Machine-learning-based approach to predict optical properties of black carbon (BC) at various aging stages

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MOTIVATION

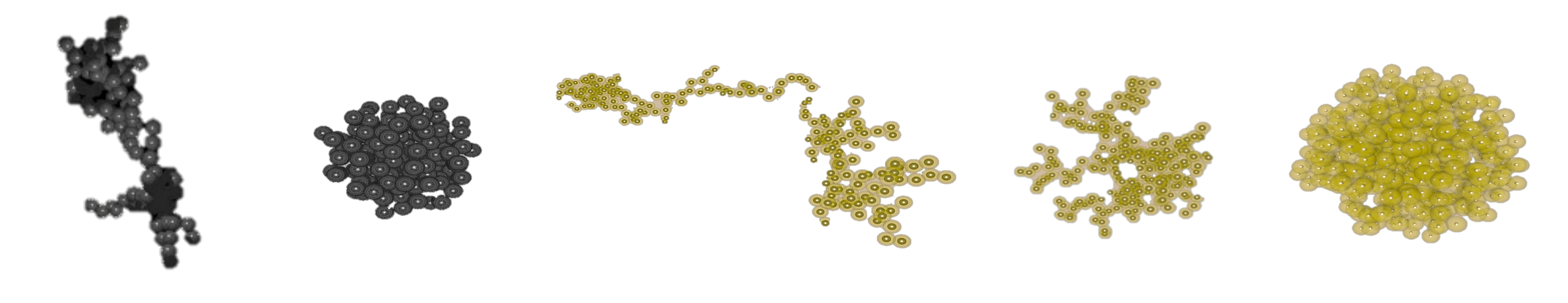
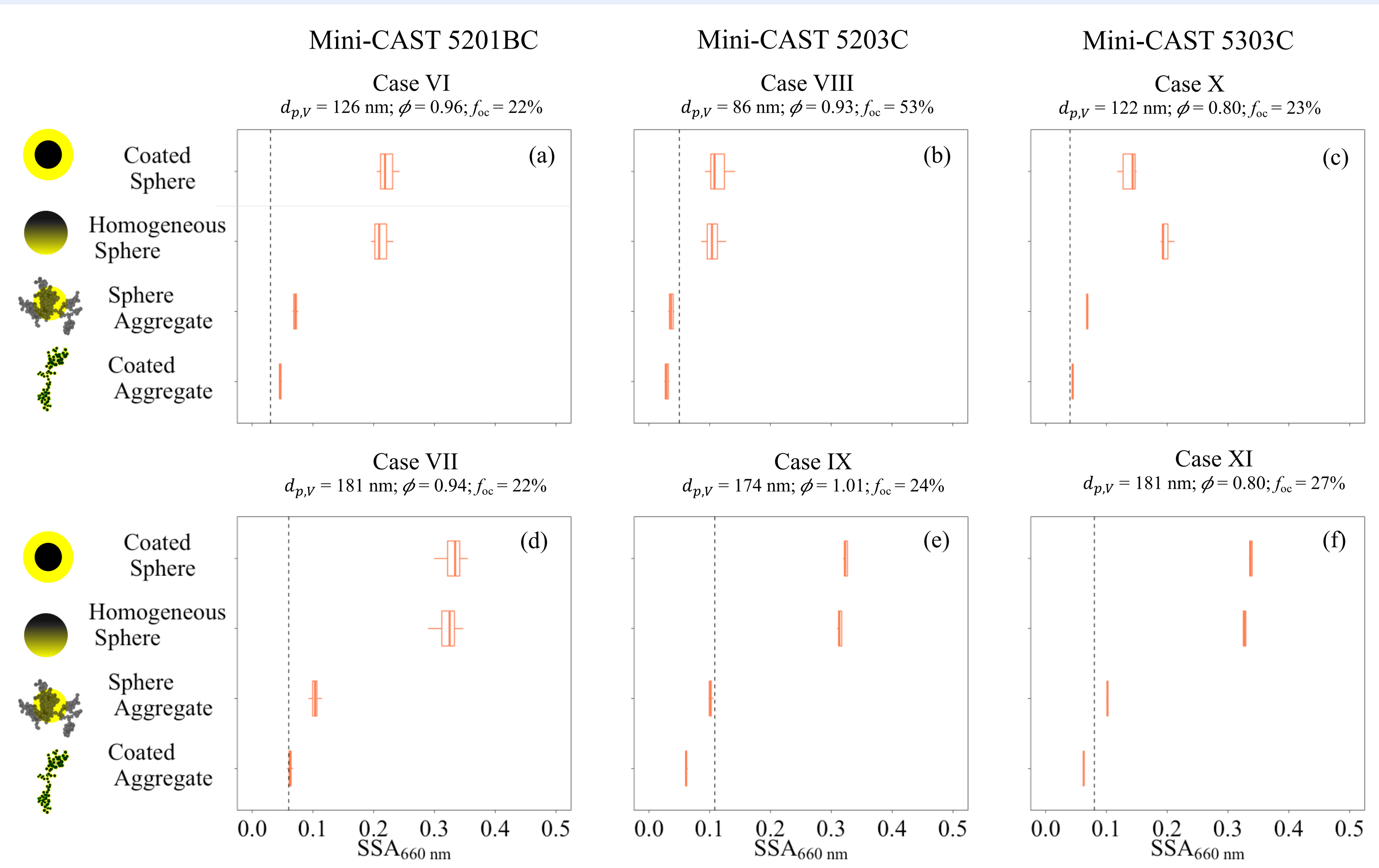


Fig.1. Visualization of the various BC aggregate particles generated in this study.

- Shortcomings of the simplified spherical assumption of BC [1,2] have led to the use of realistic fractal aggregate morphology (Fig.1) for computing the optical properties of BC.
- ML-models developed from pre-calculated databases [3,4] such as in this study save time for the construction of detailed aggregates and mitigates high computational overhead in large-scale applications.

LABORATORY EXPERIMENTS

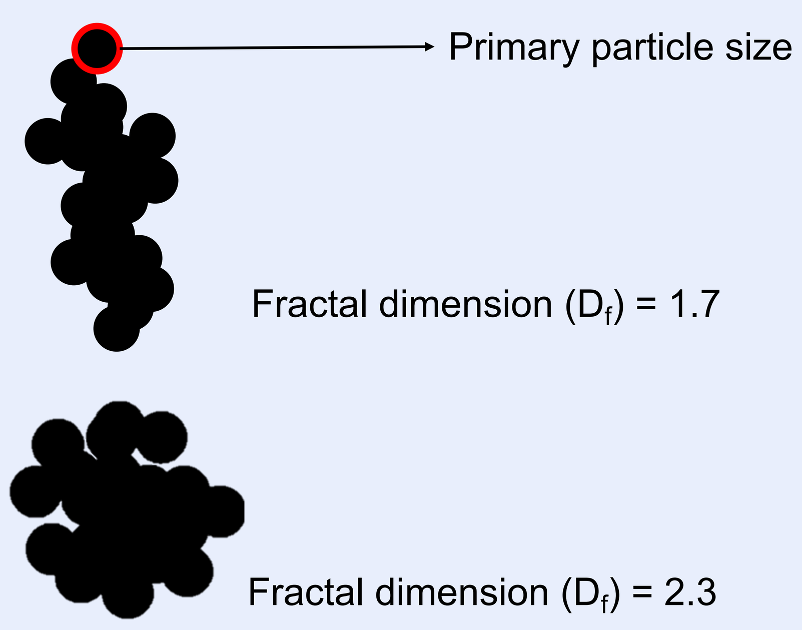


- Laboratory experiments showed that the **use of fractal aggregate morphology for BC** reproduced their optical properties most accurately [3].

DATABASE OF BC FRACTAL AGGREGATES

Physicochemical features:

- Primary particle size (a)
- Number of primary particles (N_{pp})
- Outer volume equivalent radius (r_o)
- Inner volume equivalent radius (r_i)
- Mobility diameter (D_p)
- Fractal dimension (D_f)
- Fraction of coating ($f_{coating}$)
- Total volume of particle (V_{total})
- Volume of the BC (V_{BC})
- Volume of the coating ($V_{coating}$)
- Total mass of particle (m_{total})
- Mass of the BC (m_{BC})
- Mass of the coating ($m_{coating}$)
- Mass ratio (M_R)



Radiative features:

- Wavelength (λ)
- Optical efficiencies ($Q_{ext/abs/sca}$)
- Geometric cross-section (C_{geo})
- Optical cross-sections ($C_{ext/abs/sca}$)
- Asymmetry parameter (g)
- Single scattering albedo (SSA)
- Mass absorption cross-section (MAC)

PERFORMANCE OF THE ML-BASED APPROACH

ML methods used

Kernel ridge regression (KRR) — scikit-learn

Artificial neural network (ANN) — Keras

Prediction accuracy

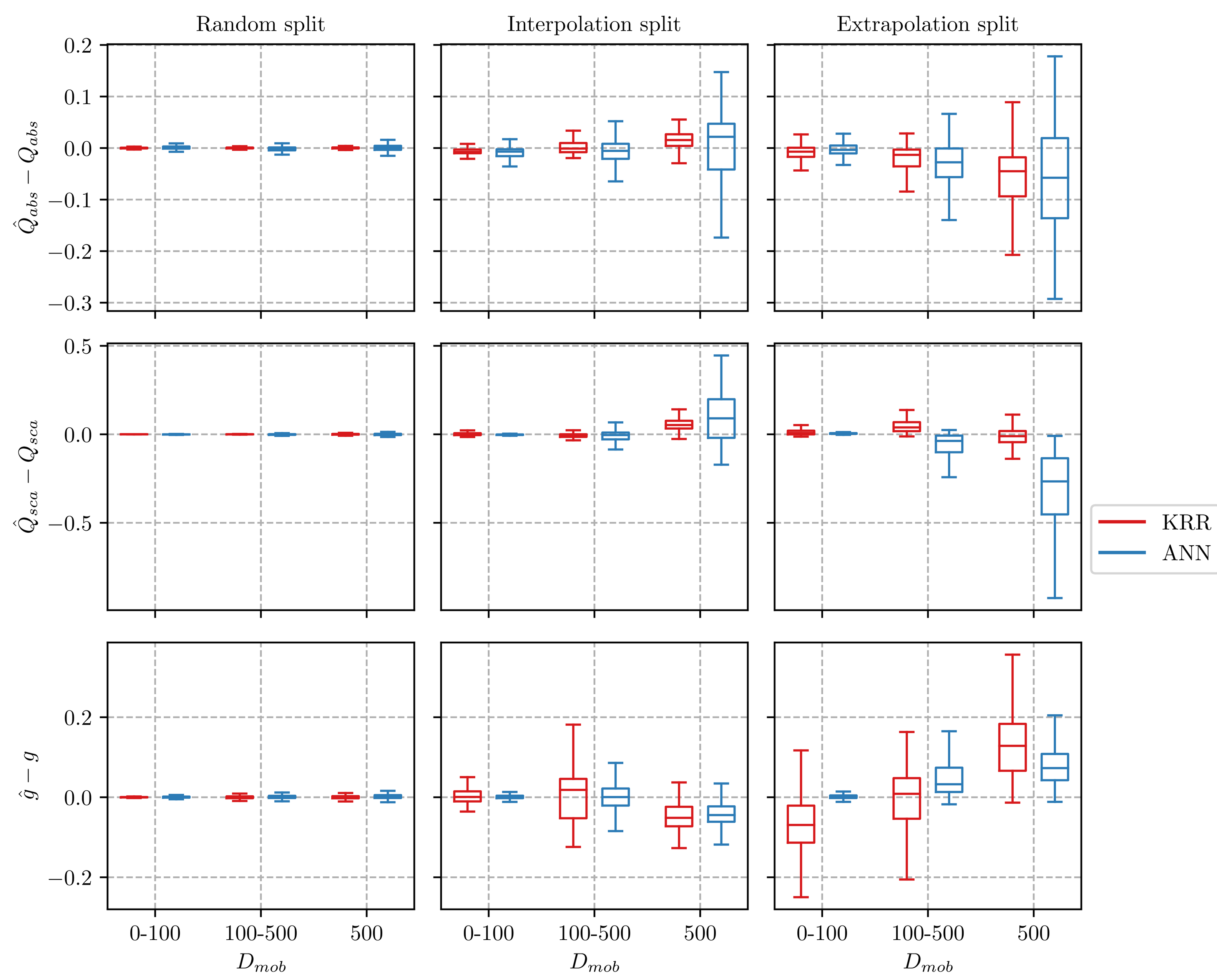


Fig. 2. Boxplots summarizing the mean absolute error between the predicted value (Q_{abs}, Q_{sca}, g) and their true value for different particle sizes using ML-methods KRR and ANN.

Table 3. Mean absolute errors of the predicted optical properties for different experiments.

Optical property	Random split		Interpolation split		Extrapolation split		Feature range
	KRR	ANN	KRR	ANN	KRR	ANN	
Q_{abs}	0.0022	0.0039	0.0122	0.0287	0.0329	0.0354	0 – 2
Q_{sca}	0.0019	0.0031	0.0224	0.0466	0.0393	0.0939	0 – 2
g	0.0044	0.0038	0.0429	0.0289	0.0879	0.0485	0 – 1

Prediction efficiency

Table 4. Training time for 18526 samples and prediction time per sample in seconds.

ML model	Training time	Prediction time
KRR	33.3s	0.0006s
ANN	1770s	0.0005s

DATA AND CODE AVAILABILITY

Database

ML experiments

Prediction script

SUMMARY

Machine-learning method to predict the optical properties of BC at various stages of ageing was developed under the following premises:

- **Active investigation area**
- **User-friendly**
- **Low-energy cost**
- **Low-computational cost**
- **Reproducibility and citability**

REFERENCES

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