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A conservative finite volume method for solving the population balance equation, and application to combustion issues

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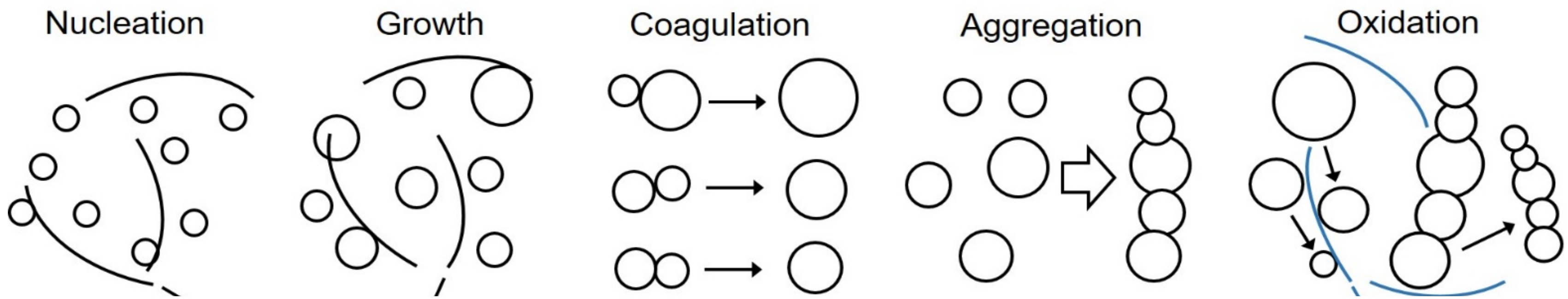
Challenges in modelling soot formation in combustion

Reacting flows carry a particulate phase in a number of engineering applications – sooting flame：

◻ Aerosol dynamics

- Nucleation
- Surface processes (growth and oxidation)
- Inter-particle processes (coagulation, aggregation)
- Breakage



◻ Aerosol-turbulence interaction

- Unknown corelations arising from interaction between particles, species and flow

Overview of this research

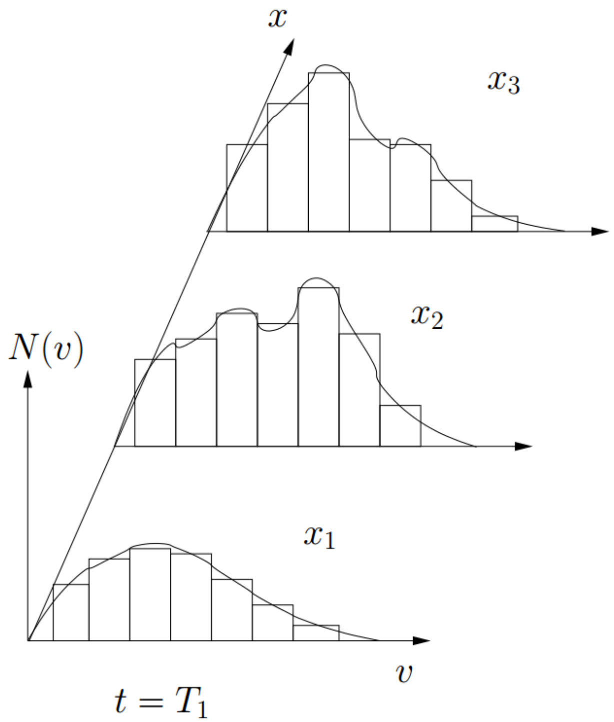
We are currently developing models for the following:

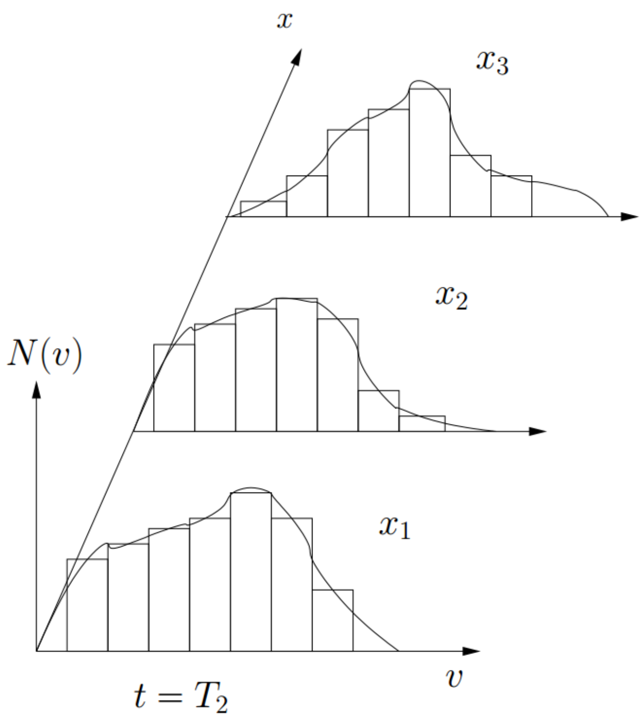
- Prediction of the particle size distribution by solving the population balance equation (PBE)
  - *Conservative finite volume method for the coagulation process*
  - Modelling of the morphology of aggregates
- Coupling of the PBE with chemical kinetics and flame dynamics
  - Simulation of laminar flames

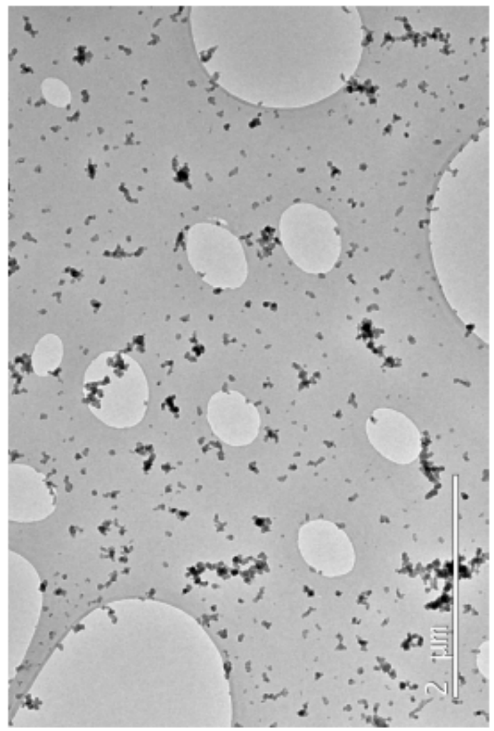
Particle size distribution

☐ Importance of particle size distribution

- Prediction of PSD is increasingly important for new regulations (PM2.5 & PM10);
- Coagulation (aggregation) rate is size-dependent;
- Growth and oxidation rates depend on surface area







Population Balance Equation (PBE)

- Define the continuous particle size distribution as density *n*(*v*) , i.e. , the number of particles of size *v* per unit size

  Let Y_a be the concentrations of chemical species

$$
\frac{\partial n(v)}{\partial t} = \underbrace{B_0(Y_a)\delta(v-v_0)}_{\text{nucleation}} - \underbrace{\frac{\partial}{\partial v}\left[G(v,Y_a)\cdot n(v)\right]}_{\text{growth}}
$$

$$
+\underbrace{\frac{1}{2}\int_0^v \beta(v-v',v')n(v-v')n(v')\,\mathrm{d}v'}_{\text{coagulation source}} - \underbrace{n(v)\int_0^\infty \beta(v-v',v')n(v')\,\mathrm{d}v'}_{\text{coagulation sink}}
$$

- Physical and chemical processes includes in the PBE above
  - Particle formation (nucleation)
  - Continuous size change (growth, oxidation)
  - Coagulation/aggregation

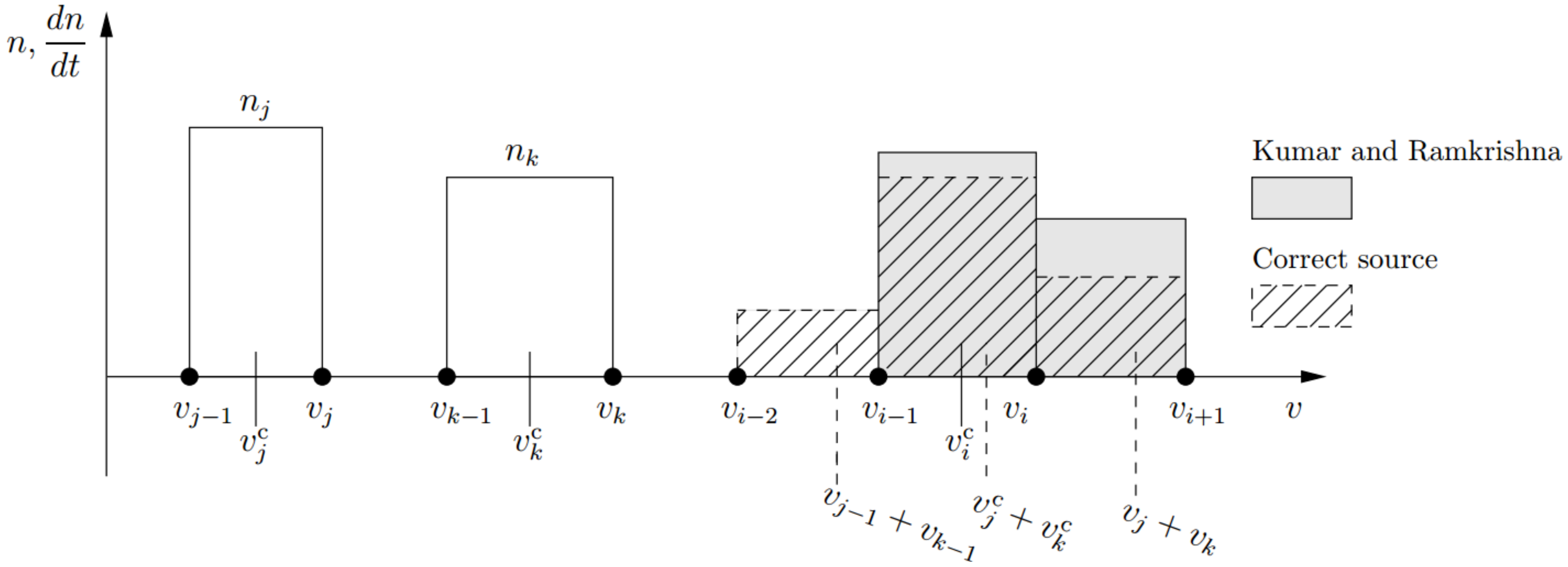
Population Balance Equation (PBE)

- ☐ Complex integral-differential equation
- ☐ Methods for solution:
  - Analytical and similarity solutions
  - Monte Carlo methods
  - Method of moments and variants~
  - **Discretisation (or sectional) methods: discrete methods, finite volume / element scheme**
- ☐ Main challenges in discretisation methods
  - Distribution can vary over several order of magnitude (10^{-27}~10^{-16}), while nucleation is localised at the minimum size;
  - **Coagulation is an integral term** while growth/oxidation term is first-order derivative with sharp fronts;
  - **Conservation of moments and accurate prediction of the change of particle size distribution in the process of coagulation**.

The problem in the discretisation of the coagulation

- Most discretisation (or sectional) methods assume that the particles are concentrated at discrete points, which is no physical；
- A non-uniform grid must be employed to cover a size range;
- However, there is no guarantee that the particle formed in a coagulation event will lie at grid points;
- Particles are redistributed so as to conserve the total volume and change of particle number at the expense of accuracy in the distribution

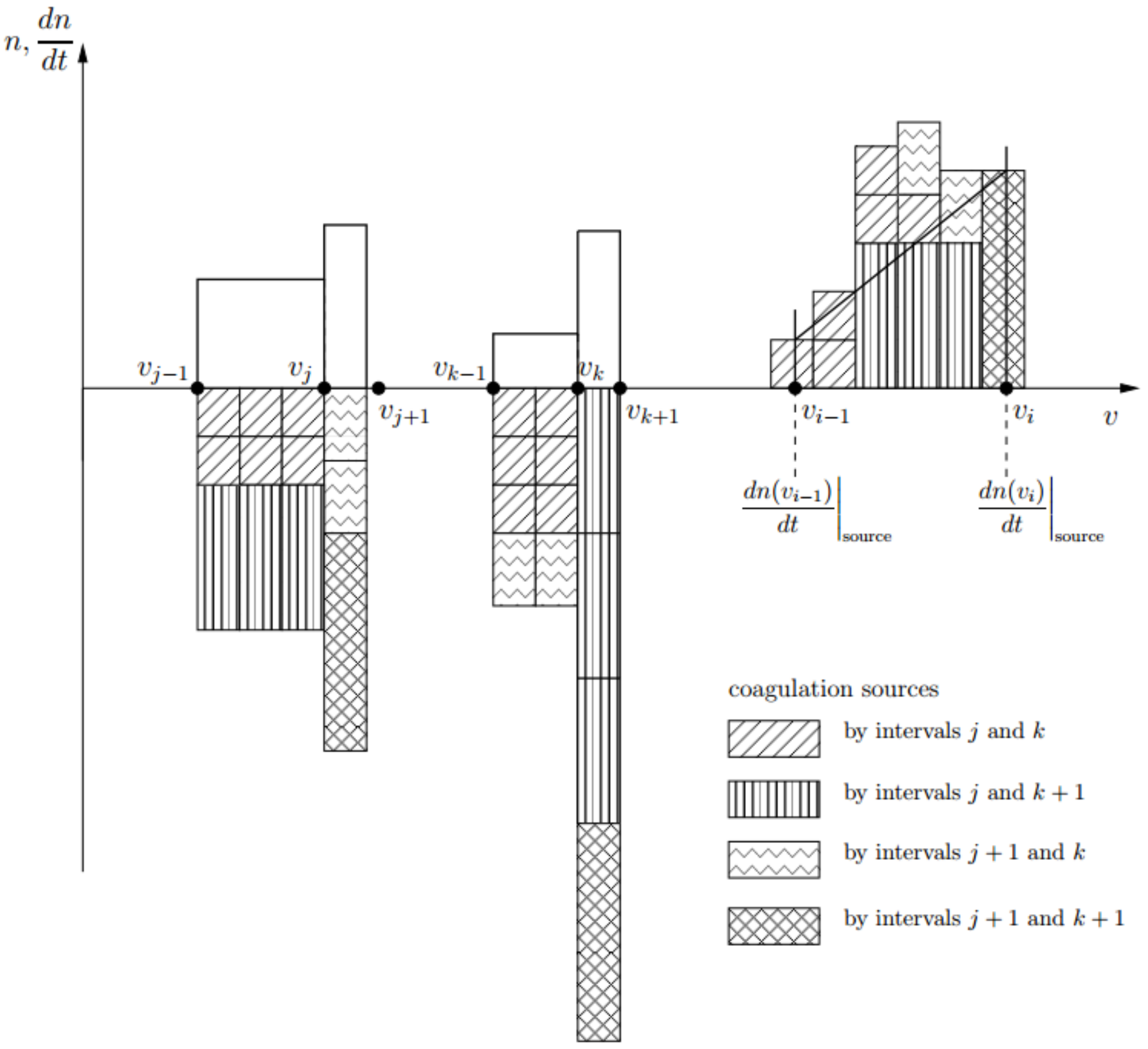
□ Kumar and Ramkrishna method



The problem in the discretisation of the coagulation

- One of the double integrations is replaced by a quadrature rule

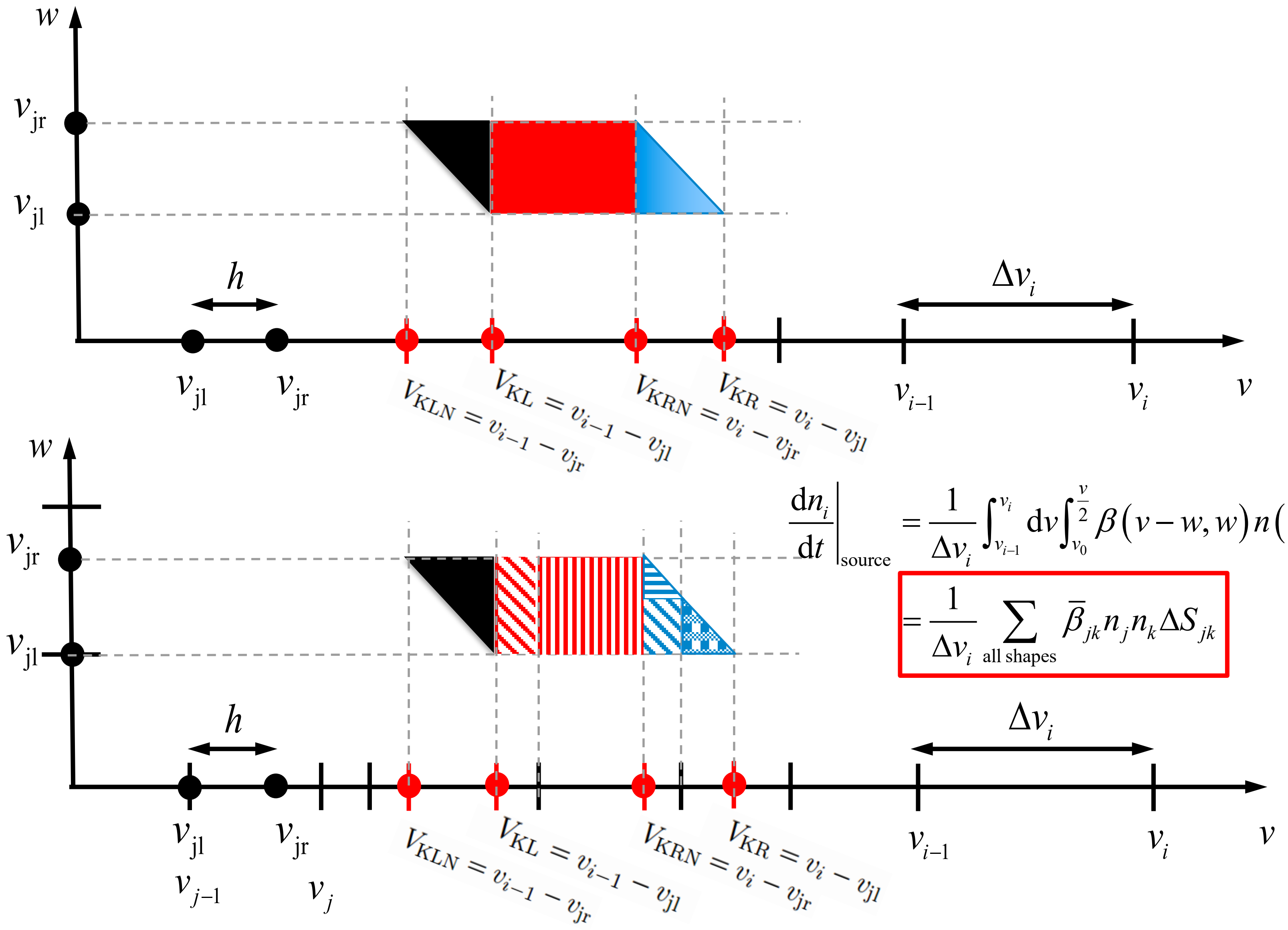
$$\left.\frac{dn_i}{dt}\right|_{\text{sourc}}$$



$$n(w)dw\Big)$$

A proposed discretisation method for the coagulation

- Each double integration is located and calculated



$$\left.\frac{\mathrm{d}n_i}{\mathrm{d}t}\right|_{\text{source}} = \frac{1}{\Delta v_i}\int_{v_{i-1}}^{v_i}\mathrm{d}v\int_{v_0}^{\frac{v}{2}}\beta(v-w,w)\,n(v-w)\,n(w)\,\mathrm{d}w$$

$$\boxed{= \frac{1}{\Delta v_i}\sum_{\text{all shapes}}\bar{\beta}_{jk}n_j n_k \Delta S_{jk}}$$

A proposed discretisation method for the coagulation

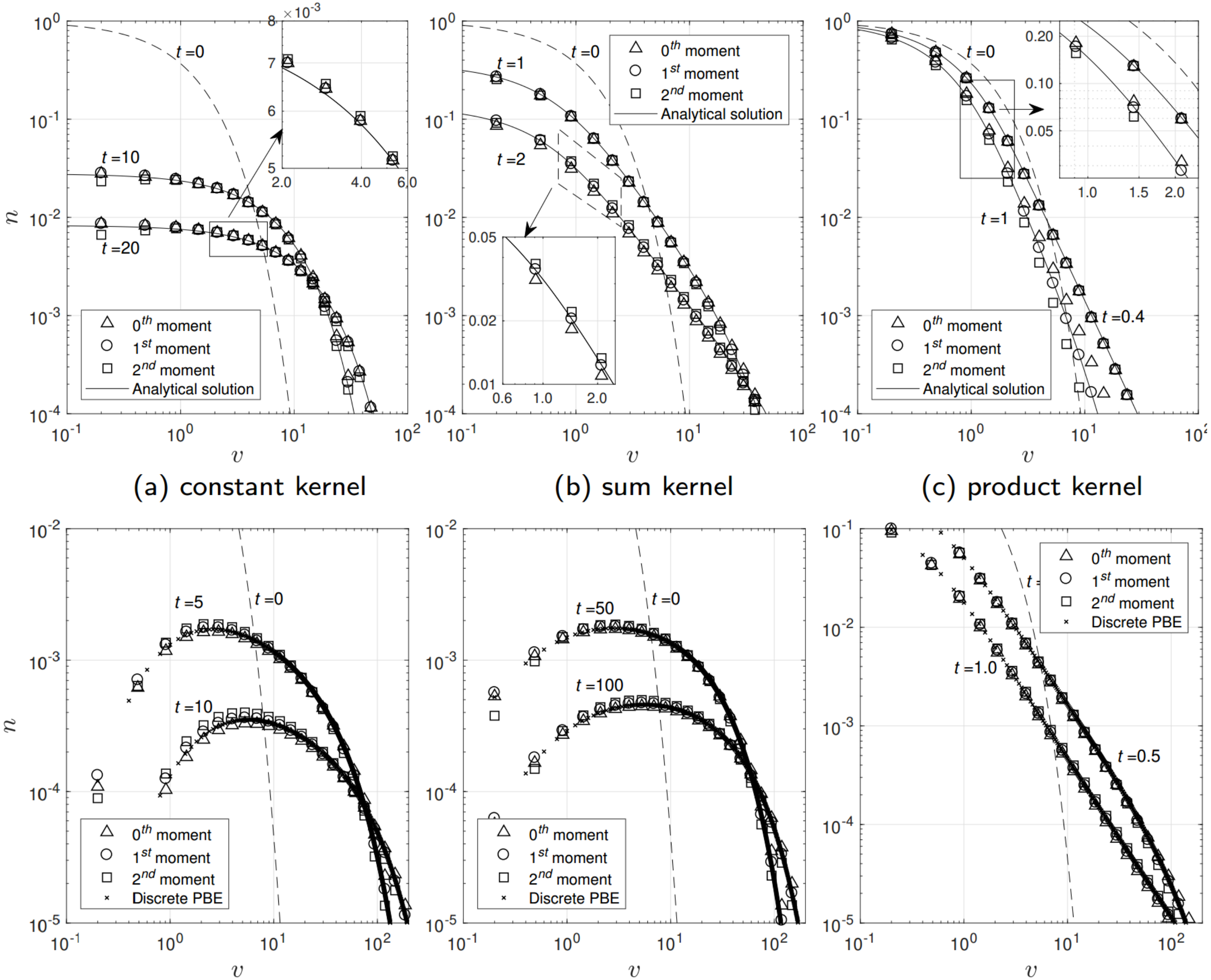
□ Each double integration is located and calculated;

- The whole algorithm is rigorous except the evaluation of coagulation kernel at each interval-pair;
- Different scenarios are likely to happen due to the non-uniformity of the grid;
- The implementation has been standardised as a solver;
- In the implementation, all geometric operations are carried out in advance and tabulated；
- Same level of time consumption as Kumar and Ramkrishna method.

	No. of subinterval pairs		No. of product operations in each subinterval pair
No. of grid	30	60	
Kumar’s method	1735	6863	3
Our method	1914	7244	3

Results of pure coagulation

- Comparison with analytical solution (a, b, c) and direct numerical solution of the discrete PBE (d, e, f), six kernels, exponential initial distribution



(a) constant kernel (b) sum kernel (c) product kernel

(d) Brownian kernel (e) Free molecule regime kernel (f) shear kernel

Spatially distributed continuous PBE

PBE must be augmented to account for:

- Convective transport in physical space;
- Thermophoresis – $\mathbf{u}^{\mathrm{T}}$: depending on μ and $\dfrac{\mathrm{d}T}{\mathrm{d}x_i}$
- Particle diffusion (much smaller than species' diffusion).

$$\frac{\partial n(v;x_j,t)}{\partial t}+\underbrace{\frac{\partial\left[(\mathbf{u}+\mathbf{u}^{\mathrm{T}})\cdot n(v;x_j,t)\right]}{\partial x_j}}_{\text{convection}}=\underbrace{\frac{\partial}{\partial x_j}\left(D_{\mathrm{P}}\frac{\partial n(v;x_j,t)}{\partial x_j}\right)}_{\text{diffusion}}\underbrace{+B_0(Y_a)\delta(v-v_0)}_{\text{nucleation}}\underbrace{-\frac{\partial}{\partial v}\left[G(v,Y_a)\cdot n(v)\right]}_{\text{growth}}$$

$$\underbrace{+\frac{1}{2}\int_0^v\beta(v-v',v')n(v-v')n(v')\mathrm{d}v'}_{\text{coagulation source}}\underbrace{-n(v)\int_0^\infty\beta(v-v',v')n(v')\mathrm{d}v'}_{\text{coagulation sink}}$$

Numerical framework

Coupling of PBE – CFD (Computational fluid dynamics)

PBE equation:
$N(v;\mathbf{x},t)$

PBE – BOFFIN
In house code

Continuity equation: $\dfrac{\partial \rho}{\partial t} + \dfrac{\partial (\rho u_j)}{\partial x_j} = 0$

Conservation equation of momentum:

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial}{\partial x_i}\left(p + \frac{2}{3}\mu \frac{\partial u_k}{\partial x_k}\right) + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \rho g_i$$

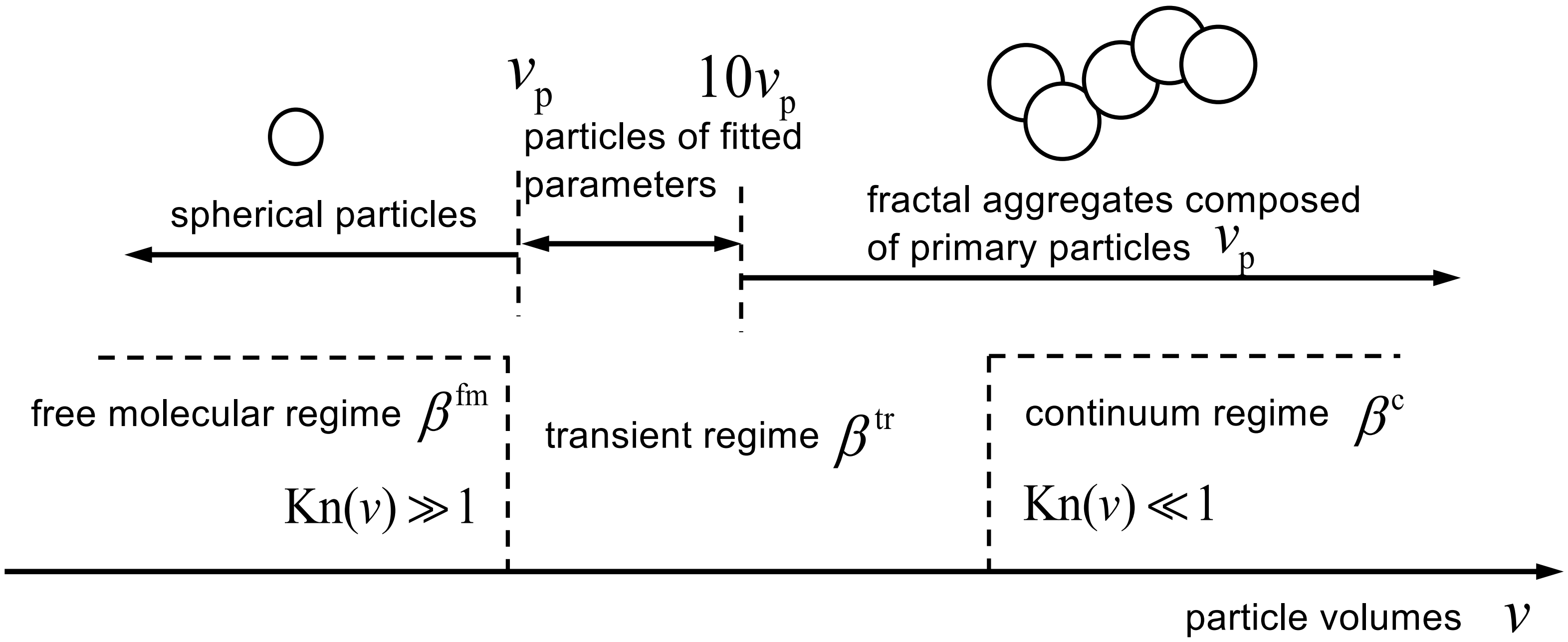
Reactive scalars transport equation (Energy & species concentrations):

$$\frac{\partial \rho \mathbf{Y}}{\partial t} + \frac{\partial (\rho u_j \mathbf{Y})}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D(\mathbf{x},t)\frac{\partial \mathbf{Y}}{\partial x_j}\right) + \rho \dot{\boldsymbol{\omega}}$$

where $\mathbf{u}(\mathbf{x},t)$ velocity $p(\mathbf{x},t)$ pressure $\mathbf{Y}(\mathbf{x},t)$ reactive scalar
$\rho(\mathbf{x},t)$ density $\mu(\mathbf{x},t)$ dynamic viscosity $D(\mathbf{x},t)$ reactive diffusivity

Soot Mechanism

- Gas phase: ABF mechanisms 101 species (up to pyrene C16H10) & 574 reactions [1]
- Nucleation: PAH dimerization
- Surface process: HACA mechanism (growth and oxidation)
  PAH condensation
- Coagulation: size-dependent kernel



[1] J. Appel, H. Bockhorn, M. Frenklach, Combustion and Flame, 2000.

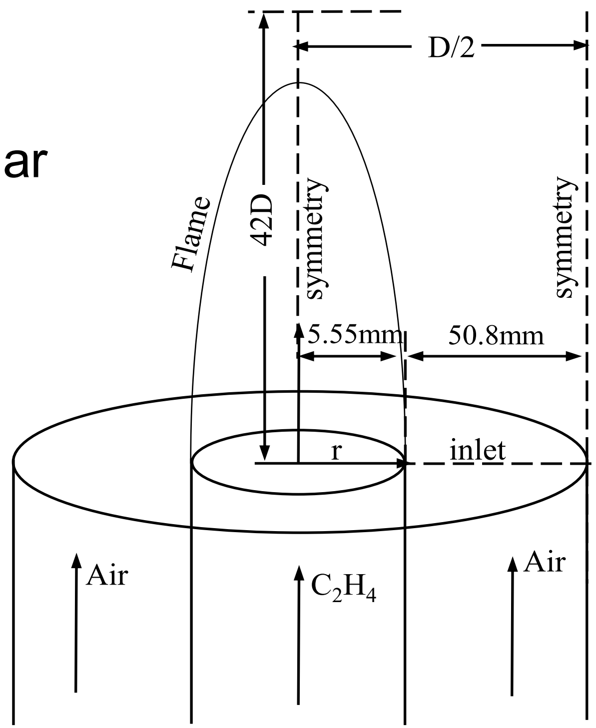
Case study: CFD simulation of Santoro flame

- ***Laminar diffusion flame*** is a simple combustion phenomenon including complete aerodynamic processes;
- ***2D physical domain*** is sufficient for simulation;
- The combustion reactions for ***ethylene fuels*** are relatively detailed and accurate;
- ***Soot emissions*** are obvious;
- ***Measurements*** for soot formation in ethylene laminar diffusion flame are available.

200 × 100 cells
physical domain
270mm × 55mm

60 cells
PBE grid
[$2.0e^{-28}m^3$, $1.0e^{-16}m^3$]

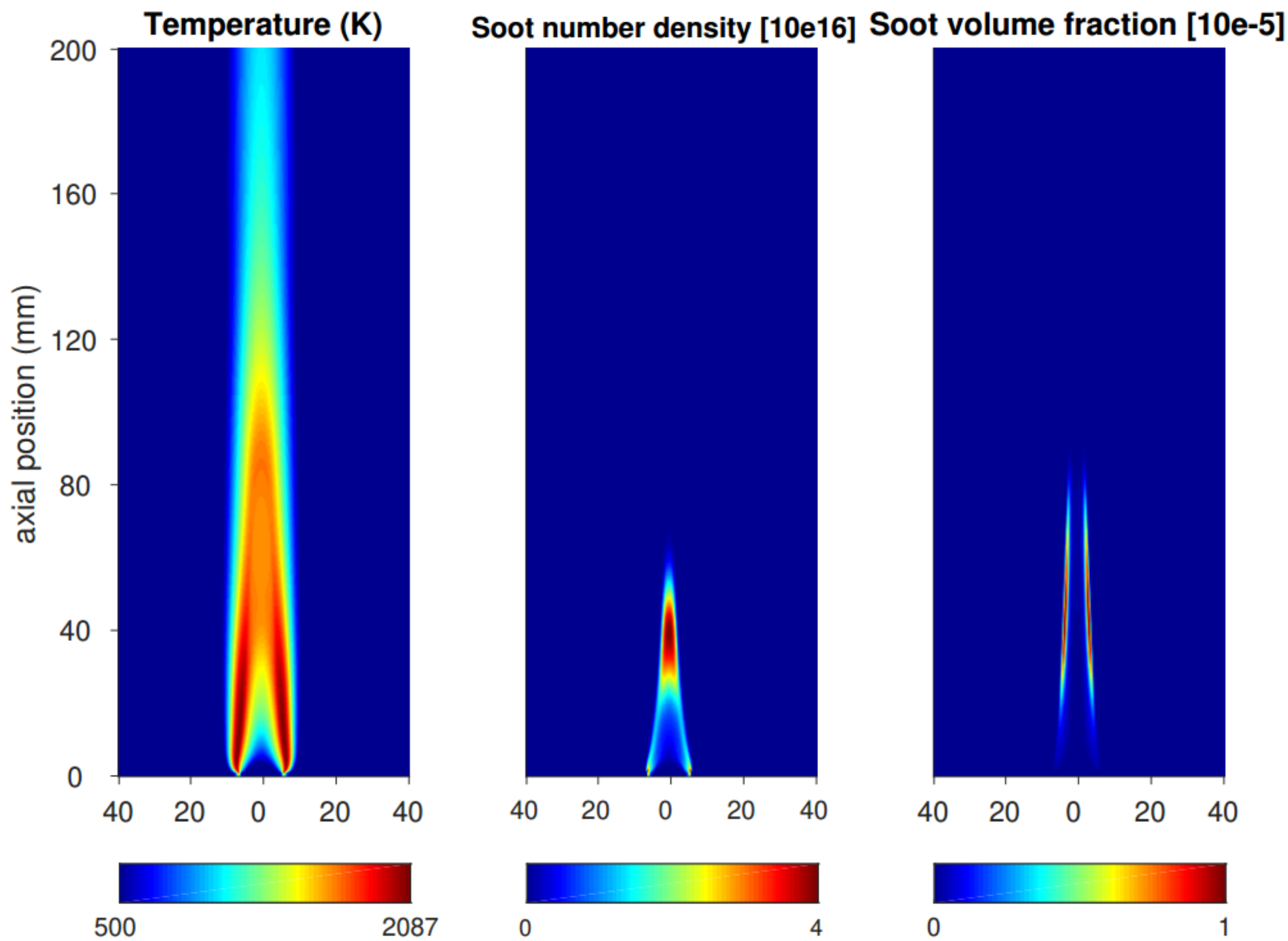
Non-smoking flame:
$v_{\text{fuel}} = 3.98\text{cm/s}, \; v_{\text{air}} = 8.98\text{cm/s}$



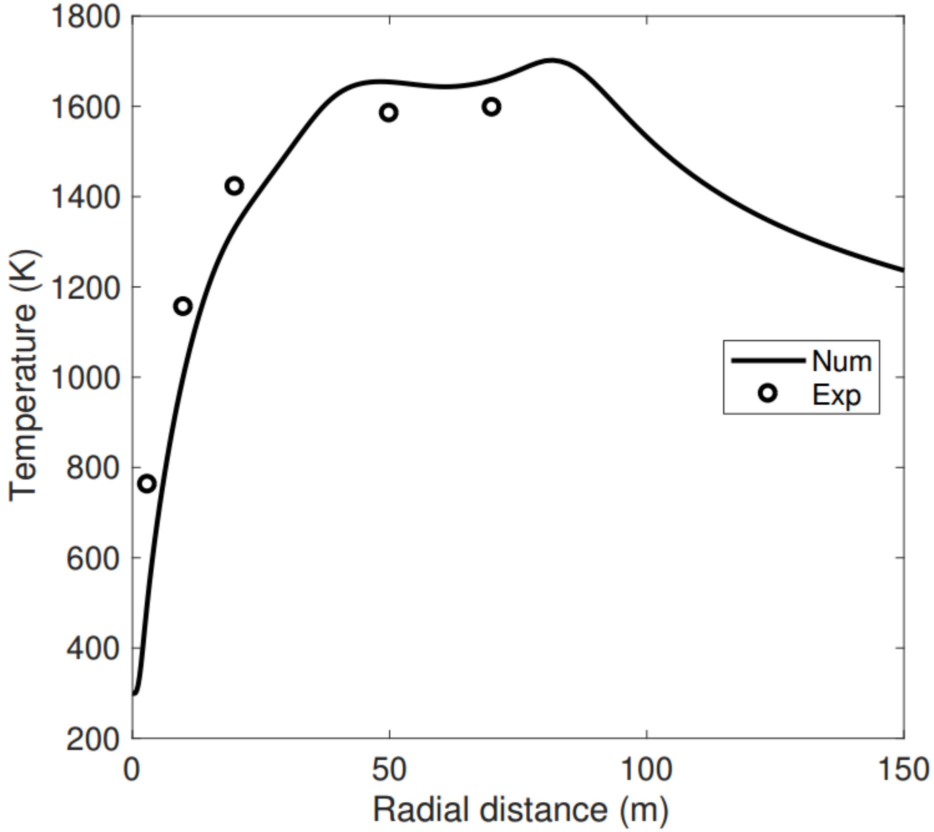
(a) Schematic plot of Santoro flame [1]

[1] R. J. Santoro, T. T. Yeh, J. J. Horvath, Combustion Science and Technology, 1987.

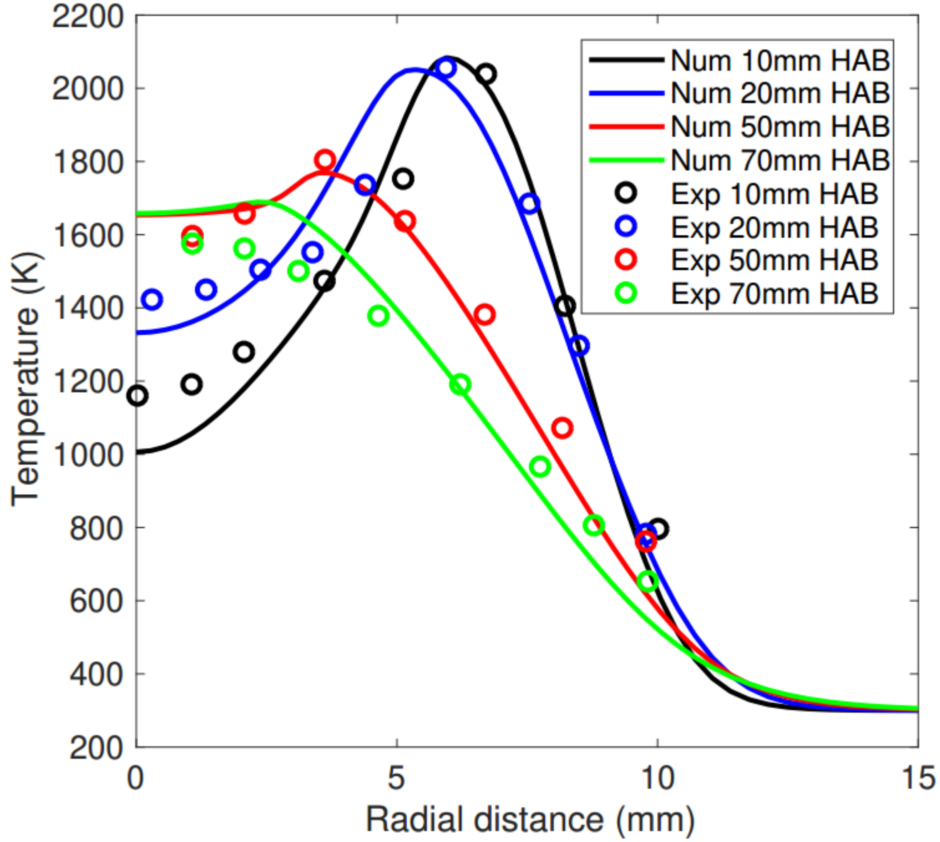
Santoro flame: contour plots



Santoro flame: temperature profiles

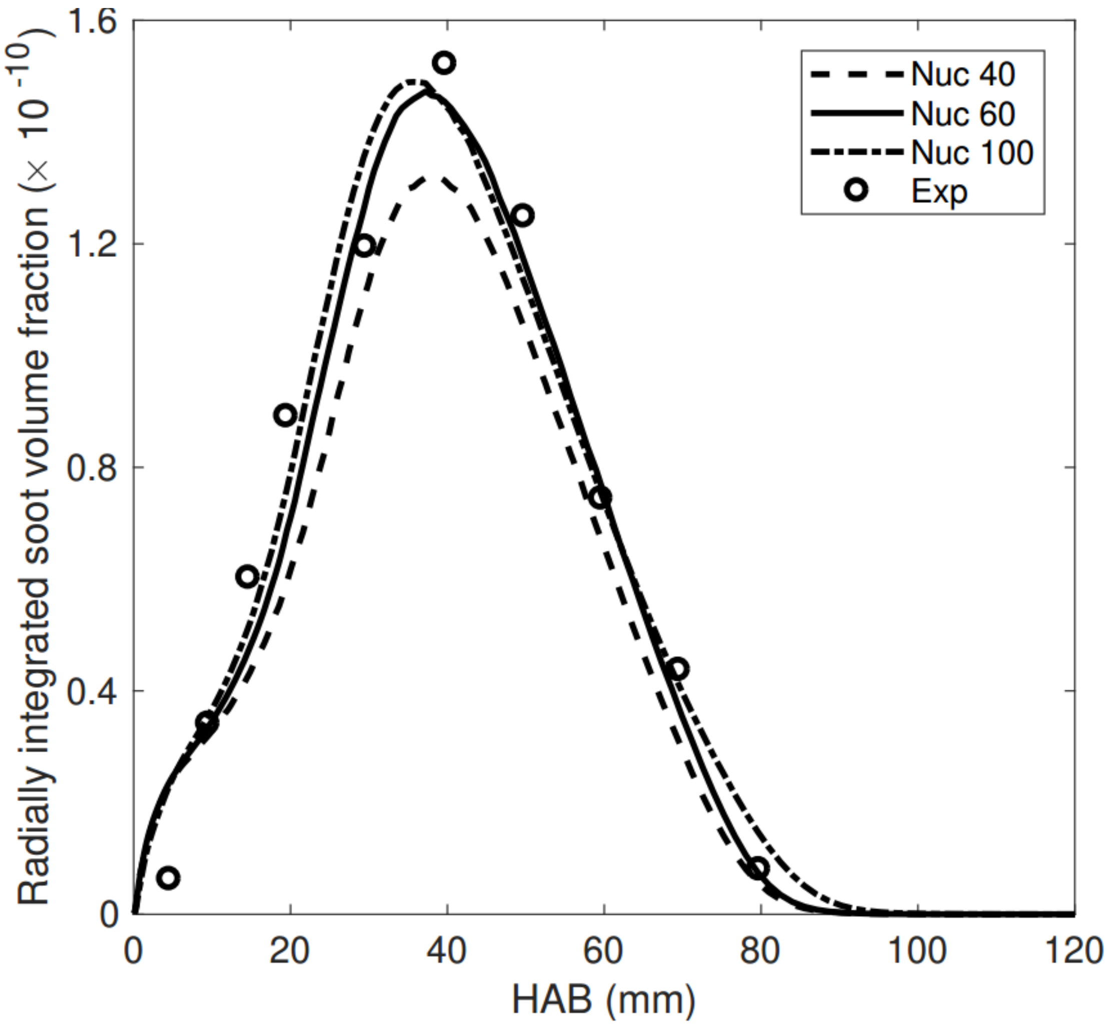


(a) Axial profile on centerline

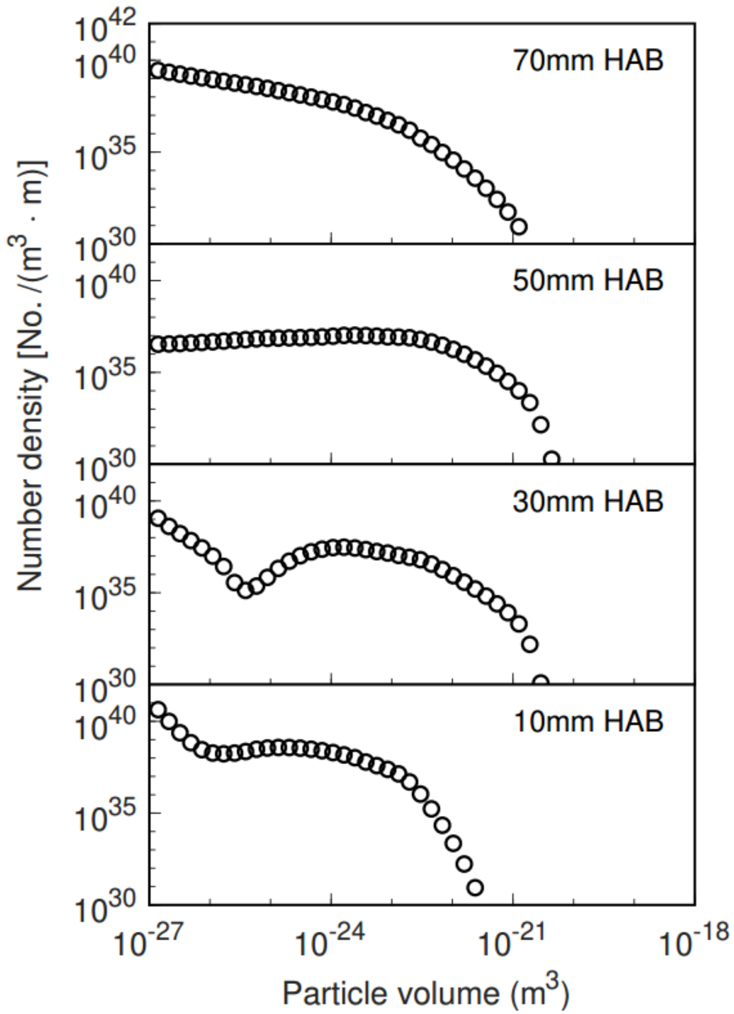


(b) Radial profile

Integrated soot volume fraction and size distribution



(a) Integrated soot volume fraction at different heights



(b) particle size distribution at different heights

CPU time breakdown

- Breakdown of the average CPU time for a time step

Subroutines	Time consumption (%)		
	40 nodes	60 nodes	100 nodes
Flow field	19.5	15.5	11.1
Scalar convection & diffusion	29.5	40.0	51.2
Chemistry	46.0	36.3	23.5
PBE (total)	5.0	8.2	14.2
Breakdown of PBE step:			
nucleation & growth	0.8	0.8	0.7
coagulation algorithm	1.6	2.8	5.1
coagulation kernel	2.6	4.6	8.4

Summary

- A conservative direct double integral method is proposed to discretize the coagulation process for the efficient and accurate solution of the PBE;
- In this work, a combined PBE-CFD model is presented to characterize the flame structure and soot formation in a laminar diffusion flame; a set of detailed gas-phase chemistry and complete soot kinetics is employed.
- The flame structure, gas phase species, soot integrated parameters and particle size distribution can be predicted by the model.

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Thank you