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MultilayerPy: a python package for creating and optimising multi-layer models of aerosol and film processes

Dr Adam Milsom

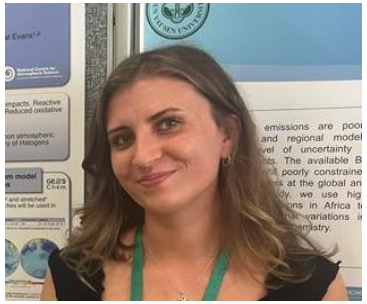
(Postdoctoral researcher in atmospheric science,

University of Birmingham, UK)

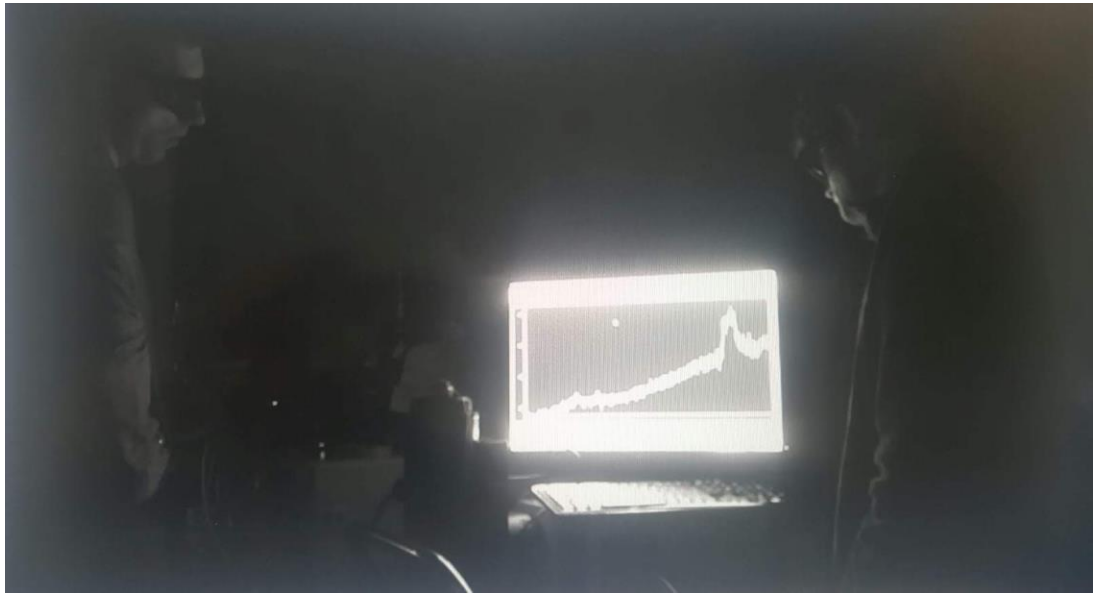
People!

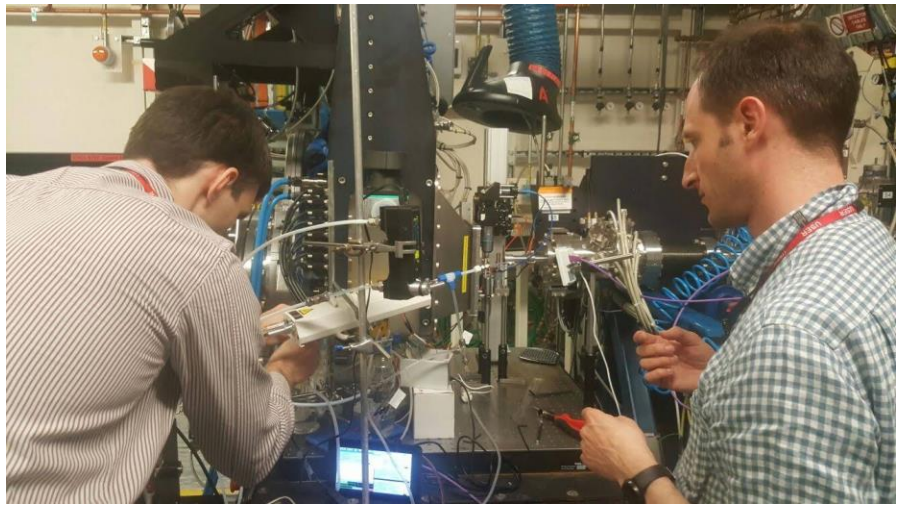
Dr Christian Pfrang (Birmingham)

Dr Adam M. Squires (Bath)



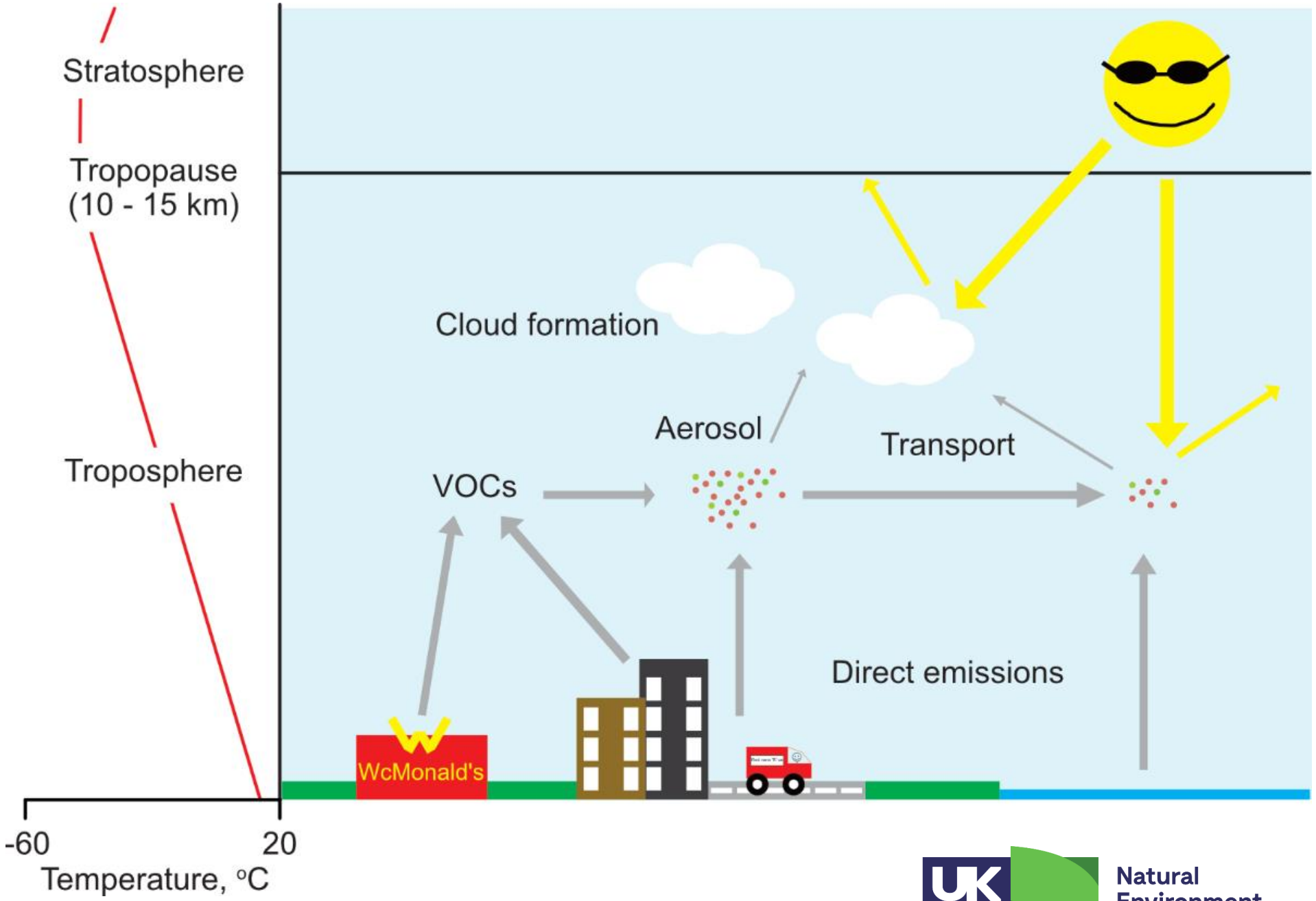
Amy Lees – MultilayerPy development (Birmingham, now York)





@adam_milsom94 | a.milsom.2@bham.ac.uk

Aerosols are important



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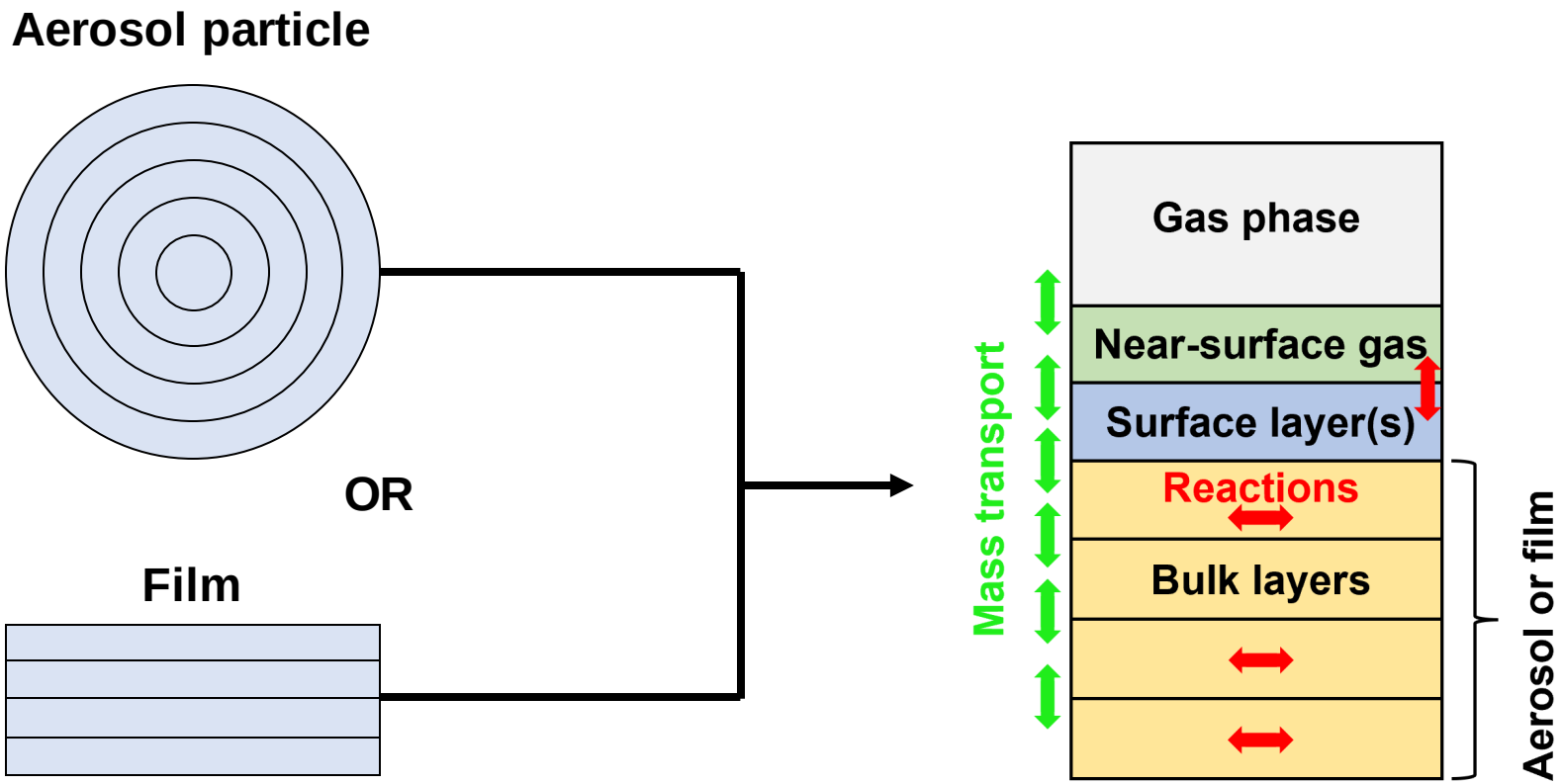
Kinetic multi-layer models



There are 2 main models I focus on:

1. Kinetic multi-layer model of aerosol surface and bulk chemistry (KM-SUB)

2. Kinetic multi-layer model of gas-particle interactions in aerosols and clouds (KM-GAP)

Shiraiwa et al., *Atmos. Chem. Phys.*, 2010 & 2012
Milsom et al., *Geosci. Model Dev.*, 2022

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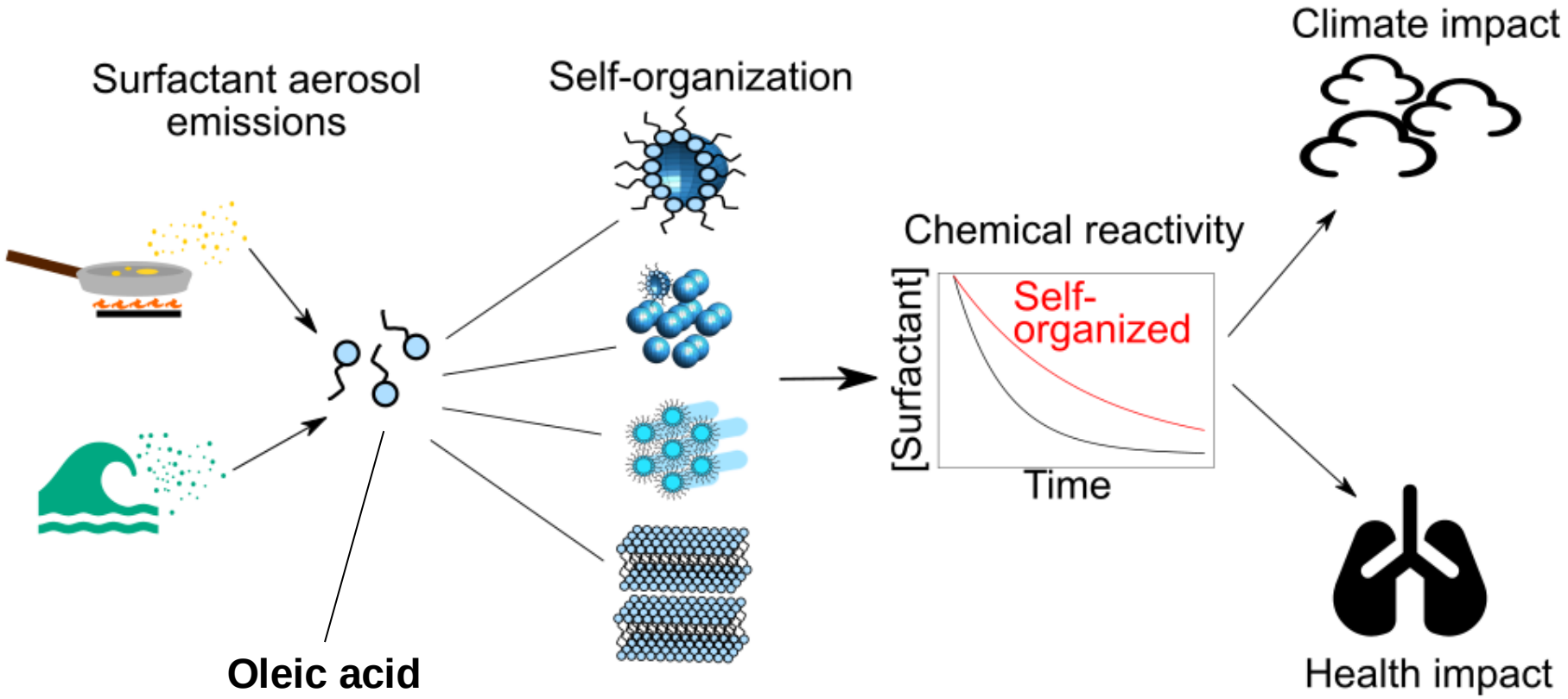
Why are these models useful?

My question (and PhD): what is the effect of molecular self-organisation on aerosol processes?



Milsom et al., *Acc. Chem. Res.*, 2023
Milsom et al., *Atmos. Chem. Phys.*, 2023
Milsom et al., *J. Phys. Chem. A*, 2022
Milsom et al., *Atmos. Chem. Phys.*, 2022
Milsom et al., *Environ. Sci.: Atmos.*, 2022
Milsom et al., *Atmos. Chem. Phys. 2021*
Milsom et al., *Faraday Discuss.*, 2021

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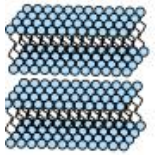
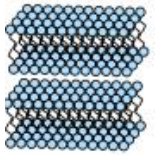
Quantifying the effect of molecular self-organisation on reaction kinetics:

Vs.



MODEL OPTIMISATION



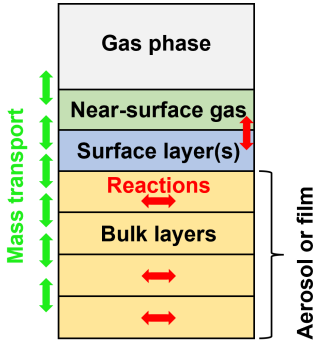
Raman

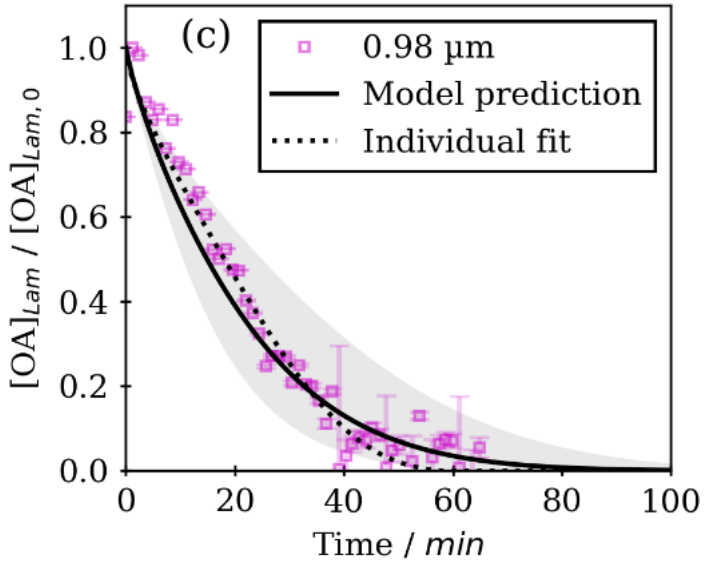
Oleic acid film

O_3

Surface

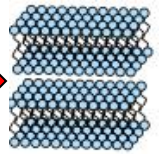
Milsom et al., Faraday Discuss., 2021.
Milsom et al., Atmos. Chem. Phys., 2022.

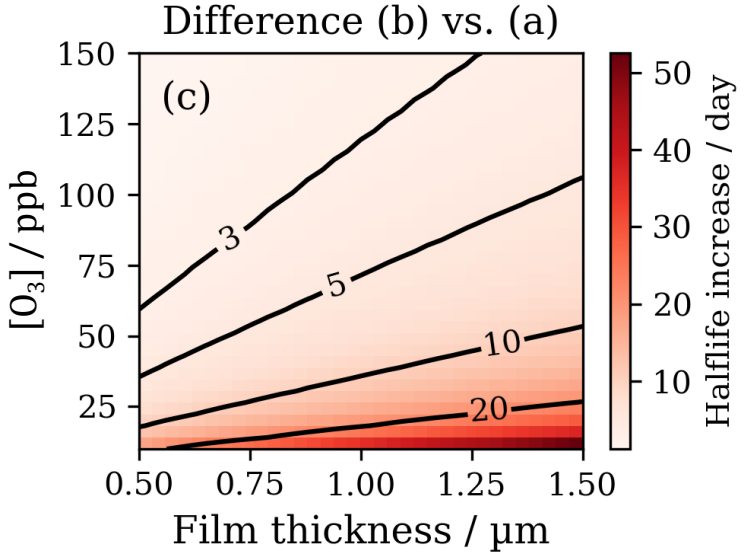




ATMOSPHERIC IMPLICATION

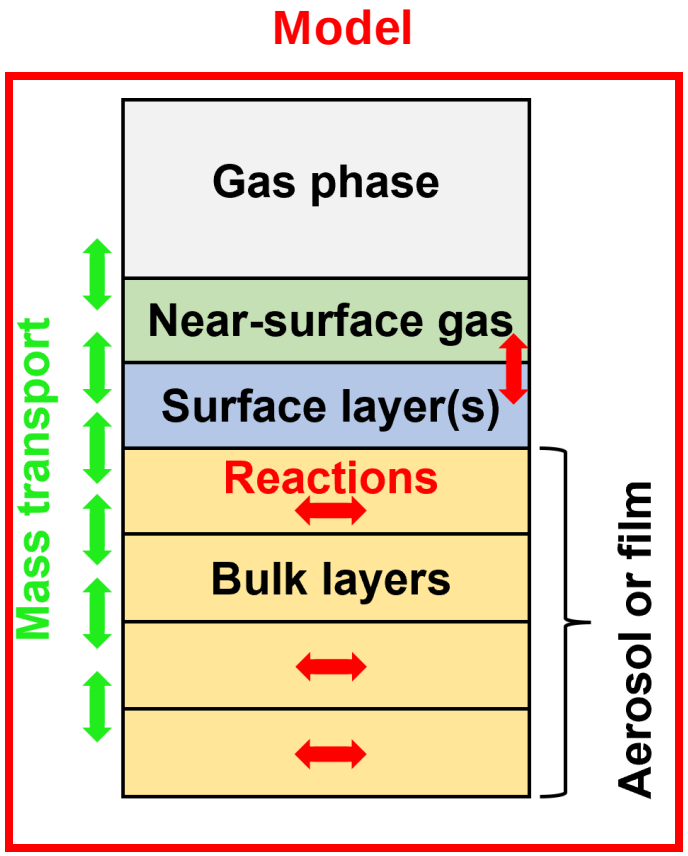
10 day half-life increase

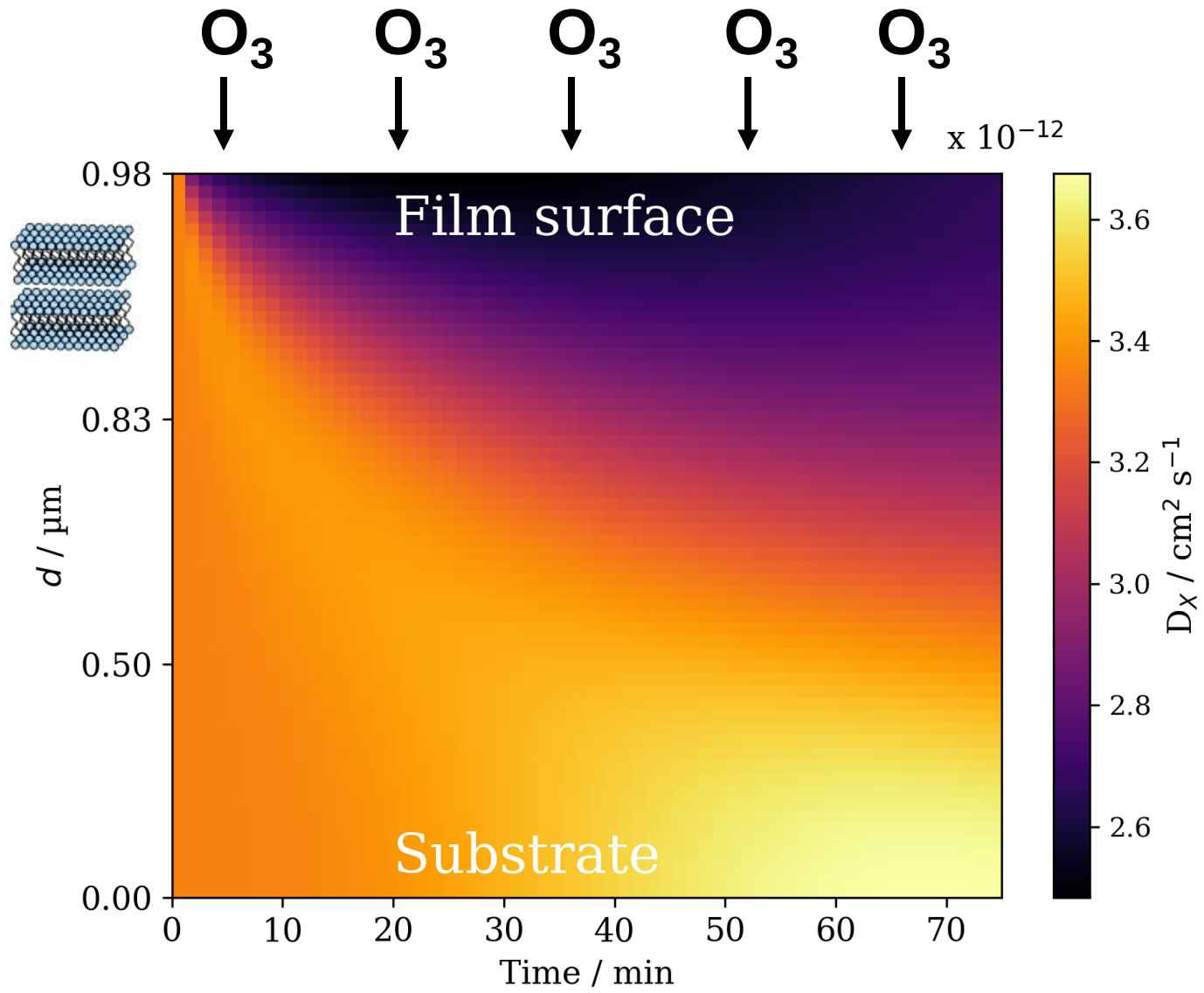




Milsom et al., Atmos. Chem. Phys., 2022.

Depth-resolved information





Milsom et al., Atmos. Chem. Phys., 2022.

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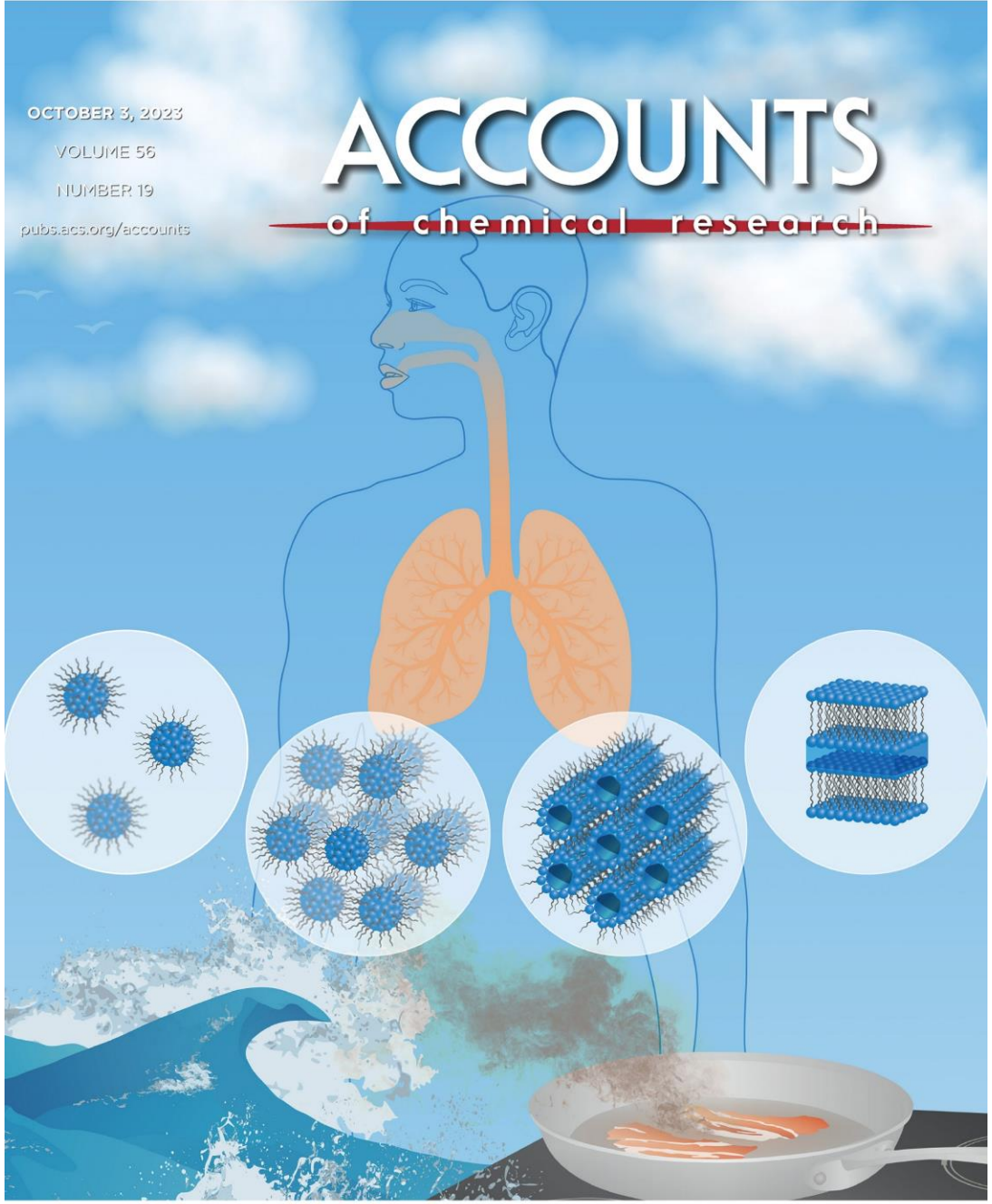
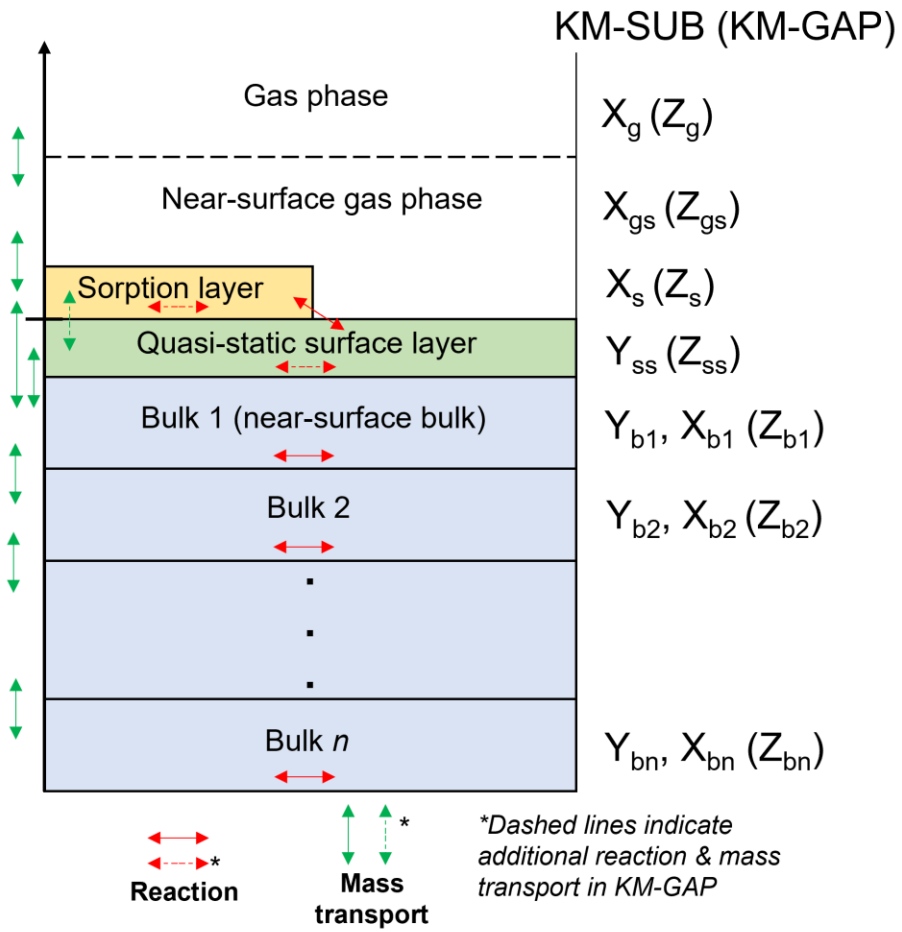


Milsom et al., *Acc. Chem. Res.*, 2023

Why make a tool to create these models?

The problem with multi-layer models



- Complicated
- Time-consuming
- Error prone
- Not always easy to modify the model
- Reproducible?

Milsom et al., *Geosci. Model Dev.*, 2022

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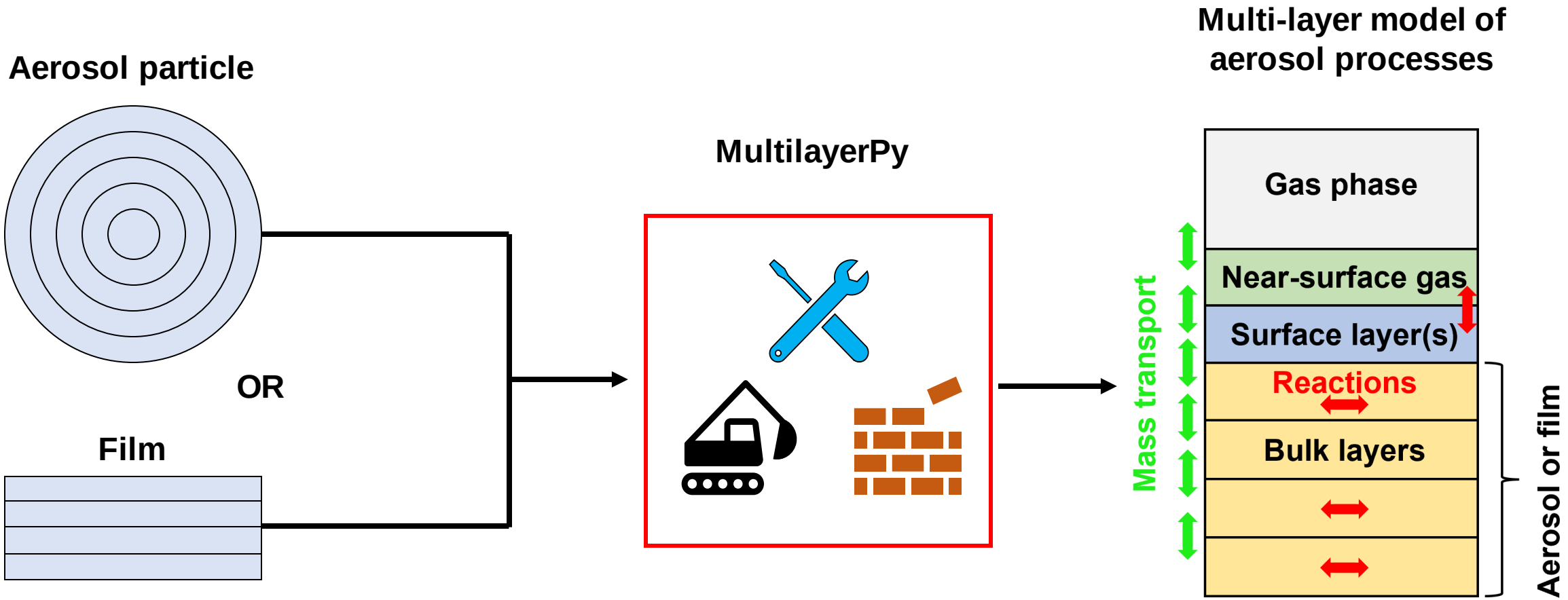
MultilayerPy: A tool for creating and optimising multi-layer models of aerosol processes



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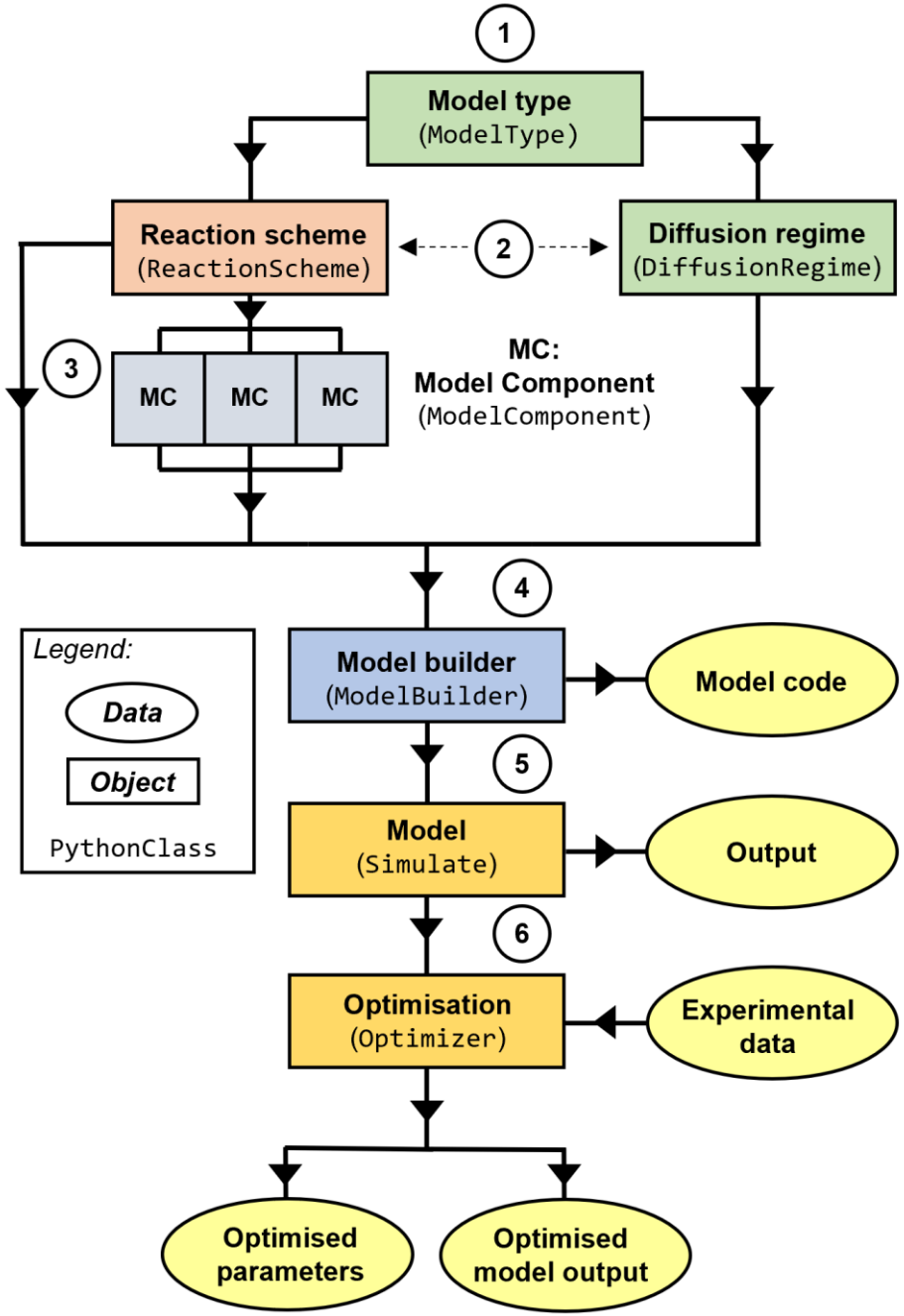
Milsom et al., *Geosci. Model Dev.*, 2022

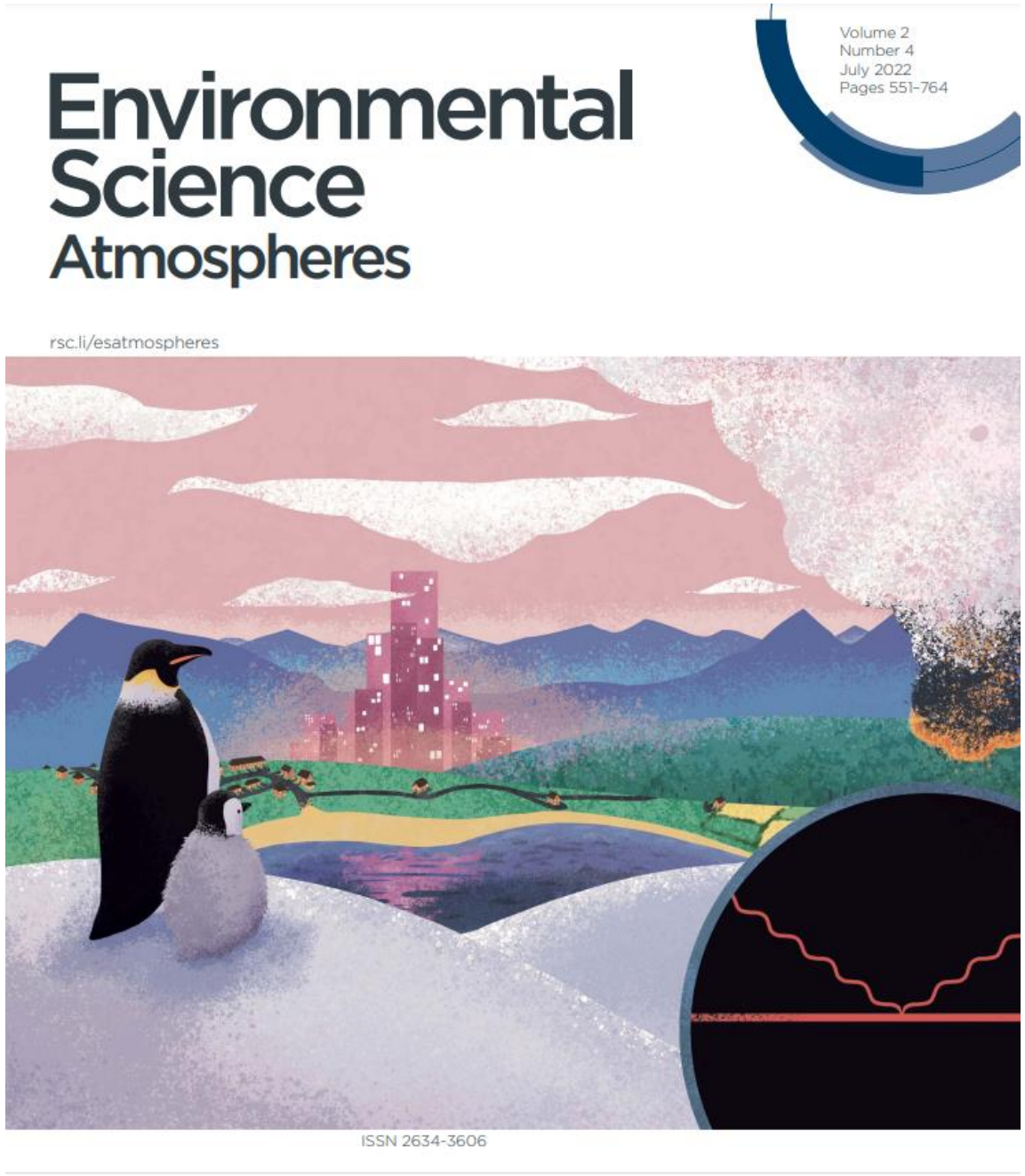
MultilayerPy: a tool for creating and optimising multi-layer models



- **Modularity** – the model building process is split into chunks so that the user can iterate through different models with ease.
- **Reproducibility** – the model output and code are generated in a readable manner, encouraging the user to share their code with e.g. a publication.
- **Open-source** – the package is released under an open-source license and collaboration on the project is encouraged.
- **Scalability** – it is possible to parallelise MultilayerPy model optimisation algorithms over many computer cores (e.g. on a supercomputer).

It has its own YouTube channel! (Search MultilayerPy)

Milsom et al., *Geosci. Model Dev.*, 2022



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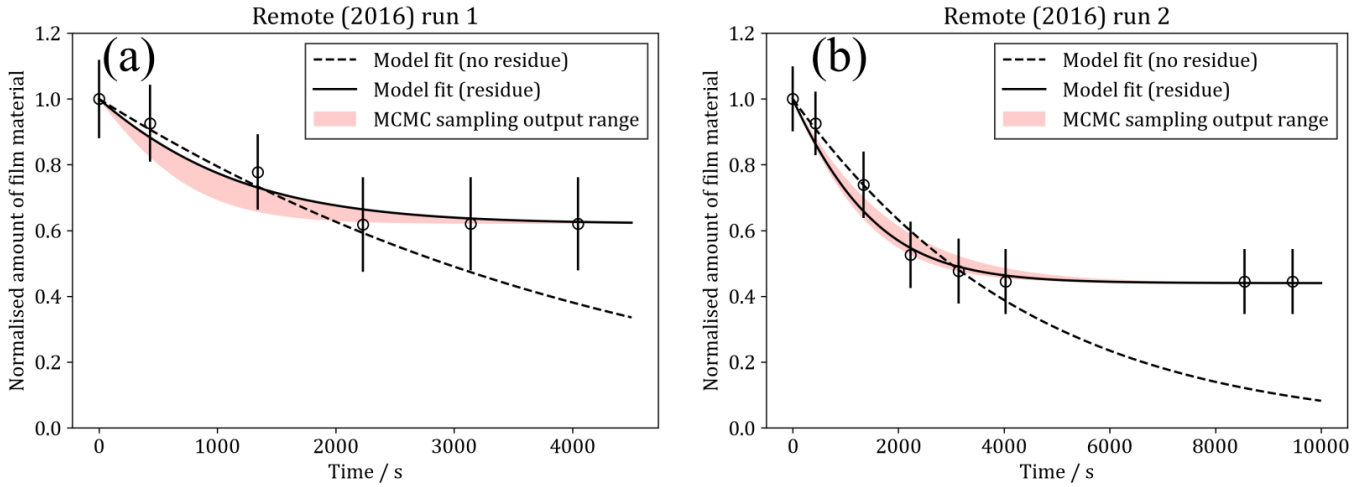
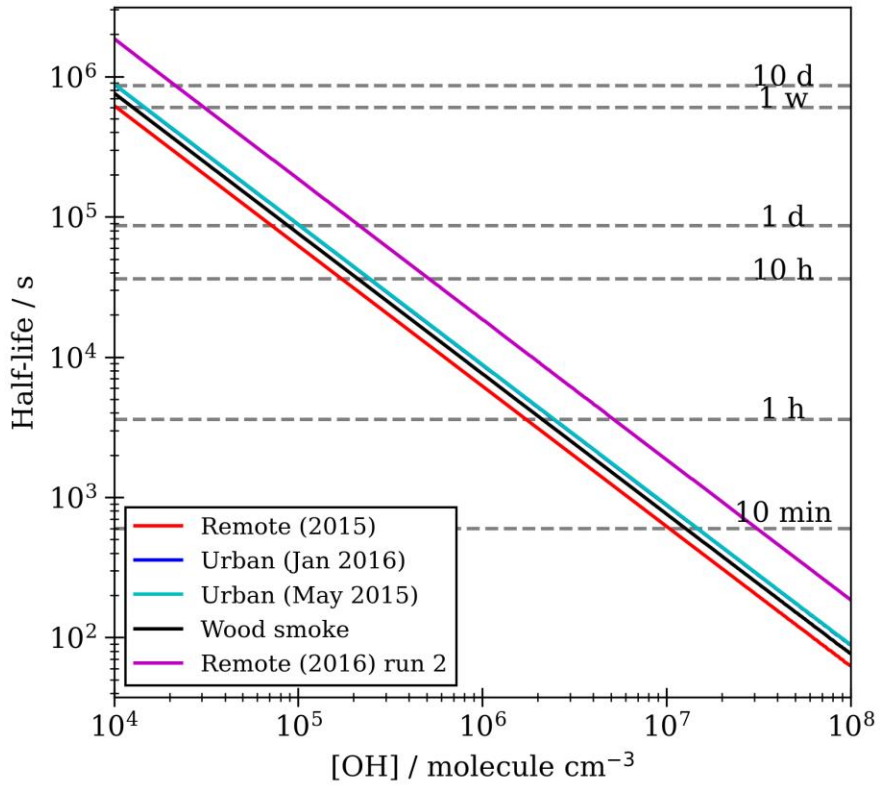
Real-life application: oxidising films of material from urban, remote and wood burning aerosols

Shepherd et al., *Environ. Sci.: Atmos.*, 2022

Societal impact award (ISIS neutron source)

Reactivity of real aerosol material





Shepherd et al., *Environ. Sci.: Atmos.*, 2022

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Building a user community

Original Article

Exploring the influence of particle phase in the ozonolysis of oleic and elaidic acid

Ravleen Kaur Kohli, Ryan S. Reynolds, Kevin R. Wilson & James F. Davies

Received 21 Feb 2023, Accepted 09 Jun 2023, Accepted author version posted online: 15 Jun 2023, Published online: 28 Jun 2023

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YouTube channel: Search “MultilayerPy” – Tutorials and a webinar for new users

GitHub: MultilayerPy

Contact email: multilayerpy@gmail.ocm

Thank you!