International Journal of Heat and Fluid Flow 52 (2015) 28–39

Contents lists available at ScienceDirect

International Journal of Heat and Fluid Flow

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

Assessment of the performances of sub-grid scalar flux models for premixed flames with different global Lewis numbers: A Direct Numerical Simulation analysis

Yuan Gao [a,1], Nilanjan Chakraborty [a,2], Markus Klein [b,*]

[a] School of Mechanical and Systems Engineering, Newcastle University, Claremont Road, Newcastle-Upon-Tyne NE1 7RU, UK
[b] Fakultät für Luft-und Raumfahrttechnik, Universität der Bundeswehr München, Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany

ARTICLE INFO

Article history:
Received 10 May 2014
Received in revised form 26 July 2014
Accepted 23 October 2014
Available online 4 December 2014

Keywords:
Sub-grid scalar flux
Global Lewis number
Large Eddy Simulations
Direct Numerical Simulations
a-priori DNS analysis

ABSTRACT

The statistical behaviours of sub-grid flux of reaction progress variable has been assessed for premixed turbulent flames with global Lewis number *Le* (=thermal diffusivity/mass diffusivity) ranging from 0.34 to 1.2 using a Direct Numerical Simulation (DNS) database of freely propagating statistically planar flames. It is known that the sub-grid scalar flux shows counter-gradient transport when the velocity jump across the flame due to heat release overcomes the effects of turbulent velocity fluctuation. The results show that the sub-grid scalar flux components exhibit counter-gradient transport for all cases considered here. The extent of counter-gradient transport increases with increasing filter width Δ and decreasing value of *Le*. This is due to the fact that flames with $Le \ll 1$ (e.g. $Le = 0.34$) exhibit thermo-diffusive instabilities, which in turn increases the extent of counter-gradient transport. The effects of heat release and flame normal acceleration weaken with increasing *Le*. Several established algebraic models have been assessed in comparison to the sub-grid scalar flux components extracted from explicitly filtered DNS data in terms of their correlation coefficients at the vector level and their mean variation conditional on the Favre-filtered progress variable. The gradient transport closure does neither capture the quantitative nor the qualitative behaviour of the different sub-grid scalar flux components for all filter widths in all cases considered here. Models which account for local flame normal acceleration perform better, especially when the flame remains completely unresolved. In particular those models that account for the alignment of local resolved velocity and scalar gradients by using a tensor diffusivity, perform relatively better than the other alternative models irrespective of *Le*.

1. Introduction

Modelling of turbulent scalar flux is one of the major challenges in the modelling of turbulent passive scalar mixing (Launder, 1976) and the development and assessment of scalar flux models remain an active field of research in the context of Reynolds Averaged Navier-Stokes (RANS) equations (e.g. Rossi, 2010) as well as in the context of Large Eddy Simulations (LES) (Fabre and Balarac, 2011; Wang and Zhang, 2013). The modelling of turbulent scalar flux in case of passive scalar mixing is usually carried out using a gradient hypothesis, which is given by: $h_i := \overline{\rho u_i Q} - \bar{\rho}\tilde{u}_i\widetilde{Q} = -(\mu_t/Sc_t)(\partial\widetilde{Q}/\partial x_i)$ where ρ is density, u_i is the ith component of velocity, μ_t is the eddy viscosity, Sc_t is the turbulent Schmidt number, Q is the scalar in question. The quantities $\overline{Q}$ and $\widetilde{Q} = \overline{\rho Q}/\bar{\rho}$ are the Reynolds-averaged/LES filtered and Favre-averaged/Favre-filtered values of a general quantity Q with the overbar suggesting a Reynolds averaging/LES filtering operation. The gradient assumption implies that the turbulent diffusivity is isotropic and that the turbulent scalar fluxes and the mean scalar gradient are aligned. In a simple shear flow, see Fig. 1a, with $\widetilde{Q} = \widetilde{Q}(y)$ and $\tilde{u} = \tilde{u}(y)$; $\tilde{v} = \tilde{w} = 0$ this results in $h_1 = 0$, $h_2 = -(\mu_t/Sc_t)(\partial\widetilde{Q}/\partial y)$. However it is known for long time from measurements (e.g. Tavoularis and Corrsin, 1981) that in fact $|h_1| > |h_2|$. Batchelor (1949) proposed a generalisation by involving a turbulent diffusivity tensor i.e. $h_i = \overline{\rho u_i Q} - \bar{\rho}\tilde{u}_i\widetilde{Q} = -\bar{\rho}D_{ij}\,(\partial\widetilde{Q}/\partial x_j)$. This tensor D_{ij} is non diagonal and asymmetric (Tavoularis and Corrsin, 1981) and therefore allows for non-alignment of scalar flux and gradient. Another problem with the standard gradient hypothesis is that the turbulent scalar flux is entirely independent of the velocity field, whereas the production terms, for example in the RANS

* Corresponding author. Tel.: +49 (0)8960042122.
E-mail addresses: yuan.gao2@ncl.ac.uk (Y. Gao), nilanjan.chakraborty@ncl.ac.uk (N. Chakraborty), markus.klein@unibw.de (M. Klein).
[1] Tel.: +44 (0)1912087532.
[2] Tel.: +44 (0)1912083570.

http://dx.doi.org/10.1016/j.ijheatfluidflow.2014.10.022
0142-727X/

Nomenclature

Arabic

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
h_i	ith component of sub-grid scalar flux
$\tilde{k}_{sgs}$	turbulent kinetic energy
Ka	Karlovitz number
l	integral length scale
M_i	ith component of resolved normal based on Favre averaged reaction progress variable
Pr	Prandtl 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 coordinate
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	viscosity of unburned gas
η	Kolmogorov length scale
ρ	density
ρ_0	unburned gas density
τ	heat release parameter
$\dot{w}$	reaction rate of reaction progress variable
Ω	volume-integrated reaction rate of progress variable

Symbol

$\bar{q}$	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
DNS	Direct Numerical Simulation
LES	Large Eddy Simulation
Pdf	probability density function
RANS	reynolds averaged Navier-Stokes equations

Subcripts

L	laminar flame condition
T	turbulent flame condition
0	unburned gas condition
∞	burned gas condition

transport equation for h_i, depend on Reynolds stresses as well as the mean velocity gradient (Younis et al., 2005).

The closure of turbulent scalar flux is further exacerbated due to the possibility of counter-gradient transport (i.e. $[\overline{\rho u_i Q} - \bar{\rho}\tilde{u}_i\tilde{Q}] \times \partial\tilde{Q}/\partial x_i > 0$ for the ith direction) which can occur in non-reacting flows (e.g. Schumann, 1987; Hattori and Nagano, 2012) and this situation is prevalent particularly in turbulent premixed flames. A number of previous analyses demonstrated that counter-gradient transport can be observed in the context of Reynolds Averaged Navier Stokes (RANS) simulations of turbulent premixed flames based on analytical (e.g. Bray et al.,1985), experimental (e.g. Moss, 1980; Shephard et al., 1982; Frank et al.,1999; Kalt et al., 2002) and computational (e.g. Rutland and Cant, 1994; Veynante et al. 1997; Swaminathan et al., 2001; Nishiki et al., 2006; Chakraborty and Cant, 2009a–c) analyses. To date, most analyses on turbulent scalar flux modelling have been carried out for RANS simulations and relatively limited effort has been directed to the sub-grid scalar flux modelling for LES (Clark et al., 1979; Boger, 2000; Boger et al., 1998; Weller et al., 1998; Rymer, 2001; Tullis and Cant, 2003; Richard et al., 2007; Pfadler et al., 2009; Huai et al., 2006; Lecocq et al., 2010). It has recently been demonstrated by Chakraborty and Cant, 2009a–c that the global Lewis number Le (i.e. ratio of thermal diffusivity to mass diffusivity) significantly affects the statistical behaviour of turbulent scalar flux in the context of RANS simulations. A detailed assessment of different LES models for sub-grid scalar flux for a range of different global Lewis numbers Le based on *a-priori* analysis of DNS data is yet to be carried out and the present analysis aims to address this gap in the existing literature. In this analysis, the sub-grid scalar flux (i.e. $\overline{\rho u_i c} - \bar{\rho}\tilde{u}_i\tilde{c}$) of reaction progress variable c (i.e. a suitably defined normalised scalar which monotonically increases from 0 in unburned gas to 1 in fully burned products) has been obtained by explicit LES filtering of DNS data of freely propagating statistically planar turbulent premixed flames with Le ranging from 0.34 to 1.2. The sub-grid scalar flux extracted from DNS data has, in turn, been compared to the predictions of different models for a

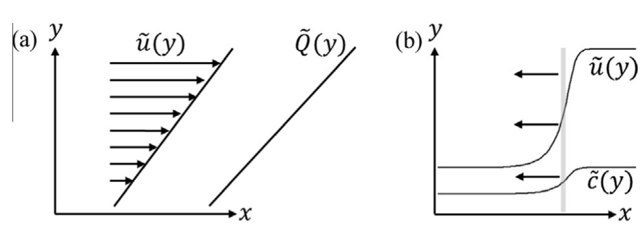

Fig. 1. (a) Sketch of a simple shear flow with transport of general passive scalar. (b) Sketch of a planar flame with indicated direction of mean flame propagation and profiles of the mean values of velocity and reaction progress variable.