

## AN ALGEBRAIC MODEL CLOSURE OF THE COUNTER GRADIENT DIFFUSION FOR THE TURBULENT FLUXES IN THEIR COMBUSTION SIMULATION

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### ABSTRACT

In modeling turbulent premixed combustion with the assumption of single step chemistry, the mass fractions of the reactive species are expressed in term of a single reduced mass fraction: the reaction progress variable  $c$ . The progress variable ranges from zero in fresh gases to unity in burnt gases.

The term of turbulent flux  $\overline{\rho u_i'' c''}$  in the transport equation for the mean reaction progress variable  $\tilde{c}$  was usually closed by simple classical gradient eddy –viscosity model :

$$\overline{\rho u_i'' c''} = -\frac{\mu_t}{\sigma} \frac{\partial \tilde{c}}{\partial x_i} . \quad (1)$$

Theoretical and experimental works (Clavin and Williams 1979 ), (Libby and Bray 1981), (Kalt et al 2002), have shown that this assumption may be wrong in some premixed turbulent flames and counter gradient turbulent transport may be observed.

Veynante et al. (1997) have analyzed the occurrence of counter gradient turbulent transport using direct numerical simulation (DNS) and the results demonstrate the power of DNS to help in the modeling of turbulent combustion.

The counter gradient diffusion phenomenon can be explained by the work of Libby and Bray (1981) which was focused on the turbulent transport term  $\overline{\rho u_i'' c''}$  . The flame was analyzed as flamelet separating fresh reactants ( $c=0$ ) and burnt products ( $c=1$ ) and the turbulent flux is expressed as:

$$\overline{\rho u_i'' c''} = \overline{\rho} \tilde{c} (1 - \tilde{c}) (\overline{u_i^b} - \overline{u_i^u}) \quad (2)$$

The expressions (1) and (2) may describe opposite fluxes: consider a left travelling one dimensional turbulent flame, because of thermal expansion the conditional velocity in the burnt gases,  $\overline{u_i^b}$  , is expected to be larger than the conditional velocity in the fresh gases,  $\overline{u_i^u}$  .

According to equation (2) the turbulent flux,  $u_i'' c''$  , is expected to be positive. On the other hand, as the mean progress variable gradient is also positive, equation (1) leads to a negative value of  $u_i'' c''$  .

This situation is known as counter gradient turbulent transport or counter gradient turbulent diffusion and it is a key point of the BML (Bray-Moss-Libby) analysis.

This paper will present an algebraic model closure of counter gradient diffusion for the turbulent fluxes. The combustion will occur in a variable equivalence ratio and as partially premixed combustion is highlighted as one of the most relevant and important modeling challenges in the field of turbulent premixed combustion, we will use the LW-P model of combustion for this situation. The resulting model is combined with the second order model of turbulence  $R_{ij} - \varepsilon$  in order to well predict the main structure of the flame zone in the case of stagnating turbulent flames. A numerical simulation is carried out in order to validate the model. The computational results are validated against the experimental measurements done by Cheng and Shepherd (1991).

The comparison of the results with the measurements were showing remarkable consistency and indicates that the model is a valid approach for predicting partially turbulent premixed flames stabilized in a stagnation flow.