European Journal of Mechanics B/Fluids 52 (2015) 97–108

Contents lists available at ScienceDirect

European Journal of Mechanics B/Fluids

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

Assessment of sub-grid scalar flux modelling in premixed flames for Large Eddy Simulations: *A-priori* Direct Numerical Simulation analysis

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HIGHLIGHTS

- Sub-grid scalar flux models for premixed turbulent combustion have been assessed.
- Assessment conducted using a-priori analysis of Direct Numerical Simulations data.
- Sub-grid scalar flux shows counter-gradient transport in all cases considered here.
- The extent of counter-gradient transport increases with increasing filter width.
- Models based on the alignment of local velocity and scalar gradients perform well.

ARTICLE INFO

Article history:
Received 9 May 2014
Received in revised form
23 September 2014
Accepted 8 December 2014
Available online 16 December 2014

Keywords:
Sub-grid scalar flux
Turbulent Reynolds number
Large Eddy simulations
Direct Numerical Simulations

ABSTRACT

The performances of different models for sub-grid scalar flux for premixed turbulent combustion in the context of Large Eddy Simulations (LES) have been assessed based on a Direct Numerical Simulation (DNS) database of freely propagating turbulent premixed flames with a range of different values of Re_t where Damköhler and Karlovitz numbers are altered independently of each other to bring about the variation of Re_t, whereas the heat release parameter τ is kept unaltered. It has been found that the sub-grid scalar flux exhibits local counter-gradient transport for all cases considered here. However, the extent of counter-gradient transport decreases with decreasing values of filter width Δ and for increasing values of the ratio of the root-mean-square turbulent velocity fluctuation to the unstrained laminar burning velocity u'/S_L. The performance of several algebraic models has been assessed with respect to explicitly filtered DNS data. The standard gradient hypothesis based model does not adequately capture both the qualitative and quantitative behaviours of sub-grid scalar flux for all cases for all filter widths. The models which account for local flame normal acceleration perform better than the standard gradient hypothesis model. In general the performance of the models, which account for the alignment of local resolved velocity and scalar gradients, remains relatively better than the performance of the other existing models. Detailed physical explanations have been provided for the observed model performances.

1. Introduction

Modelling of turbulent scalar flux poses one of the major challenges in the analysis of turbulent scalar transport [1,2]. A gradient type closure is often employed for the closure of turbulent scalar flux in the case of passive scalar mixing [1,2] but several previous analyses (e.g. Refs. [2–5]) suggested that an isotropic description of eddy viscosity may not be sufficient for modelling turbulent scalar flux in both Reynolds Averaged Navier–Stokes (RANS) and Large Eddy Simulations (LES). The challenge of modelling turbulent scalar flux is further exacerbated by the possibility of counter-gradient transport (CGT) in some flow configurations. Although a number of recent analyses (e.g. Refs. [6,7]) demonstrated the presence of CGT for turbulent passive scalar mixing, the presence of CGT is well-established and its closure plays a key role in the modelling of turbulent premixed combustion [8–28]. A recent LES analysis [29] demonstrated that the exact nature of sub-grid flux closure plays a key role in determining the turbulent flame thickness and the extent of flame wrinkling (thus the overall heat release rate) predicted by the simulation. Thus, it is important to have high fidelity models for turbulent scalar flux in simulations

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http://dx.doi.org/10.1016/j.euromechflu.2014.12.003
0997-7546/

Nomenclature

Arabic

a_0	Acoustic velocity in the unburned gas
A_T	Turbulent flame area
A_L	Laminar flame area
c	Reaction progress variable
C_P	Specific heat at constant pressure
C_V	Specific heat at constant volume
D	Reaction progress variable diffusivity
D_t	Eddy diffusivity
Da	Damköhler number
F_i^{sg}	ith component of sub-grid scalar flux
$\tilde{k}_{sgs}$	Turbulent kinetic energy
Ka	Karlovitz number
l	Integral length scale
Ma	Mach number
M_i	ith component of resolved normal based on Favre filtered reaction progress variable
Pr	Prandtl number
Re_t	Turbulent Reynolds number
S_L	Unstrained laminar burning velocity
t	Time
t_c	Chemical time scale
t_f	Initial turbulent eddy turnover time
t_{sim}	Simulation time
T	Temperature
T_{ad}	Adiabatic flame temperature
T_0	Reactant temperature
u_i	ith component of non-dimensional fluid velocity
u'	Root mean square fluctuation of velocity
u'_Δ	Sub-grid fluctuation of velocity
V_{hr}	Velocity jump across the flame
x_i	ith Cartesian co-ordinate
Y_R	Reactant mass fraction
Y_{R0}	Reactant mass fraction in unburned gas
$Y_{R\infty}$	Reactant mass fraction in burned gas
Y_P	Product mass fraction
Y_{P0}	Product mass fraction in unburned gas
$Y_{P\infty}$	Product mass fraction in burned gas

Greek

α_T	Thermal diffusivity
α_E	Model parameter
α'_E	Efficiency function
β_Z	Zel'dovich number
γ_g	Ratio of specific heats ($= C_P/C_V$)
γ_c	Coefficient for burning rate probability density function
δ_{th}	Thermal flame thickness
Δ	Filter width
μ	Viscosity
μ_0	Unburned gas viscosity
η	Kolmogorov length scale
ρ	Density
ρ_0	Unburned gas density
τ	Heat release parameter

Symbols

$\bar{q}$	Filtered value of a general quantity q
$\overline{(q)}_R$	Conditional filtered value of a general quantity q in reactants
$\overline{(q)}_P$	Conditional filtered value of a general quantity q in products
$\tilde{q}$	Favre filtered value of a general quantity q

Acronyms

BML	Bray–Moss–Libby
CGT	Counter-gradient transport
DNS	Direct Numerical Simulation
GT	Gradient transport
LES	Large Eddy Simulation
Pdf	Probability density function
RANS	Reynolds averaged Navier–Stokes equations

Subscripts

L	Laminar flame condition
T	Turbulent flame condition
0	Unburned gas condition
∞	Burned gas condition

of turbulent premixed combustion. The modelling of turbulent scalar flux in premixed flames has been analysed extensively based on analytical [8], experimental [9–11] and computational [12–16] studies in the context of RANS simulations. Relatively limited effort has been directed to the modelling of turbulent scalar flux in the context of LES of turbulent premixed combustion [17–27]. The performances of different possible models of turbulent scalar flux have been assessed based on explicitly filtered experimental data by Pfadler et al. [26,27]. Recently, Lecocq et al. [25] carried out a combined *a-priori* DNS and *a-posteriori* assessment of turbulent scalar flux models. However, a detailed assessment of different LES models for turbulent scalar flux for a range of different turbulent Reynolds numbers Re_t is yet to be carried out based on *a-priori* analysis of DNS data and the present analysis aims to address this gap in the existing literature. In this analysis, the turbulent scalar flux (i.e. $F_i^{sg} = \overline{\rho u_i c} - \bar{\rho}\tilde{u}_i\tilde{c}$) of reaction progress variable c has been obtained by explicit LES filtering of DNS data of freely propagating turbulent premixed flames where ρ is the gas density, u_i is the ith component of velocity and $\tilde{q} = \overline{\rho q}/\bar{\rho}$ represents the Favre-filtered value of a general quantity q with the overbar indicating an LES filtering operation. The turbulent scalar flux extracted from DNS data has, in turn, been compared to the predictions of different models for a range of different filter widths Δ. An ideal model is expected to capture the correct qualitative and quantitative variations of F_i^{sg} with $\tilde{c}$ across the flame brush and the model prediction needs to be well correlated with F_i^{sg} obtained from DNS to capture the correct local variation. To carry out the aforementioned assessment a DNS database of statistically planar turbulent premixed flames with a range of different turbulent Reynolds numbers $\mathrm{Re}_t = \rho_0 u' l/\mu_0$ has been considered where ρ_0 and μ_0 are the unburned gas density and viscosity respectively, u' is the root-mean-square turbulent velocity fluctuation and l is the integral length scale of turbulence. The main objectives of this study are:

(a) To analyse the statistical behaviours of $[\overline{\rho u_i c} - \bar{\rho}\tilde{u}_i\tilde{c}]$ for a range of different values of Δ and Re_t.
(b) To assess the performances of different models in the directions along, and normal to, the mean direction of flame propagation using a-*priori* DNS analysis.

The rest of the paper will be organised as follows. The mathematical background and numerical implementation pertaining to the current analysis will be presented in the next two sections. Following this, results will be presented and subsequently discussed. The main findings will be summarised and the conclusions will be drawn.