Effects of overlapping in the evaluation of volume and surface area of complex soot aggregates in flames

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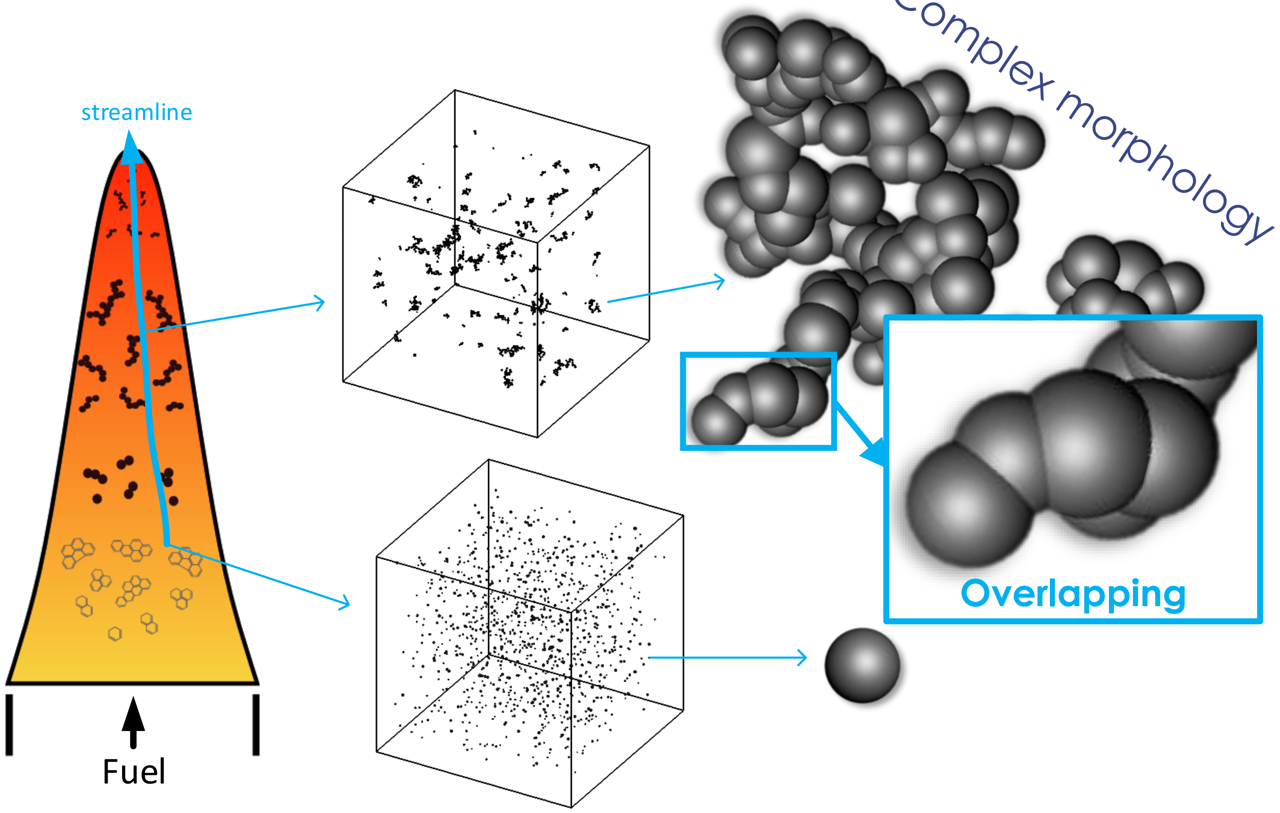
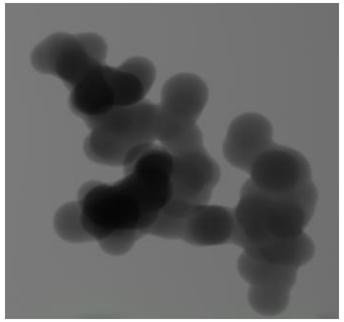
1. Challenge

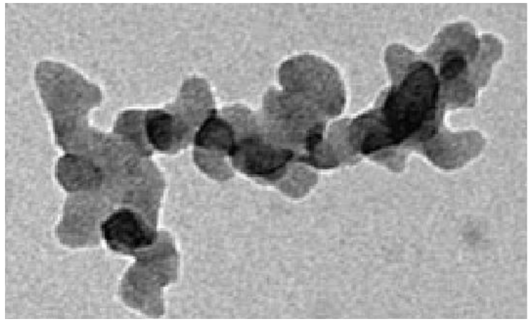
Monte Carlo simulations have shown soot particles are formed under the competition of agglomeration and surface growth[1]



Simulations[1]



Experiments[2]



- **No codes** (excepting mesoscale simulations) considers primary particle **overlapping**.
- Total volume and surface area should be **corrected**.
- Impact: particle dynamics and coagulation kinetics. Surface reaction and mass transfer modeling.

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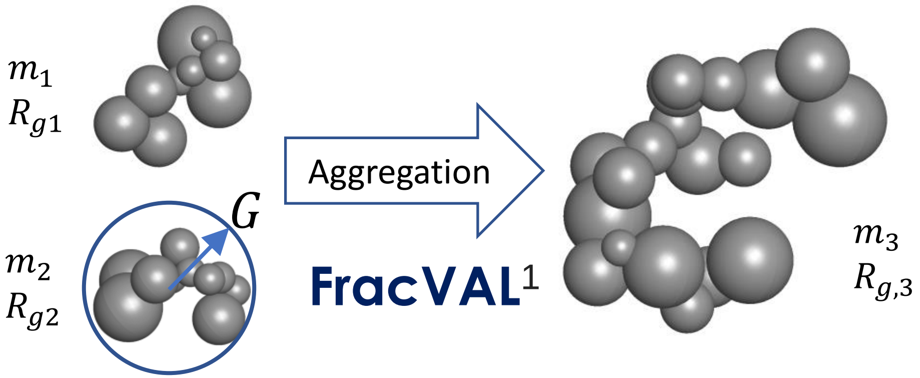
[1]Morán, J., Poux, A., & Yon, J. (2021). *J. Aerosol Sci.*, *152*, 105690.
[2]De Iuliis, S., *et al.* (2011). *Appl. Phys. B*, *102*(4), 891-903.

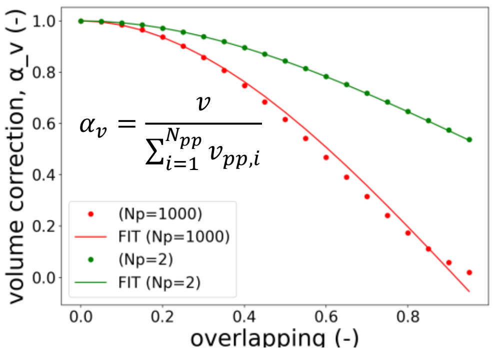
2. Methods

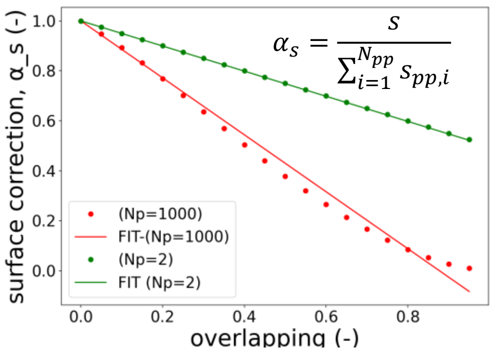
2.1. Aggregates generation



Parameters: $D_f = 1.78$, $k_f = 1.30$, $N_p = [2, 1000]$, $c_{ov} = [0, 0.95]$

2.2. Aggregates processing





$$\alpha_v = 1 - \frac{1}{4}\overline{n_c c_{ov}}^2(3 - \overline{c_{ov}})\phi \qquad \alpha_s = 1 - \frac{1}{2}\overline{n_c c_{ov}}\phi$$

$$\overline{n_c} = \overline{n_c}(N_{pp}); \; \phi = \phi(N_{pp})$$

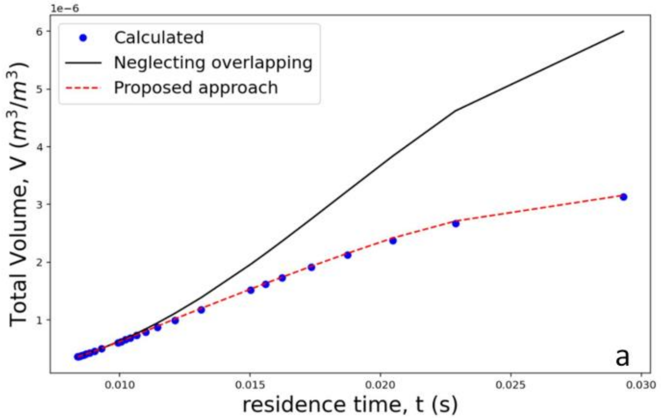
2.3. Determining overlapping

$$\overline{c_{ov}}(t) = f(D_{pp}; u; k_{ij})$$ } Population average

- Primary particle diameter (D_{pp})
- Surface growth rate (u)
- Collision frequency (k_{ij})

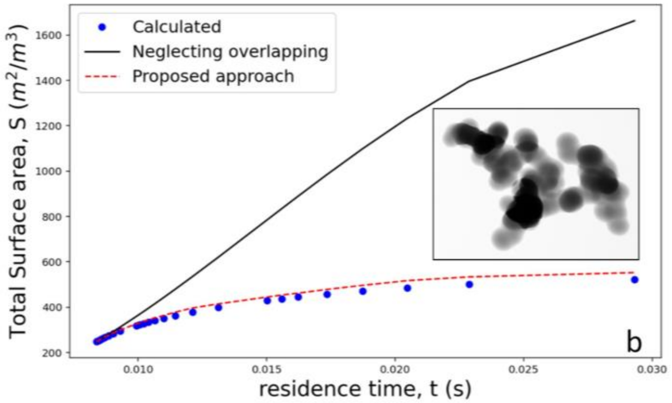
3. Results

3.1. Test case: ethylene premixed flame (C/O=0.94)



Neglecting overlapping:
maximum error total:
Volume 91%
Surface area 218% for total

Proposed method:
maximum error total
Volume 0.6%
Surface area 5.75%



[1] Morán, J., Fuentes, A., Liu, F., & Yon, J. (2019). *Comp. Phys. Commun.*, *239*, 225-237.

3. Conclusions

- A new method to determine the volume and surface area of aggregates with overlapping primary particles is introduced. This method is in good agreement and extends the works of[1,2].
- These methods are combined to accurately predict total soot volume (<0.6% error) and surface area (<5.75% error) in a premixed ethylene flame.
- This method can be **easily implemented in current** Population Balance (macroscopic) or discrete element (mesoscale) codes to improve accuracy and/or computational time.

Acknowledgments

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[1]Morán, J., Poux, A., & Yon, J. (2021). *J. Aerosol Sci.*, *152*, 105690.
[2]Brasil, A. M., Farias, T. L., & Carvalho, M. G. (1999). *J. Aerosol Sci.*, *30*(10), 1379-1389.

A. Volume and Surface area correction factors

$$\alpha_v = 1 - \frac{1}{4}\overline{n_c c_{ov}}^2(3 - \overline{c_{ov}})\phi$$

$$\alpha_s = 1 - \frac{1}{2}\overline{n_c c_{ov}}\phi$$

$$\phi(N_p) = \frac{a}{b + (a-b)\exp[-a(N_p - 2)]} + c, \qquad N_p \geq 2$$

$$\overline{n_c} = 2(1 - 1/N_p)$$

$$a = 0.0642$$
$$b = 0.0565$$
$$c = 0.0061$$

In the case of surface area ϕ is quite close to the one proposed by Brasil et al.[1] in the limit $N_p \to \infty$

B. Determining overlapping

$$\overline{c_{ov}}(t) = \frac{\int_{t_0}^{t} c_{ov}(t_0, t)B_{t_0}\ dt'}{\int_{t_0}^{t} B_{t_0}\ dt'}$$

Population average

$$B_t = \int_0^{\Delta t}\left(\frac{dn}{dt}\right)_{coag} dt = \text{Total number of collisions}$$

$$c_{ov}(t_0, t) = 2D_{pp,0}\int_{t_0}^{t}\frac{u}{D_{pp,t}^2}\ dt' = \text{Time accumulated overlapping}$$

[1]Brasil, A. M., Farias, T. L., & Carvalho, M. G. (1999). *J. Aerosol Sci.*, *30*(10), 1379-1389.