Imperial College London

Combining LES with a detailed population balance model to predict soot formation in a turbulent non-premixed jet flame

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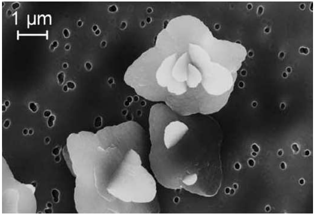
Outline

Introduction

Our objective is to model turbulent reacting flows with particle formation.

(a) A sooting jet flame [2].

(b) Cloud formation.



(c) $BaSO_4$ particles [1].

(d) Coal combustion.

Particle characteristics

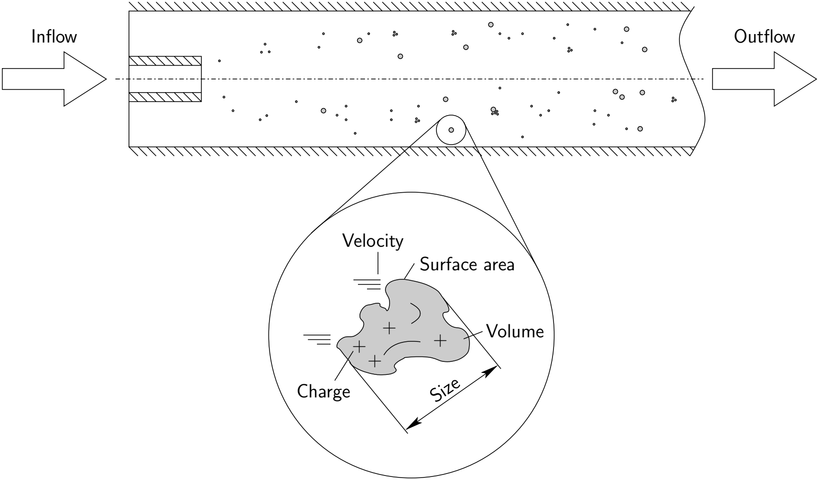


Figure: Polydisperse particles forming within a carrier flow through a pipe mixer.

Fluid and particulate phase

The evolution of the distribution $N(v, \mathbf{x}, t)$ can be described by the PBE

$$\frac{\partial N}{\partial t} + \frac{\partial\left(u_j N\right)}{\partial x_j} + \frac{\partial\left(GN\right)}{\partial v} = \frac{\partial}{\partial x_j}\left(\gamma_p \frac{\partial N}{\partial x_j}\right) + \dot{s} \qquad (1)$$

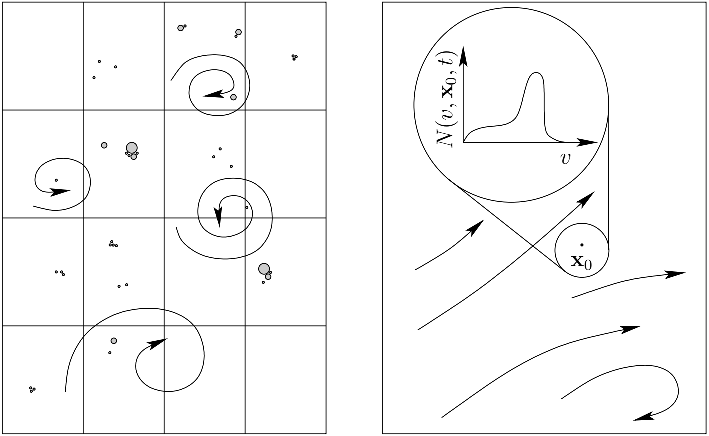
while the fluid phase composition $\mathbf{Y}(\mathbf{x}, t)$ evolves according to

$$\frac{\partial \rho \mathbf{Y}}{\partial t} + \frac{\partial\left(\rho u_j \mathbf{Y}\right)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho\gamma \frac{\partial \mathbf{Y}}{\partial x_j}\right) + \rho\dot{\boldsymbol{\omega}} \qquad (2)$$

where

- $\mathbf{u}(\mathbf{x}, t), G(\mathbf{Y}, v)$ Velocity field and particle growth rate
- $\gamma(\mathbf{x}, t)$, $\gamma_p(\mathbf{x}, t)$ Diffusivities
- $\dot{s}(\mathbf{Y}, N, v)$, $\dot{\boldsymbol{\omega}}(\mathbf{Y}, N)$ Production/destruction rates
- $\rho(\mathbf{x}, t) = \hat{\rho}(\mathbf{Y}(\mathbf{x}, t))$ Mixture density

Two main challenges



(a) PBE and turbulence model

(b) Discretization in v-space

Figure: Polydisperse particles forming within a carrier flow.

Turbulence-chemistry interaction

Based on the mass-based number density

$$N_\rho(v, \mathbf{x}, t) \equiv \frac{N(v, \mathbf{x}, t)}{\rho(\mathbf{x}, t)} \tag{3}$$

we consider the Joint scalars-number density *pdf*

$$f(\mathbf{y}, n; v, \mathbf{x}, t) = \langle \delta\left(\mathbf{y} - \mathbf{Y}(\mathbf{x}, t)\right) \delta\left(n - N_\rho(v, \mathbf{x}, t)\right) \rangle \tag{4}$$

Its density-weighted counterpart $\tilde{f}(\mathbf{y}, n; v, \mathbf{x}, t)$ obeys

$$\begin{aligned} \langle\rho\rangle \frac{\partial \tilde{f}}{\partial t} + \langle\rho\rangle \tilde{u}_j \frac{\partial \tilde{f}}{\partial x_j} + G \frac{\partial \tilde{f}}{\partial v} &= \frac{\partial}{\partial x_j}\left(\langle\rho\rangle \Gamma \frac{\partial \tilde{f}}{\partial x_j}\right) \\ &- \langle\rho\rangle \frac{\partial}{\partial y_i}\left(\dot{\omega}_i + \mathcal{M}_i\right) \tilde{f} - \langle\rho\rangle \frac{\partial}{\partial n}\left(\frac{\dot{s}}{\hat{\rho}} - n\frac{\partial G}{\partial v} + \mathcal{M}_p\right) \tilde{f} \end{aligned} \tag{5}$$

Statistically, Eq. (5) is equivalent to the stochastic process

$$\frac{\partial \boldsymbol{\theta}}{\partial t} = -\left(\tilde{u}_j + \sqrt{2\Gamma}\dot{W}_j\right) \frac{\partial \boldsymbol{\theta}}{\partial x_j} - G\frac{\partial \boldsymbol{\theta}}{\partial v} - \ldots + \mathbf{s} \tag{6}$$

LES-PBE-PDF framework

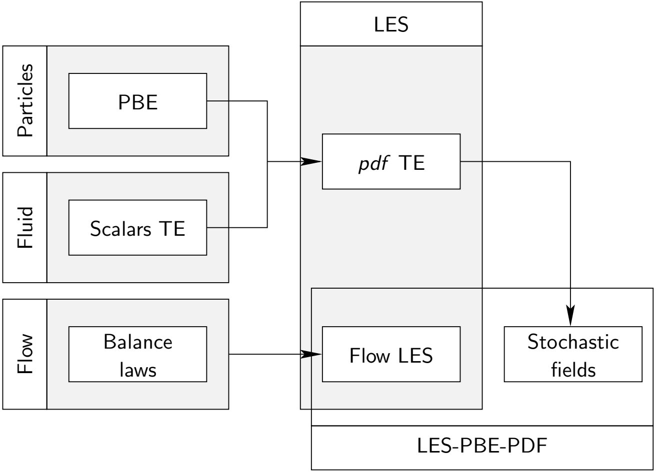


Figure: Illustrating the LES-PBE-PDF model (TE: Transport Equation).

Discretizing particle property space

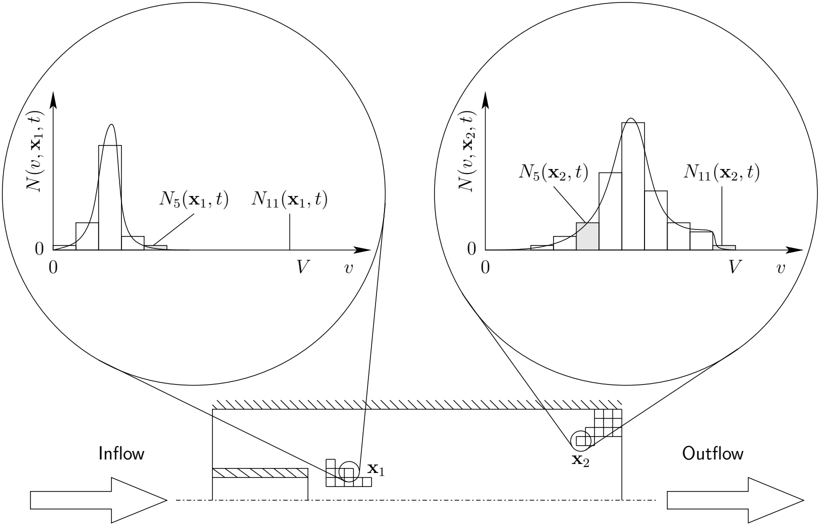


Figure: Illustrating the discrete number density fields $N_i(\mathbf{x}, t)$, $i = 1, \ldots, n + 1$.

An adaptive PBE discretization

- Construct a coordinate transformation $\bar{v} : (\tau, \mathbf{x}, t) \mapsto v$.
- Discretize the stochastic field equations on a fixed grid in τ-space.

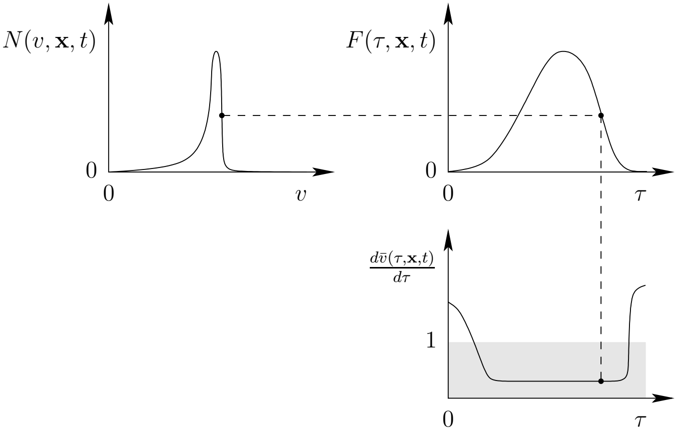


Figure: Illustrating the effect of a coordinate transformation.

Delft flame III

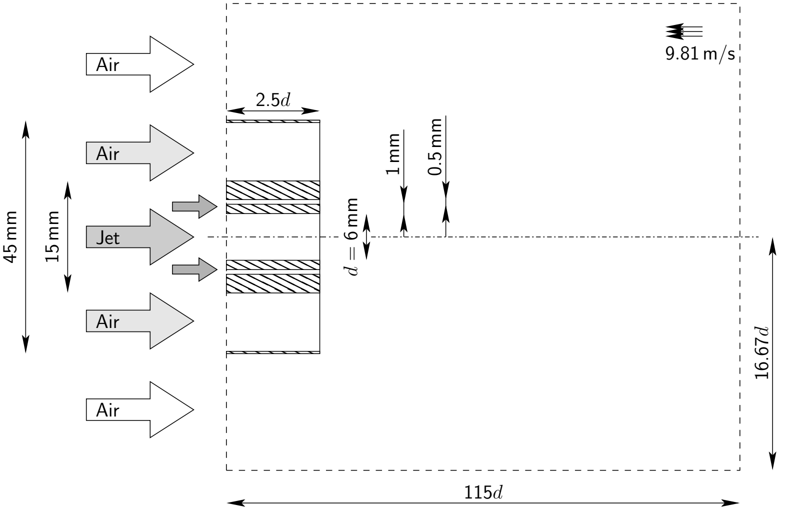


Figure: Schematic representation of the flow domain for the Delft flame III ($Re \approx 8370$).

Instantaneous fields

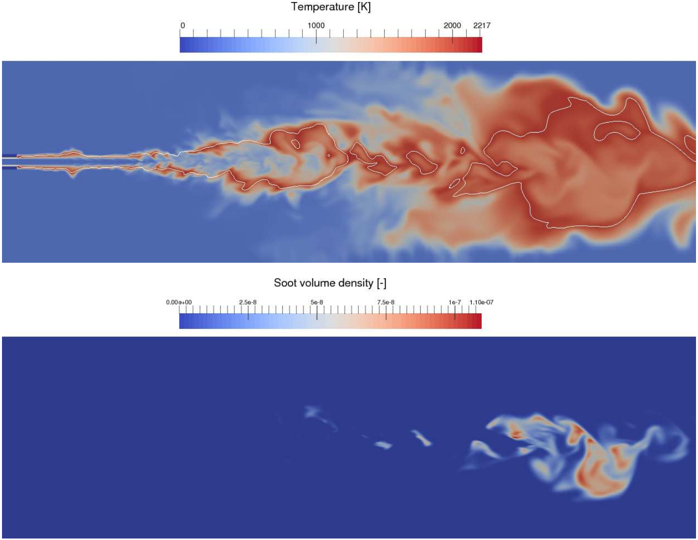


Figure: Temperature and stoichiometric mixture fraction as well as soot volume density.

Velocity and temperature in the near-field

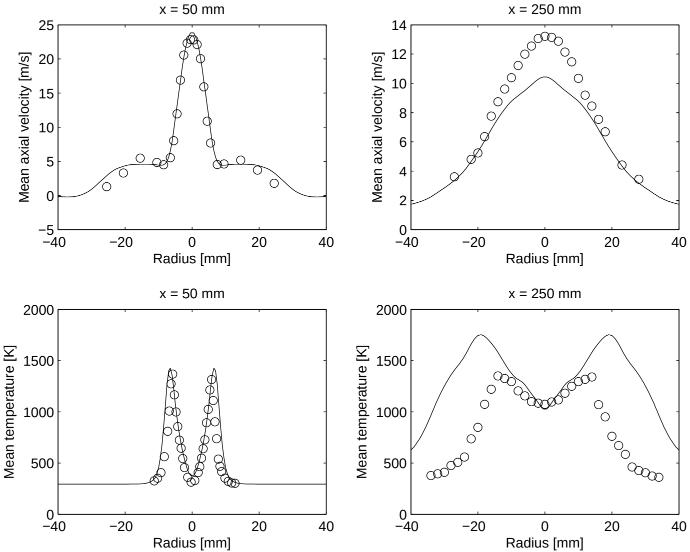


Figure: Comparing mean axial velocity and temperature with measurements.

Radially integrated soot volume fraction

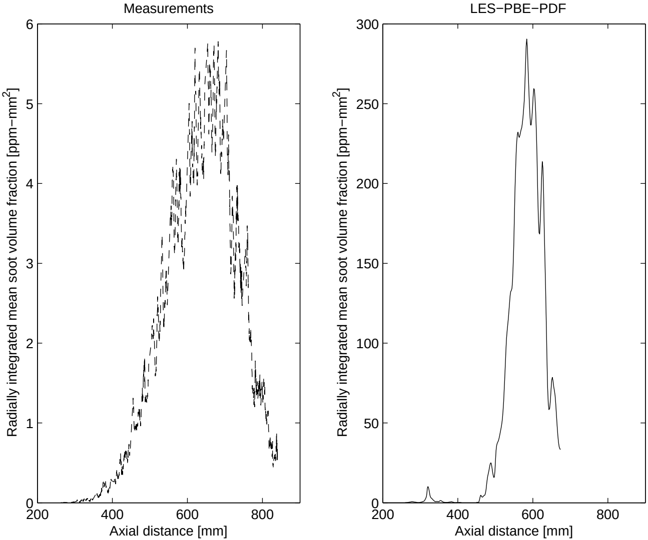


Figure: Comparing the radially averaged soot volume fraction with measurements.

Sample particle size distributions

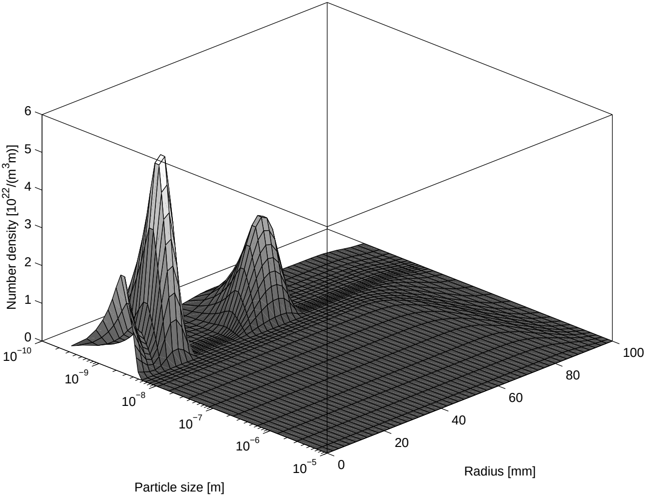


Figure: Instantaneous particle size distributions along the radius at $x = 480\,\text{mm}$.

Time measurements

Physical process	Average runtime
Scalar convection/diffusion	1.589 s
Gas-phase reaction	2.476 s
Particle phase reaction	2.411 s
Flow field	1.696 s
All processes	8.172 s

Table: Average runtime for advancing the LES-PBE-PDF model by one time step of $\Delta t = 10^{-6}$ s on an Intel Xeon E5-2660 v2 processor.

Concluding remarks

Advantages of the LES-PBE-PDF model:

- Fully Eulerian solution scheme
- Easy to implement (or to combine with existing software)
- Physical model distinct from numerical solution scheme
- Predict entire particle property distribution
- Accommodate fluid/particle phase kinetics without approximation

Advantages of our explicit adaptive grid approach:

- Easy to implement
- Can be combined with any direct discretization scheme in τ-space
- Can be combined with any time integration scheme
- Resolves sharp features
- Converges at an accelerated pace

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Selected references

[1] B. Judat and M. Kind. “Morphology and internal structure of barium sulfate–derivation of a new growth mechanism”. In: *Journal of Colloid and Interface Science* 269.2 (Jan. 2004), pp. 341–353.

[2] M. Köhler, K. P. Geigle, W. Meier, B. M. Crosland, K. A. Thomson, and G. J. Smallwood. “Sooting turbulent jet flame: characterization and quantitative soot measurements”. In: *Applied Physics B: Lasers and Optics* 104.2 (2011), pp. 409–425.