

Response to Reviewers for ar-2025-40 “Soot growth by monodisperse particle dynamics model coupled with Computational Fluid Dynamics” by Fakharneshad, Berry and Goudeli. The Reviewers’ comments are shown in *italics*. The responses (blue) and changes in the revised manuscript (red), are given below. Corrections made on this new revision were highlighted in red.

Reviewer 1

The manuscript compares molecular-dynamics-derived nucleation, coagulation, and surface growth rates with empirical rate models in a premixed ethylene burner-stabilized stagnation (BSS) flame, focusing on their influences on the modeled particle number concentration and volume fraction. This is accomplished by solving the coupled mass, energy, and momentum transport equations using Fluent. Overall, this study is potentially interesting and relevant to the Aerosol Research. However, the presentation would benefit from significant improvement to better highlight the value of the work. The following comments are provided for the authors’ consideration and focus on selected aspects, although the authors are encouraged to carefully revise the manuscript as a whole, beyond the specific points listed below.

1. The methodology section would benefit from a more structured organization, for example by clearly separating geometry, governing equations, boundary conditions, and initial conditions. In addition, the descriptions should be more complete. For instance, although the temperature conditions can be inferred from Figure 1, all initial and boundary conditions for the flow, energy, and transport equations should be explicitly stated in the text. The manuscript provides the transport equations. It would also be beneficial to provide the exact flow and energy equations, as they are critical.

1. Thank you for this suggestion. The geometry, governing equations, and boundary conditions are separated in the methodology section, and the governing equations section has been modified in page 4 of the revised manuscript:

“2.1.2 Governing equations

The steady-state Navier-Stokes equations were solved using a pressure-based solver that ensures mass conservation through a pressure correction equation. The equation for conservation of momentum (Batchelor, 2000) is:

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\bar{\tau}) + \rho \vec{g} + \vec{F} \quad (1)$$

where ρ is the gas density, \vec{v} is the velocity vector, p is the static pressure, and $\bar{\tau}$ is the viscous stress tensor. The terms $\rho \vec{g}$ and \vec{F} represent the gravitational and external body forces, respectively. The energy equation was also included to capture thermal variations:

$$\frac{\partial}{\partial t} \left(\rho \left(e + \frac{v^2}{2} \right) \right) + \nabla \cdot \left(\rho v \left(h + \frac{V^2}{2} \right) \right) = \nabla \cdot \left(k_{eff} \nabla T - \sum_j h_j \vec{J}_j + \bar{\tau}_{eff} \cdot \vec{v} \right) + S_h \quad (2)$$

The e and h on the left-hand side of eq. 2 denote the internal energy and the enthalpy, respectively. On the right-hand side, k_{eff} is the effective thermal conductivity, \vec{J}_j is the diffusion flux of species j , and S_h accounts for volumetric heat sources including the heat released by chemical reactions.”.

A new “Initial conditions” section has also been added in page 6 of the revised manuscript:

“2.1.4 Initial conditions

All simulations were first initialized using the Hybrid Initialization method used to generate a physically representative initial flow field through boundary-based interpolation. Then, Fluent simulations were performed at cold-flow conditions (no combustion chemistry considered) until the flow reaches steady state. Upon convergence of the cold-flow solution, the volumetric reactions were activated, and a temperature of 2000 K was imposed in the entire region above the burner surface. This temperature patch acts as an ignition source to initiate flame formation in the combustion zone.

This two-step procedure ensured numerical stability and provided a physically realistic initial condition for the reacting flow simulations.”.

2. *The manuscript would benefit from a clearer description of how the MD-derived rates are obtained. While readers may refer to the cited literature for details, it would be helpful to briefly summarize the underlying chemical and physical mechanisms, the types of systems used to derive these rates, and the conditions under which the rates are applicable.*

2. Thank you for this suggestion. The following sentences have been added to the 3rd paragraph of the section 2.2 of the revised manuscript: “... were described using MD-derived expressions. The expression for the MD-derived nucleation rate (Model II) was developed from MD simulations of isothermal acetylene pyrolysis conducted at a flame-relevant temperature range of 1200–1800 K and high-pressure of 189–568 atm (Fakharneshad et al., 2025). The nucleation rate was determined by monitoring the temporal evolution of incipient soot cluster formation relating it to the initial acetylene concentration (Table 1: $S_{N, Nucl.}$ of Model II).”.

3. *The capabilities and limitations of the monodispersed model should be clarified. As currently described, it appears that the model is able to represent only the total particle number concentration, rather than size-resolved particle distributions. It would be beneficial to have more structured and involved discussions on this.*

3. Indeed, the particle size distribution is not resolved as the present model assumes a monodisperse population of particles/agglomerates/aggregates at each time (or height above the burner), as described in the fourth paragraph of the Introduction of the original manuscript: “The particle dynamics equation can be greatly simplified ... for coupling with multidimensional CFD simulations in realistic geometries.”. This simplification increases the computational performance of the PD model when implemented in CFD as equations are solved only for one size class. However, the self-preserving mobility size distribution can be generated based on the average mobility diameter (Fig. 7) if the self-preserving geometric standard deviation is known.

To further address the Reviewer’s comment, the following discussion has been added in page 16 of the revised manuscript: “... mobility particle sizer (SMPS) measurements in premixed ethylene flames [1]. Even though the present PD model does not account for the agglomerate/aggregate polydispersity, the mobility-based self-preserving size distribution can be derived based on the average d_m (Fig. 7) and the mobility-based self-preserving geometric standard deviation of soot ($\sigma_{g,m} = 1.48 \pm 0.03$), obtained by discrete element method simulations (Kelesidis and Goudeli, 2021: Fig. 2).”.

4. *In Line 105, Section 3.1.1, the text shows “Error! Reference source not found.” Please provide the correct reference.*

4. It has been fixed.

5. *In Line 124, the parameter C is introduced without a clear definition. In Equation (3) as well. Please clarify if C represents the total concentration of carbon species, or is individual concentration for different carbons.*

5. We thank the reviewer for pointing this out. Here, C represents total molar concentration of carbon contained in soot particles (obtained by converting the soot mass concentration using the molar mass

of carbon, $MW_c = 12$ g/mol), rather than the concentration of individual gas-phase carbon species. To clarify this, we have modified 1st paragraph of Section 2.2 of the revised manuscript: "... the total carbon molar concentration C of carbon contained in soot particles (obtained by the soot mass concentration using the molar mass of carbon, $MW_c = 12$ g/mol) was modelled using CFD ...".

6. In Equations (2) and (3), the notation used for the source terms on the right-hand side may be misleading, as they resemble derivatives of the variables N and C , although they are not (they are source terms). Please consider revising the notation to avoid potential confusion.

6. The notation for source terms in Equations (2) and (3) has been changed in the revised manuscript: "...the transport of total particle number density N is described by:

$$\frac{\partial(\rho u_i N)}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\Gamma_{k,N} \frac{\partial N}{\partial x_i} \right) = S_{N, Nucl.} + S_{N, Coag.} \quad (4)$$

and the transport of carbon molar concentration C is defined by:

$$\frac{\partial(\rho u_i C)}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\Gamma_{k,C} \frac{\partial C}{\partial x_i} \right) = S_{C, Nucl.} + S_{C, SG} \quad (5)$$

The terms on the left-hand side of equations (4) and (5) represent convection and diffusion in the flow, where u_i denotes the velocity, and $\Gamma_{k,N}$ and $\Gamma_{k,C}$ are the effective diffusion coefficients for number density and carbon concentration, respectively. The right-hand side of eq. (4) includes the nucleation term, $S_{N, Nucl.}$, which describes the formation of new particles, and the coagulation term, $S_{N, Coag.}$, which describes the reduction in the number of particles due to agglomeration. In eq. (5), the source terms correspond to carbon addition due to newly formed particles by nucleation, $S_{C, Nucl.}$, which can be obtained by:

$$S_{C, Nucl.} = S_{N, Nucl.} \frac{n^*}{N_{Av}} \quad (6)$$

where n^* is the number of carbon atoms within the soot critical nucleus and N_{Av} is Avogadro's number. $S_{C, SG}$ is the accumulation of carbon on existing particles due to surface growth.".

7. In Line 140, the variables Wc and M should be defined when they are introduced.

7. Thank you. The MW_c is one variable corresponding molar mass of carbon. To avoid confusion, the clause has been modified in the revised manuscript: "... volume of a primary soot particle, $V = \frac{C \cdot MW_c}{\rho_{soot}}$ is the total soot volume concentration of the whole particle population and $MW_c = 12$ g/mol), and ...".

8. Several variables listed in Table 1 have not been defined elsewhere in the manuscript. Please ensure that all variables appearing in the table are clearly defined.

8. A Nomenclature section has been added in the revised manuscript.

Reviewer 2

This paper presents a simulation of a laminar premixed sooting flame with a CFD code coupled with a monodisperse soot model whose kinetics are derived by molecular dynamics (MD). The main contribution of the paper is in employing MD-derived kinetics in the context of a CFD simulation of a laminar flame. I applaud the authors' attempt, as I also think that the involvement of MD kinetics in soot and aerosol simulations is the way to go in the future. However, I think that the manuscript requires considerable revision in order to do justice to its cause. In the present form, the conclusions drawn do not seem to be adequately supported by the simulation results. This does not mean that the results are not publishable, but the discussion and conclusions should reflect the results and acknowledge the shortcomings, given that this is an early attempt, otherwise the aim of the authors in promoting the use of MD in sooting flame simulations will be compromised. I provide below a list of major points.

1. There is no detail at all on how the MD kinetics are derived, with the paper citing instead two works by the authors (one of them on surface growth still unpublished, so I cannot know how that model is derived). Even with the papers published, I feel that a summary of these works is required here, otherwise the paper cannot be comprehended without reading the other papers. This is important because the use of MD kinetics is the main contribution here and MD for soot is at a very early stage, so there are many open questions as to how MD kinetics could be derived and what would be their range of validity.

1. We thank you the Reviewer for this Comment. As the manuscript on surface growth is still under review we have now cited its preprint, made publicly available at https://papers.ssrn.com/sol3/papers.cfm?abstract_id=6348218. In addition, more information on the derivation of the molecular dynamics (MD) surface growth rate has been added to the 3rd paragraph of Section 2.2 of the revised manuscript: "...were described using MD-derived expressions. The MD-derived nucleation rate (Model II) was developed from MD simulations of isothermal acetylene pyrolysis at temperatures of 1200–1800 K and high-pressure of 189–568 atm in Fakharneshad et al. (Fakharneshad et al., 2025). The nucleation rate was determined by monitoring the temporal evolution of the number of incipient soot clusters for various initial acetylene concentration using a single lumped rate expression (Table 1: $S_{N, Nucl}$ of Model II). This MD-derived rate equation corresponds to the overall nucleation rate and does not require the identification of specific intermediates or tracking their concentration. As such, in contrast to traditional approaches where existing kinetic models are interfaced with CFD, here a detailed PAH-based mechanism does not need to be employed.

Similarly, the MD-derived surface growth rate, $k_{MD, SG}$ (Goudeli et al., 2026) in Model III, was obtained during isothermal surface growth of incipient soot nanoparticles by acetylene pyrolysis at a comparable temperature (1350–1800 K) and pressure range (106–568 atm). The steady-state particle mass growth rate, $\left(\frac{dm}{dt}\right)^{SG}$, was obtained by distinct simulations with different initial acetylene concentrations $[C_2H_2]$ and particle sizes (or surface areas, a), and the rate constant $k_{MD, SG}$ was determined by (Goudeli et al., 2026):

$$k_{MD, SG} = \frac{\left(\frac{dm}{dt}\right)^{SG}}{MW_c \cdot [C_2H_2] \cdot a} \quad (8)$$

resulting in an Arrhenius dependence with temperature (Goudeli et al., 2026):

$$\ln(k_{MD, SG}) = 3.946 - \frac{2017.3}{T} \quad (9)$$

Equation (8) originates from the HACA equation (Frenklach and Wang, 1991) where $k_s \cdot \chi_{soot}/N_{Av}$ has been replaced by the MD-derived lumped rate constant, $k_{MD, SG}$ (Goudeli et al., 2026). ”.

2a. Related to point 1, in the abstract (and possibly elsewhere) it is implied that MD kinetics are superior in predictive power ('...does not rely on reaction kinetic modeling').

2a. We would like to clarify that we do not suggest superiority of MD-based kinetics over reaction kinetic modeling in terms of predictive power but rather on computational efficiency, as also mentioned in the abstract: “is computationally efficient compared to detailed population balance equation models as it does not rely on reaction kinetic modeling”, at the end of Section 3: “It should be noted that even though the lumped MD-derived nucleation rate employed in Model II cannot capture the level of chemical detail accounted for in sectional models interfaced with chemical kinetic reaction mechanisms, it does capture f_v and d_m measurements with reasonable accuracy at significantly lower computational cost.”, and in the Conclusions: “Even though the developed MD-informed CFD-PD framework does not include the detail accounted for in chemical kinetic mechanisms, it captures the measured f_v and d_m reasonably well...”.

In fact, the motivation of the present work is exactly this: to evaluate how well MD kinetics and other *reduced* models can predict soot volume fraction and particle size when implemented in a simple CFD-monodisperse particle dynamics model. We do use the sectional model with the detailed kinetic mechanism as the state-of-the-art soot model and benchmark against it. To clarify this, we have added the following sentence in the 7th paragraph of Section 3.2: “...and experiments (Camacho et al., 2015). The sectional model (Model V) shows the best agreement with number density and soot volume fraction measurements, outperforming all reduced models, as expected. The soot number...”.

2b. However, while MD simulations do indeed employ Newton’s laws at the basic level, they involve parametrised potentials that bring their own assumptions. In addition, there are many assumptions involved in the way statistical mechanics is used to relate the outcomes of MD simulations to macroscopic kinetics. At present, only very small sets of molecules can be simulated, often under conditions that are far from what would be encountered in real situations such as flames, and many more choices and assumptions are involved regarding boundary conditions etc.,...

2b. We agree with the Reviewer that there is a number of assumptions and limitations related to the interaction potentials, system size, and simulation conditions in MD, as they have been acknowledged in the corresponding papers [2, 3] where the MD rate constants were originally proposed.

However, the motivation of the present work is to assess the performance of those MD-obtained rate constants in soot modeling, rather than to treat them as inherently reliable. To clarify this, the following clause has been added at the end of the Abstract of the revised manuscript: “reaction kinetic modeling. To the best of our knowledge, this work is the first systematic assessment of the potential of MD-derived nucleation and surface growth rate constants for soot modeling. In addition, the proposed CFD-coupled monodisperse PD framework can serve as a predictive tool for soot modeling and design-oriented simulations of practical combustion and aerosol systems.”.

2c. ...so there is no consensus as to how reliable ab initio kinetics can be obtained with MD.

2c. Indeed. Even though we have validated some MD-obtained reaction paths and energy barriers with density functional theory (DFT) in the past [4], an assessment of the overall kinetics would be extremely challenging, to the best of our knowledge. So, the present work is the first systematic assessment of the potential of MD for soot modeling with respect to other reduced models and serves as a basis for benchmarking its performance in the employed BSS flames. Generalization of the conclusions would require validation across additional flames and operating conditions, which we now explicitly acknowledge in the Conclusions of the revised manuscript: “...lower computational cost. Even though this framework is benchmarked in premixed ethylene BSS flame where the centerline temperature is mostly within the range that the MD rate constants were derived, it provides a promising foundation for predictive, design-oriented simulations of combustion and aerosol

synthesis systems. **Additional benchmarking would be necessary before application to different flame configurations.**”.

2d. Given the fact that the MD model is not described at all here, the reader is left with uncertainty as to what is its range of validity.

2d. Here, we have provided the range of validity of the MD-derived equations in the end of Section 2: “...encompass a range of physical assumptions. **For example, the MD-derived nucleation (Fakharneshad et al., 2026) and surface growth rates (Goudeli et al., 2026) have been obtained at high pressures and within a narrow temperature range of approximately 1200–1800 K. All are systematically benchmarked against experiments in Section 3.**”.

3. In the same vein, it seems that the MD model used here relates soot to acetylene. This was the assumption of early soot models, such as the Brookes and Moss model, but now it is established that soot is mechanistically formed via PAH routes and the dependence on acetylene is a rather crude and indirect correlation. This does not mean that one cannot base a model on this correlation (after all early soot models had considerable success with it), but the deficiencies must be acknowledged given that MD is proposed here as an approach with predictive power. The lack of discussion of the derivation and assumptions of the MD model is again the root of the problem.

3. Thank you for raising this. Indeed, PAHs may contribute to soot nucleation and this is accounted for implicitly in reactive MD simulations as PAHs and other cyclic and non-cyclic molecules form during nucleation [5]. In principle, more elaborate expressions could be developed from MD accounting for several species involved. However, this is impractical to the best of our knowledge as thousands of reactive species can emerge with a currently unknown contribution to soot formation [6]. In addition, as employing PAH-based nucleation models can be computationally prohibitive in multidimensional CFD simulations, we believe that correlating the growth rate with initial fuel concentrations (here acetylene) is an easy-to-use alternative. It should also be noted that reactive MD at high temperature can also account for chemical nucleation, a pathway not accounted for in traditional PAH dimerization pathways. The deficiencies associated with MD-derived nucleation rates lie primarily in the much higher pressures compared to those encountered in experiments. This has been added to the 3rd paragraph of the Section 2.2 of the revised manuscript: “...were described using MD-derived expressions. **The MD-derived nucleation rate (Model II) was developed from MD simulations of isothermal acetylene pyrolysis at temperatures of 1200–1800 K and high-pressure of 189–568 atm in Fakharneshad et al. (Fakharneshad et al., 2026).**”.

4. Again on the same point, given that the MD model is based on a crude correlation, the results on a single premixed flame leave open the question of the range of validity. This should also be acknowledged.

4. The following has been added to the conclusion section of the revised manuscript: “...**Even though this framework is benchmarked in premixed ethylene BSS flame where the centerline temperature is mostly within the range that the MD rate constants were derived, it provides a promising foundation for predictive, design-oriented simulations of combustion and aerosol synthesis systems. Additional benchmarking would be necessary before application to different flame configurations.**”.

5. The base case that the MD is compared with, the Brookes and Moss kinetics, is a very old model, which should be acknowledged. Having said that, comparison is made also with a detailed kinetic-sectional model which is closer to the state of the art.

5. Indeed, yet it remains one of the most widely used C_2H_2 -based formulations in commercial CFD tools such as ANSYS Fluent [7, 8], which was a driving reason to use it as a benchmark. We have added the following in the last paragraph of Section 2.2 of the revised manuscript: “For comparison, the Moss-Brookes soot model (Brookes and Moss, 1999), an early model developed in 1999, implemented in Fluent (Model V) is also considered as it is widely used in design applications (Wang, 2020).”.

6a. The main results do not seem to support the discussion that follows. The discussion outlines various improvements in several models that use different combinations of MD-derived kinetics (nucleation only, growth only or both) and the conclusions mention that "... it [the MD-derived] captures the measured f_v and d_m reasonably well, resulting in even comparable predictions to those by a detailed sectional model in the post-nucleation flame region, at significantly lower computational cost'. However, this is not the impression one gets from Fig. 6. In (a) (number density) the detailed model is clearly seen to be the only one reasonably close to the experimental results with considerable difference from all the others, of which the early Brookes-Moss-HACA gives the best results. In (b) (volume fraction) again the detailed model follows closer the trend, although here it is difficult to draw conclusions as most models either overpredict or underpredict by a similar amount. These results should be better reflected in the discussion and conclusions.

6. We thank the Reviewer for this Comment. As the sectional model is not only most chemically detailed but also accounts for the primary particle and aggregate size polydispersity, it is expected to be more accurate than any of the reduced models (Models I-V), as discussed in response to Comment 2a. Hence, the above discussion was aiming to assess the performance of Model II compared to experiments and to the detailed sectional model. To avoid confusion, we have added the following sentence in the 7th paragraph of Section 3.2: "...and experiments (Camacho et al., 2015). The sectional model (Model V) shows the best agreement with number density and soot volume fraction measurements, outperforming all reduce models, as expected. The soot number...”.

In addition, to better reflect the results of the reduced models of Figures 6 and 7, we have rephrased the last paragraph of Section 3 of the revised manuscript: “Among the reduced models (Models I-IV), the baseline framework (Model I), accounting for the semi-empirical nucleation rate and the HACA surface growth rate, captures the overall trend of the soot number density (Fig. 6a), volume fraction (Fig. 6b), and particle size (Fig. 7). Accounting for the MD-derived nucleation rate, Model II improves the d_m predictions and nicely matches the soot volume fraction and SMPS measurements in this flame. Model II predicts comparable N (within one order of magnitude) with the detailed sectional model across all H_p , but is outperformed by Models I (Moss-Brookes nucleation rate and HACA-predicted surface growth rate) and V (Moss-Brookes nucleation and surface growth rates). It should be noted that even though the Moss-Brookes nucleation rate in Model I and the lumped MD-derived nucleation rate employed in Model II cannot capture the level of chemical detail accounted for in sectional models interfaced with chemical kinetic reaction mechanisms, they do capture f_v and d_m measurements with reasonable accuracy, especially at $HAB > 5$ mm, at significantly lower computational cost.”.

7. Fig. 5 is not informative and even obfuscates the conclusions to be drawn from this study. To begin with, the information contained in these histograms is redundant as it is wholly contained in the radial profiles of Fig. 6. More importantly, histograms do not show trends unless one juxtaposes the two positions and tries to look at correlations. Since the radial profiles (the common way of presenting this information in sooting flame studies) are shown in Fig. 6, I think that this figure does not serve its purpose and this is aggravated by the fact that it is shown and discussed before Fig. 6.

7. This is probably a misunderstanding. Even though the results of the reduced models (I-IV) in Fig. 5 are identical to those presented in Fig. 6 at $HAB = 4$ and 8 mm, the results of Model V in Fig. 5 correspond to 2D sectional model of Saggese et al. [9], while the results of Model V in Fig. 6 correspond to 1D sectional model reported in a preceding paper by the same group (Saggese et al. [10]). The 2D results are available only at two burner-to-stagnation plate separations (4 and 8 mm) and distinct from each other (e.g., at $HAB = 4$ mm the 1D and 2D models predict soot volume fractions of 0.51 (Fig. 6) and 0.23 ppm (Fig. 5), respectively). To clarify this further, we have modified the 7th paragraph of Section 3.2: “The performance of the **reduced models** is assessed across a broader range of burner-to-stagnation plate separations investigated experimentally, as shown in Fig. 6. The results are **now** compared against the 1D sectional model of Saggese et al. (Saggese et al., 2015), which employed the same soot sub-model as **in 2D simulations (Fig. 5) but covers a wider range of H_p values from 4 to 12 mm.**” and have included the corresponding references in Figures 5, 6 and 7 of the revised manuscript.

8. In Fig. 7, results for the detailed model are not shown. Are results for mobility diameter not available for that model? If they are, they should be shown, otherwise a reason should be provided.

8. We thank the Reviewer for this recommendation. Even though the average mobility diameters are not provided in Saggese et al. [10], we have calculated them based on their reported mobility-based size distributions [10], as shown in Figure R1.

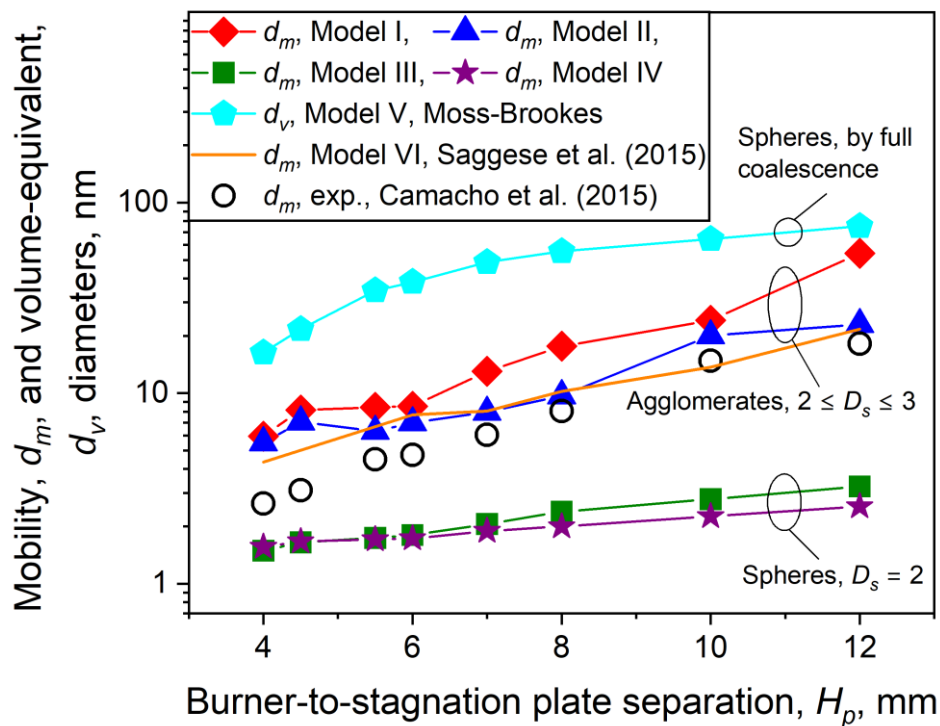


Figure R1. Soot mobility diameter (d_m) predicted by the CFD-coupled monodisperse PD framework (Models I-IV) and volume-equivalent diameter (d_v) predicted by the Moss-Brookes soot model (Model V; full coalescence) (filled symbols). The model predictions are compared to 1D sectional model (Model VI) reported in [10] (line) and to the average d_m from SMPS measurements in premixed ethylene flames (circles) [1].

Similar to soot volume fraction and number concentration predictions, the mobility size predicted by the section model shows the best agreement with experiments. To address the Reviewer’s Comment, Figure 7 in the revised manuscript has been replaced with Figure R1 and the following discussion has been added to the second to last paragraph of Section 3.2 of the revised manuscript: “...The model

predictions are compared with the average d_m from the detailed 1D sectional model (Model VI: orange line) derived from the reported mobility size distributions in Saggese et al. (Saggese et al., 2015: Fig. 11), as well as with the average d_m obtained by scanning mobility particle sizer (SMPS) measurements in premixed ethylene flames (Camacho et al., 2015: symbols). Even though the present PD model does not account for the agglomerate/aggregate polydispersity, the mobility-based self-preserving size distribution can be derived based on the average d_m (Fig. 7) and the mobility-based self-preserving geometric standard deviation of soot ($\sigma_{g,m} = 1.48 \pm 0.03$), obtained by discrete element method simulations (Kelesidis and Goudeli, 2021: Fig. 2). All models capture the expected increase in particle size with increasing burner-to-stagnation plate separation. Similarly to soot volume fraction and number concentration (Fig. 6), the 1D sectional model predicts most accurately the mobility diameter measurements. Among the reduced models, the MD-informed nucleation model (Model II) shows the best agreement with the measured mobility diameters and with the 1D sectional model (Model VI) predictions, esp. for $H_p \geq 6$ mm, followed by the baseline Model I...”.

There also some minor points and typos:

- The model referred to as 'Moss-Brookes' would be better written as 'Brookes-Moss' given that this is the order of the names in the publication.
Indeed, but even though the original publication lists the authors in this order, the term 'Moss-Brookes' is the form most commonly used in the literature, and we have therefore retained it for consistency.
- Title: I would recommend '...by a monodisperse...'
We thank the Reviewer for the recommendation. We have removed “model” from the title.
- There is an undefined reference 'Section 3.1.1Error! Reference source not found..' '
It has been fixed.
- End of p. 4: 'd... iffusion'
It has been fixed.
- p.5 'denotes the velocity' there is a formatting issue there
It has been fixed.
- p.6 'detailed in (... - no parenthesis needed'
It has been fixed.

References

1. Camacho, J., et al., *Mobility size and mass of nascent soot particles in a benchmark premixed ethylene flame*. Combustion and Flame, 2015. **162**(10): p. 3810–3822.
2. Fakharneshad, A., et al., *Nucleation, surface growth and coagulation of soot by hierarchical modeling*. Powder Technology, 2026. **469**.
3. Goudeli, E., et al., *Surface growth rate of soot by reactive Molecular Dynamics*. SSRN Electronic Journal, 2026.
4. Schmalz, F., et al., *Reaction path identification and validation from molecular dynamics simulations of hydrocarbon pyrolysis*. International Journal of Chemical Kinetics, 2024.

5. Ganguly, A., Mukut, K. M., Roy, S., Kelesidis, G., & Goudeli, E., *Investigation of soot precursor molecules during inception by acetylene pyrolysis using reactive molecular dynamics*. *Aerosol Research*, 2025. **3**(1): p. 185–203.
6. Schmalz, F., et al., *Reaction path identification and validation from molecular dynamics simulations of hydrocarbon pyrolysis*. *International Journal of Chemical Kinetics*, 2024. **56**(9): p. 501–512.
7. Wang, C., *The Development and Implementation of a Population Balance Method-Based Soot Model in Diffusion Flames*. 2020, UNSW Sydney.
8. *Ansys Fluent Theory Guide*, ed. I. Ansys. 2023, Canonsburg, PA: Ansys Inc.
9. Saggese, C., et al., *Probe effects in soot sampling from a burner-stabilized stagnation flame*. *Combustion and Flame*, 2016. **167**: p. 184–197.
10. Saggese, C., et al., *Kinetic modeling of particle size distribution of soot in a premixed burner-stabilized stagnation ethylene flame*. *Combustion and Flame*, 2015. **162**(9): p. 3356–3369.
11. Kelesidis, G.A. and E. Goudeli, *Self-preserving size distribution and collision frequency of flame-made nanoparticles in the transition regime*. *Proceedings of the Combustion Institute*, 2021. **38**(1): p. 1233–1240.