Modelling Soot Formation in a Benchmark Ethylene Stagnation Flame with a New Detailed Population Balance Model

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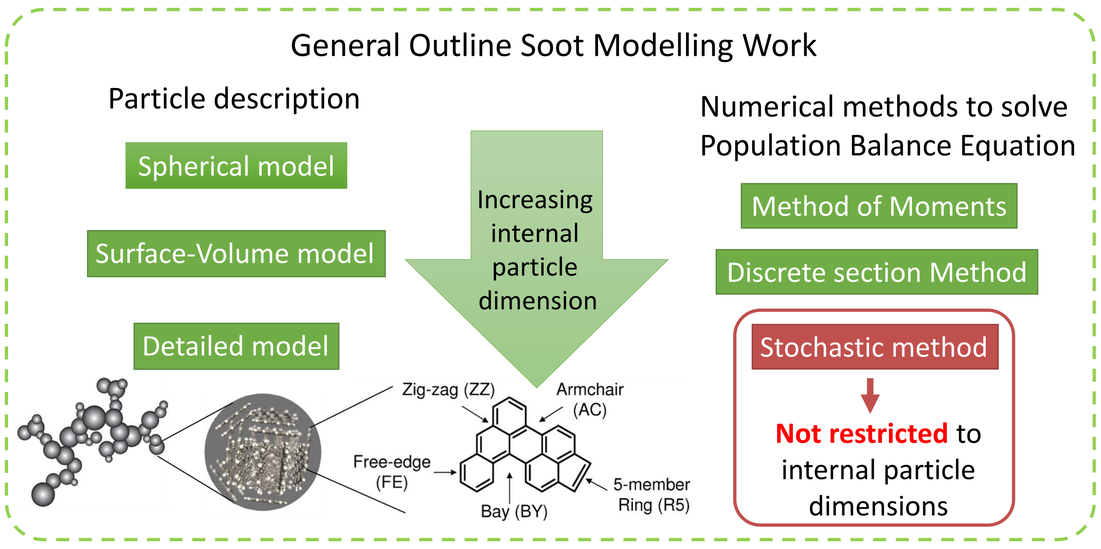
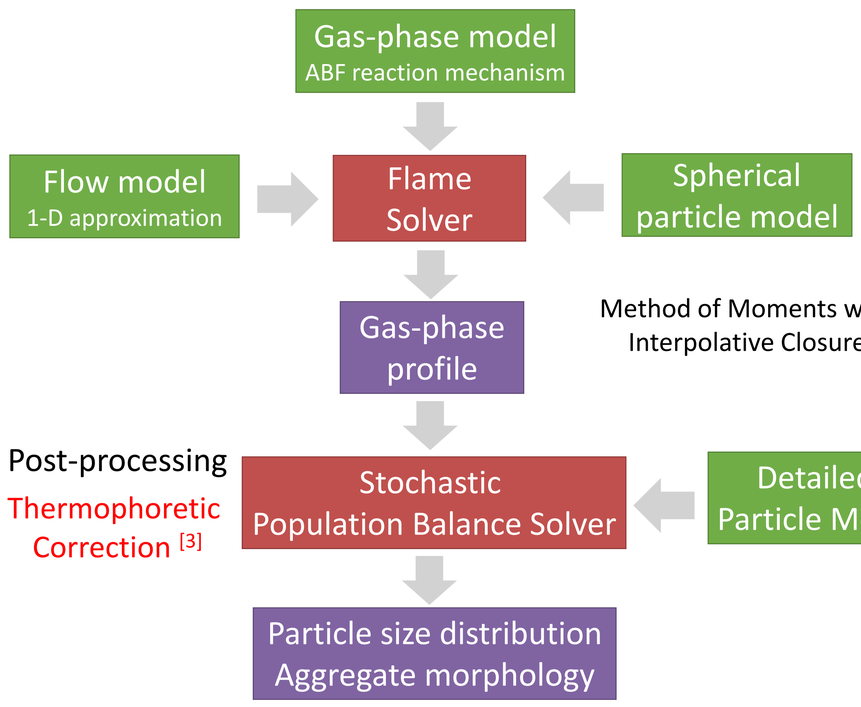
Numerical simulation of soot formation in a premixed C_2H_4 BSS flame was performed with a new detailed population balance model using a two-step method. The new model is capable of tracking aggregate morphology during simulation. Thermophoretic transport effect due to the large temperature gradient near the stagnation plate is accounted for in the post-processing. A thorough parametric sensitivity study is carried out to investigate the influence of key model parameters on the computed PSDs and soot morphology. The capability of the new model to predict PSDs in BSS flame is studied by comparing simulated PSDs with the measured ones in the literature. We provide insight into individual soot formation process and suggest future work which are imperative to make further progress on soot modelling.

1. Introduction

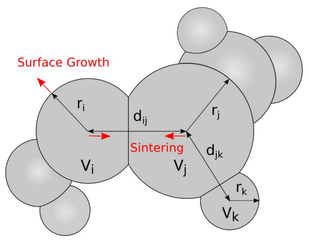


- Problems in previous work [4] on modelling soot formation in a C_2H_4 BSS flame
  - Particle morphology was not modelled.
  - Thermophoretic transport effect was not accounted for in the post-process.

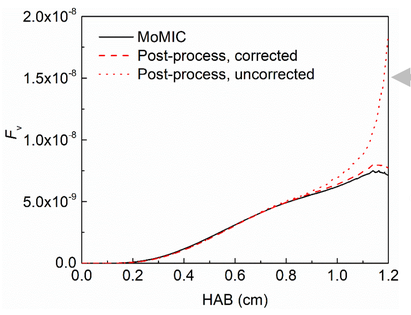
2. Modelling Methodology



- Detailed Particle Process
  - Inception
  - Coagulation
  - Surface growth
  - Condensation
  - Coalescence
  - Sintering
- Detailed Type Space [2]

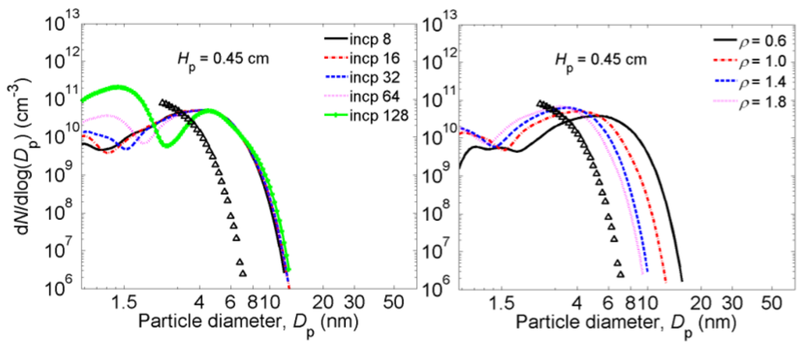


3. Results and Discussion

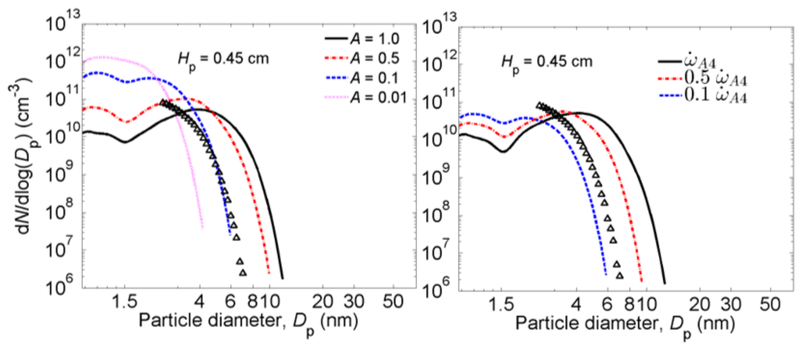


Thermophoretic transport effect on post-processed soot volume fraction F_v

- Thermophoretic correction is necessary when temperature gradient is large.



Sensitivity of computed PSDs to inception threshold and density



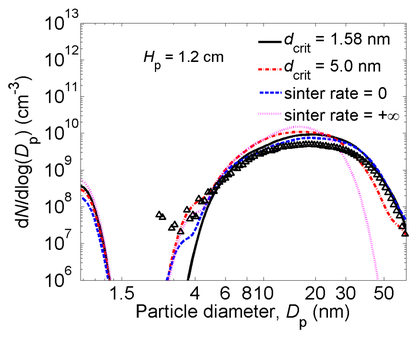
Sensitivity of computed PSDs to collision efficiency and the rate of production of the inception species.

- The computed PSDs are most sensitive to the **rate of production of A4** and **collision efficiency**, while not sensitive to inception threshold, condensation threshold, inception mode, sintering rate.

- Sintering model

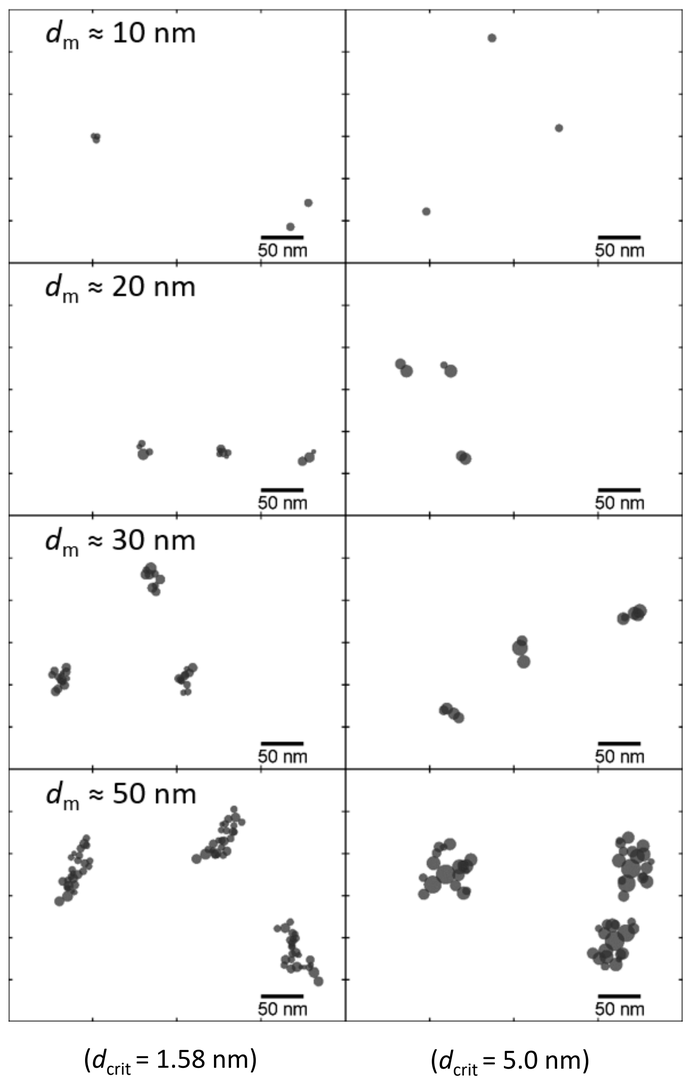
$$\tau_s = A_s d_{i,j} \exp\left[\frac{E_s}{T}\left(1 - \frac{d_{crit}}{d_{i,j}}\right)\right]$$

d_{crit} (nm): below which soot is assumed to be liquid-like and will "sinter" instantaneously.



Sensitivity of computed PSDs to sintering rate

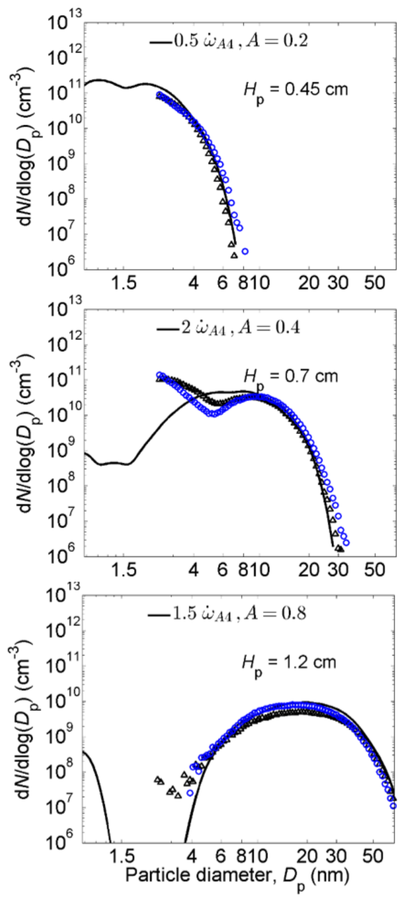
- The simulated PSDs are not very sensitive to sintering rate, yet aggregate morphology (primary particle size) is very sensitive to sintering rate.



(d_{crit} = 1.58 nm) (d_{crit} = 5.0 nm)

Simulated TEM Images with mobility diameter ≈ 10, 20, 30, 50 nm for a burner-stagnation plate separation (H_p) of 1.2 cm.

Simulated PSDs vs Measured PSDs [1]



Computed PSDs (solid lines) compared to experimental measurements (blue and black symbols) [1]

- Good agreements between simulation and experiment results can be achieved for d_m > 6 nm.
- Collision efficiency is suggested to be increasing with particle size.

4. Conclusions and Future Work

- A new detailed population balance model for soot **capable of tracking aggregate morphology** is presented.
- A thorough **parametric sensitivity** is performed to understand the influence of some key parameters to the computed **PSDs** and particle **morphology**.
- The **capability to track aggregate morphology** will facilitate further study on soot process relating to morphology evolution, such as sintering and coalescence.
- More fundamental work on **collision efficiency** of nascent soot particles and **gas-phase PAH chemistry** are imperative to make further progress on soot modelling work.

5. Key Reference

[1] J. Camacho, C. Liu, C. Gu, H. Lin, Z. Huang, Q. Tang, X. You, C. Saggese, Y. Li, H. Jung, L. Deng, I. Wlokas, and H. Wang. Mobility size and mass of nascent soot particles in a benchmark premixed ethylene flame. Combustion and Flame, 162: 3810 – 3822, 2015. .
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[3] C. Lindberg, M. Y. Manuputty, J. Akroyd, and M. Kraft. A two-step simulation methodology for modelling stagnation flame synthesised aggregate nanoparticles. 2018. Manuscript submitted for publication.
[4] E. K. Yapp, D. Chen, J. Akroyd, S. Mosbach, M. Kraft, J. Camacho, and H. Wang. Numerical simulation and parametric sensitivity study of particle size distributions in a burner-stabilised stagnation flame. Combustion and Flame, 162:2569 – 2581, 2015.

Acknowledgements
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