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Implementations of bivariate population balance equations in CFD codes for modelling nanoparticle formation in turbulent flames

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Introduction

Formation of nanoparticles in flames

- High pressurized and hypersonic flames (high equivalence ratio)
- In the situations in which the combustion process cannot be computed with elementary equations

Soot formation

- Production of soot formation via: nucleation, aggregation, growth, and oxidation

Soot formation (undesired particulate matter)

- Epidemiological studies have demonstrated that particulate matter has an impact on human health even at low concentrations
- Both aggregates with size of the order of nanometer and smaller also formed in the early stages of the process (nucleation) can be toxic
- Radiative properties of soot nanoparticles increase with size

It is important to be able to accurately predict the evolution of the size distribution and morphology of soot particles during the combustion process.

The Population Balance Equation (PBE)

\[
\frac{d n_i}{d t} + \nabla \cdot (n_i \mathbf{u}) = \mathcal{K}_i - \mathcal{D}_i \frac{d}{d x} \left( \frac{n_i}{\beta p} \right) + \mathcal{S}_i
\]

- \( n_i \) is the number density function of the size class
- \( \mathcal{K}_i \) is the production rate due to partial differential source terms
- \( \mathcal{D}_i \) is the coagulation coefficient
- \( \mathcal{S}_i \) is the growth rate due to chemical reactions

The solution of the PBE is not trivial. When it has to be coupled with CFD computations, the solution technique has to be adapted to have low computational cost (number of additional transport equations to be solved).

Only methods based on the moments approach are suitable to be coupled with CFD for the solution of PBE.

The bivariate PBE, in terms of particle volume and surface area, is important to model the evolution of soot particle morphology.

When the monovariate PBE is solved, we have to make some simplifying assumptions:
- Superposition of constant C, in the white domain
- No use of an algebraic model to take into account changes in C, due to aggregation and restructuring (Kreisheit et al. 2007)

Modelled of particle morphology

- Aggregation time: \( t_{agg} = \frac{1}{k_{agg}} \)
- Restructuring time: \( t_{rstr} = \frac{1}{k_{rstr}} \)

The source term (1/4) determines the evolution of moments due to nucleation, aggregation, molecular growth, oxidation, and restructuring.

The Direct Quadrature Method of Moments (DQ MOM)

- The accurate modelling of soot formation requires the accurate modelling of velocity, temperature and composition profiles in the flame: Computational Fluid Dynamics

The accurate solution of the PBE is a challenging task. The Direct Quadrature Method of Moments (DQ MOM) is a very promising approach for solving the PBE in CFD codes, for simple homogeneous aggregating and restructuring systems.

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The knowledge of the probability distribution function of composition and temperature allows to compute the averaged chemical source term.

The Bivariate Population Balance

\[
\begin{align*}
\frac{d n_{11}}{d t} &= \mathcal{K}_{11} - \mathcal{D}_{11} \frac{d}{d x} \left( \frac{n_{11}}{\beta_{11}} \right) + \mathcal{S}_{11} \\
\frac{d n_{12}}{d t} &= \mathcal{K}_{12} - \mathcal{D}_{12} \frac{d}{d x} \left( \frac{n_{12}}{\beta_{12}} \right) + \mathcal{S}_{12} \\
\frac{d n_{21}}{d t} &= \mathcal{K}_{21} - \mathcal{D}_{21} \frac{d}{d x} \left( \frac{n_{21}}{\beta_{21}} \right) + \mathcal{S}_{21} \\
\frac{d n_{22}}{d t} &= \mathcal{K}_{22} - \mathcal{D}_{22} \frac{d}{d x} \left( \frac{n_{22}}{\beta_{22}} \right) + \mathcal{S}_{22}
\end{align*}
\]

The Bivariate Population Balance

- Two independent variables: Particle Volume (\( V \)) and Surface Area (\( S \))
- The number density function is approximated as follows:

Appr: \[ n(V, S) \approx n_{11}(V, S) + n_{12}(V, S) + n_{21}(V, S) + n_{22}(V, S) \]

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- The number density function is approximated as follows:

\[ n(V, S) \approx n_{11}(V, S) + n_{12}(V, S) + n_{21}(V, S) + n_{22}(V, S) \]

The source terms for weights and oblique are calculated solving a linear algebraic system obtained from the population balance written as a balance equations for moments, after the application of the quadrature approximation:

\[ (1 - k) \sum_{i} n_i = \sum_{i} \mathcal{K}_i - \sum_{i} \mathcal{D}_i \frac{d}{d x} \left( \frac{n_i}{\beta p} \right) + \sum_{i} \mathcal{S}_i \]

Simplified kinetics for nucleation, growth, oxidation and aggregation lead to good results in the flame under investigation.

Conclusions

- The DQ MOM is a valid approach for the solution of the population balance equation within a CFD code, both in the monovariate and in the bivariate case.
- Simplified kinetics for nucleation, growth, oxidation and aggregation lead to good results in the flame under investigation.
- In order to take into account properly the evolution of particle morphology (fractal dimension) is it important to solve the bivariate population balance, i.e., to follow the evolution of both particle volume and surface area.
- Future Developments

- More detailed investigation of nucleation, growth, oxidation and aggregation rates, with particular attention to the dynamics of nanoparticles, and validation with other turbulent flames.
- Validation of the model with experimental data on soot particle size distribution in laminar flows.