Responsive Aerosol: A Design Framework for Aerosol with Required Properties

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1. Background

- Aerosol are naturally responsive to their environment. Changes in temperature, relative humidity (RH), gas phase composition and many other conditions can illicit changes in the aerosol such as size, rheology, composition, and phase. There is therefore an opportunity to design aerosol to have a desired response to a specific stimuli.
- Hydrogels are three-dimensional polymeric networks that have hydrophilic groups attached to the polymeric backbone and can therefore swell to retain large amounts of water.
- Initially poly(N-isopropylacrylamide) (**PNIPAM**), a thermoresponsive hydrogel, will be aerosolized and studied.
- PNIPAM exhibits a clear, measurable response to temperature at its lower critical solution temperature (LCST). Below 32 °C the hydrogel is in a solution state, and above 32 °C the polymer chains collapse into their globular state, and the hydrogel transitions from solution-to-gel.

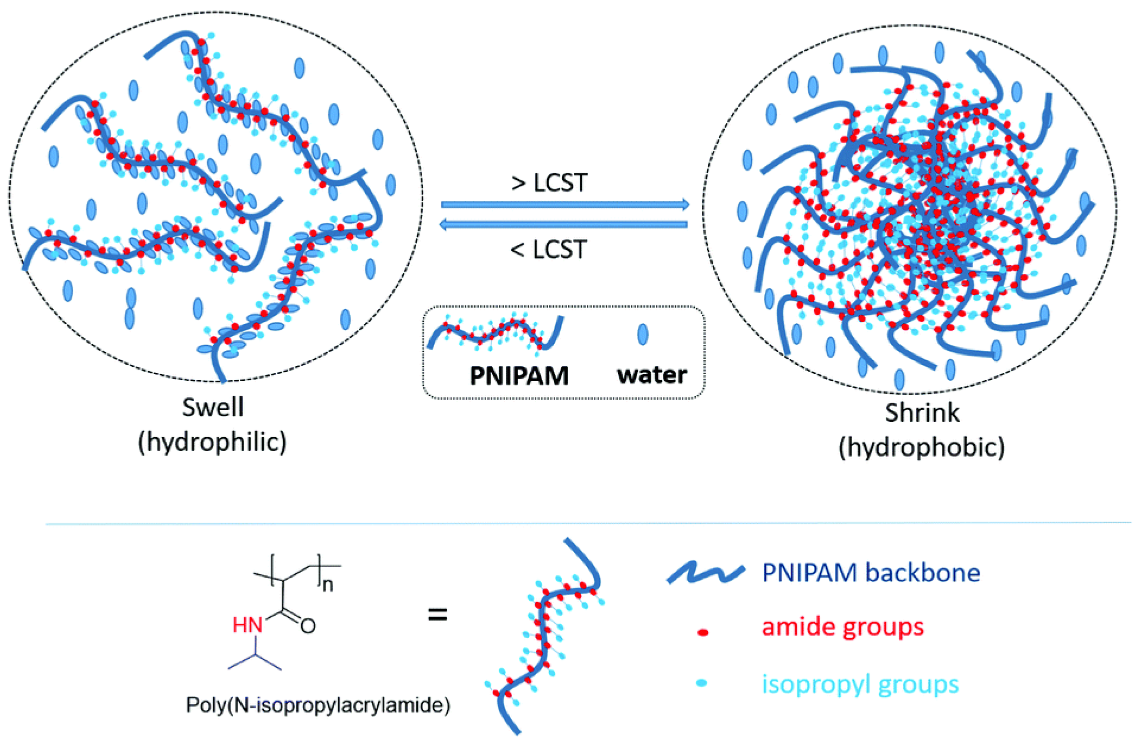

Figure 1—Graphical representation of the swollen and collapsed state of PNIPAM below and above the LCST. Figure taken from Doberenz et al.

2. Motivation

- The ability to design an aerosol to have a required response to its environment has potential applications in many areas. For example, the aerosol could be used to report on changes in temperature, pH, or RH in the environment, and they could also be designed for controlled release of an API in aerosol drug delivery (shown in figure 2).

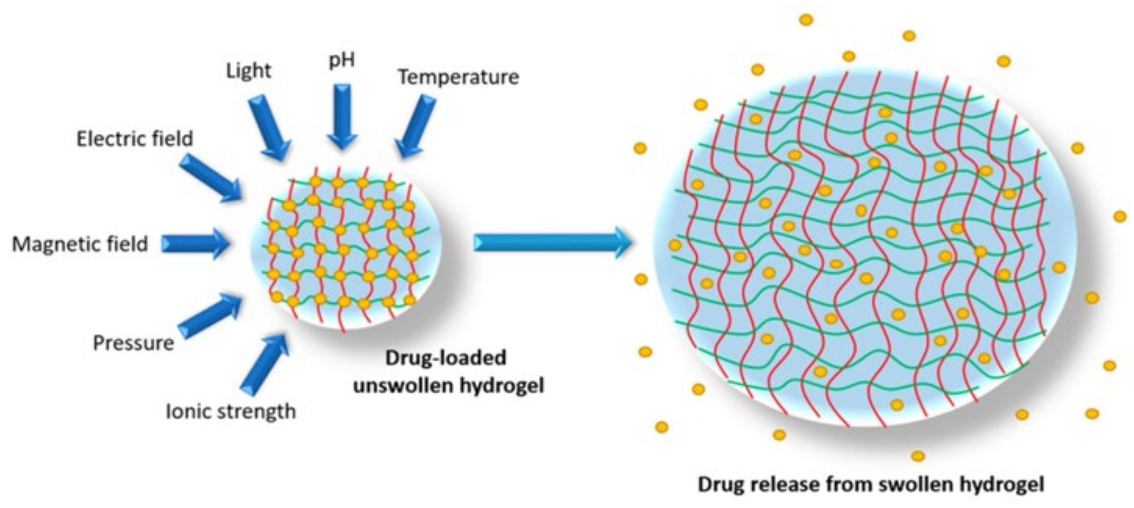

Figure 2—schematic showing release of drug molecules in a hydrogel triggered by external stimuli.

3. Aims

- To characterise changes in an aerosol's properties in response to an external stimulus.
- To build a framework to allow the design of aerosol that have a desired response to stimuli.
- To create a model to understand how changes in the environment can be detected from the corresponding change in size and viscosity of the aerosol and to allow a prediction of one from the other.

4. Research Methodology

- **Comparative-kinetic electrodynamic balance** will be used to measure the size dependance of the droplets on temperature and RH.

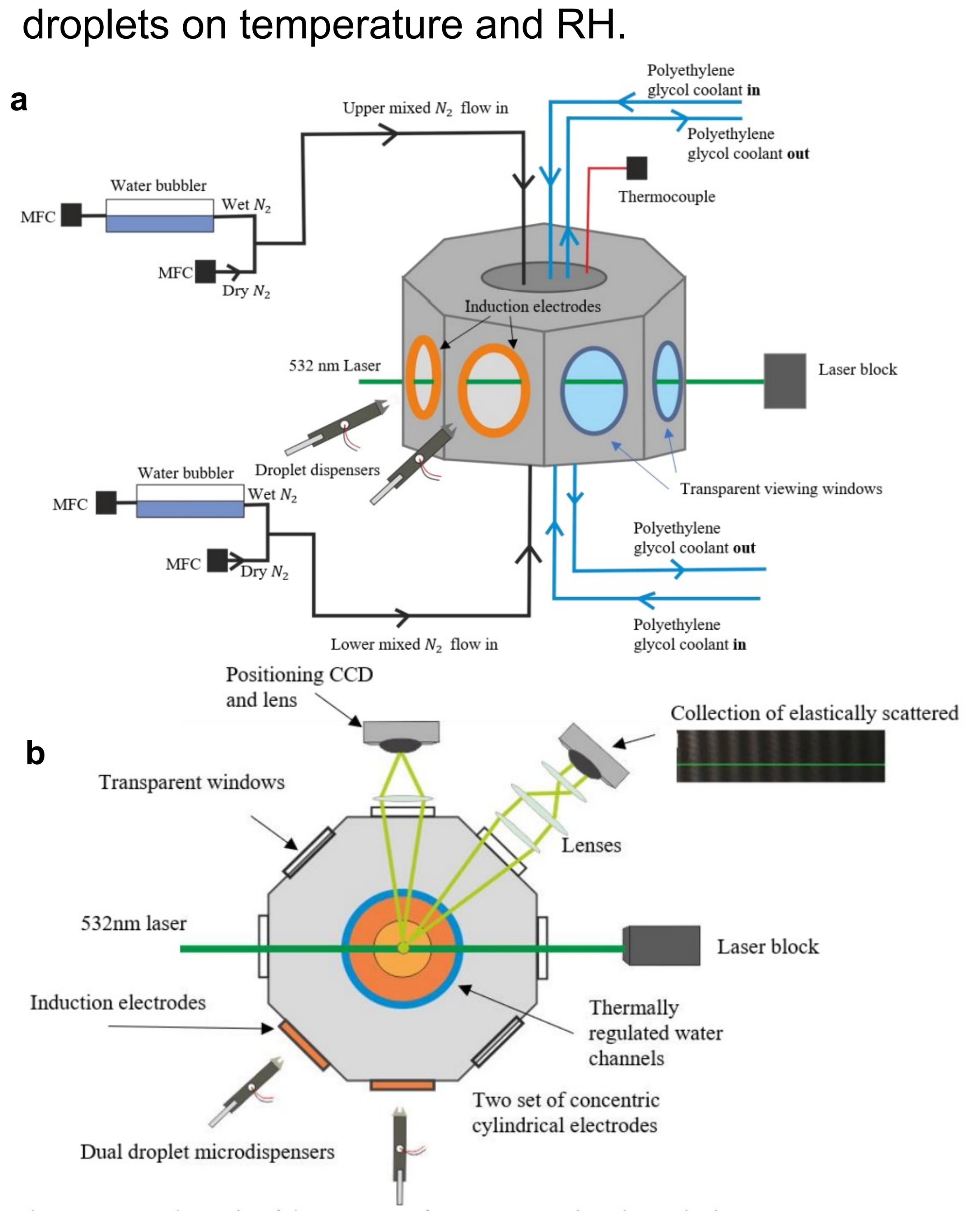

Figure 3—A schematic representation of a CK-EDB from (a) a side view and (b) a view looking down into the instrument. Figures taken from N.C. Green PhD thesis.

- **Optical tweezers** will be used to measure the change in viscosity of the droplet with respect to temperature.

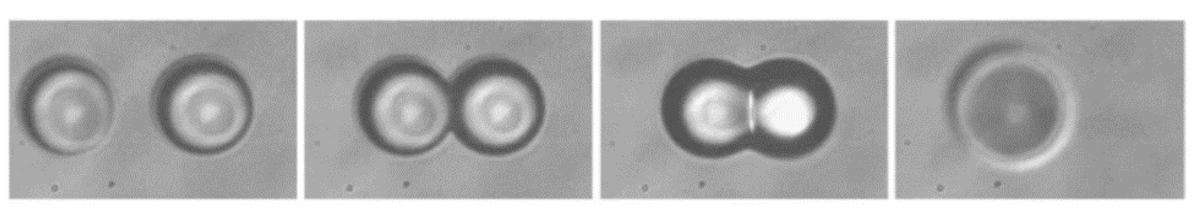

Figure 4—Two droplets coalescing in an optical tweezer. Figure taken from Reid et al.

- Experimental data will be used to parameterise models that will aim to predict how the properties of the aerosol will change with respect to temperature.
- It will describe the change in size of the droplet of PNIPAM by modelling the loss of interstitial water in the polymer matrix.

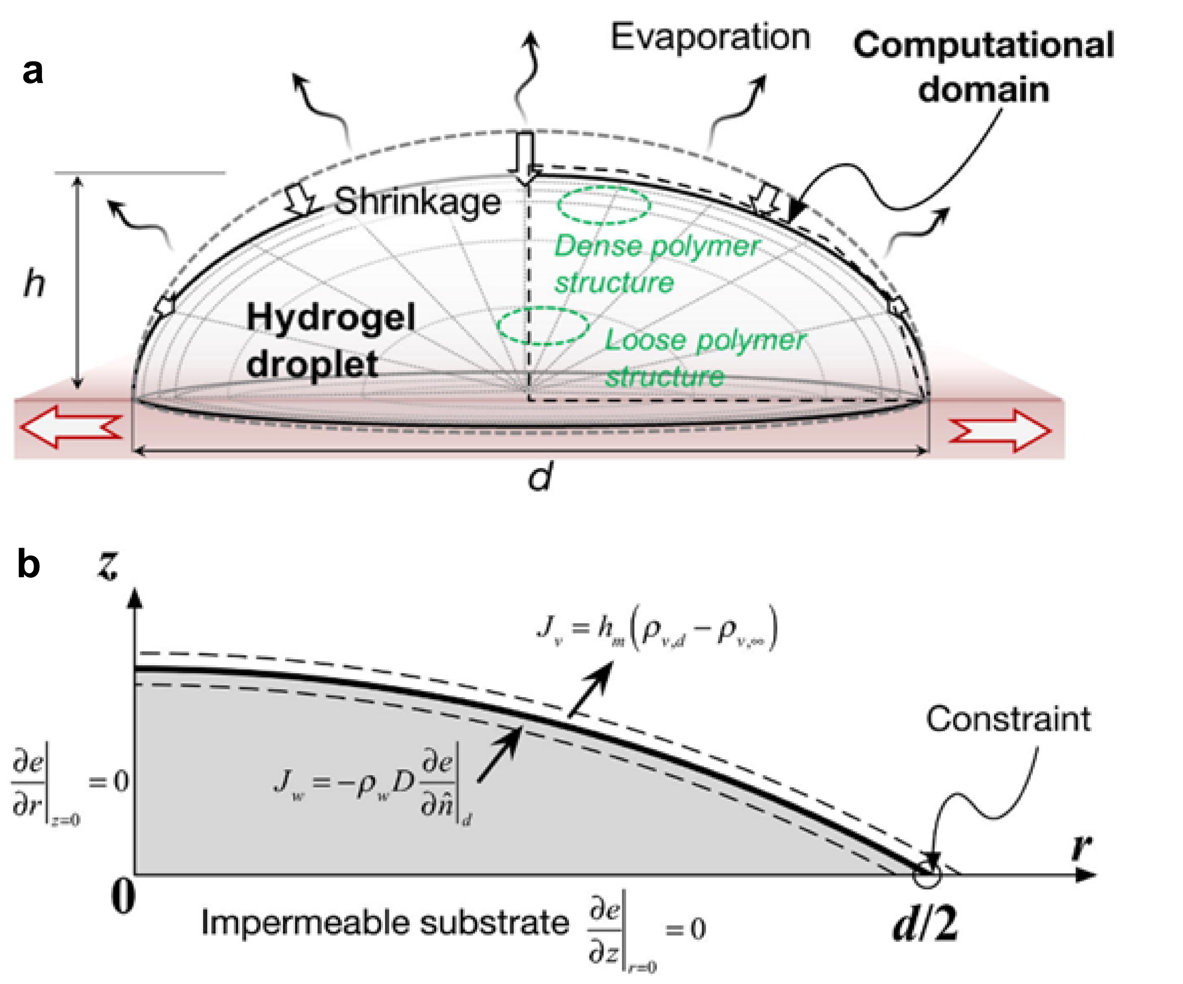

Figure 5— Schematic showing theoretical dehydration on a droplet on a substrate. (a) Evaporation of interstitial water at the droplet-air interface. (b) Computational domain and corresponding boundary conditions. Figure taken from Han et al.

- Using the model's predictions, experiments will be run to investigate the size distribution of a plume of aerosol when exposed to changes in its environment. These data will be used to validate and improve the model.

5. Challenges

- Aerosolising hydrogels– hydrogels can have a high viscosity which could cause a problem when producing droplets with a droplet-on-demand generator.
- How will the hydrogel behave in aerosol phase:
  - Will the properties be the same as in the bulk phase?
  - Will evaporation take place on a faster timescale than the solution-to-gel phase change?

References

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