Mechanics of Soft Aerosols

Engineering and Physical Sciences Research Council

UNIVERSITY OF BATH

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Motivations and Aims

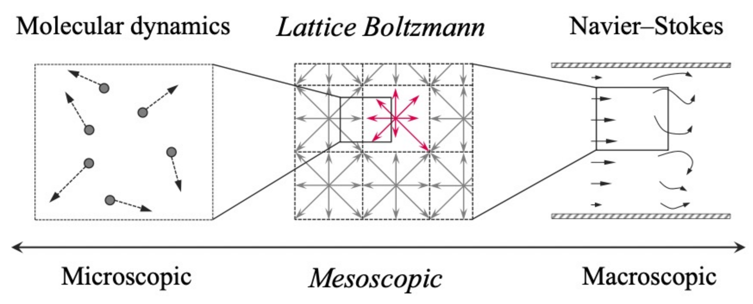
- Lack of models of soft aerosols as they interact dynamically with each other and surfaces. Relevant for many processes.
- Models particularly topical given Covid-19, where soft respiratory aerosols act as vectors for disease.
- Generic soft aerosol models may have many applications.

Aims:

- Develop models for soft aerosols using Computational fluid dynamics (CFDs) – focusing on individual droplet interactions
- Experimentally probe soft materials, make model materials and test simulations
- Apply models to relevant applications- e.g. soft respiratory droplet - mask

Computational Fluid Dynamics

- Lattice Boltzmann Methods (LBMs) give an effective method to simulate viscoelastic droplets. LBMs take place on a mesoscopic scale and rely on kinetic principles to replicate fluid behaviour. Droplet simulated from smaller particles on discrete lattice. Particles move between lattice nodes and collide. [4]



- Particles distributions on lattice sites evolve with some collision operator Ω giving particles discrete velocities $\underline{c}$.

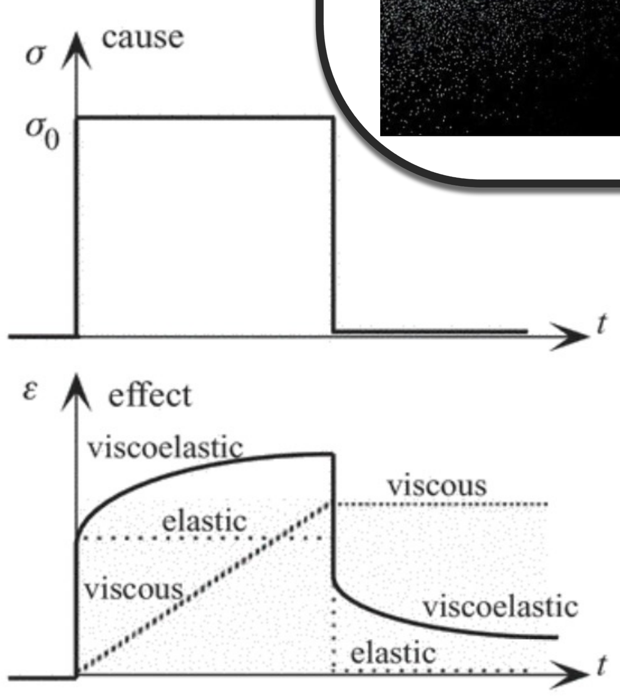
$$f_i(\underline{x} + \delta t \underline{c_i}, t + \delta t) = f_i(\underline{x}, t) + \Omega_i$$

- Ω is scenario specific with initial conditions, boundary conditions can specify specific interaction type.
- Method will be implemented via waLBerla framework in C++

What are Soft Aerosols?

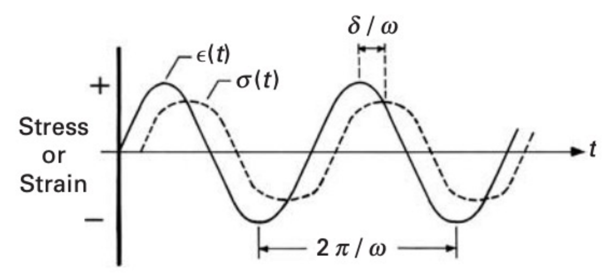
- Soft materials exhibit complex behaviour laying somewhere between a solid and a fluid.
- They are soft to the touch and easily deformed by mechanical / thermal stress. Many common systems are considered soft, like polymers, colloids and gels.
- Examples of soft aerosolized material are rife in everyday life: Respiratory droplets, spray paint, superheated sand and more!

- These aerosols have non-Newtonian, viscoelastic properties that differ from purely elastic solid or viscous fluid systems
- This gives complex stress - strain $(\sigma - \varepsilon)$ relationships. As seen here [1]:
- $\sigma \propto \epsilon$ Elastic solid
- $\sigma \propto \frac{d\epsilon}{dt}$ Viscous fluid
- Viscoelastic materials exhibit both properties leading to interest behaviour when they experience forces.



Experimental Methods

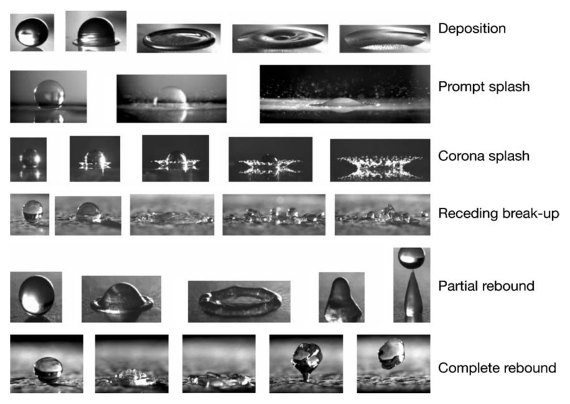
- Oscillatory shear rheometers induce a sinusoidal deformation in a material causing a stress response. Phase difference between stress -strain can quantify rheology. (If $\delta = 0$ purely elastic [1])



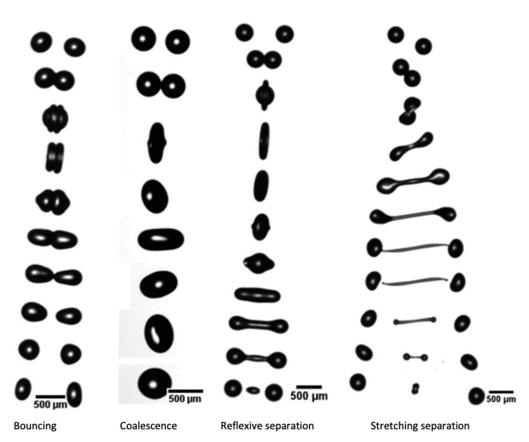
- Pendant drop methods can measure surface tension by optically measuring droplet deformation under gravity.
- These techniques will be used to gather material properties of soft items created from polymers surfactants etc.
- Droplet on demand systems will be used to create droplets of these substances.
- Experiments to probe the dynamics of these droplets will then be developed to test simulated models.

Aerosol Mechanics

- Droplets impact surfaces with a variety of outcomes such as depositing, splashing and bouncing [2].



- Outcomes determined by droplet inertia, surface properties, impact parameters and material properties such as surface tension.
- Similar quantification of outcomes in droplet -droplet interactions with: separation, bouncing and coagulation all possible [3].



- Interactions can be assessed in terms of impact parameters and dimensionless numbers of the Weber and Reynolds numbers. The ratio of inertia / surface tension and inertia / viscosity.

Responsible Innovation and Challenges

- Since 2019, 500 million people have been infected with Covid-19, - massive amounts of research. Models could feed into research - best materials for mask, or contact points for infection etc.
- Other applications in engineering and industry. Example models for viscoelastic hot sand particles hitting jet engine blades in deserts.

Challenges:

- Ability to create very viscous aerosols may be limited by droplet on demand system
- Conditions to replicate mask like surface may be complicated as non fully solid on aerosols scale.
- Linking up the two separate parts of the project on relevant time scales

References:

[1] R Lakes. Viscoelastic Materials. Cambridge University Press, 1st edition, 2009

[2] R Rioboo, M Marengo, and C Tropea. Outcomes from a drop impact on solid surfaces. Atomization and Sprays, 11:155–166, 2001.

[3] K Al-Dirawi and A Bayly. A new model for the bouncing regime boundary in binary droplet collisions. Physics of Fluids, 31:027105, 2019.

[4] S Saito, Y Abe, and K Koyama. Lattice boltzmann modeling and simulation of liquid jet breakup. Physical Review E, 96:013317, 2017