Discrete Element Method Model for Restructuring of Soot Aggregates

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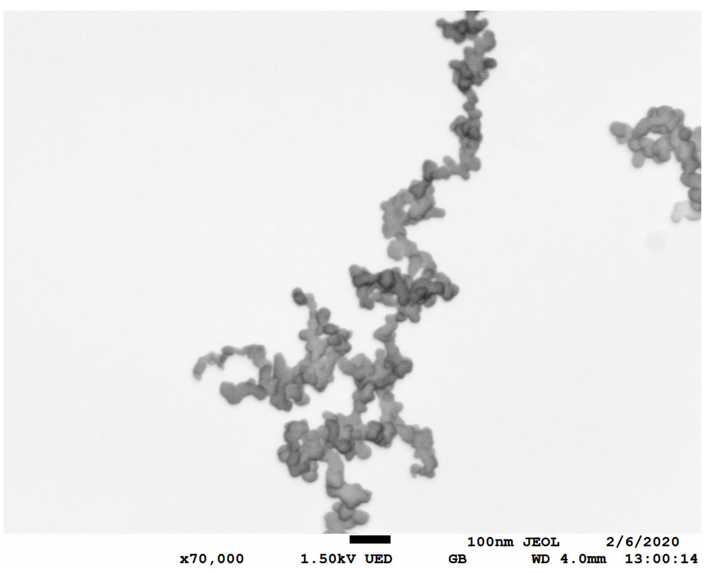
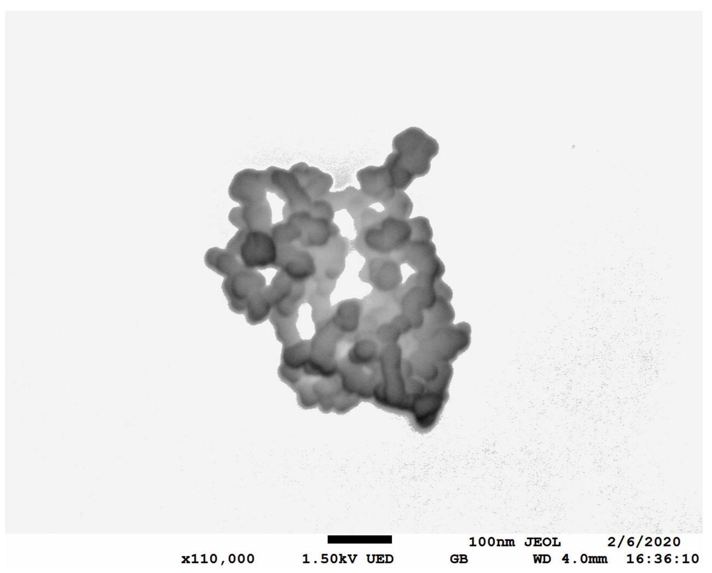
Introduction

- Soot particles are aggregates of carbon spherules
- Soot particles age in the atmosphere by internal mixing with other compounds through condensation or coagulation
- Internally mixed with liquid coatings soot aggregates restructure due to capillary forces and this change in morphology affects climate forcing properties of soot
- We developed a discrete element method (DEM) contact model for soot aggregate mechanics and restructuring



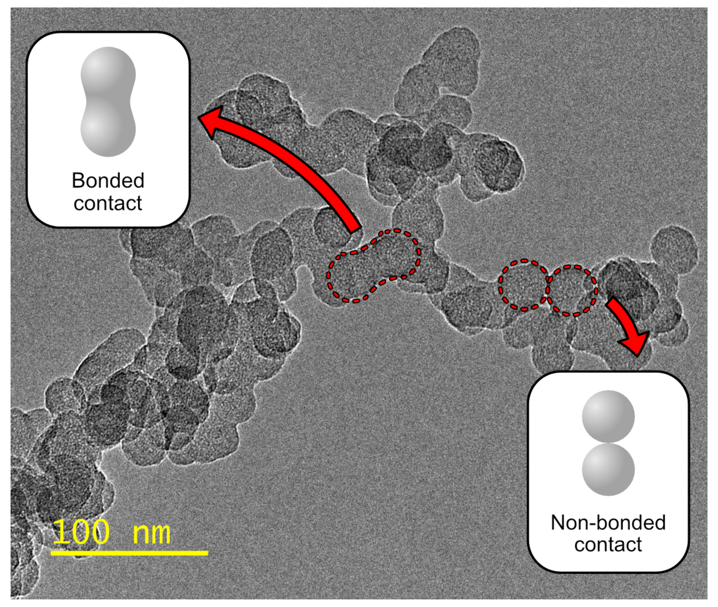
Fresh aggregate



Restructured aggregate

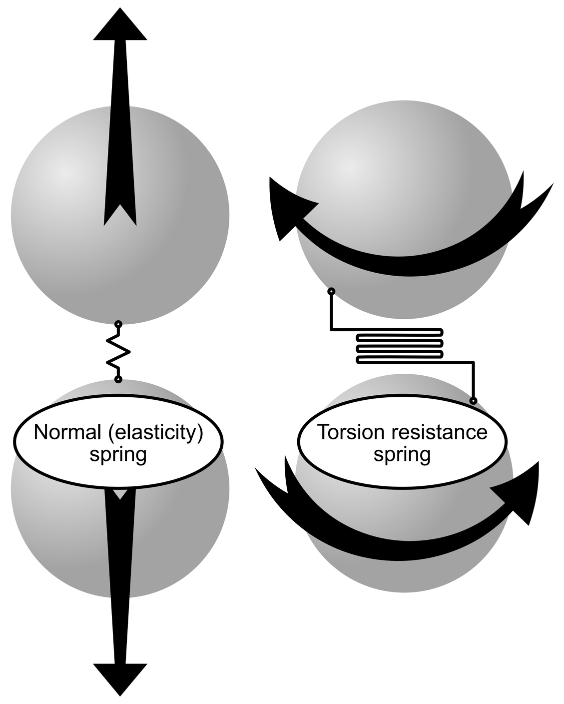
Background

- An aggregate can be represented as a collection of spherical particles
- Neighboring particles are bonded with solid necks in fresh soot aggregates
- Coating-induced forces can fracture necks, thus creating frictional non-bonded contacts

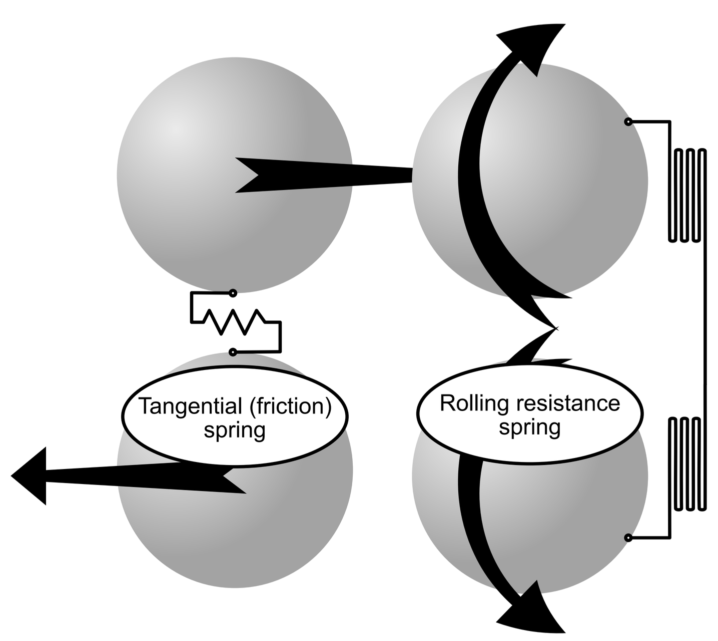


Contact model

$$m\mathbf{a}_i = \sum_{\substack{j=1 \\ j\neq i}}^{N} \mathbf{f}_{c,ij} + \mathbf{f}_{b,i} \qquad I\boldsymbol{\alpha}_i = \sum_{\substack{j=1 \\ j\neq i}}^{N} \boldsymbol{\tau}_{c,ij}$$



Normal degrees of freedom



Tangential degrees of freedom

Contact model (continued)

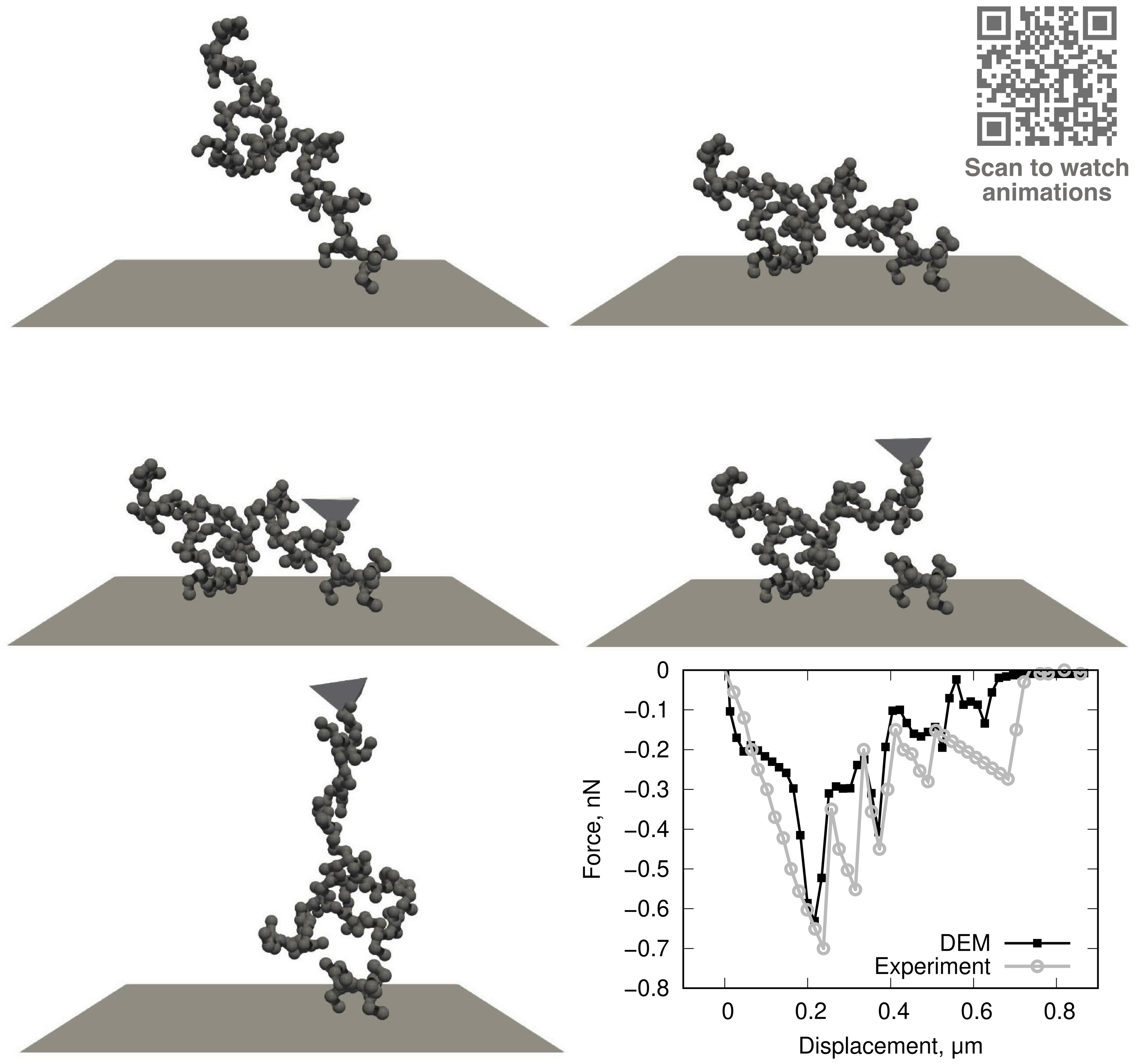
- Four springs are inserted in every contacting pair of particles to constrain four degrees of freedom
- To model elastic necks:
  - Springs are incremented throughout the simulation
- To model frictional contacts:
  - Springs are incremented for the duration of contact
  - Limited sliding is allowed to simulate friction
- To model van der Waals attraction:
  - Hamaker equation is used:

$$\mathbf{f}_{ij} = -\frac{A}{6}\left[\frac{(4r+2\delta_{ij})}{(4r+\delta_{ij})\delta_{ij}} - \frac{2}{(2r+\delta_{ij})} - \frac{4r^2}{(2r+\delta_{ij})^3} - \frac{2r^2(4r+2\delta_{ij})}{(4r+\delta_{ij})^2\delta_{ij}^2}\right]\mathbf{n}_{ij}$$

where δ_{ij} is separation between particles, r is particle radius, and A is Hamaker constant

Model validation - aggregate mechanics

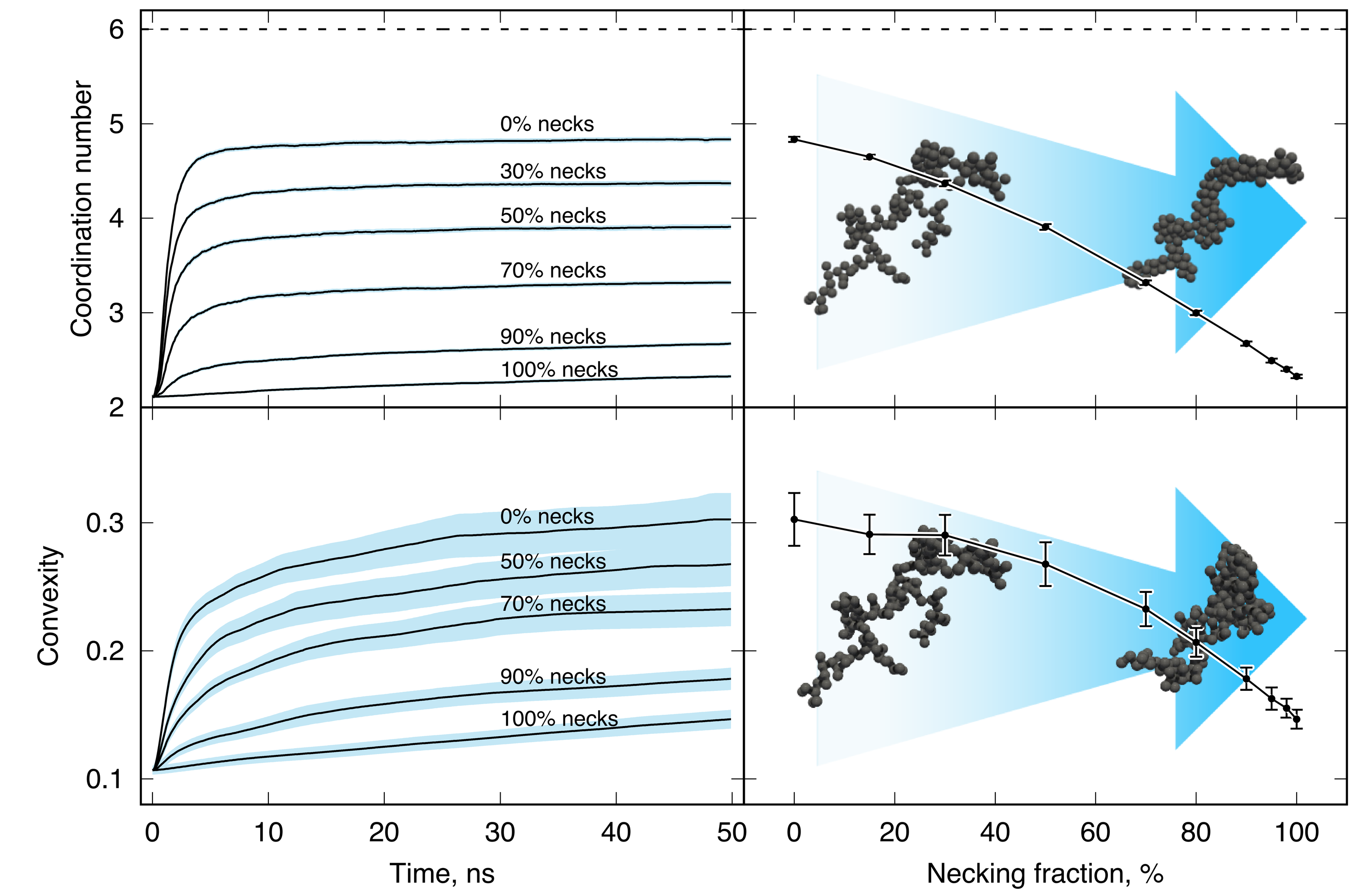
- The soot mechanics model was validated by reproducing AFM force spectroscopy experiments
- Aggregates were deposited on a substrate, indented, and stretched with a probe
- Force was recorded as a function of displacement



- The characteristic sawtooth pattern was reproduced
- The magnitude of force and the number of sawtooth features, on average, match experimental data

Model application - aggregate restructuring

- Coating-induced force was simulated with a cut off pair potential
- Restructuring outcome as a function of necking fraction was investigated



- Coordination number was computed to quantify the degree of local restructuring
- Coordination number approaches the random jammed packing value of 6 with decreasing necking fraction
- Convexity was computed to quantify the degree of global restructuring
- 3D convexity reported here can be related to 2D convexity reported in experimental studies by projecting the aggregates onto xy, xz, and yz planes
- 2D convexity of compact aggregates was estimated to be 0.80 ± 0.03, which lies in the range from 0.75 to 0.87, reported for restructured aggregates in experimental studies

Conclusions

- A DEM contact model for soot aggregates was developed
- The model reproduces mechanical behavior of aggregates under AFM spectroscopy
- The model can be used to simulate restructuring of aggregates

Future work

- Parametrize neck fracture taking into account the microstructure of carbonaceous material
- Develop a more rigorous representation of the coating material
  - A pair potential is a valid approximation for thinly coated soot
  - Some many-body potential is needed to simulate thickly coated soot

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