MODELING OF TURBULENT CHEMICAL REACTION

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Modeling Turbulent Reacting Flows

Model for Turbulent Flows

Model for Effects of Turbulence on Chemical Reactions

Model for Chemical Kinetics
Regimes of Turbulent Combustion

Regimes of Premixed Turbulent Combustion

\[ K_{\alpha} = \frac{1}{\sqrt{D_{\alpha \gamma}}} \]
Regimes of Non-Premixed Turbulent Combustion

Chemical Closure Models

1. Laminar Chemistry
   \[ \langle \rho w_i \rangle = \rho w_i (\overline{Y}_i, \overline{T}) \]

2. Fast Chemistry
   \[ \langle \rho w_i \rangle = -\frac{1}{2} \rho \chi_f \frac{\partial^2 Y^c (f)}{\partial f^2} \]

3. Flamelet model
   \[ \langle \rho w_i \rangle = \int \int \rho w_i (\eta, \chi_f) P_{\chi, \chi_f} (\eta, \varepsilon_f) d\eta d\varepsilon_f \]

4. Assumed PDF:
   \[ \langle \rho w_i \rangle = \int \int \rho w_i (\phi_1) \cdot P_{\phi} d\phi_1 d\phi_2 \ldots d\phi_n \]
   Assumed the shape of \( P_{\phi} \).

5. Scalar PDF method:
   Solve for \( P_{\phi} \) directly.

6. Conditional Moment Closure (CMC)
   \[ \langle \rho w_i \rangle = \int \rho w_i \cdot \eta > \cdot P_{\eta} (\eta) d\eta \]
Flamelet library with one side being burned premixed flame $= 1.4$

Flamelet Model: 69%H₂ + 31%CH₄

Turbulent Jet Flame, Rey. = 10,000

Flamelet Model: 69% H₂ + 31% CH₄
Turbulent Jet Flame, Rev. = 10,000

Conditional Moment Closure (CMC)

Definition:

\[ < Y, \eta > = \int Y(\bar{x}, t) f(\bar{x}, t) = \eta > \]

Equation:

\[ \frac{\partial < Y, \eta >}{\partial t} + \rho \frac{\partial < Y, \eta >}{\partial t} = \nabla \cdot (\rho \frac{\partial Y}{\partial \eta} > P_r(\eta)) \]

\[ = < \rho w, \eta > + < \rho D, \nabla f \cdot \nabla f > \frac{\partial ^2 < Y, \eta >}{\partial \eta ^2} \]

Modeling:

\[ < w, \eta > = w_i (< T_i \eta >, < Y_i \eta >, ...) \]

\[ < \rho D, \nabla f \cdot \nabla f > = < \rho D, \nabla f \cdot \nabla f > = \frac{1}{2} \rho \chi_i \]

\[ < \rho u \eta > = \rho u \]

\[ < \rho u ' \eta > = 0 \]

\[ < \rho \eta > = \rho (< Y, \eta >, < T \eta >) \]
Conditional Moment Closure (CMC)

![Graph showing mole fraction vs mixture fraction for various components like N₂, H₂, O₂, and H₂O, with predictions and equilibrium lines.]

NOx Emissions from Turbulent H₂ Jet Flames

![Graph showing log(EnoX/m) vs log(U/D) with data points and lines for measurement, scalar PDF, CMC, and assumed PDF.]

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Conditional Moment Closure (CMC)

Applications:

- Incorporated into existing moment closure CFD codes for complex geometry flows
- Realistic Chemistry - Detailed or reduced

Research issues:

- Modeling of conditional statistics
- Preferential diffusion
- Parallel computing algorithms

Probability Density Function (PDF)

Applications:

- NO\textsubscript{x} from methane jet flames with reduced chemistry
- Sooting flames
- 2-D flows

Research Topics:

- Mixing model
- Extension to droplet spray & particle laden flows
- Preferential diffusion
- Efficient stochastic algorithm
- Construction of chemical tables
- Parallel computing - 3D Flows or 2D flows with complex chemistry
Departures From Chemical Equilibrium

(r) Hydrogen

Methane

Methanol
Mixing Models for PDF Methods

- Modified Curl's Model (stochastic)

$$\frac{k}{\alpha=1,\beta=1} \frac{\partial^2}{\partial \psi \partial \psi'} \left( \left[ \frac{\partial \phi}{\partial \psi'} \frac{\partial \phi}{\partial \psi} \right] \dot{P}_\phi (\psi, t) \right) =$$

$$\frac{1}{\tau_{mix}} \left\{ \int_{\psi'}^{\psi'} \frac{\dot{P}_\phi (\psi', t) \dot{P}_\phi (\psi'', t) H(\psi', \psi'' | \psi) - \dot{P}_\phi (\psi, t)}{\partial \psi'} \right\}$$

- IEM (Interaction-by-Exchange-with-the-Mean) Model (deterministic)

$$\frac{k}{\alpha=1,\beta=1} \frac{\partial^2}{\partial \psi \partial \psi'} \left( \left[ \frac{\partial \phi}{\partial \psi'} \frac{\partial \phi}{\partial \psi} \right] \dot{P}_\phi (\psi, t) \right) = \frac{C_0}{\tau_{mix}} \frac{\partial}{\partial \psi} \left( \psi \dot{P}_\phi (\psi, t) \right)$$

Mixing Frequency: $\omega_{mix} = \frac{1}{\tau_{mix}}$

PaSR: H2/NOx Detailed Chemistry $\phi=1$ $\tau=1ms$
Comparison of Predicted and Measured H2O Mass Fractions
Turbulent Nonpremixed Jet Flames

Fuel: (CO/H2/N2: 0.30/0.10/0.6)

Experimental Evidence of Preferential Diffusion in Turbulent Jet Flames
(Fuel: 36% H2+64% CO2)

INTRODUCTION TO TURBULENCE SUBPROGRAM

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OBJECTIVES

- A means for CMOTT to interact with industry
- A vehicle for technology transfer to industry

CONCEPT OF TURBULENCE MODULE

- Exact CFD equations:

\[
\frac{D\rho U_i}{Dt} = \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right) - \rho \overline{u_i u_j} \right] - \frac{\partial P}{\partial x_i}
\]

- Reynolds stresses will be recasted as:

\[
-\rho \overline{u_i u_j} = \mu_T \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right) + \left( \mu_T + \frac{u_i u_j}{\partial x_j} - \frac{2}{3} \frac{u_k u_k}{\partial x_k} \delta_{ij} \right) \overline{T_{ij}}
\]

\[
\mu_T \equiv C_k \frac{k^2}{\varepsilon}
\]

- CFD equations become:

\[
\frac{D\rho U_i}{Dt} = \frac{\partial}{\partial x_j} \left[ (\mu + \mu_T) \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right) \right] + \frac{\partial T_{ij}}{\partial x_j} - \frac{\partial P}{\partial x_i}
\]

- The task of turbulence module: Provide \( \mu_T \) and \( T_{ij} \)
- Turbulence Module:
  
  ◦ Input: \( U_i, \rho \) and \( \mu \) ... from the mean flow solver
  
  ◦ Output:

  \[
  \mu_T = C_\mu \frac{k^2}{\varepsilon} \left[ \frac{Dk}{Dt} = \ldots, \quad \frac{D\varepsilon}{Dt} = \ldots \right]
  \]

  \[
  T_{ij} = -\rho \bar{u}_i \bar{u}_j - \mu_T \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right)
  \]

  ◦ Models for \( \rho \bar{u}_i \bar{u}_j \):

    - One- and two-equation eddy viscosity models
    - Reynolds stress algebraic equation models
    - Reynolds stress transport equation models
Module with CMOTT research code (incompressible)

- CFD equations in CMOTT research code:
  \[
  \frac{D\rho U_i}{Dt} = \frac{\partial}{\partial x_j} \left[ (\mu + \mu_T) \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \right] + \frac{\partial}{\partial x_j} T_{ij} - \frac{\partial P}{\partial x_i}
  \]

- Turbulence module: provide \( \mu_T \) and \( T_{ij} \)
  - Built-in models without wall function:
    - Launder-Sharma and Chien \( k - \varepsilon \) models
    - CMOTT \( k - \varepsilon \) model
  - Built-in models with wall function:
    - \( k - \omega \) model, standard \( k - \varepsilon \) model
    - CMOTT \( k - \varepsilon \) model
    - CMOTT Reynolds stress algebraic equation model

Module with NPARC code

- CFD equations in NPARC code:
  \[
  \frac{D\rho U_i}{Dt} = \frac{\partial}{\partial x_j} \left[ (\mu + \mu_T) \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right) \right] - \frac{\partial P}{\partial x_i}
  \]

- Turbulence module (present time): provide isotropic \( \mu_T \)
  - Build-in models without wall function:
    - Baldwin-Lomax model and Chien \( k - \varepsilon \) model
    - CMOTT \( k - \varepsilon \) model
  - Further development:
    - Models with wall function
    - Reynolds stress algebraic equation models
    - Reynolds stress transport equation models
Joint Program with Industry
on Turbulence Module

- For those who want to use the available modules:
  - Need interface program for particular industry codes
    - Grid informations, Boundary treatment, ...
- For those who want a module for their own codes:
  - Need modules exclusively for particular industry codes
- Maintain and update the turbulence modules along with model development.
General Transport Equations

\[ \frac{\partial}{\partial t}(rJ^{-1}\rho \phi) + \frac{\partial}{\partial \xi_i}(C_i \phi - D_i \phi) = rJ^{-1}S_\phi \]

- Non-dimensional form \((\mu, \mu_t \Leftrightarrow \mu/Re, \mu_t/Re)\)
- Conservative form
- Cartesian velocity components
  1. Easy to transform (chain rule)
  2. No curvature terms
Discretization

- Finite-volume method
- Source term
  \[ S_\phi = S_1 + S_2 \phi, \quad S_1 \geq 0 \text{ and } S_2 \leq 0 \]
- Transient term
  1. 1st-order fully implicit scheme
  2. 2nd-order three-level fully implicit scheme
- Diffusion term
  Standard central differencing scheme

- Convection term: HLPA scheme
  (Hybrid Linear/Parabolic Approximation)

\[ \phi_w = \phi_W + \gamma (\phi_C - \phi_W) \hat{\phi}_W, \quad \hat{\phi}_W = \frac{\phi_W - \phi_{WW}}{\phi_C - \phi_W W} \]

\[ \gamma = \begin{cases} 
1 & \text{if } |\hat{\phi}_W - 0.5| < 0.5 \\
0 & \text{otherwise} 
\end{cases} \]

- Second-order accurate
- Bounded (non-oscillatory)
- Diagonally dominant matrix
Example 1

Initial profile at $t = 0$

Predicted profiles at $t = 100$ (201 x 2 grid, $\Delta t = 0.4$)

Predicted profiles at $t = 100$ (1001 x 2 grid, $\Delta t = 0.1$)

Example 2

$S$-profiles at outer ($O$, exact solution)
Solution Procedure

- Non-delta form
  Positiveness ($\phi \geq 0$ but $\Delta \phi$ may < 0)
  Simple linearization

- Algebraic equations
  \[ A_C \phi_C = A_W \phi_W + A_E \phi_E + A_S \phi_S + A_N \phi_N + S \]
  $A$'s, $S \geq 0$

- Decoupled solution

- Alternating direction TDMA solver

Boundary Conditions

- Inflow: $\phi$ specified

- Outflow: Fully-developed condition

- Symmetry: $\partial \phi / \partial n = 0$

- Wall:
  1. Low-Reynolds number turbulence models
  2. Standard wall-function approach
Sub-Programs

- NPARC2D version
  Plane or axisymmetric, without swirling
  Compressible
  Non-vectorized

- FAST2D version
  Plane or axisymmetric, with or without swirling
  Incompressible
  Vectorized

NPARC2D Version

- Grid arrangement
  Control volume centers
  Boundary nodes
  Embedded bodies

J-Patches

K-Patches
- Input from the main code
  1. Geometric quantities: \( x, y, \xi_x, \xi_y, \eta_x, \eta_y, J \)
  2. Flow variables: \( \mu, J^{-1}\rho, J^{-1}\rho U, J^{-1}\rho V, J^{-1}E \)
  3. Patch control: \( 5 \times 2 \) parameters
  4. Boundary conditions: \( 7 \times 2 \) parameters

- Output
  1. To the main code: \( \mu_t \)
  2. For post-processing: \( K, \epsilon, y^+, y_n, f_\mu \)

**FAST2D Version**

- Grid arrangement
  - CV centers
  - Boundary nodes
  - Embedded bodies
• Vectorization

Single-index:

\[ ii = i + (j-1)ni \]
\[ \phi(i,j) = \phi(ii) \]
\[ \phi(i+1,j) = \phi(ii+1) \]
\[ \phi(i,j-1) = \phi(ii-ni) \]

Control parameter:

\[ K_{BLK} = \begin{cases} 1 & \text{for computational nodes} \\ 0 & \text{otherwise} \end{cases} \]

\[ \phi = K_{BLK} \cdot \phi_c + (1-K_{BLK}) \phi_b \]

• Input from the main code

1. Geometric quantities:  \( x, y, x_\xi, x_\eta, y_\xi, y_\eta, J \)
2. Flow variables:  \( \mu, \rho, U, V, W, C_w, C_s \)
3. Vectorization parameters
4. Boundary parameters

• Output

1. To the main code:  \( \mu_t, T_{ij} \)
2. For post-processing:  \( K, \epsilon, y^+, y_n, f_\mu \)
OVERVIEW OF PROBABILITY DENSITY FUNCTION (PDF) MODELING AT LeRC

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OBJECTIVE
Accurately model the effect of turbulence on chemical reactions in a fluid flow

APPROACH
Use Probability Density Function (PDF) model -
Express dependent variables as functions representing statistically realizable events

POSSIBLE MODELING STRATEGIES

1. Evolution PDF - solve for function
   a. Joint PDF for velocities and chemical species
   b. Joint PDF for only chemical species & energy

2. Assumed PDF - function prescribed
   Limited range of applicability -
   reaction time \(< \) or \(>\) turbulence time scale
CURRENT APPROACH

- Develop evolution PDF model for compressible reacting flows & extend to spray combustion
- Solve for joint PDF for species and energy using Monte-Carlo technique
- Couple with conventional CFD codes

AREAS OF IMPACT

- NOx Prediction - HSCT and AST application
- Spray combustion - swirling turb. reacting flows
- Scramjet flow path analysis
- Ignition kinetics - prediction of blow-off, etc.
- Combustion instability studies
CODE FEATURES

- Modular - can be coupled with any CFD code
- Applicable for compressible flows with discontinuities
- Monte-Carlo solver for generalized curvilinear coordinate system
- Easily adaptable for parallel computation (currently under progress)

CURRENT STATUS

- 2-D and axisymmetric version released
  (default H2-air chemistry - 5 species)
  - parallel version to be released
- 3-D version demonstrated for supersonic combustion (jet in cross flow)
  - validation planned for HSCT-type configurations
- General chemistry (CHEMKIN)
  - Hydrocarbon spray combustion case currently under study
- CFD codes used - RPLUS, ALLSPD, & SIMPLE-type
FUTURE PLANS

• Further application/validation of 3-D model

• Improved closure models - mixing and turbulence (use available DNS data)

• Parallel processing - workstation clusters

• Unsteady applications - long-term

• Extend scope of impact