MODELING OF TURBULENT CHEMICAL REACTION

J.-Y. Chen
Department of Mechanical Engineering
University of California, Berkeley
Berkeley, California

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

\[ K_{\alpha} = \sqrt{\frac{\text{Da}}{\text{Ka}}} \]

Regimes of Non-Premixed Turbulent Combustion

![Diagram showing regimes of non-premixed turbulent combustion]


Chemical Closure Models

(1) Laminar Chemistry
\[ \langle \rho w_i \rangle = \rho w_i (Y_i, T) \]

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

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

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

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

(6) Conditional Moment Closure (CMC)
\[ \langle \rho w_i \rangle = \int \langle \rho w_i \rangle \eta \cdot P_\varepsilon (\eta) d\eta \]
Flamelet Model: 69%H₂+31%CH₄
Turbulent Jet Flame, Reₜ = 10,000

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


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


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Advanced Flamelet Approach

**Conditional Moment Closure (CMC)**

**Definition:**
\[ < Y_i | \eta >= < Y (x, t) | f(x, t) = \eta > \]

**Equation:**
\[ \frac{\partial < Y_i | \eta >}{\partial t} + \rho_i u_i \nabla < Y_i | \eta > + \nabla \cdot \left( \rho_i u_i < Y_i | \eta > \right) = \frac{\partial^2 < Y_i | \eta >}{\partial \eta^2} \]

**Modeling:**
\[ < w_i | \eta > = w_i (< T | \eta >, < Y_i | \eta >, ...) \]
\[ < pD_i \nabla f | \nabla v_i > = < pD_i \nabla f | \nabla v_i > = \frac{1}{2} \rho_i \chi_i \]
\[ < \rho_i u_i | \nabla > = \rho_i u \]
\[ < \rho_i u' y' | \eta > = 0 \]
\[ < \rho i | \eta > = \rho (< Y_i | \eta >, < T | \eta >) \]
Conditional Moment Closure (CMC)

Nox Emissions from Turbulent H2 Jet Flames
**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

Hydrogen

Methane

Methanol
Mixing Models for PDF Methods

- Modified Curl's Model (stochastic)

\[- \sum_{\alpha=1}^{32} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left\{ \left( \delta_{ij} \phi = \psi \right) \tilde{P}_\phi (\psi, t) \right\} = \frac{1}{\tau_{mix}} \int \psi' \psi'' \left[ \tilde{P}_\phi (\psi', t) \tilde{P}_\phi (\psi'', t) H(\psi', \psi'' | \psi) - \tilde{P}_\phi (\psi, t) \right] d\psi' d\psi'' \]

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

\[- \sum_{\alpha=1}^{32} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left\{ \left( \delta_{ij} \phi = \psi \right) \tilde{P}_\phi (\psi, t) \right\} = \frac{C_o}{\tau_{mix}} \frac{\partial}{\partial \psi_\alpha} \left( \tilde{P}_\phi (\psi, t) \right) \]

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

PaSR: H2/NOx Detailed Chemistry \(\phi = 1\) \(\tau = 1\)ms
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)

Computation of Turbulent Reacting Flows

Development

Direct Numerical Simulation → Large Eddy Simulation → Turbulence Model → Stochastic Simulation

Reduced Mechanisms

Laminar Flames with Detailed Mechanisms

Practical Interests

Combustion in Compressible Turbulence

Soot in Turbulent Flames

Flame Extinction & Re ignition

NOx in Turbulent Flames
INTRODUCTION TO TURBULENCE SUBPROGRAM

T.-H. Shih and J. Zhu
Institute for Computational Mechanics in Propulsion
and Center for Modeling of Turbulence and Transition
NASA Lewis Research Center
Cleveland, Ohio

OBJECTIVES

• A means for CMOTT to interact with industry

• A vehicle for technology transfer to industry

CONCEPT OF TURBULENCE MODULE

• Exact CFD equations:

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

• Reynolds stresses will be recast as:

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

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

• 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:**
  - \( \diamond \) **Input:** \( U_i, \rho \) and \( \mu \) ... from the mean flow solver
  - \( \diamond \) **Output:**
    \[
    \mu_T = C_\mu \frac{k^2}{\varepsilon} \quad \left[ \frac{Dk}{Dt} = \ldots, \quad \frac{D\varepsilon}{Dt} = \ldots \right] \\
    T_{ij} = -\rho \overline{u_i u_j} - \mu_T \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right)
    \]
  - \( \diamond \) **Models for** \( \rho \overline{u_i u_j} \)
    - One- and two-equation eddy viscosity models
    - Reynolds stress algebraic equation models
    - Reynolds stress transport equation models

![Diagram of Turbulence Module]
Module with CMOTT research code (incompressible)

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

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

- 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

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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)

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

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

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

Initial profile at $t = 0$

Predicted profiles at $t = 100$ (201x2 grid, $\Delta t = 0.4$)

Predicted profiles at $t = 100$ (1001x2 grid, $\Delta t = 0.1$)

Example 2

$S$-profiles at outlet ($O$, 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: \( K, \epsilon, y^+, y_n, f_\mu \)
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