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Arab Academy for Science, Technology & Maritime Transport

Turbulent Combustion Modeling in CFD

PROSPECTS AND CHALLENGES

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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 he 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

Turbulent flow
- Mixing
- Diffusion
- Dissipation

Combustion
- Chemical reaction rate (local and global)

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

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla.\left(\bar{\rho}\,\tilde{\vec{U}}\right) = 0$$

$$\frac{\partial(\bar{\rho}\,\tilde{Y}_i)}{\partial t} + \nabla.\left(\bar{\rho}\,\tilde{\vec{U}}\,\tilde{Y}_i\right) = \nabla.\left(\mu_{eff}\nabla\tilde{Y}_i\right) + \frac{\partial \bar{p}}{\partial t} + \dot{\omega}_i$$

$$\frac{\partial\left(\bar{\rho}\,\tilde{\vec{U}}\right)}{\partial t} + \nabla.\left(\bar{\rho}\,\tilde{\vec{U}}\,\tilde{\vec{U}}\right) = -\nabla\bar{p} + \nabla.\left(\tilde{\vec{\vec{\tau}}}_{eff}\right) + \bar{\rho}\vec{g}$$

$$\frac{\partial(\bar{\rho}\,\tilde{h}_s)}{\partial t} + \nabla.\left(\bar{\rho}\,\tilde{\vec{U}}\,\tilde{h}_s\right) = \nabla.\left(\alpha_{eff}\nabla\tilde{h}_s\right) + \frac{\partial \bar{p}}{\partial t} + \dot{\omega}_c + \dot{\omega}_r$$

Reaction rate

Stress tensor

Sensible enthalpy

Heat of reaction

Heat transfer due to radiation

The turbulence-combustion coupling problem appear in these equations in the stress tensor → 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

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla.\left(\bar{\rho}\,\tilde{\vec{U}}\right) = 0$$

  - Species transport

$$\frac{\partial(\bar{\rho}\,\tilde{Y}_i)}{\partial t} + \nabla.\left(\bar{\rho}\,\tilde{\vec{U}}\,\tilde{Y}_i\right) = \nabla.\left(\mu_{eff}\nabla\tilde{Y}_i\right) + \frac{\partial \bar{p}}{\partial t} + \dot{\omega}_i$$

  - Momentum equation

$$\frac{\partial\left(\bar{\rho}\,\tilde{\vec{U}}\right)}{\partial t} + \nabla.\left(\bar{\rho}\,\tilde{\vec{U}}\,\tilde{\vec{U}}\right) = \nabla.\left(\overline{\overline{\tau_{eff}}}\right) - \nabla\bar{p} + \bar{\rho}\vec{g}$$

  - Sensible enthalpy equation

$$\frac{\partial(\bar{\rho}\,\tilde{h}_s)}{\partial t} + \nabla.\left(\bar{\rho}\,\tilde{\vec{U}}\,\tilde{h}_s\right) = \nabla.\left(\alpha_{eff}\nabla\tilde{h}_s\right) + \frac{\partial \bar{p}}{\partial t} + \dot{\omega}_c + \dot{\omega}_r$$

Local acceleration (time derivatives)

Convective acceleration (spatial derivatives

Diffusion terms (Laplacial derivatives)

Turbulent Combustion: A CFD Approach

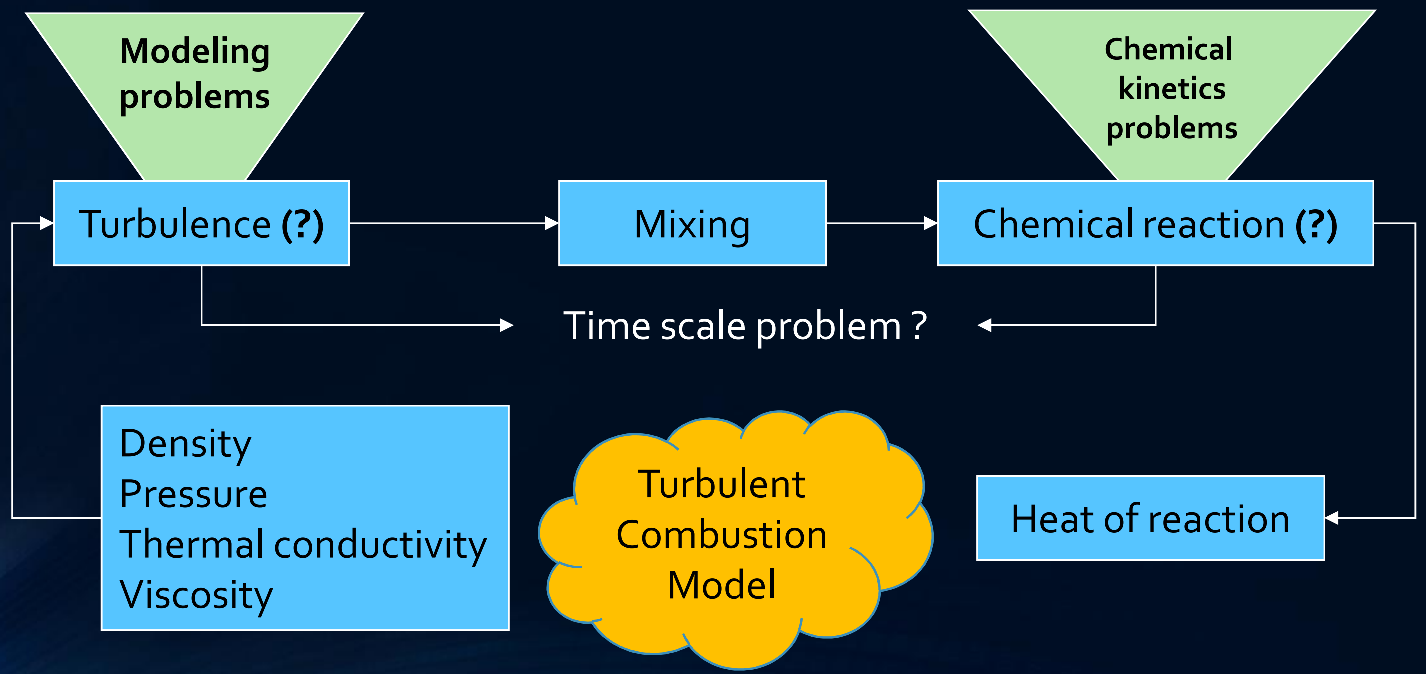
- Modeling goals of an ideal CFD turbulence combustion model are basically to achieve accurate predictions of:

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**



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	Mixing controlled models	Detailed chemistry models

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)

Coupling

Technique

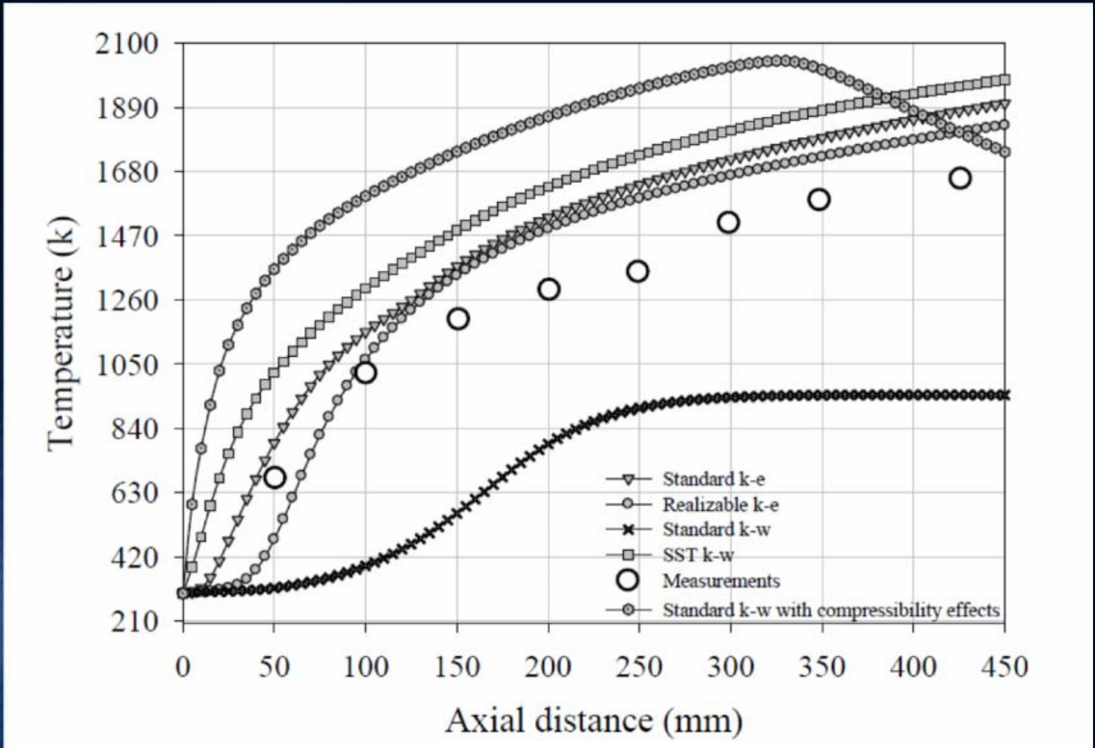
Eddy break-up theory
- EDM
- EDC

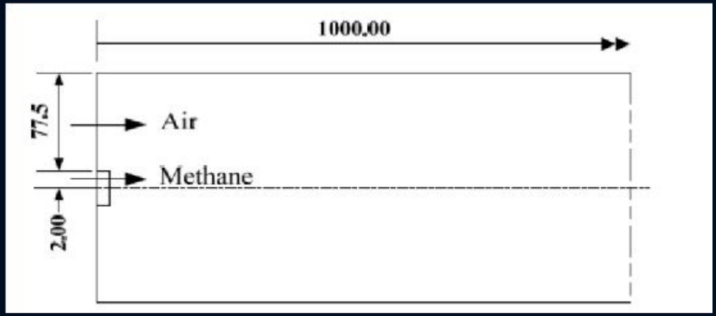
Flamelet theory
- Flamelet model

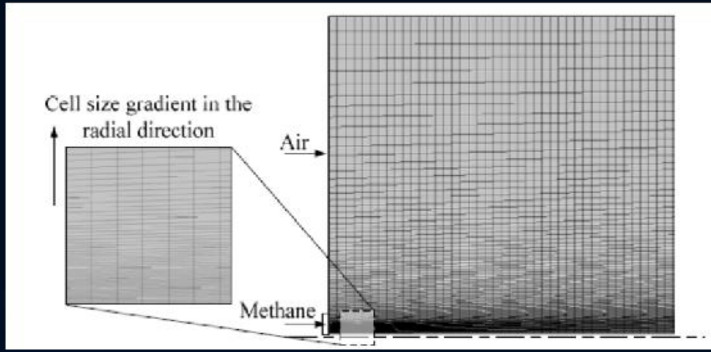
Detailed chemistry
- PDF model
- Detailed chemical kinetics

Chemical Reaction modeling approaches

EDM with RANS for Jet Flame Modeling







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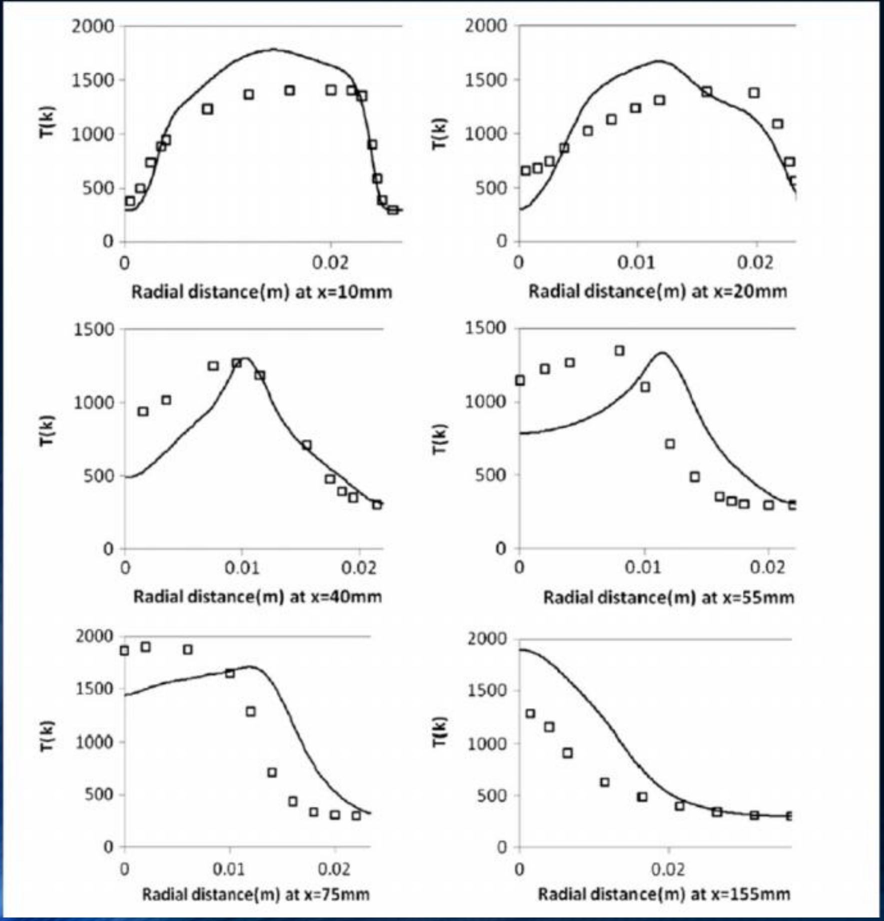
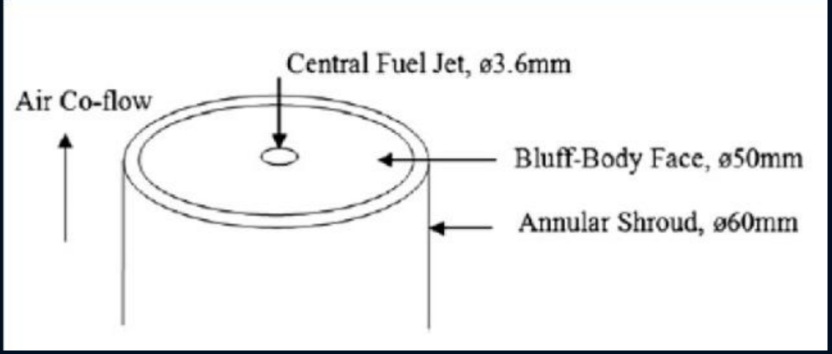
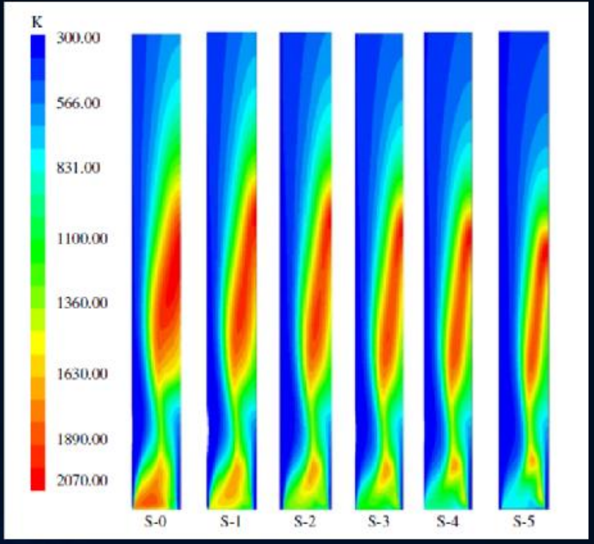
Flamelet Model with RANS for Hydrogen-Enriched Swirl Flame







Challenges and Prospects

Turbulence	Multiphase flow	Chemical reaction
- 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