PRESENTATION TOPICS

- Introduction;
- Combustion Phenomenology;
- Combustion Modeling;
- Reaction Mechanism;
- Radiation;
- Case Studies;
Introduction

• Combustion has many important applications in industry;

• The correct phenomenon representation is important to predict equipment efficiency and non-desired behavior;

• There are several models in both FLUENT and CFX for different combustion regimes;

• The challenge in combustion modeling is to describe reaction and fluid flow, which evolution happens in different timescales;
Combustion Phenomenology

- Chemistry
  - stoichiometry
  - chemical kinetics
- Heat transfer
  - conduction, convection, radiation
  - buoyancy
- Mass transfer
- Turbulence
  - turbulence-chemistry interaction
- Compressibility
- Particle transport
Combustion Phenomenology

- The mixing between oxidant and fuel in the domain controls the decision of which model can be applied;
Combustion Phenomenology

• Combustion depends directly on Mixing and Chemistry. The relative speed of chemical reaction to mixing is crucial;
  – Fast Reactions: reaction progress is limited by turbulent mixing;
  – Slow Reactions: reaction progress is limited by chemical kinetics;

• The Damköhler Number (Da) represents the ratio of the characteristic turbulent mixing time to the characteristic chemical reaction time

\[
Da = \text{Mixing Time} / \text{Chemical Time}
\]

– For Da >> 1, Chemical reaction rates are fast
– For Da << 1, Chemical reaction rates are slow
Combustion Modeling

- Fast Chemistry (Da >> 1)
  - Non-premixed Combustion
    - PDF Flamelet Model
    - Eddy-Dissipation/Finite-Rate Chemistry Model
    - Eddy-Dissipation Model
  - Premixed Combustion
    - BVM: Burning Velocity Model
    - Eddy-Dissipation/Finite-Rate Chemistry Model
    - Eddy-Dissipation Model
  - Partially Premixed Combustion
    - BVM: Zimont sub-model
    - Eddy-Dissipation/Finite-Rate Chemistry Model
    - Eddy-Dissipation Model

- Slow Chemistry (Da << 1)
  - Detailed Kinetic
    - Eddy-Dissipation-Concept Model (FLUENT)
    - Finite-Rate Chemistry Model
    - Eddy-Dissipation/Finite-Rate chemistry
  - Non-Detailed Kinetic
    - Finite-Rate Chemistry Model

- Slow Chemistry (Da <= 1)
  - BVM: Zimont sub-model
    - Eddy-Dissipation/Finite-Rate Chemistry Model
    - Eddy-Dissipation Model

- Premixed Combustion
  - BVM: Burning Velocity Model
  - Eddy-Dissipation/Finite-Rate Chemistry Model
  - Eddy-Dissipation Model
Combustion Modeling: Reaction Rate-Based Models

- Finite Rate Chemistry Model: the effect of turbulent fluctuations are ignored, and reaction rates are determined by Arrhenius kinetic expressions.

- Eddy-dissipation model: reaction rates are assumed to be controlled by the turbulence
  - Expensive Arrhenius chemical kinetic calculations can be avoided.
  - The model is computationally cheap
  - For realistic results, only one or two step heat-release mechanisms should be used.

- Eddy-dissipation-concept model: detailed Arrhenius chemical kinetics can be incorporated in turbulent flames
  - Note that detailed chemical kinetic calculations are computationally expensive.
  - FLUENT

- Eddy-dissipation/Finite-Rate chemistry model: reaction rate is evaluated by both models and the smallest is chosen
Combustion Modeling: PDF Flamelet

- The combustion is assumed to occur in thin sheets called flame-lets. The turbulent flame is treated as an ensemble of laminar flame-lets;

- Species transport equations not solved;

- Only applicable to a two-feed system (Fuel and Oxidizer);

- Only two scalar quantities (Mixture Fraction and Mixture Fraction Variance) solved along with the momentum and energy equations;

- The combustion species extracted from a pre-calculated library as a function of mixture fraction and strain rate;

- Can model a large number of intermediate species and radicals involved in the combustion process (cinéticas complexas).
Combustion Modeling: Burning Velocity Model

- In premixed and partially premixed flames, the flame-lets have a discontinuity between the burnt and the un-burnt regions;
- A Flame Front Tracking approach is needed;
- A scalar (Reaction Progress) subdivides the flow field in two different areas, the burnt and the un-burnt mixture;
- The reaction progress is the probability of the reacted state of the fluid along the time;
- Burnt regions are treated similar to a diffusion flame whereas un-burnt region is represented by the cold mixture;
- The effect of turbulent fluctuations on the combustion process is taken into account statistically;
Reaction Mechanism

- Kinetic plays an important role in flame discretization and emission evaluation;

- Both ANSYS CFX and ANSYS Fluent present single-step and two-step reactions;

- There are also special reaction mechanisms for NOx-based species;

- ANSYS Fluent can import detailed kinetic mechanisms from Reaction Design’s Chemkin;
Radiation

- Radiation modeling is important to represent temperature and heat flux fields accurately in combustion simulation;

- The main heat transfer mechanism in equipments like furnaces in near walls is radiation;

- There are many radiations models in ANSYS CFX and ANSYS Fluent;

- Some models can predict the absorption and reemission of radiation intensity performed by the burned gases like CO2 and H2O;
Case Studies

- IFRF Swirling Pulverized Coal Flame
  - IFRF industrial scale furnace;
  - Eddy Dissipation model (fuel: pulverized coal);
  - Standard $k-\varepsilon$ turbulence model, standard wall functions;
  - $P1$ with gas-phase absorption coefficient dependence;
  - Thermal and Fuel NOx mechanism;
  - Unstructured hexahedral mesh
    - 70k cells before adaption;
    - 260k cells after region adaption near inlet;
Case Studies
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Tracks of 1μm particles, colored by particle temperature (K)
Case Studies

- GE LM-1600 Gas Turbine Combustor
  - Non-premixed, natural gas;
  - 12.8 MW, 19:1 pressure ratio;
  - Multi-block hexahedral mesh (286 K);
  - Standard $k-\varepsilon$ turbulence model;
  - Laminar Flamelet model: 22 species, 104 reactions reduced GRI-MECH 1.22 mechanism;
  - Differential diffusion ($Le$ effects) included;
Case Studies
Case Studies

- Mean NO ppm, wet
- Mean mass fraction of OH
- Path ribbons colored by temperature (K)
Case Studies

\[ \text{NO exit flux} = 10^6 \frac{\int \rho X_{\text{NO}} \vec{V} \cdot d\vec{A}}{\int \rho \vec{V} \cdot d\vec{A}} \]