CFD Modelling of Thermal Conversion of Biomass in Residential Stoves

First Meeting with Industry Sponsor

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Outline

Physical Model of Combustion Chamber in a Stove

Volatile (Gas Phase) Region

CFD Models for Combustion

Modelling of Solid Phase Region

Collaborations

Physical Model of Combustion Chamber in a Stove

- Multi-region model is needed:
  1. Volatile region (gas phase)
  2. Wood log region
  3. Char region
- Different equations for different volume fields (regions) and for different surface fields (region boundaries) to be solved
- Modelling challenges: multi-region, multiphase (modelling of soot), multi-component, eq. stiffness, high CPU effort, validation procedure (experimental part), uncertainty of log parameters (composition, moisture, wood log form and orientation, etc.), conjugate heat transfer, radiation, etc.

Modelling of Volatile (Gas Phase) Region

CFD Models for Combustion: Laminar Flames

- Equations (PDEs) to be solved iteratively:
  1. Navier-Stokes Equations: Continuity (ρ) & Momentum (ρu_j) - equations for non-reactive flows $+$
  2. Energy Equation (one of various forms) $+$
  3. either:
     - Species continuity equations (Y_k) (k equations for k species)
     - Transport equation for mixture fraction (Z) ($Z = 1$ - fuel stream; $Z = 0$ - oxidiser stream)
- Species continuity equations contain source terms (species chemical reaction rate, $\dot{\omega}_k$)

Calculating Reaction Rate, $\dot{\omega}_k$

- Finite-rate kinetics
- The species chemical reaction rate calculated through the sum of the Arrhenius reaction sources over N reactions:

$$\dot{\omega}_k = M_{x,k} \sum_{r=1}^{N} \bar{R}_{k,r} \tag{1}$$

where

$$\bar{R}_{k,r} = (\nu''_{k,r} - \nu'_{k,r}) \left[k_{f,r} \prod_{j=1}^{N} [C_{j,r}]^{\nu'_{k,r}} - k_{b,r} \prod_{j=1}^{N} [C_{j,r}]^{\nu''_{k,r}} \right] \tag{2}$$

CFD Models for Combustion: Turbulent Flames

- Unclosed terms in PDEs to be modeled:
  1. In momentum eq.: Reynolds stresses ($\widetilde{u_i'' u_j''}$)
  2. either:
     - species continuity eq., species turbulent fluxes ($\widetilde{u_i'' Y_k''}$)
     - mixture fraction eq., mixture fraction turbulent fluxes ($\widetilde{u_i'' Z''}$)
  3. In enthalpy eq., enthalpy turbulent fluxes ($\widetilde{u_i'' h_s''}$)
- Source terms in PDEs to be modelled:
  1. In species continuity eq., species mean chemical reaction rates ($\bar{\dot{\omega}}_k$); heat release term in energy eq. ($\bar{\dot{\omega}}_T = -\sum_{k=1}^{N} \Delta h_{f,k}^o \bar{\dot{\omega}}_k$) is known from tabulations

CFD Models for Combustion: Turbulent Flames

- Modelling (closing) the unclosed terms:
  1. Reynolds stresses ($\widetilde{u_i'' u_j''}$): by classical turbulence models: zero, one and two-equation models (RANS approach)
  2. Turbulent fluxes (scalar transport) ($\widetilde{u_i'' Y_k''}$ and $\widetilde{u_i'' Z''}$): by using a gradient assumption
  3. Chemical reaction rate term ($\bar{\dot{\omega}}_k$): key difficulty for non-premixed combustion

RANS of Turbulent Non-premixed flames

- Two basic approaches for modelling:
  1. **Primitive variable method**: solve for $\tilde{Z}$, $\widetilde{Z''^2}$, ... and for flow variables ($\bar{\rho}$, $\tilde{u}_i$, ...) and deduce T and Y_k from library (for flamelets or for laminar flames)
     - Balance equations for species mass fractions and for temperature are not needed
     - Reaction rates $\bar{\dot{\omega}}_k$ are not present and, therefore, do not need to be modelled
     - Less time consuming
     - Valid only under restrictive conditions
  2. **Reaction rate approach**: Solve balance eq. for species mass fractions and temperature. Reaction rates $\bar{\dot{\omega}}_k$ need modelling

Reaction Rate Approach: Modelling the Mean Reaction Rates, $\overline{\dot{\omega}}_k$

- Infinitely fast chemistry (*"mixed is burnt"*)
  1. Eddy Break-Up model (EBU)
  2. Eddy Dissipation Model (EDM)
- Finite rate chemistry
  1. Eddy Dissipation Concept (EDC)
  2. Presumed PDF flamelet model
  3. Flame surface density flamelet models
  4. Full statistical point models

Eddy Dissipation Concept

- Often used in industry for modelling combustion of biomass volatiles
- Introduced by Magnussen in 1981, [1]. Many variations are made for specific cases since then
- Based on Kolmogorov's energy cascade model; the combustion takes place in *fine structures*, i.e. on dissipating scales
- Convenient to account for both *Infinitely Fast Chemistry* and *Finite-Rate Chemistry*

Modelling of Solid Phase Region

Solid Phase Region (Wood + Char)

- Wood pellets and wood chips are mostly modelled
- Modelling of thermally thick biomass particles (Mehrabian et al., [2])
  - Wood particles modelled as cylinders and spheres
  - Each particle contains four layers (subregions) (from centre outwards):
    1. moist wood,
    2. dry wood,
    3. char and
    4. ash
- Other notable research by: Di Blasi, Galgano, ...

Collaborations

- Graz, Austria: Bioenergy2020+ & TU Graz
  - Bioenergy2020+:
    - Research, development and demonstration in the field of biomass combustion
    - Experimental facilities
    - `https://www.bioenergy2020.eu/`
- Possible:
  - Politecnico di Milano
  - ...

References

B. F. Magnussen. On the structure of turbulence and a generalized eddy dissipation concept for chemical reaction in turbulent flow. *19th Americal Institute of Aeronautics and Astronautics Aerospace Science Meeting*, 1981.

R. Mehrabian, S. Zahirovic, R. Scharler, I. Obernberger, S. Kleditzsch, S. Wirtz, V. Scherer, H. Lu, and L. L. Baxter. A CFD model for thermal conversion of thermally thick biomass particles. *Fuel Processing Technology*, 95:96–108, 2012.