MODELING OF FLUCTUATING MASS FLUX IN VARIABLE DENSITY FLOWS

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Abstract

In practical combustion systems, the assumption of chemical equilibrium is not always appropriate. This is especially true in regard to predicting various critical combustion processes including ignition, flame stability, smoke and gaseous emissions. In order to estimate combustor performance accurately, it is important to calculate combustor internal profiles of temperature, species and velocities to reasonable accuracy. This, in turn, requires realistic assumptions concerning the turbulent transports of heat, mass and momentum and their interaction with chemical reactions.

Conventional combustion models assume the scalar transport process can be described adequately by an assumed two/three parameter probability density function (pdf) and that the transport of heat and mass is essentially identical. These models give reasonably well correlated results for simple flows. However, their applications to complex flows involving strong recirculation and swirl do not appear promising. Since such flows are of common occurrence in any combustion systems, straight forward extension of conventional combustion models to combustor flow calculations is not adequate.

The present approach is formulated to investigate some of the problems that are common to both reactive and non-reactive variable density flows. Such problems are mass transport in a variable density flow, validity of

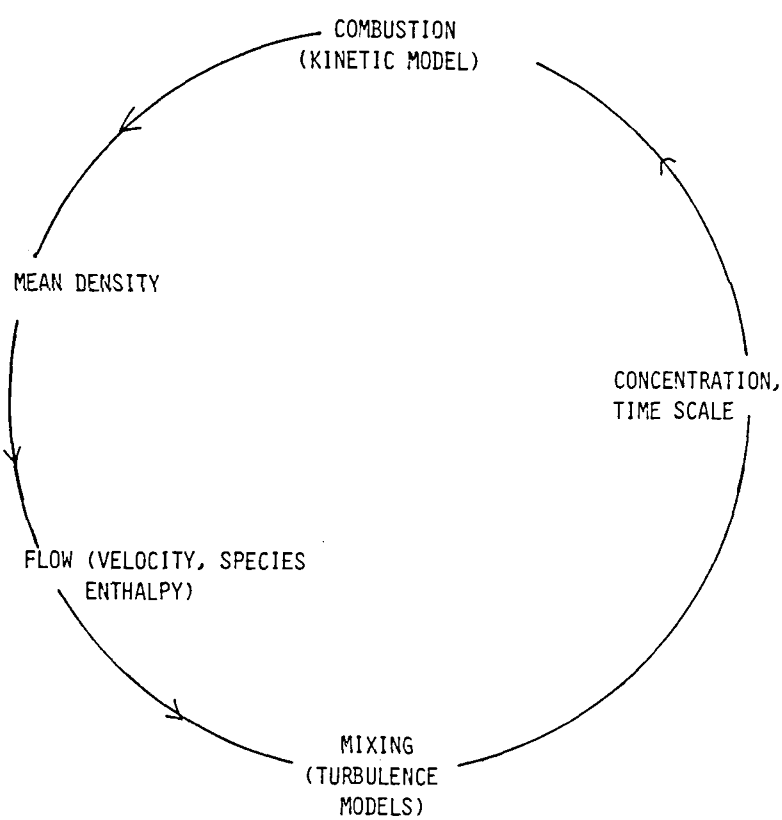
constant density turbulence models, relative merits of Reynolds versus Favre average and calculated versus assumed pdf for the scalar. The approach solves for both Reynolds and Favre averaged quantities and calculates the scalar pdf. Turbulent models used to close the governing equations are formulated to account for complex mixing and variable density effects. In addition, turbulent mass diffusivities are not assumed to be in constant proportion to turbulent momentum diffusivities.

The governing equations are solved by a combination of finite-difference technique and Monte-Carlo simulation. Some preliminary results on simple variable density shear flows are presented. The differences between these results and those obtained using conventional models are discussed.

MOTIVATION

- UNDERSTANDING OF TURBULENT REACTIVE FLOWS
- MODELING OF TURBULENT REACTIVE FLOWS
- COMBUSTOR FLOW MODELING
- DEVELOPMENT OF SUITABLE COMBUSTOR DESIGN GUIDES

TURBULENT REACTIVE FLOWS



MAIN PROBLEM IN COMBUSTION MODELING

NON-REACTIVE FLOW MODELING

- CONTINUITY
- MOMENTUM (TURBULENT MOMENTUM FLUXES, $-\overline{\rho u_i' u_j'}$, ETC.)
- ENTHALPY (TURBULENT HEAT FLUXES, $\overline{h' u_i'}$, ETC.)
- SCALAR (TURBULENT SCALAR FLUXES, $\overline{\phi' u_i'}$, ETC.)
- FLUCTUATING MASS FLUXES ($\overline{\rho' u_i'}$, ETC.)
- QUESTION OF REYNOLDS VS. FAVRE AVERAGE
- VALIDITY OF CONSTANT DENSITY MODEL FOR VARIABLE DENSITY FLOWS.

REACTIVE FLOW MODELING

- EVALUATION OF MEAN FORMATION RATES

  $$- \overline{\dot{R}} (\Phi, h, p, ---) \overset{?}{=} \dot{R} (\bar{\Phi}, \bar{h}, \bar{p}, ---)$$

  - FAST/FINITE CHEMISTRY

- VALIDITY OF CONSTANT DENSITY TURBULENCE MODEL FOR REACTIVE FLOWS

ASSUMPTIONS

- FAST CHEMISTRY

  (IF IT MIXES, IT REACTS)

- ONE STEP FORWARD REACTION

  (FUEL + OXIDANT → PRODUCTS)

- TURBULENT TRANSPORT OF DIFFERENT SPECIES IS THE SAME

  (TURBULENT SCHMIDT NUMBER FOR ALL SPECIES IS IDENTICAL)

- EDDY DIFFUSIVITIES FOR MASS AND HEAT ARE IDENTICAL

  (LEWIS NUMBER EQUALS UNITY)

CONSERVED SCALAR, f

$$f = \text{MIXTURE FRACTION}$$

$$= \frac{\text{MASS OF SPECIES i}}{\text{MIXTURE MASS}}$$

RELATED TO OTHER CONSERVED SCALAR, SUCH AS ENTHALPY, h, BY

$$h = (h_{fu} - h_{ox})f + h_{ox}$$

EQUATIONS SOLVED IN CONVENTIONAL REACTIVE FLOW MODELING

- MEAN CONTINUITY
- MEAN MOMENTUM (CLOSURE VIA TURBULENCE MODELING)
- MEAN CONSERVED SCALAR (CLOSURE VIA TURBULENCE MODELING AND SCHMIDT NO.)
- MEAN VARIANCE OF CONSERVED SCALAR ($\overline{f'^2}$, WHERE $f' = f-\overline{f}$)

CONVENTIONAL APPROACH

- SOLVE EQUATIONS USING FINITE DIFFERENCE SCHEME
- ASSUME A TWO-PARAMETER PDF FOR f TO ACCOUNT FOR SCALAR FLUCTUATIONS
- DETERMINE THE PARAMETERS BY REQUIRING FIRST AND SECOND MOMENTS TO AGREE WITH $\overline{f}$ AND $\overline{f'^2}$

PRESENT MEASUREMENT AND PREDICTION CAPABILITIES FOR TURBULENT REACTIVE FLOWS

	Physical Quantities	Measurement Capabilities: Probe Data	Measurement Capabilities: Optical Data	Measurement Capabilities: Difficult ?	Prediction Capabilities: Assumed pdf	Prediction Capabilities: pdf Transport	Prediction Capabilities: Difficult ?	Remarks
Flow Field	$\overline{\rho u^2}$	X			X			
	$\overline{u_i}$	X	X		X			Hot-wire/LDA technique
	$\overline{u_i'u_j'}$	X	X	X $\overline{V},\overline{W}$ $\overline{U}$				Hot-wire/LDA technique; Need to improve model
	$\overline{\rho' u_i'}$				X		X	"
	$\overline{h' u_i'}$	X			X		X	"
Combustion Field	pdf of	X	X	X (Major Species)	X	X		Raman scattering tech. need to improve model
	$\overline{\phi_\alpha' u_i}$		X	X (Major Species)	X (Model)	X (Model)	X	
	$\bar{\rho}$		X (Rayleigh)	X	X	X		Deduced from meas.; Rayleigh scattering
Pollutants	$\overline{O_2' N_2'}$		X (N_2)	X		X		Raman Scattering, O_2 difficult
	$\phi_{O_2}' T'$, Etc		X (N_2)	X		X		"
	$\overline{\phi_{O_2}' \phi_{N_2}'}$ $\overline{T'}$			X		X		

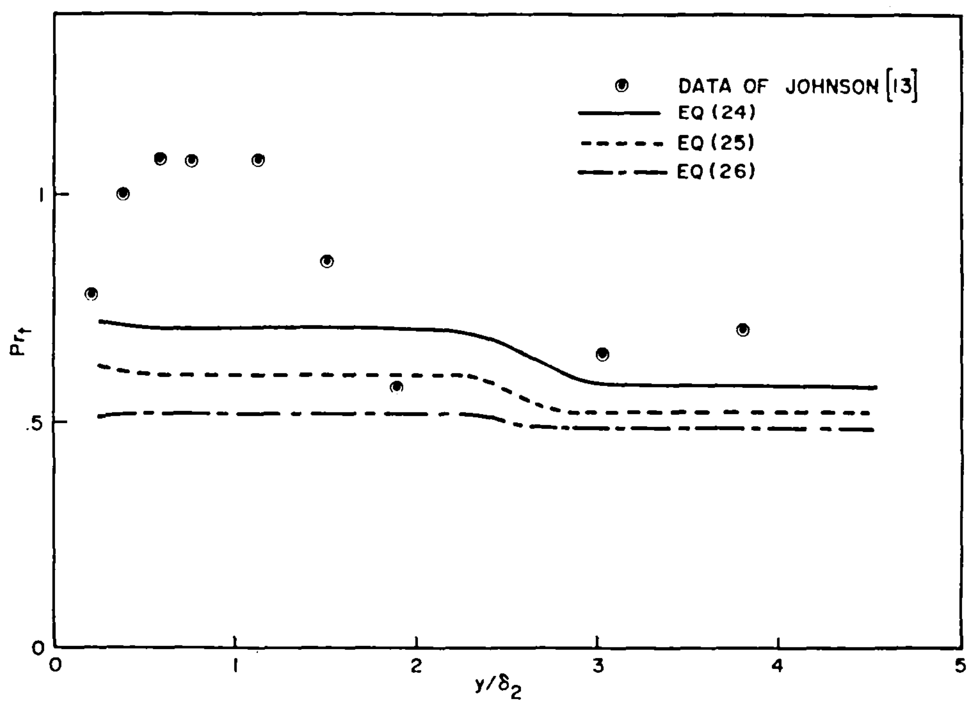
CONVENTIONAL APPROACH TO

COMBUSTION MODELING

- REDUCE PROBLEM TO EQUIVALENT SCALAR MIXING PROBLEM

LIMITATIONS OF CONVENTIONAL APPROACH

- INFINITELY FAST CHEMISTRY
- ONE/TWO STEP REACTIONS ONLY
- SCALAR FLUCTUATIONS DETERMINED BY ASSUMED PDF
- ALL SPECIES DIFFUSE AT SAME RATE
- HEAT/MASS DIFFUSE AT SAME RATE



PRESENT APPROACH ADDRESSES THE FOLLOWING PROBLEMS

- PDF OF SCALAR
- MASS DIFFUSION IN TURBULENT FLOWS
- REYNOLDS OR FAVRE AVERAGE
- CALCULATION OF FLUCTUATING MASS FLUXES

NOMENCLATURE

U_i , Φ, etc.	–	FAVRE AVERAGE
$\bar{U}_i$, $\bar{\Phi}$, etc.	–	REYNOLDS AVERAGE
u_i , ϕ, etc.	–	FLUCTUATING PART OF FAVRE DECOMPOSITION
u_i' , ϕ', ρ' , etc.	–	FLUCTUATING PART OF REYNOLDS DECOMPOSITION
$F(\tilde{\phi}_\alpha)$	–	PDF.OF $\tilde{\phi}$
$\langle\ \ \rangle$	–	TIME AVERAGE
$\sim$	–	INSTANTANEOUS QUANTITIES

GOVERNING EQUATIONS

- **CONTINUITY**

$$\frac{\partial}{\partial x_i}\left(\bar{\rho}\, U_i\right) = 0$$

- **MOMENTUM**

$$\frac{\partial}{\partial x_i}\left[\bar{\rho}\, U_i\, U_j + \bar{\rho}\,\langle u_i\, u_j\rangle\right] = -\frac{\partial P}{\partial x_i}$$

- **PDF OF $F(\tilde{\phi}_\alpha)$**

$$U_i \frac{\partial F(\tilde{\phi}_\alpha)}{\partial x_i} = \frac{1}{\bar{\rho}} \frac{\partial}{\partial x_i}\left[\Gamma \frac{\partial F(\tilde{\phi}_\alpha)}{\partial x_i}\right] - \frac{\partial}{\partial \phi_\alpha}\left[F(\tilde{\phi}_\alpha)\, S(\tilde{\phi}_\alpha)\right] + E\,(\tilde{\phi}_\alpha\,,\, x_i)$$

TURBULENT CLOSURE

TWO-EQUATION PLUS NON-EQUILIBRIUM ALGEBRAIC STRESS MODEL

$$\bar{\rho}\, U_i \frac{\partial k}{\partial x_i} = \frac{\partial}{\partial x_i}\left[C_k \frac{k}{\varepsilon}\, \bar{\rho}\, \langle u_i\, u_j\rangle \frac{\partial k}{\partial x_j}\right] - \bar{\rho}\, \langle u_i\, u_j\rangle \frac{\partial U_i}{\partial x_j}$$

$$- \bar{\rho}\varepsilon + \frac{\langle \rho' u_i\rangle}{\bar{\rho}} \frac{\partial P}{\partial x_i}$$

$$\bar{\rho}\, U_i \frac{\partial \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_i}\left[C_\varepsilon \frac{k}{\varepsilon}\, \bar{\rho}\, \langle u_i\, u_j\rangle \frac{\partial \varepsilon}{\partial x_j}\right] -$$

$$C_{\varepsilon 1} \frac{\varepsilon}{k}\, \bar{\rho}\, \langle u_i\, u_j\rangle \frac{\partial U_i}{\partial x_j} - C_{\varepsilon 2}\, \bar{\rho}\, \frac{\varepsilon^2}{k}$$

$$+ \frac{\varepsilon}{k} \frac{\langle \rho' u_i\rangle}{\bar{\rho}} \frac{\partial P}{\partial x_i} + \bar{\rho}\varepsilon \frac{\partial Ui}{\partial x_i}$$

$$0 \simeq - \left[\langle u_i\, u_k\rangle \frac{\partial U_j}{\partial x_k} + \langle u_j\, u_k\rangle \frac{\partial U_i}{\partial x_k}\right]$$

$$- \frac{2}{3}\, \delta_{ij} \left[- \langle u_i\, u_m\rangle \frac{\partial U_i}{\partial x_m}\right] + \left\langle \frac{p}{\bar{\rho}} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \right\rangle$$

MODEL FOR $\overline{\rho}$ AND $\langle \overline{\rho' u_i'} \rangle$

CONSIDER MIXING OF TWO FLUIDS WITH DIFFERENT DENSITIES.

$$\frac{1}{\overline{\rho}} = \alpha_1 + \alpha_2 \Phi$$

$$\overline{U}_i = U_i + \alpha_2 \overline{\rho} \langle u_i \phi \rangle$$

$$\langle \rho' u_i' \rangle = - \alpha_2 \overline{\rho} \langle u_i \phi \rangle$$

$$\alpha_1 = \frac{1}{\overline{\rho}_2}$$

$$\alpha_2 = \frac{1}{\overline{\rho}_1} - \frac{1}{\overline{\rho}_2}$$

Φ FROM PDF $F(\tilde{\phi}_\alpha)$ AND $\langle u_i \phi \rangle$ FROM TURBULENCE MODEL

MODEL FOR $\langle u_i \phi \rangle$

NON-EQUILIBRIUM ALGEBRAIC FLUX MODEL

$$- \langle u_i \, u_j \rangle \frac{\partial \Phi}{\partial x_j} - \langle u_j \phi \rangle \frac{\partial U_i}{\partial x_j} + \langle \frac{p}{\overline{\rho}} \frac{\partial \phi}{\partial x_i} \rangle \simeq 0$$

SOLUTION PROCEDURE

- FINITE DIFFERENCE SOLUTION OF ALL GOVERNING EQUATIONS

- OPERATOR-SPLITTING TECHNIQUE APPLIED TO PDF EQUATION

ASSUME $F(\tilde{\phi}_\alpha) = F^*(\tilde{\phi}_\alpha) + F'(\tilde{\phi}_\alpha)$

F^* AND F' GIVEN BY SOLVING

$$U_i \frac{\partial F^*}{\partial x_i} = \frac{1}{\bar{\rho}} \frac{\partial}{\partial x_i} \left[\Gamma \frac{\partial F^*}{\partial x_i} \right]$$

$$\frac{dF'}{dt} = U_i \frac{\partial F'}{\partial x_i} = - \frac{\partial}{\partial \phi_\alpha} \left[F^* S \right] + E(\tilde{\phi}_\alpha , x_i)$$

$$E = 2^\sigma \beta_t \int F^* (\tilde{\phi}'_\alpha) \rho^* (2\tilde{\phi}_\alpha - \tilde{\phi}'_\alpha) \, d\phi'_\alpha$$

$$- 2\beta_t F^* (\tilde{\phi}_\alpha)$$