Available online at www.sciencedirect.com
ScienceDirect
Energy Procedia 51 (2014) 253 – 258
Energy Procedia

7th Trondheim CCS Conference, TCCS-7, June 4-6 2013, Trondheim, Norway

Numerical simulation of differential molecular diffusion effects in a hydrogen-rich turbulent jet using LEM3D

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Abstract

The LEM3D stochastic model for numerical simulation of turbulent mixing is used to simulate differential molecular diffusion effects in an isothermal jet of hydrogen and Freon 22 issued into air. The computations are compared with a published experimental study of the flow configuration. Salient features of the measured results are reproduced qualitatively, but the absence of spatial variation of the smallest eddy motion in LEM3D omits the streamwise variation of this length scale in the experimental configuration, resulting in a systematic deviation from the experimental trend. A first-principles basis for incorporating this missing physics into LEM3D is described, indicating the path forward for physically based quantitative prediction of differential diffusion effects, and turbulent combustion phenomenology more generally, using LEM3D.

Selection and peer-review under responsibility of SINTEF Energi AS
Keywords: pre-combustion capture, turbulent combustion, turbulent mixing

1. Introduction

Accurate predictions of mixing and reaction in turbulent reactive flows require high-resolution computational tools. Such simulation tools are essential in the design of combustion technology with improved efficiency and reduced emissions, and in particular in the development of new combustor configurations in connection with CO_2 capture. In the pre-combustion CO_2 capture concept, the carbon is removed from the fossil fuels prior to combustion, leaving a hydrogen-rich gas as the burnable fuel. Hydrogen is a fuel with distinct thermo-physical

Selection and peer-review under responsibility of SINTEF Energi AS
doi:10.1016/j.egypro.2014.07.029

properties compared to conventional fuels, and is characterized by a high flame speed, wide flammability limits, and a higher diffusivity than any other gas. This calls for special care in the development of hydrogen combustion technology, and issues such as flame holding, flashback, auto-ignition, and safety must be resolved in the design of new burner configurations for hydrogen gas turbine combustors.

Another critical requirement is the ability to operate in the lean premixed mode. The adiabatic flame temperature of hydrogen is much higher than that for natural gas, and the elevated flame temperature is likely to cause high emissions of NO_x, as well as increased thermal stresses on the combustor equipment. In the premixed combustion mode, in which the fuel and oxidizer is mixed prior to ignition, the flame temperature can be lowered for premixed lean mixtures of hydrogen and air. Hence, lean premixed operating conditions lead to reduced NO_x emissions compared to conventional non-premixed designs. However, the development of high efficiency, hydrogen-fueled gas turbines with low NO_x-combustion remains a great challenge, since a stable and efficient operation requires a rapid and homogeneous mixing of fuel and air. In particular, there is a need for numerical design tools that resolve the small-scale mixing and reaction of the turbulent flows since the small-scale structures are important for the overall behaviour.

Conventional numerical methods for studying turbulent reacting flows in industrial applications are based on the Reynolds Averaged Navier-Stokes (RANS) equations. However, these methods employ turbulence and mixing models that rely on the large-scale characteristics of the turbulent flow and do not resolve the smallest scales at which the molecular mixing and chemical reactions take place. Such tools, based on state-of-the-art combustion models, therefore have limited predictive capabilities in many practical engineering applications. Direct Numerical Simulation (DNS), which resolves the entire range of turbulent length scales, falls at the opposite end of the fidelity spectrum. DNS is computationally very expensive, however, and out of reach for complex geometries or flow configurations. In the present work an alternative modeling approach, in which small-scale resolution is provided at an affordable cost compared to DNS, is pursued and applied to a cold-flow mixing configuration involving hydrogen. The approach, named LEM3D [1], is a 3D construction based on the Linear Eddy Model (LEM) [2], involving three orthogonally intersecting arrays of 1D LEM domains, and coupled so as to capture the 3D characteristics of the fluid flow. LEM3D provides small-scale resolution in all three spatial directions of the turbulent flow field, and is by construction applicable as a subgrid scalar closure both for RANS and Large Eddy Simulation (LES) applications.

The present study reports the first validation of LEM3D against measurements [3, 4] of the differential molecular diffusion of hydrogen mixed with a heavier gas in a turbulent round jet. These measurements isolate the effects of the high molecular diffusivity of hydrogen from other complicating factors involved in the turbulent combustion of hydrogen. A complete description of the experimental technique for measuring differential diffusion in a turbulent jet has been given in [5].

Interesting effects that were observed experimentally were interpreted qualitatively using LEM [6]. That LEM formulation involved some specialized features needed to represent the specific flow geometry, including the introduction of cylindrical geometry on the 1D domain in a non-conservative way. Recent advances in LEM methodology [7] enable a conservative cylindrical formulation. Nevertheless, this remains a specialized formulation whose validation would not imply broad applicability of LEM to turbulent mixing configurations involving differential diffusion effects, or more generally to turbulent combustion processes.

The present study applies LEM3D to a flow configuration resembling the experimental setup. This study is a step in the development and validation of LEM3D, targeting future application to hydrogen-rich combustion and other low-emission combustion technologies.

2. Differential diffusion measurement and modeling

The relevance of differential diffusion effects in turbulent combustion was highlighted by the proposal, supported by LEM simulations and scaling analysis, that the decrease of these effects with increasing Reynolds number Re in simple configurations is expected to be slower than previously supposed [8]. This motivates efforts to represent these effects in computational models of turbulent combustion. For this purpose, the available experimental evidence of these effects, as summarized in [5], plays an essential role in the validation of turbulent combustion models.

In the present study, physical assumptions and quantitative formulations are the same as those in [6], where a mixture of 90% H_2 and 10% Freon 22 (on a molar basis) issued into air from a round jet at jet Reynolds number 20,000. (Freon 22 is $CHClF_2$.) The mixture was formulated to allow a simple inference of the differential diffusion variable z from a Rayleigh scattering signal. The quantity z is given by

$$z = \xi_F - \xi_H,$$

where ξ_F and ξ_H are the mixture fractions of Freon and H_2, respectively.

The molecular diffusivities of the configuration constituents are assumed to be $D_{H_2} = 0.77$ cm^2/sec for H_2 and $D_F = 0.12$ cm^2/sec for Freon. Owing to the qualitative rather than quantitative correspondence of the case to the experiment, the constituents were treated as trace contaminants in an ambient air flow, as was also the case in [6]. As in [3, 4, 6], the jet Reynolds number is based on the estimated viscosity of the jet mixture rather than the viscosity of air because the former is the best choice for model representation of the turbulent flow behaviour.

3. LEM3D application to the differential diffusion measurements

As explained in [1], LEM3D involves coarse cubic control volumes (CVs) intersected by a lattice-work of 1D LEM domains oriented in the respective coordinate directions in 3D space. Each LEM domain time advances with a small sub-cycling time step, reflecting LEM spatial refinement, within a time interval corresponding to the larger time step associated with domain coupling at the coarse-grained spatial scale.

LEM3D involves several free parameters that have some degree of configuration dependence. For the present application, the CV face area was set equal to the cross-sectional area of the gas flow issuing from the jet nozzle. (The numerical value of this area is immaterial due to jet similarity scaling that allows all distances to be expressed as multiples of the nozzle diameter, as in the plots shown below.) On this basis, the jet inflow was represented in the LEM3D flow domain as a flux of jet fluid through one CV face at the bottom of the flow domain. Thus, the species constituents, which are mixed at the nozzle, were issued from the same CV. The flow domain was a cuboid extending 38 CV lengths in the streamwise (nominally upward) direction and 23 CV lengths in each of the two lateral directions. The mean velocity field and the spatial distribution of turbulent viscosity, which are required inputs to LEM3D, were the same (in a normalized sense) as in the round jet application in [1]. The largest allowed LEM eddy size was twice the CV length.

The lower bound of the range of LEM eddy sizes has more effect on differential diffusion than on the large-scale-dominated quantities examined in [1]. There is no quantitative empirical guidance in this regard, but a relevant qualitative guideline is that the turbulent round jet is a constant-Reynolds-number flow (while it remains fully turbulent) and spreads linearly, so the smallest relevant mixing scale (the Batchelor scale [1]) increases linearly with downstream distance. LEM3D is presently implemented with no streamwise variation of the size of the smallest allowed LEM eddy, so the systematic variation of the Batchelor scale in the jet flow is not reflected in the current LEM3D formulation. Appropriate streamwise variation of the size of the smallest allowed LEM eddy would provide the needed variation of the Batchelor scale, but this has not yet been implemented. Consequences for comparison of computed and measured results are noted in Sec. 4.

4. Comparison of computations and measurements

Computed radial profiles of the root-mean-square (r.m.s.) fluctuation z' of the quantity z at various streamwise locations are shown in Figure 1, while the measured radial profiles of z' are shown in Figure 2. For the results shown here the simulation runs were over 50,000 time-advancement cycles, with data collection every 50 cycles starting at 10,000 cycles so that initial transient relaxation is excluded. As noted in Sec. 3, differential diffusion is sensitive to the spatial refinement of the turbulent eddy motions, so cases were run for various choices of the LEM spatial resolution, which controls the smallest eddy size in the present model implementation. The illustrated results correspond to resolution of 0.030, 0.012, and 0.003 jet diameters, respectively. The most time-consuming computation, corresponding to a fine-scale resolution of 300 LEM wafers within each CV and for each direction, took about 3 weeks of real cpu time on a single Intel Xeon 3.0 GHz processor. It is noted in Sec. 3 that one fixed value of the smallest eddy size cannot be applicable at all streamwise locations, so results are shown for which LEM3D gave reasonable agreement at the indicated streamwise locations. Note that due to the chosen coarse-grid size, the computed radial profiles are shown at downstream locations x/D = 9.7, 20.4, and 30.1, rather than at x/D = 10, 20, and 30 used for the measured profiles. Thus, for the locations x/D = 20.4 and 30.1, there is good agreement between the computed and measured results for LEM resolutions of 0.012 and 0.030, respectively. In the latter case, the results are higher than measured values upstream of x/D =30.1 (Figure 1; left), caused by insufficient LEM activity that allows for excessive differential diffusion. In the former case (Figure 1; center), the results are higher than measured values upstream of the location x/D =20.4 (due to insufficient LEM eddy activity) but lower than measured values downstream of that location, due to excessive LEM eddy activity that causes too much suppression of differential diffusion effects.

Figure 1 (right) shows that an LEM resolution of 0.003 jet diameter is not quite enough to bring the computed results down to the level of the measured profile at x/D = 10. Hence, in the relative near field of the jet, further reduction of the smallest eddy size is required to obtain good agreement between computations and measurements. However, near-field z fluctuations in the jet are influenced by deviations from the self-similar jet structure assumed in the present LEM3D implementation [1]. In this regard, the envisioned future implementation of LEM3D as a subgrid mixing model coupled to RANS or LES will be a more suitable formulation for jet (and other) applications. Nevertheless, the present results based on the assumed self-similar structure suggest that the present formulation (as well as subgrid formulations) will be substantially improved by future incorporation of local variation of the smallest eddy size in LEM3D. The observed spikes in Figure 1 (right), also present but less predominant in Figure 1 (center), seem to be a generic artifact of LEM3D resulting from the domain coupling. However, the artifact does not necessarily adversely impact the LEM3D performance, as indicated by the results reported in [1].

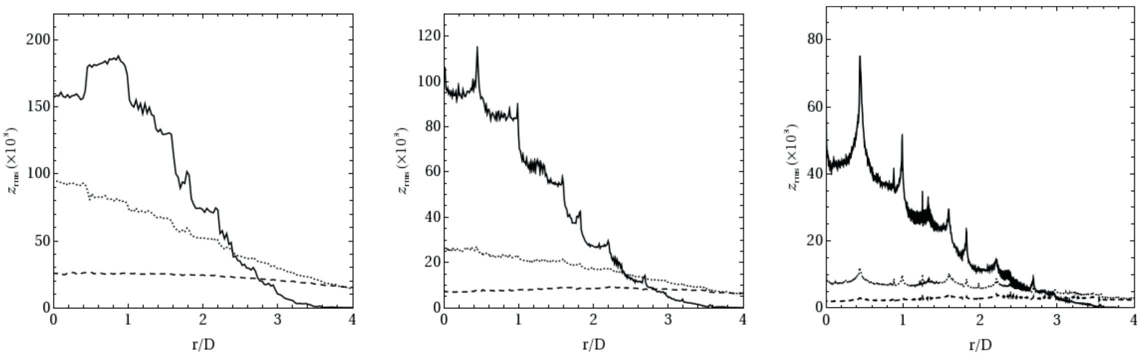

Figure 1. Computed radial profiles of r.m.s. differential diffusion z' for a jet of H_2 and Freon into air at Re_{jet}=20,000. The profiles correspond to resolution of 0.030 (left), 0.012 (center), and 0.003 (right) jet diameters, respectively. ——— , x/D = 9.7 ; ········ , x/D = 20.4; - - - - - , x/D = 30.1.

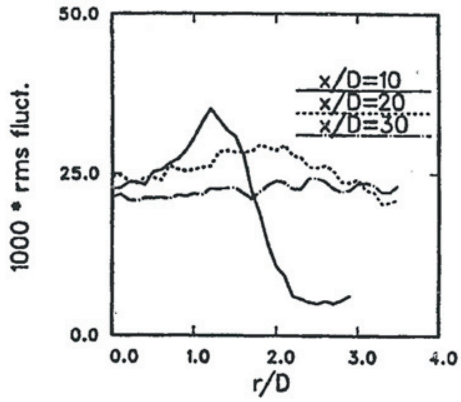

Figure 2. Measured [4] radial profiles of r.m.s. differential diffusion z' for a jet of H_2 and Freon into air at Re_{jet}=20,000.

5. Discussion

The comparisons shown in Sec. 4 suggest that incorporation of local variation of the smallest eddy size is an important extension of LEM3D that should be implemented in the future. In principle this should be straightforward because the local eddy viscosity is a needed model input, so for known kinematic viscosity, the local Reynolds number Re is obtained as the ratio of the former to the latter. The smallest eddy size should then scale relative to the turbulence integral scale as $Re^{3/4}$ based on standard inertial-range phenomenology.

Based on the results presented here and their physical implications, it thus appears that LEM3D has the capability in principle to provide a physically sound, quantitatively accurate representation of technologically relevant regimes of differential molecular diffusion. Moreover, since the requirements for accurate representation of differential molecular diffusion are much the same as for accurate representation of flame structure and evolution in turbulent combustion, the present study highlights the path forward toward high-fidelity turbulent combustion simulations using LEM3D.

Acknowledgements

This work forms part of the CAMPS project supported by the Research Council of Norway (215707). The authors also acknowledge support from the Research Council of Norway through the CRAFTS project (216035). The work has additionally been produced with support from the BIGCCS Centre, performed under the Norwegian research program Centres for Environment-friendly Energy Research (FME). The authors acknowledge the following partners for their contributions: Aker Solutions, ConocoPhillips, Gassco, Shell, Statoil, TOTAL, GDF SUEZ and the Research Council of Norway (193816/S60).

References

[1] Sannan S, Weydahl T, Kerstein AR. Stochastic simulation of scalar mixing capturing unsteadiness and small-scale structure based on mean-flow properties. Flow Turbul Combust 2013; 90:189-216.

[2] Kerstein AR. Linear-eddy modeling of turbulent transport. Part 6. Microstructure of diffusive scalar mixing fields. J Fluid Mech 1991; 231:361-394.

[3] Kerstein AR, Dibble, RW, Long, MB, Yip B, Lyons K. In: Proc. 7th Symposium on Turbulent Shear Flows, Stanford University, August 21-23; 1989, pp. 14.2.1-14.2.6.

[4] Dibble RW, Kerstein AR, Long MB, Yip B, Lyons K. In: Takeno T (Editor). Turbulence and molecular processes in combustion. Elsevier Science, Amsterdam; 1993, pp. 303-310.

[5] Dibble RW and Long MB. Investigation of differential diffusion in turbulent jet flows using planar laser Rayleigh scattering. Combust Flame 2005; 143:644-649

[6] Kerstein AR. Linear-eddy modeling of turbulent transport. Part 3. Mixing and differential molecular diffusion in round jets. J Fluid Mech 1990; 216:411-435.

[7] Lignell DO, Kerstein AR, Sun G, Monson EI, Mesh adaption for efficient multiscale implementation of one-dimensional turbulence. Theor Comput Fluid Dyn 2013; 27:273-295

[8] Kerstein AR, Cremer MA, McMurtry PA. Scaling properties of differential molecular diffusion effects in turbulence. Phys Fluids 1995; 7:1999-2007.