interest lies in power generation applications or in fire safety. The seminal work of Liñán [1] has provided the mathematical foundations for the study of non-premixed flame extinction in laminar counter-flow configurations. Several authors have since then extended the extinction analysis to different non-premixed flame configurations [2–4], with various level of heat losses [4,5], and turbulent conditions [6]. Further references and descriptions are provided in the reviews by Williams [7,8]. These studies have shown that extinction can be explained by the concept of a critical value of a Damköhler number, defined as the ratio of a characteristic mixing time divided by a characteristic chemical time.

Direct Numerical Simulations (DNS) provide a valuable platform for the understanding of the physics of flames. Several past DNS works and analysis using DNS data have focused on non-premixed flame extinction in various environments [9–17]. Dependence of local extinction and reignition on the overall mixing in CO/H_2 non-premixed turbulent jet flames were studied using the one-dimensional turbulence model by Hewson and Kerstein [9]. It was shown that the actual probability of extinguished fluid (taken as local condition with temperature lower than 1000 K) is

* Corresponding author. Fax: +1 301 405 9383.
E-mail address: vlecous1@umd.edu (V.R. Lecoustre).

http://dx.doi.org/10.1016/j.combustflame.2014.05.016
0010-2180/

greater than the probability that the critical extinction scalar dissipation rate, obtained from laminar steady-state flamelet consideration, is exceeded. It was also concluded that the rate of reignition scales with the global mixing rate, as the mixing increases the rate of heat transfer between stoichiometric regions. An extension of the flamelet model was proposed by Pitsch et al. [10] to account for flame reignition, and compared with DNS data. The updated model includes the transport terms along the stoichiometric iso-surface – which are usually neglected in the flamelet approach – to account for the heat exchange between flamelets. The model assumed reignition by edge-flame propagation along the stoichiometric iso-surface. Analysis on the *S* curve show that the addition of these extra terms allows to predict flame reignition with satisfactory agreements with DNS data.

Sripakagorn et al. [11] performed DNS of 3D, non-premixed flame immersed in an isotropic, decaying turbulent field to study the mechanisms of flame extinction and reignition. Single step chemistry and Lagrangian flame element tracking technique were employed to examine the dynamics response of chosen flame elements with turbulence. The observed extinction events were attributed to be principally caused by excessive heat losses for local scalar dissipation rate exceeding values of extinction of steady state flames. Extinguished flame elements were identified as those with stoichiometric temperature lower than that possible for a steady-state flamelet at elevated scalar dissipation rate. Their results show that while the 1D flamelet model predicts extinction very well, it does not predict most of the re-ignition events. Three different flame reignition scenarios were identified, each involves different levels of neighboring flame interaction. The independent flamelet scenario does not involve any interaction with the neighboring flame elements, while edge flame propagation and engulfment scenarios involve strong interactions with the neighboring, either through important lateral positive diffusion of heat from a hot neighboring stoichiometric region toward the cold region, or heat transport to the cold region via turbulence motion, respectively.

Two dimensional DNS investigations of extinction and re-ignition were performed by Venugopal and Abraham [13]. Their numerical configuration was that of a n-heptane laminar non-premixed flame at 40 bar interacting with counter-rotating vortex pairs. Effects of unsteadiness and curvature on flame extinction and reignition were explored. Using an irreversible single-step reaction model, they show that extinction are well captured with 1D transient diffusion flamelet libraries that account for the time history of the scalar dissipation rate, while reignition involves flame-flame interactions and is affected by the local flame topology. A local Damköhler number was defined and extinction was identify when the Damköhler number reached 1. Analysis of the extinction mechanisms has shown that the heat losses by convection along the direction normal to the stoichiometric iso-surface is the dominant mode of heat losses followed by the diffusive heat losses along this direction. Further analysis show that while extinction is a 1D phenomenon, the curvature has a significant effect on the rate of increase of the stoichiometric scalar dissipation rate.

Lignell et al. [14] performed a parametric study of flame extinction and reignition in non-premixed ethylene/air flames using a 3D DNS configuration with detailed chemistry similar to that of Hawkes et al. [12]. Varying Damköhler number at fixed Reynolds was considered. They predicted that flames with increased level of extinction have increased stoichiometric scalar dissipation rate and have shown that the probability density function of the stoichiometric scalar dissipation rate is very close to that of a log-normal distribution, with however some deviation from it at low and high scalar dissipation rate. A positive correlation between scalar dissipation rates and flame curvature was exhibited, with extinction occurring preferentially in flame region with the center of curvature being located in the fuel stream. Mechanisms for flame reignition were identified and were very similar to that of [11], with the addition of flame reignition mechanism due to premixed flames propagation. In contrast to the work of Sripakagorn, access to detailed flame structure allows to distinguish between edge-flame propagation and premixed flames.

Past work by our group was focused on flame extinction diagnostics in different flame extinction configurations: by convective cooling due to flame interactions with a cold wall [15], by thermal radiation losses due to high soot loading [16], by evaporative cooling due to water-spray [17]. Narayanan et al. [18], have studied a Damköhler-number-based flame extinction criterion using large activation energy asymptotic (AEA) analysis and explored the extinction limits of laminar counter-flow diffusion flames as a function of flame stretch and radiant losses due to soot and gas-phase species. A parametrization of this Damköhler number criterion was performed in subsequent work for diffusion flame conditions with various levels of stretch, radiation losses, and air or fuel vitiation [19]. These studies confirm the early concept of a critical value of a Damköhler number for flame extinction; note, however, that they are limited to a global single-step representation of the combustion chemistry.

The objectives of this present work are to perform DNS of non-premixed flame extinction resulting from sustained high mixing intensities, and to study the applicability of the AEA-based critical Damköhler number flame extinction criterion to turbulent-like flames described with detailed chemistry.

Different cases are simulated in order to achieve different combustion regimes: from extinction-free flames under high Damköhler number conditions to flames with frequent extinction events under low Damköhler number conditions. Changes in Damköhler number conditions are implemented using a modified viscosity and changing pressure (MVCP) scheme: the MVCP scheme allows simulating cases with identical flow conditions and flames that are weakened or strengthened at will. The simulated flames are first analyzed using the classical AEA-based flame Damköhler number. Next, they are analyzed using a more elaborate flame Damköhler number provided by a Chemical Explosive Mode Analysis (CEMA) [20]. The comparison between DNS, AEA, and CEMA provides an evaluation of our ability to predict diffusion flame extinction under turbulent flow conditions.

2. Numerical methods

2.1. Navier–Stokes solver

The DNS solver employs an explicit 4th order Runge–Kutta (ERK) time integration scheme [21] and an 8th order central finite-differencing scheme [22] for accurate integration of the compressible form of the Navier–Stokes equations. Spatial filtering is performed using a purely-dissipative 10th order filter [22]. Boundary conditions are treated using Navier–Stokes Characteristic Boundary Conditions (NSCBCs) described in Ref. [23]. Further information and discussion on the governing equations and the boundary conditions can be found in Refs. [15,24,17,14] and references therein.

Transport properties are evaluated using a mixture averaged model, calculated from the transport libraries provided by wrappers to the CHEMKIN package [25]. The code is highly modular, incorporating advanced multi-physics such as radiation [15], soot models [16], water droplet dynamics [17], that have previously been used.

2.2. Reduced chemical model

The detailed mechanism used was first proposed by Appel et al. [26]. It is a C_2H_4-air combustion model featuring 101 species and