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Parametric study of the Incompletely Stirred Reactor modeling

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ABSTRACT

The Incompletely Stirred Reactor (ISR) is a generalization of the widely-used Perfectly Stirred Reactor (PSR) model and allows for incomplete mixing within the reactor. Its formulation is based on the Conditional Moment Closure (CMC) method. This model is applicable to nonpremixed combustion with strong recirculation such as in a gas turbine combustor primary zone. The model uses the simplifying assumptions that the conditionally-averaged reactive-scalar concentrations are independent of position in the reactor: this results in ordinary differential equations in mixture fraction space. The simplicity of the model permits the use of very complex chemical mechanisms. The effects of the detailed chemistry can be found while still including the effects of micromixing. A parametric study is performed here on an ISR for combustion of methane at overall stoichiometric conditions to investigate the sensitivity of the model to different parameters. The focus here is on emissions of nitric oxide and carbon monoxide. It is shown that the most important parameters in the ISR model are reactor residence time, the chemical mechanism and the core-averaged Probability Density Function (PDF). Using several different shapes for the core-averaged PDF, it is shown that use of a bimodal PDF with a low minimum at stoichiometric mixture fraction and a large variance leads to lower nitric oxide formation. The 'rich-plus-lean' mixing or staged combustion strategy for combustion is thus supported.

1. Introduction

The Incompletely Stirred Reactor (also known as the Imperfectly Stirred Reactor), (ISR), originally investigated by Smith [1] and later studied by Mobini [2], is a generalized version of the widely-used Perfectly Stirred Reactor (PSR) model [3]. In this model, unlike the PSR, the inlet flow is not completely premixed, and spatial inhomogenity in mixing and its turbulent fluctuation with time are taken into account. The ISR can also be viewed as a zero-dimensional approximation of the Conditional Moment Closure (CMC) method for turbulent reacting flows [4–6]. It is defined as a reaction zone in which conditional averages of reactive scalars, conditioned on mixture fraction, are assumed to be independent of position or time. This assumption transforms the complicated partial differential equations of CMC into simple ordinary differential equations in mixture fraction space, and hence reduces computational cost. On the other hand it limits application of ISR to strongly recirculating flows, like the gas turbine primary zone. Also the reactor condition should be far from ignition or extinction or for which the flow is highly time dependent. This model has been applied to experimental combustors by Mobini et al. [7], Gough et al. [8] and Mobini and Bilger [9] and the comparisons have shown acceptable levels of accuracy. Klimenko and Bilger [6] have reviewed CMC methods, including their application to the ISR.

The Conditional Moment Closure (CMC) method was proposed by Klimenko [4] and Bilger [5]. The CMC method has been successfully applied to experimental reacting flows. Smith et al. [10] applied CMC and PDF methods to predict NO formation in a turbulent nonpremixed hydrogen jet flame and compared the results with the data from laser measurements. Recent successful applications of the CMC method include prediction of NO formation in turbulent jet flames of methane in air [11], prediction of extinction and reignition in jet flames [12], prediction of lifted jet flames [13] and prediction of flames in a hot co-flow [14].

Turbulence-chemistry interaction is an important issue in turbulent diffusion flames. Use of detailed chemical mechanisms is as important as accurate prediction of turbulent mixing. Application of CMC to ISR, permits use of very complex chemical mechanisms which can be solved in a fraction of computational time used by other methods [1]. This great advantage compensates for limitations and inaccuracies made by the approximations. Here a skeletal methane mechanism [16], the full Miller–Bowman methane mechanism [17] and the GRI mechanism for natural gas [18] have been used. The last two mechanisms include detailed chemistry with more than 250 reaction steps.

In an ISR, turbulent mixing, which is represented by scalar dissipation rate, is highly dependent on the core-volume-averaged

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Nomenclature

A	inlet or outlet area	V	core volume
D_ξ	diffusivity of mixture fraction	Y_i	mass fraction of species i
$\dot{m}$	mass flow rate	δ	Dirac delta function
N	scalar dissipation rate	$\vec{\nabla}$	gradient
N_η^{**}	core-averaged conditional mean scalar dissipation	$\vec{\nabla}.$	divergence
P_η	mixture fraction PDF	η	mixture fraction
P_η^*	mass-flow-rate-weighted mixture fraction PDF	η_s	stoichiometric mixture fraction
P_η^{**}	core-averaged mixture fraction PDF	ξ	random variable mixture fraction
Q_i	conditional mean mass fraction of species i	$\tilde{\xi}$	mean mixture fraction
$Q_{i,in}$	conditional mean mass fraction of i at the inlet	ρ	mass density
$Q_{i,out}$	conditional mean mass fraction of i at the outlet	$\bar{\rho}^{**}$	core-averaged mass density
t	time	τ_r	residence time
T	temperature	ω_i	production rate of species i
$\vec{u}$	velocity vector	$\langle X\|Y=y\rangle$	mean of X on the condition that $Y = y$

PDF. Therefore, prediction of the PDF shape is very important. PDF shapes for some experimental burners have been derived in previous investigations [7–9] using CFD, and species concentrations were predicted by ISR. These results are used as a guideline for this work.

After derivation of the ISR equations, a parametric study has been performed using assumed PDF shapes in order to evaluate the effects of different parameters involved in the ISR equations. Then, to obtain more realistic PDF shapes, the effects of the core-averaged PDF shape on the combustion products have been studied and are reported in the next section. The conclusions are summarized in the last section.

2. Derivation of the ISR equations

The derivation of the ISR equations is available in [6]. The derivation is summarized here for completeness and also because more general treatment of the inflow and outflow streams is needed. The ISR equations are derived from the CMC equations [4,6],

$$\frac{\partial}{\partial t}(\langle\rho Y_i|\eta\rangle P_\eta) + \vec{\nabla}.(\langle\rho\vec{u}Y_i|\eta\rangle P_\eta) = P_\eta\langle\rho\omega_i|\eta\rangle + \frac{\partial}{\partial\eta}\left[\langle\rho N|\eta\rangle P_\eta\frac{\partial Q_i}{\partial\eta} - Q_i\frac{\partial}{\partial\eta}\langle\rho N|\eta\rangle P_\eta\right] \quad (1)$$

in which, $$Q_i = \langle Y_i|\xi=\eta\rangle \equiv \langle Y_i|\eta\rangle \quad (2)$$

and $$N = D_\xi\vec{\nabla}\xi\cdot\vec{\nabla}\xi \quad (3)$$

Considering statistically stationary flow, integration of this equation over the core volume V and using the flux divergence theorem leads to,

$$\int_{A_{out}}\langle\rho\vec{u}|\eta\rangle P_\eta Q_i\cdot d\vec{A} - \int_{A_{in}}\langle\rho\vec{u}|\eta\rangle P_\eta Q_i\cdot d\vec{A} = \int_V\left[P_\eta\langle\rho\omega_i|\eta\rangle + \langle\rho N|\eta\rangle P_\eta\frac{\partial^2 Q_i}{\partial\eta^2} - Q_i\frac{\partial^2}{\partial\eta^2}(\langle\rho N|\eta\rangle P_\eta)\right]dV \quad (4)$$

In this equation, terms involving fluctuations about the conditional mean in the inlet and outlet flows are ignored. Since, according to definition of the ISR, all conditional reactive scalar statistics are uniform inside the core, they can be moved outside of the integrals on the right hand side (RHS) of Eq. (4). Moving them outside, making similar assumptions for the inlet and outlet streams, and using the following definitions, for the mass-flow-rate-weighted mixture fraction PDF in inlet and outlet streams:

$$P_\eta^* \equiv \frac{1}{\dot{m}}\int_A(P_\eta\langle\rho\vec{u}|\eta\rangle)\cdot d\vec{A} \quad (5)$$

for the core-averaged mixture fraction PDF:

$$P_\eta^{**} \equiv \frac{1}{V}\int_V P_\eta dV \quad (6)$$

and for the core-averaged conditional mean scalar dissipation rate:

$$N_\eta^{**} \equiv \frac{1}{VP_\eta^{**}\langle\rho|\rho\eta\rangle}\int_V(\langle\rho N|\eta\rangle P_\eta)dV \quad (7)$$

Eq. (4) can be written as:

$$\dot{m}\left[Q_{i,out}(P_\eta^*)_{out} - Q_{i,in}(P_\eta^*)_{in}\right] = V\left[P_\eta^{**}\left(\langle\rho\omega_i|\eta\rangle + \langle\rho|\eta\rangle N_\eta^{**}\frac{d^2Q_i}{d\eta^2}\right) - Q_i\frac{d^2}{d\eta^2}(N_\eta^{**}P_\eta^{**}\langle\rho|\eta\rangle)\right] \quad (8)$$

$Q_{i,in}$ is specifically retained, since the condition at the inlet is different from that in the core. As a result it is possible to have a range of conditions from completely unmixed to partly premixed flow at the inlet. In what follows, $Q_{i,out}$ is taken as being equal to Q_i in keeping with stirred reactor concepts. This assumption is also necessary since it is unreasonable to make any other assumption for Q_i that would be needed to allow solution of the ISR equations. It is noted in passing that it is not necessary to assume that the outlet stream PDF $[(P_\eta^*)_{out}]$ is identical to the core PDF P_η^{**}. This will be discussed later.

In Eq. (8) a large part is played by the core-averaged scalar dissipation N_η^{**} and this needs to be realistically modeled. An essential component of the ISR model is that N_η^{**} may be determined from the mixing assumed for the inlet flow, core volume and the outlet as is defined by the PDFs assumed for these. The transport equation for the mixture fraction PDF is [6]:

$$\frac{\partial}{\partial t}(\langle\rho|\eta\rangle P_\eta) + \vec{\nabla}.[\langle\rho\vec{u}|\eta\rangle P_\eta] - \nabla^2[\langle\rho D_\xi|\eta\rangle P_\eta] + \vec{\nabla}.\left[\langle\vec{\nabla}(\rho D_\xi)\eta\rangle P_\eta\right] = -\frac{\partial^2}{\partial\eta^2}[\langle\rho N|\eta\rangle P_\eta] \quad (9)$$

Integrating this equation over the core volume, considering statistically stationary flow with negligible contributions of molecular diffusion to the fluxes, and using the flux divergence theorem we get,

$$\int_{A_{out}}\langle\rho\vec{u}|\eta\rangle P_\eta\cdot d\vec{A} - \int_{A_{in}}\langle\rho\vec{u}|\eta\rangle P_\eta\cdot d\vec{A} = -\frac{d^2}{d\eta^2}\int_V(\langle\rho N|\eta\rangle P_\eta)dV \quad (10)$$