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

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1 Introduction

Formation of nanoparticles in flames

- High premixed and counter-rotated flames (high equivalence ratio)
- In the situations in which the combustion process cannot be computed separately

- Soot formation (undesired particulate matter)

- Formation of soot nuclei produces soot aggregates and aggregates

- 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 micrometers and smaller and also formed in the early stages of the process (nanoaggregates) can be toxic.

- Radiative properties of soot nanoparticles (e.g., extinction)

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

2 Turbulent combustion and CFD

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

The turbulence model is Reynolds Averaged Navier-Stokes equations.

3 The Population Balance Equation (PBE)

\[ \frac{d n_i(x,t)}{dt} = \frac{1}{\epsilon} \int_0^\infty \int_0^\infty \int_0^\infty \frac{n_j(x',t')}{n_j(x,t')} \left( \frac{\partial n_j(x,t')}{\partial t} + \frac{\partial \mathbf{u}_j(x,t')}{\partial x} \cdot \nabla n_j(x,t') - \epsilon \frac{\partial n_j(x,t')}{\partial x} \right) \delta(x-x') \delta(t-t') \frac{dx'dt'}{2\pi} \]

- \( n_i(x,t) \) is the number density function of the particle population.
- \( \mathbf{u}_j(x,t) \) are the properties identifying the status of each aggregate, e.g., diameter, volume, surface area, velocity, composition, age.

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 PBEs.

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

4 Modelling of particle morphology

The algorithm generates and tracks the computational cell distribution of a lattice of cubes (in 1D), and 3D) with a computational cell size controlled by the size of the particle.

- Soot aggregates have fractal properties: fractal dimension, \( D_f \) (scaling exponent)

The solution of a finite 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:

a) Superposition of constant \( D_f \) in the whole domain

b) \( D_f \) constant

5 The Direct Quadrature Method of Moments (DQ MOM)

The number density function is approximated as follows:

\[ n_i(x,t) \approx \sum_{k=1}^N A_k \rho_k(x,t) \]

where \( A_k \) and \( \rho_k(x,t) \) are the moments of the particle population.

The source terms for weights and significance 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.

6 The Bivariate Population Balance

The number density function is approximated as follows:

\[ n_{ij}(x,t) \approx \sum_{k=1}^N A_{ijk} \rho_{ijk}(x,t) \]

where \( A_{ijk} \) and \( \rho_{ijk}(x,t) \) are the bivariate moments of the particle population.

7 Results

Case study: the non-premixed ethylene-air turbulent flame A (Kirt & Horiuti, 1937)

- Soot volume fraction

- Soot volume fraction in the reaction zone

8 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) it is important to solve the bivariate population balance, i.e., to follow the evolution of both particle volume and surface area.

- \( D_f \) is not a unique number of the character of the moments to be tracked, and affects both accuracy and numerical stability.

- The method has been validated by comparison with the results of a Direct Simulation Monte Carlo code, for simple homogeneous aggregating and restructuring systems.

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 flames.