

Abstract

A review is presented of some modelling techniques to predict mean rates of chemical reaction for use in theoretical models of turbulent combustion. Emphasis is placed on laminar flamelet models for combustion of premixed reactants. Brief descriptions of some other models are also included.

1. Introduction

In order to predict the progress of chemical reactions in a reacting flow it is necessary to solve transport equations of the form ⁽¹⁾

$$\frac{\partial}{\partial t}(\rho Y_i) + \frac{\partial}{\partial x_k}(\rho u_k Y_i) = \frac{\partial}{\partial x_k} \left(\mathcal{D} \frac{\partial Y_i}{\partial x_k} \right) + \dot{w}_i \quad (1.1)$$

where Y_i is the mass fraction of a reacting species i , whose mass rate of formation per unit volume is \dot{w}_i , \mathcal{D} is a molecular diffusion coefficient, ρ is density and u_k is the component of velocity in direction x_k . However, for practical turbulent combustion problems, it is not feasible to solve the set of equations of this form, together with the Navier-Stokes equations for turbulent flow, with the necessary space and time resolution to resolve the smallest scales of flow and chemical change. Direct numerical simulations (DNS) of turbulent reacting flows⁽²⁾ are a valuable research tool but can be attempted only in circumstances of extreme simplification. Calculations involving discrete vortex dynamics and calculations with large eddy simulations (LES) are also restricted to being research tools.

For realistic geometries and for practical engineering problems it is necessary to resort to averaging. Equation (1.1) and the Navier Stokes equations are averaged, prior to their solution, and the resulting loss of information is compensated by the introduction of closure assumptions which lead to empirical models.

Here we are concerned with the average value of the chemical source term \dot{w}_i in Equation (1.1). See Refs.^(1,3,4) for reviews. For statistically stationary flows the

average, denoted by an overbar, may be defined as

$$\bar{w}_i(\underline{x}) = \frac{1}{\Delta t} \int_t^{t+\Delta t} w_i(\underline{x}, t) dt \quad (1.2)$$

where Δt is a suitably long interval of time. If the process is not statistically stationary (examples include combustion in a reciprocating engine and the growth in time of a fire or explosion) ensemble averaging must be used. Then

$$\bar{w}_i(\underline{x}, t) = \frac{1}{N} \sum_{n=1}^N w_{in}(\underline{x}, t) \quad (1.3)$$

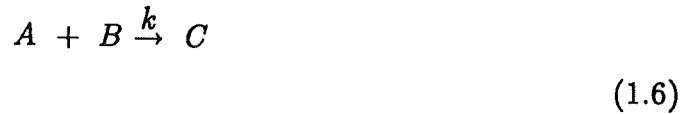
In this review we consider statistically stationary flows for which time averaging is appropriate. The instantaneous source term w_i is a highly nonlinear function of composition and state, of the form

$$w_i = w_i(\rho, T, Y_j \dots) \quad (1.4)$$

We shall assume this function to be known. Because of nonlinearity we cannot in general replace \bar{w}_i by Equation (1.4) evaluated at the mean values of its arguments, i.e.

$$\bar{w}_i \neq w_i(\bar{\rho}, \bar{T}, \bar{Y}_j \dots) \quad (1.5)$$

If a chemical reaction of the form



takes place in a turbulent flow of liquid, at constant temperature, and the reaction rate coefficient k can be assumed constant, then it may sometimes be useful to expand the reactant concentrations in the form $Y_A(\underline{x}, t) = \bar{Y}_A(\underline{x}) + Y'_A(\underline{x}, t)$ and $Y_B(\underline{x}, t) = \bar{Y}_B(\underline{x}) + Y'_B(\underline{x}, t)$. Then the mean chemical source term for C is

$$\bar{w}_c = k\rho^2 \bar{Y}_A \bar{Y}_B \left(1 + \frac{\overline{Y'_A Y'_B}}{\bar{Y}_A \bar{Y}_B} \right) \quad (1.7)$$