Improving the Evaporative Light Scattering Detector using experiments and modelling

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Introduction

- The Evaporative Light Scattering Detector (ELSD) uses light scattering to detect analyte concentration.
- The device uses three main stages to analyse sample:
  (i) spray formation
  (ii) solvent evaporation
  (iii) detection via light scattering
- The physics and mechanics of the ELSD are, at present, poorly understood [1,2,3]. Making it difficult to optimize the device.
- An empirical correlation is currently used to obtain and interpret data, taking the form:

$$S = k \cdot c^{\alpha} \qquad \text{(Eq. 1)}$$

where S is the ELSD signal, c is the sample mass concentration, and k and α are experimentally determined constants [4] .

Objectives

- Characterise physics of each stage of device:
  ☞ Atomization/spray formation
  ☞ Losses through impaction and diffusion
  ☞ Droplet vaporization
  ☞ Particle aggregation and breakage
  ☞ Light-scattering of final particle distribution
- Derive a transfer function for the entire system, linking inputs and outputs from each stage of the device.
- Use elucidated understanding to optimize the device.

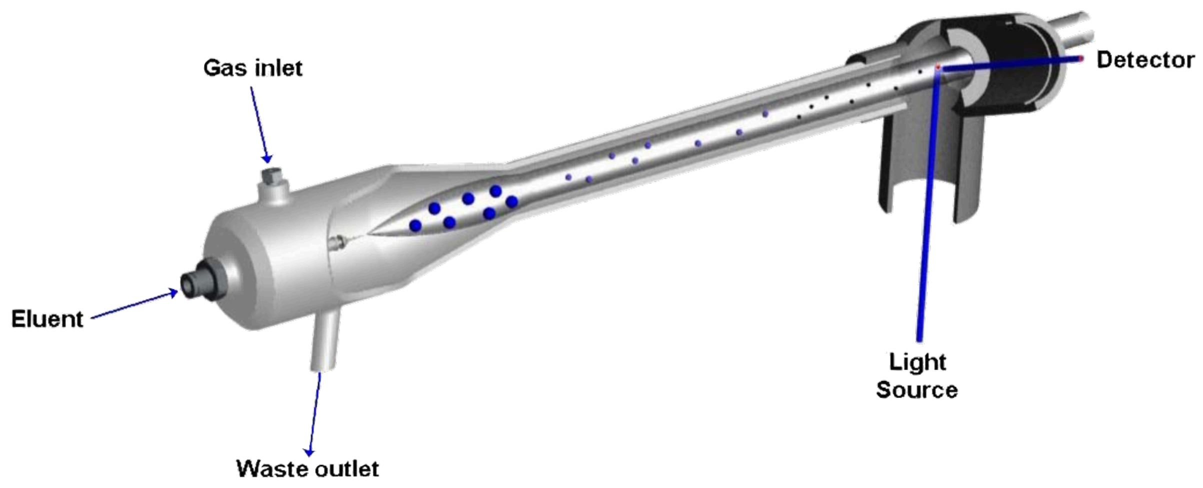

Fig 1: Diagram of ELSD, depicting different stages of detection.

Methods

- Obtain information about particle distributions (size, velocity, number) through experiments at different points of device using Phase Doppler Particle Analysis (PDPA) and Electrical Low Pressure Impaction (ELPI).
- Use optical tweezers for single particle experiments, allowing for the determination of particle size, refractive index, and composition.
- Create a database from experiments using different experimental conditions with the ELSD, allowing the wide-ranging response to be documented.
- Create a transient computational model which recreates the phenomena in the ELSD and allows for the elucidation of the physics in the device.

Results

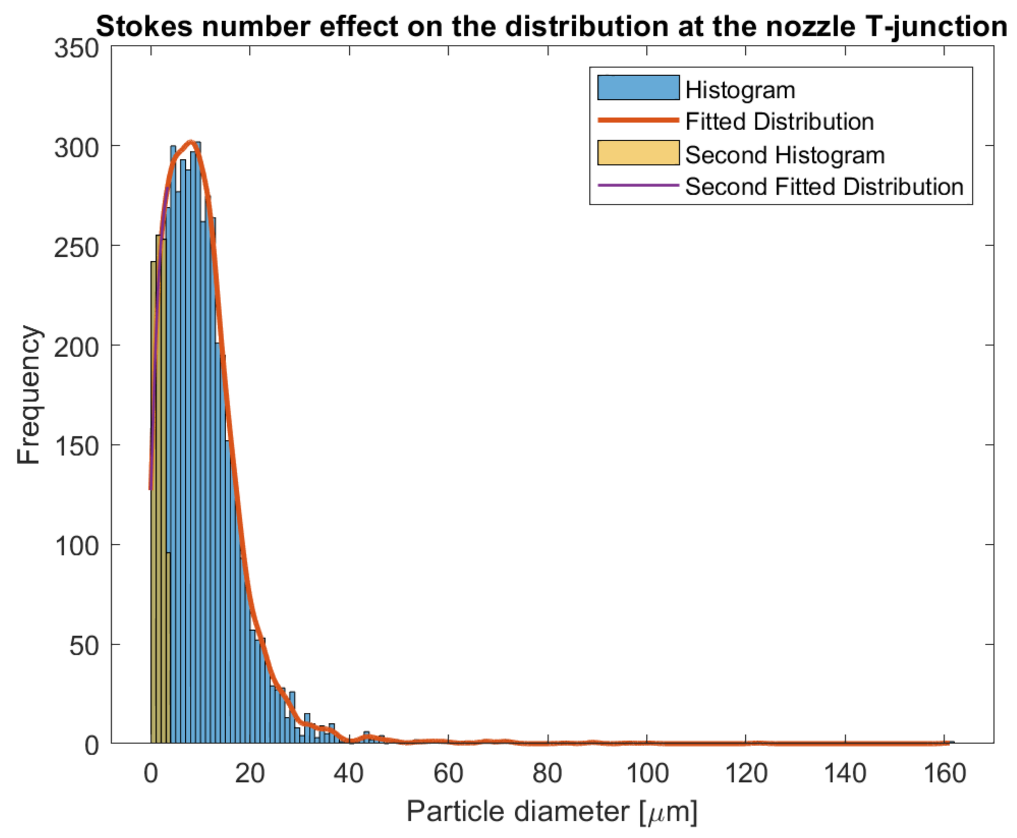

Fig 2: PDPA-acquired particle distribution and the effect of inertial impaction upon it.

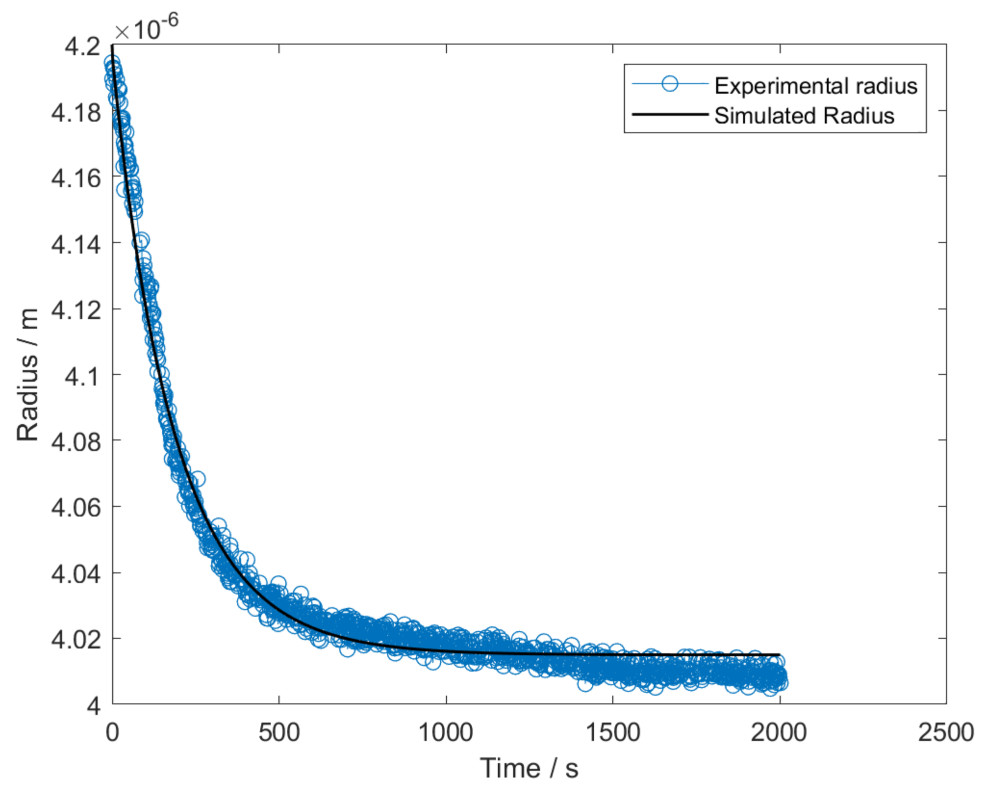

Fig 3: Evaporation model overlaid on experimental data of single droplet trapping using the optical tweezers.

- The PDPA set-up was successfully employed to characterise the atomizer at different axial and radial distances from the nozzle, with a variety of flow conditions.
- Data from the ELSD allowed for the construction of a database for different experimental conditions and their relation to signal outputs.
- An evaporation model based on the equations of Sirignano was created [5], and validated against values from the literature as well as single-droplet experiments using the optical tweezers.
- Consideration of the geometry of the device allowed for the calculation of the inertial loss of the distribution.
- Data from the PDPA experiments was used to get an estimate of the dried droplet distribution immediately before detection.
- The use of a Mie scattering algorithm was employed to simulate the light scattering signal of the ELSD to allow for the modelling of the final signal output.
- Construction of a preliminary population balance model for the system has begun, which allows for more general physical processes of the system to be simulated (i.e. aggregation, fragmentation, diffusional losses, etc.). The conservation equation takes the form:

$$\frac{\partial n(v,t)}{\partial t} + \frac{\partial}{\partial v}(\dot{v}(v,t)n(v,t)) + u\frac{\partial n(v,t)}{\partial z} = \mathfrak{D}_p\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial n(v,t)}{\partial r}\right) + \frac{\partial^2 n(v,t)}{\partial z^2}\right) + \left[\frac{\partial n(v,t)}{\partial t}\right]_{agg} + \left[\frac{\partial n(v,t)}{\partial t}\right]_{frag} \qquad \text{(Eq. 2)}$$

where n is the number density, t is time, v is the discretized volume, u is the velocity, $\mathfrak{D}_p$ is the diffusion constant, and r and z are the radial and axial coordinates respectively.

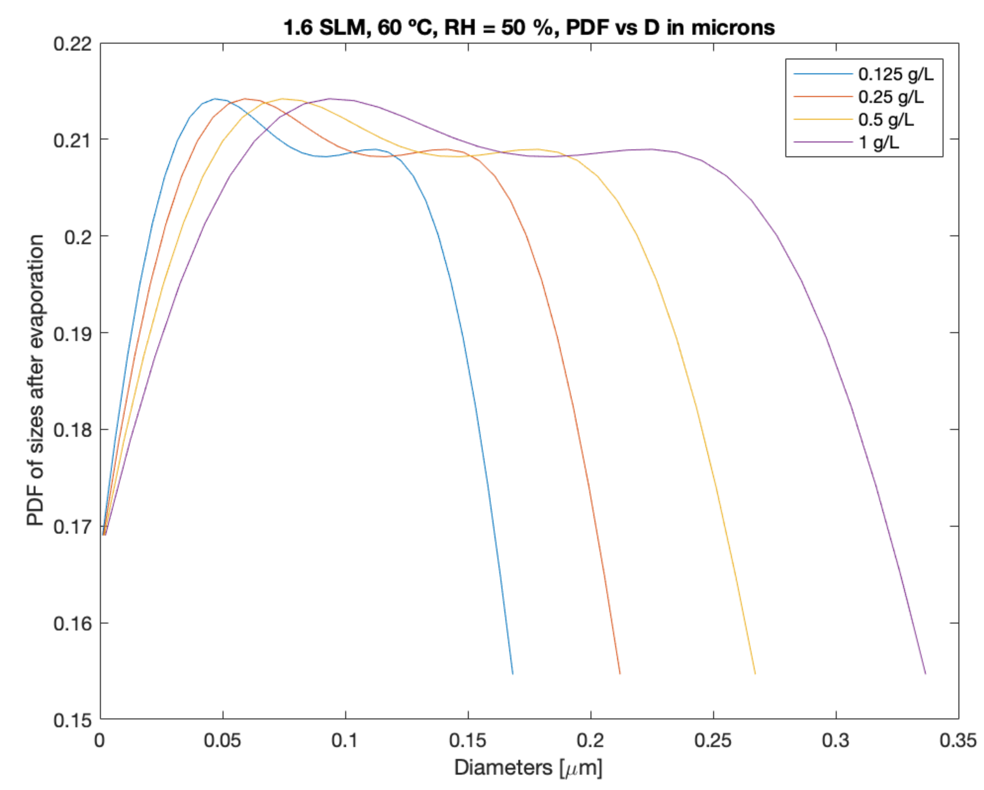

Fig 4: Simulation of final dry particle distributions for different initial concentrations, using PDPA data as initial conditions.

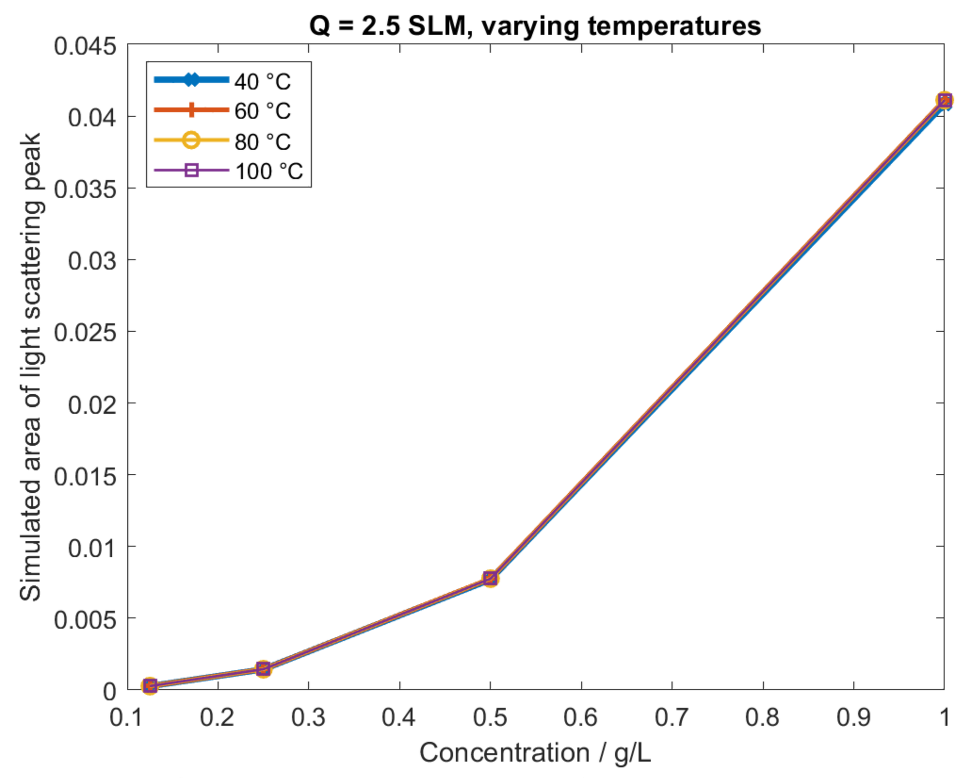

Fig 5: Current Lagrangian (no interaction) model output for fixed gas flowrate and varying evaporation temperatures.

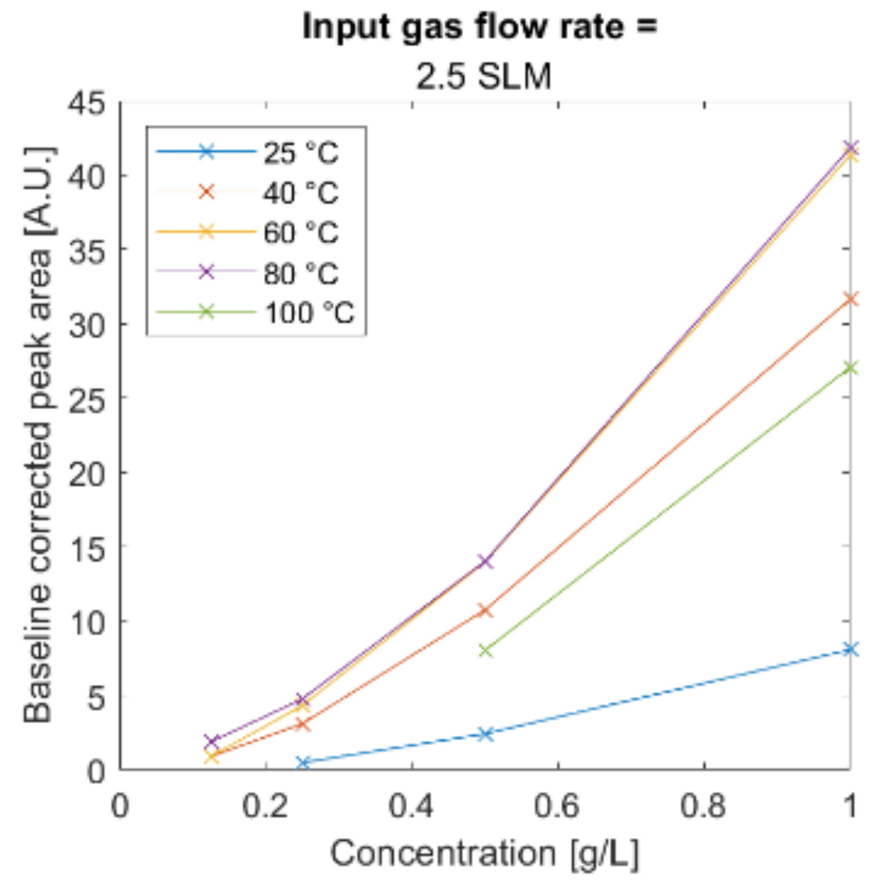

Fig 6: Actual ELSD data showing effect of temperature on signal for a fixed input gas flow-rate.

Conclusion and next steps

- First results are advancing with results from experimental techniques and simple computational models.
- Computational model for evaporation shows good agreement with literature values and single-droplet trapping experiments.
- Exploratory model simulating ELSD signal as a function of initial solute concentration has been established, replicating shape of experimental results but lacking dependence of temperature and input gas flow on signal.
- Initial population balance model of system has begun; needs to be expanded to incorporate more physical phenomena.
- Still to collect more particle distribution data for anywhere but the atomizer nozzle.
- Still to collect ELSD data for different compounds – only caffeine in water has been attempted so far.

References

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