Efficient Engine CFD with Detailed Chemistry

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Digital Analysis of Reaction Systems
Challenges in CFD engine modeling

- The flow is turbulent
  - Turbulence modeling required
- Spray injection and evaporation occurs
  - Spray modeling is required
- Autoignition, combustion, pollutant formation chemistry
  - Kinetic modeling required for various fuels
  - Soot, NOx models required
Efficient Engine CFD with Detailed Chemistry

Problem: Multidimensional modeling of turbulent reactive flow

Turbulent flowfield

Combustion

Navier-Stokes equations

?
Outline

• Species transport models
  - "Laminar"
  - Techniques for speed-up
  - Incorporation of turbulence interactions

• Flamelet models
  - Transient interactive flamelets
  - Transient flamelet progress variable model

Requirements for industrial production simulations:
Efficient handling of combustion chemistry
Fully parallel flow simulation capabilities
STAR-CD and DARS-CFD

Problem: Multidimensional modeling of turbulent reactive flow

Solution I:

- Turbulent flowfield
- Combustion
- Navier-Stokes equations
- Species transport
DARS-CFD – STAR-CD coupling

\[
\begin{align*}
\frac{\partial}{\partial t} \rho Y_k + \frac{\partial}{\partial x_j} (\rho u_j Y_k + F_{k,j}) &= 0 \\
\frac{\partial}{\partial t} \rho h + \frac{\partial}{\partial x_j} (\rho u_j h + F_{h,j}) &= \frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} + \tau_{ij} \frac{\partial u_i}{\partial x_j}
\end{align*}
\]

Species \( Y_i^0 \)  
Enthalpy \( h \)

Species \( Y_i^* \)

Transport data \( D_{ij}, \lambda, \nu \)

DARS-CFD
\[
\frac{dY_i}{dt} = \frac{\omega_i W_i}{\rho}
\]
DARS-CFD – STAR-CD coupling with DOLFA

STAR-CD:
\[
\begin{align*}
\frac{\partial}{\partial t} \rho Y_k + \frac{\partial}{\partial x_j} (\rho u_j Y_k + F_{k,j}) &= 0 \\
\frac{\partial}{\partial t} \rho h + \frac{\partial}{\partial x_j} (\rho u_j h + F_{h,j}) &= \frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} + \tau_{ij} \frac{\partial u_i}{\partial x_j}
\end{align*}
\]

- Species $Y_i^0$
- Enthalpy $h$
- Species $Y_i^*$
- Transport data $D_{ij}, \lambda, \nu$

DOLFA Database

DOLFA

\[
\frac{dY_i}{dt} = \frac{\omega_i W_i}{\rho}
\]
Two options for considering turbulence interactions:

- Kong-Reitz model:

\[ s_i^t = \frac{\tau_{\text{kin}}}{\tau_{\text{kin}} + f \tau_{\text{turb}}} s_i^l \]

\[ \tau_{\text{turb}} = c \cdot k \varepsilon \]

\[ f = \frac{(1 - e^{-r})}{0.632} \]

\[ r = \frac{m_{\text{CO}_2} + m_{\text{H}_2\text{O}} + m_{\text{CO}} + m_{\text{H}_2}}{1 - m_{\text{N}_2}} \]

- User coding:
  - Scaling of reaction rates
  - User can modify the reaction rates for all species
STAR-CD and Transient Flamelet Models

Problem: Multidimensional modeling of turbulent reactive flow

Solution II:

- Turbulent flowfield
  - Navier-Stokes equations

- Combustion
  - Flamelet modeling
    - Interactive
    - Transient library
Basics of the flamelet model

Physical Coordinates $\Rightarrow$ Mixture fraction coordinate $Z_i$

$t, x_1, x_2, x_3 \rightarrow \tau, Z, Z_2, Z_3$

Flame: Surface of Stoichiometric mixture
Basics of the flamelet model

Transport of a generic scalar

\[ \rho \frac{\partial \psi}{\partial t} + \rho v \frac{\partial \psi}{\partial x} - \rho D \frac{\partial^2 \psi}{\partial x^2} = S_\psi \]

Def. Scalar dissipation rate

\[ \chi = 2D \left( \frac{\partial Z}{\partial x} \right)^2 \]

Equations in flamelet space

\[ \rho \frac{\partial \psi}{\partial \tau} = \rho \frac{\chi}{2} \frac{\partial^2 \psi}{\partial Z^2} + S_\psi - R(\psi) \]

\[ R(\psi) = \rho v \frac{\partial \psi}{\partial Z} + \frac{\partial}{\partial x} \left( \rho D \frac{\partial \psi}{\partial Z} \right) - \rho D \sum_{k=2}^{3} \left( \frac{\partial Z}{\partial x_k} \frac{\partial^2 \psi}{\partial Z \partial Z_k} + \frac{\partial^2 \psi}{\partial Z^2_k} \right) \]
STAR-CD – TIF coupling

STAR-CD
Transport of $Z$, $Z^\prime\prime$, $h$, $l$

Get cell local $T$ and $W_q$

Perform species pdf integration

$Y_i(Z)$

Update $h$ and $\chi$

\[
\frac{\partial Y_i}{\partial t} = \frac{\rho}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \omega_i W_i
\]
Soot modeling with TIF

- Turbulent diffusion flame (J. B. Moss et al. 1991) test case
- Flowfield post-processed with TIF
- Detailed kinetic soot model
  - Soot precursors: cyclopentapyrene and larger PAH
  - Surface growth: HACA with separate ring closure
  - Oxidation: $O_2$ and OH
  - Condensation and coagulation
- Particle size distribution
  - Method of moments with interpolative closure (4 moments)
  - Sectional method (100 sections)

Soot modeling with TIF

Centerline soot volume fraction

Soot modeling with TIF

Particle size distributions in the turbulent diffusion flame

Transient flamelet progress variable model

- Progress variable defined using chemical enthalpy integrated over the flamelet

\[
C = \frac{\int_0^1 \sum_{i=1}^{N_s} h_{298,i} \,(Y_i(Z), \tau) \,dZ - \int_0^1 \sum_{i=1}^{N_s} h_{298,i,u} \,(Y_i(Z), 0) \,dZ}{\int_0^1 \sum_{i=1}^{N_s} h_{298,i,b} \,(Y_i(Z), \tau_\infty) \,dZ - \int_0^1 \sum_{i=1}^{N_s} h_{298,i,u} \,(Y_i(Z), 0) \,dZ}
\]

Transport eqn for chemical enthalpy

\[
\rho \frac{\partial h_{298}}{\partial t} + \rho v_\alpha \frac{\partial h_{298}}{\partial x} - \rho D \frac{\partial^2 h_{298}}{\partial x_\alpha^2} = \sum_{i=1}^{N_s} \omega_i h_{i,298}
\]

Transport eqn for the progress variable

\[
\rho \frac{\partial C}{\partial t} + \rho v_\alpha \frac{\partial C}{\partial x_\alpha} - \rho D \frac{\partial^2 C}{\partial x_\alpha^2} = \rho \frac{\partial C}{\partial C} \frac{\partial h_{298}}{\partial h_{298}} \frac{\partial h_{298}}{\partial t}
\]

Transform to \(Z - C\) space

\[
\begin{aligned}
\frac{\partial \psi}{\partial t} &= \frac{\partial \psi}{\partial Z} \frac{\partial Z}{\partial t} + \frac{\partial \psi}{\partial C} \frac{\partial C}{\partial t} + \frac{\partial \psi}{\partial t} \\
\frac{\partial \psi}{\partial x_\alpha} &= \frac{\partial \psi}{\partial Z} \frac{\partial Z}{\partial x_\alpha} + \frac{\partial \psi}{\partial C} \frac{\partial C}{\partial x_\alpha}
\end{aligned}
\]

TFPV – Coupling to STAR-CD

To library

\[ \text{IdentifyFlamelet} \]
\[ EGR, p(t), T_{ox}(x,t), \tilde{\chi}(x,t), \tilde{C}(x,t) \]

\[ \tilde{Z}(x,t), \tilde{Z}^2(x,t) \]

\[ \tilde{T}(x,t)_{\text{guess}}, \tilde{h}(x,t) \]

To CFD

\[ \tilde{T}(x,t), \tilde{C}(x,t) \]

Flamelet library module

\[ \sum \left( h_i(\tilde{T}) \cdot \int_{0}^{1} Y_i \cdot \tilde{P}(Z; \tilde{Z}, \tilde{Z}^2) dZ \right) \]

\[ \tilde{h}_{\text{flamelet}}(\tilde{T}) \]

\[ \tilde{T}(x,t) = f(\tilde{T}_{\text{guess}}(x,t), \tilde{h}(x,t), \tilde{h}_{\text{flamelet}}(\tilde{T})) \]

\[ \tilde{T}(x,t) \]
### TFPV – Sample engine calculation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Swept volume</td>
<td>2.0 L</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>15.3</td>
</tr>
<tr>
<td>Number of nozzle holes</td>
<td>6</td>
</tr>
<tr>
<td>Nozzle hole diameter</td>
<td>0.2 mm</td>
</tr>
<tr>
<td>Speed</td>
<td>1176 rpm</td>
</tr>
<tr>
<td>Fuel type</td>
<td>Diesel</td>
</tr>
<tr>
<td>Fuel amount</td>
<td>74.35 mg</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>1.24</td>
</tr>
<tr>
<td>Start of injection</td>
<td>361 CA</td>
</tr>
<tr>
<td>EGR ratio</td>
<td>0.32</td>
</tr>
</tbody>
</table>

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TFPV – Sample engine calculation

Combustion progress

Pressure and rate of heat release

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Temperature

Mixture fraction

<table>
<thead>
<tr>
<th>T [K]</th>
<th>Z [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2300</td>
<td>0.4</td>
</tr>
<tr>
<td>300</td>
<td>0</td>
</tr>
</tbody>
</table>
TFPV – Sample engine calculation, CA 395

Temperature  Mixture fraction

T [K]  Z [-]

2300  0.4

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Summary

- Strategies for efficiently incorporating detailed chemistry in multidimensional simulations were presented:
  - Direct integration of chemistry with DARS-CFD
  - Flamelet approach
    » Transient interactive flamelet (TIF)
    » Transient flamelet progress variable model (TFPV)

- The DARS-CFD model allows for
  - Turbulence interactions (Kong-Reitz) or user
  - Coupling to DOLFA
  - Full parallelism
Summary

- The TIF model allows for
  - Efficient treatment of chemistry
  - Consistent handling of turbulence interactions
  - Efficient treatment of complex soot and emission chemistry
  - Fully parallel simulations

- The TFPV model allows for
  - Consideration of effects of local inhomogeneities and local variations of scalar dissipation rate on the chemistry
  - Arbitrary large chemistry can be used in the tabulation without influencing the CFD simulation CPU time
  - Coupling to library based emission models
  - Fully parallel simulations