Turbulent Combustion Modeling in CFD

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Turbulent Combustion: The Physics

- Turbulent combustion can be defined as a chemical reaction that takes place within turbulent flow.
- Turbulent flow affects the mixing of chemical species → thus affects the rate of reaction.
- The reaction produces thermal energy which in turn affects the flow velocity, pressure and temperature → thus affects turbulence behavior.
- This two way coupling between the two phenomena imposes a great deal of complexity!
Turbulent Combustion: The Physics

Due to such coupling, a number of phenomena become very important for the study of turbulent combustion:

- **Combustion efficiency**: The efficiency of the chemical reaction to produce thermal energy.
- **Reaction zone structure**: The morphology of the flow region where chemical reaction occurs.
- **Combustion stability**: The tendency of chemical reaction to stop due to thermal, aerodynamic, acoustic or magnetic effects.
**Turbulent Combustion: The Mathematics**

- The governing equations are:
  - Conservation of mass & species
  - Species transport
  - Momentum equation
  - Sensible enthalpy equation

\[
\frac{\partial (\bar{p} \bar{U})}{\partial t} + \nabla \cdot (\bar{p} \bar{U} \bar{U}) = \nabla \cdot (\mu_{eff} \nabla \bar{Y}_i) + \frac{3\bar{p}}{\partial t} + \bar{\omega}_i
\]

\[
\frac{\partial (\bar{p} \bar{h}_s)}{\partial t} + \nabla \cdot (\bar{p} \bar{h}_s \bar{h}_s) = \nabla \cdot (\alpha_{eff} \nabla \bar{h}_s) + \frac{\partial \bar{p}}{\partial t} - \bar{\omega}_c + \bar{\omega}_r
\]

The turbulence-combustion coupling problem appears in these equations in the stress tensor \( \omega \) \( \rightarrow \) In order to evaluate the velocity field, this tensor must be modelled (turbulence modelling)!
Turbulent Combustion: The Mathematics

- The governing equations are:
  - Conservation of mass & species
  - Species transport
  - Momentum equation
  - Sensible enthalpy equation

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{U}) &= 0 \\
\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \vec{U} Y_i) &= \nabla \cdot (\mu_{\text{eff}} \nabla Y_i) + \frac{\partial P}{\partial t} + \omega_i \\
\frac{\partial (\rho \vec{U})}{\partial t} + \nabla \cdot (\rho \vec{U} \vec{U}) &= \nabla \cdot (\tau_{\text{eff}}) - \nabla P + \rho \vec{g} \\
\frac{\partial (\rho h_s)}{\partial t} + \nabla \cdot (\rho \vec{U} h_s) &= \nabla \cdot (\alpha_{\text{eff}} \nabla h_s) + \frac{\partial P}{\partial t} + \omega_c + \omega_r
\end{align*}
\]
Turbulent Combustion: A CFD Approach

• Modeling goals of an ideal CFD turbulence combustion model are basically to achieve accurate predictions of:

1. Species transport including pollutants
2. Heat of reaction and enthalpy
3. Flame aerodynamics
4. Combustion stability

But of course to achieve all these goals, one must have enormous computational resources which are not practical for engineering applications. That is why modelling turbulent combustion must be optimized for every application!
Turbulent Combustion: A CFD Approach

- How the coupling between turbulence and combustion is manifested in CFD

- Modeling problems
  - Turbulence (?)
  - Density
  - Pressure
  - Thermal conductivity
  - Viscosity

- Mixing
  - Time scale problem?

- Chemical reaction (?)
  - Chemical kinetics problems
  - Heat of reaction

Turbulent Combustion Model
Classification to turbulent combustion models

- Turbulent combustion models are classified according to:
  1. The linking method between turbulence scalars and reaction rate
  2. The level of details of chemical reaction

Chemistry controlled models
- Arrhenius models
  - Reaction rate depends on temperature

Mixing controlled models
- Eddy dissipation model
- Eddy dissipation concept
- Laminar flamelet models

Detailed chemistry models
- Chemical kinetics mechanisms
  - Require DNS / LES
Turbulent Combustion Modeling

Turbulence modeling approaches

- Isotropic turbulence
  - Algebraic models
  - Eddy viscosity models (2 equations, 4 equations)
- DNS
- Anisotropic turbulence
  - Reynolds stress models
  - Filtering approaches (LES, DES, VLES)

Chemical Reaction modeling approaches

- Eddy break-up theory
- Flamelet theory
- Detailed chemistry

Coupling Technique

- EDM
- EDC
- Flamelet model
- PDF model
- Detailed chemical kinetics
EDM with RANS for Jet Flame Modeling
Flamelet Model with RANS for Hydrogen-Enriched Swirl Flame
Challenges and Prospects

- Highly strained flows
- Atmospheric flow modeling
- Transitional flow regimes

- Interaction between primary and secondary phase
- Integration with new turbulence models

- Optimize between physical assumptions and correct chemical kinetics
- Efficient coupling with turbulence models
Challenges and Prospects

Computational requirements
- Faster processors and larger memories
- Smarter software algorithms

![Diagram showing computational requirements for different turbulence models: RANS, LES, DES, DNS. DNS has the highest computational requirements.](diagram.png)