[Proceeding] Novel modelling approaches for turbulence-chemistry interaction and particle formation in flames

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Novel modelling approaches for turbulence-chemistry interaction and particle formation in flames

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Introduction

The accurate modelling of particle formation in flames is becoming important in a wide range of applications:

- Soot formation (undesred particulate matter)
- Flame aerosol synthesis (production of tailored materials, e.g. TiO_2)

Modelling of turbulent combustion requires an accurate description of turbulence-chemistry interaction in order to obtain reliable temperature and composition profiles

In order to obtain detailed information on particle features (size, morphology, composition, etc.) it is necessary to model particle dynamics

The stochastic nature of both turbulence and some processes involved in particle dynamics suggests to statistically solve these problems in terms of the fluid probability density function (PDF) and of the particle number density function (NDF)

Turbulence-chemistry interaction

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

Turbulence modelling (Reynolds Averaged Navier-Stokes equations)

- continuity $$\frac{\partial \overline{\rho}}{\partial t}+\frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{U}_i\right)=0$$
- momentum $$\frac{\partial}{\partial t}\overline{\rho}\tilde{U}_i+\frac{\partial}{\partial x_.}\overline{\rho}\tilde{U}_i\tilde{U}_j+\frac{\partial}{\partial x_.}\overline{\rho}\widetilde{u_i u_j}=-\frac{\partial \overline{p}}{\partial x_.}+\nu\frac{\partial^2\overline{\rho}\tilde{U}_i}{\partial x_.\,\partial x_.}$$
- scalars $$\frac{\partial}{\partial t}\overline{\rho}\tilde{\Phi}_\alpha+\frac{\partial}{\partial x_i}\overline{\rho}\tilde{\Phi}_\alpha\tilde{U}_i+\frac{\partial}{\partial x_i}\overline{\rho}\widetilde{\phi_\alpha u_i}=\Gamma_t\frac{\partial^2\overline{\rho}\tilde{\Phi}_\alpha}{\partial x_i\partial x_i}+\widetilde{S(\Phi)}$$

The chemical reaction is affected by turbulent fluctuactions of both temperature and concentration. → The knowledge of the **probability density function** of composition and temperature allows to compute the averaged chemical source term.

Presumed PDF methods: the functional shape of the PDF is assumed

Particle formation

The accurate modelling of particle formation in flames requires the solution of the **Population Balance Equation (PBE)**, in order to describe the evolving distribution of the particle state variables of interest:

$$\frac{\partial\tilde{n}(\xi;\mathbf{x},t)}{\partial t}+\frac{\partial}{\partial x_i}\widetilde{U}_i\tilde{n}(\xi;\mathbf{x},t)-\frac{\partial}{\partial x_i}\left[(\Gamma+\Gamma_t)\frac{\partial\tilde{n}(\xi;\mathbf{x},t)}{\partial x_i}\right]=\widetilde{S(\xi;\mathbf{x},t)}$$

where $\tilde{n}(\xi;\mathbf{x},t)$ is the **number density function** of the particle population, in terms of a number of **internal coordinates (ξ)**, which are properties identifying the status of each particle (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 simple and 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.

$$\widetilde{m_k}(\mathbf{x},t)=\int_0^{+\infty}\tilde{n}(\xi;\mathbf{x},t)\,\xi^k d\xi \quad\rightarrow\quad \frac{\partial\widetilde{m_k}(\mathbf{x},t)}{\partial t}+\widetilde{U_i}\frac{\partial\widetilde{m_k}(\mathbf{x},t)}{\partial x_i}-\frac{\partial}{\partial x_i}\left[\Gamma_t\frac{\partial\widetilde{m_k}(\mathbf{x},t)}{\partial x_i}\right]=\widetilde{S(\mathbf{x},t)}$$

The source term $\widetilde{S(\mathbf{x},t)}$ determines the evolution of moments due to **nucleation**, **aggregation**, **molecular growth**, **oxidation** and **restructuring**.

The Finite-Mode PDF model

The PDF is described by a sum of Dirac delta functions (each representing a reacting or non-reacting environment):

$$f_\Phi(\mathbf{\Psi};\mathbf{x},t)=\sum_{n=1}^{N_e}p_n(\mathbf{x},t)\prod_{\alpha=1}^{N_s}\delta\left[\psi_\alpha-\langle\phi_\alpha\rangle_n(\mathbf{x},t)\right]$$

Probabilities (volume fractions) of modes (environments)

$$\frac{\partial p_n}{\partial t}+\tilde{U}_j\frac{\partial p_n}{\partial x_j}-(\Gamma+\Gamma_t)\frac{\partial^2 p_n}{\partial x_j\partial x_j}=G_n(\mathbf{p})+c_n^p$$

Molecular mixing

Spurious terms due to the finite-mode representation

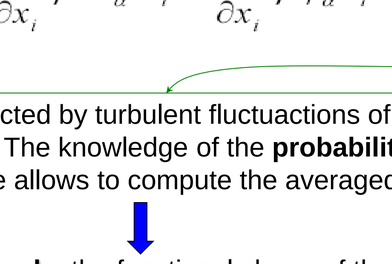
Weighted concentrations

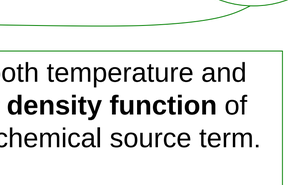
$$\langle s_\alpha\rangle_n=p_n\langle\phi_\alpha\rangle_n$$

$$\frac{\partial\langle s_\alpha\rangle_n}{\partial t}+\tilde{U}_j\frac{\partial\langle s_\alpha\rangle_n}{\partial x_j}-(\Gamma+\Gamma_t)\frac{\partial^2\langle s_\alpha\rangle_n}{\partial x_j\partial x_j}=M_{n,\alpha}(\mathbf{p},\mathbf{s})+p_nS(\langle\varphi\rangle_n)+c_{n,\alpha}^s$$

N=3

The reaction occurs only in the mixed environment (3).





The Direct Quadrature Method of Moments (DQMOM)

Closure of the source term → Quadrature approximation

$$\tilde{n}(\xi;\mathbf{x},t)\approx\sum_{\alpha=1}^{N}w_\alpha(\mathbf{x},t)\prod_{i=1}^{M}\delta\left[\xi_i-\xi_{i\alpha}(\mathbf{x},t)\right]$$

$$m_{k_1,k_2,\ldots,k_M}=\int_{-\infty}^{\infty}\xi_1^{k_1}\int_{-\infty}^{\infty}\xi_2^{k_2}\cdots\int_{-\infty}^{\infty}\xi_M^{k_M}\tilde{n}(\xi;\mathbf{x},t)\,d\xi_1 d\xi_2\cdots d\xi_M\approx\sum_{\alpha=1}^{N}w_\alpha\prod_{i=1}^{M}\xi_{i\alpha}^{k_i}$$

It is possible to calculate the values of **weights** and weighted **abscissas** $\varsigma_{i,\alpha}=w_\alpha\xi_{i,\alpha}$ of the delta functions, forcing them to yield known values of the moments, directly solving the transport equations:

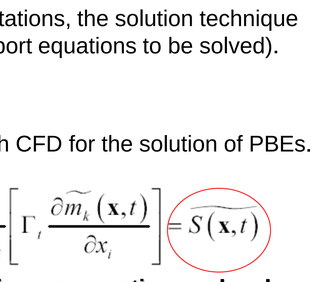
$$\frac{\partial w_\alpha}{\partial t}+\frac{\partial}{\partial x_j}\left(\tilde{U}_j w_\alpha\right)-\frac{\partial}{\partial x_j}\left[(\Gamma+\Gamma_t)\frac{\partial w_\alpha}{\partial x_j}\right]=a_\alpha \qquad \frac{\partial\varsigma_{i,\alpha}}{\partial t}+\frac{\partial}{\partial x_j}\left(\tilde{U}_j\varsigma_{i,\alpha}\right)-\frac{\partial}{\partial x_j}\left[(\Gamma+\Gamma_t)\frac{\partial\varsigma_{i,\alpha}}{\partial x_j}\right]=b_{i,\alpha}$$

The source terms for weights and abscissas are calculated solving a ***linear algebraic system*** obtained from the population balance written as a balance equation for moments, after the application of the quadrature approximation; in the bivariate case:

$$\sum_{\alpha=1}^{N}\left[(1-k-l)\xi_{1,\alpha}^k\xi_{2,\alpha}^l a_\alpha+k\xi_{1,\alpha}^{k-1}\xi_{2,\alpha}^l b_{1,\alpha}+l\xi_{1,\alpha}^k\xi_{2,\alpha}^{l-1}b_{2,\alpha}\right]=\bar{C}_{k,l}+S_{k,l}^{(N)}$$

Spurious terms due to the finite-mode representation

Source terms for moments



Turbulent combustion: Results

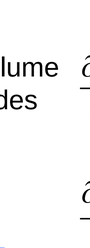
Flames studied in the framework of the International Workshop on Turbulent Non-premixed Flames

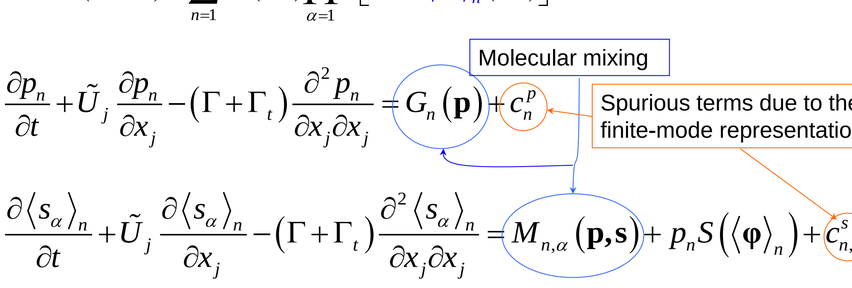
3E-Finite Mode PDF (4-step mechanism by Jones and Lindsted)
β-PDF (chemical equilibrium)
laminar flamelets (skeletal mechanism 17 species)

Location: 30 mm above the burner

Non Swirling Flame (Bluff body)

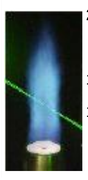
Fuel	CH_4/H_2 1:1
Jet velocity	118 m/s
Coflow velocity	40 m/s

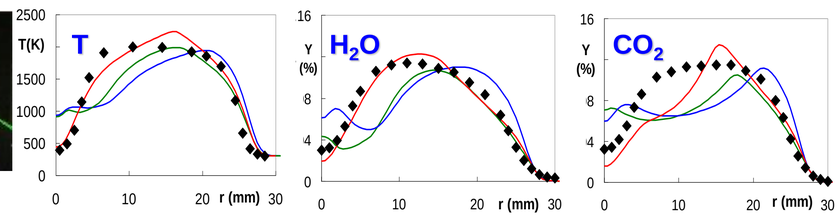




Swirling Flame (Sydney, Partially Premixed)

Fuel	CH_4/Air1 :2
Jet velocity	66.3 m/s
Air axial vel	16.26 m/s
Coflow velocity	20 m/s

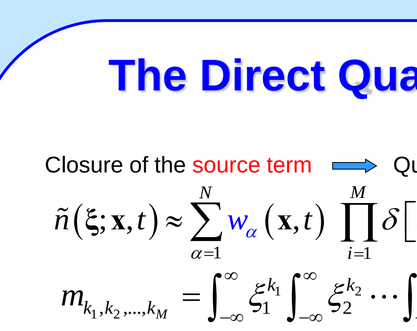


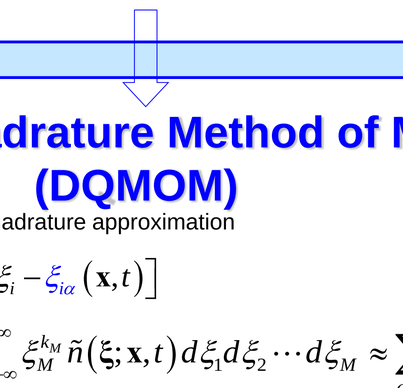


Soot formation: Results (bivariate PBE)

Case study: the non-premixed ethylene-air turbulent flame A (Kent & Honnery, 1987(*))

Soot volume fraction

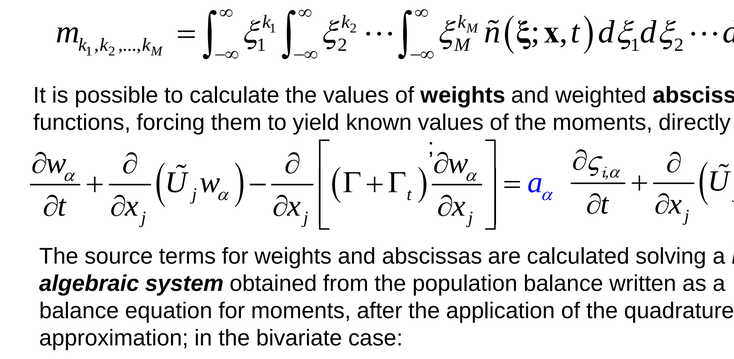




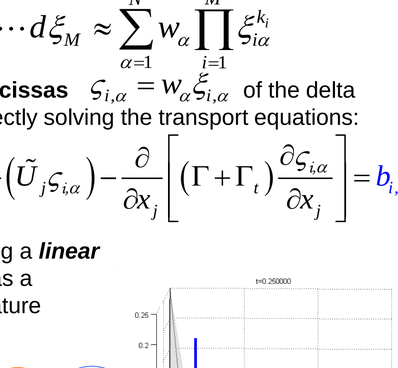
Bivariate simulation (V and A)

Monovariate simulation with algebraic model for fractal dimension

Artelt C., Schmid H.J., Peukert W. (2003). On the relevance of accounting for the evolution of the fractal dimension in aerosol process simulations. *Journal of Aerosol Science*, **34**, 511-534.



Projections of the nodes along the internal coordinates



(*) Kent J. H., and Honnery D. (1987). Soot and mixture fraction in turbulent diffusion flames. *Combustion Science and Technology*, **54**, 383-397.

Conclusions

In this work, two methods based on a similar description of the PDF and the NDF, represented by a finite sum of Dirac delta functions, were successfully employed to solve the problem of turbulence-chemistry interaction in turbulent flames (finite-mode PDF method), and the population balance for modelling soot formation (Direct Quadrature Method of Moments, DQMOM).

Both methods appeared to be versatile and reliable tools, particularly suitable for CFD computation, presenting a good trade-off between accuracy and computational cost.

In particular:

- The **Finite-Mode PDF** model is suitable for modelling turbulence-chemistry interaction in flames
- The implementation of **finite rate chemistry** can be crucial to obtain good results, especially in the case of partially premixed flames.
- The **DQMOM** 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 soot **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.