Some examples where Maths can help progressing my research

Dr Nuno M Reis

Chemical Engineering, Bath

1. Simulation of bubble formation in pulsating reactor systems

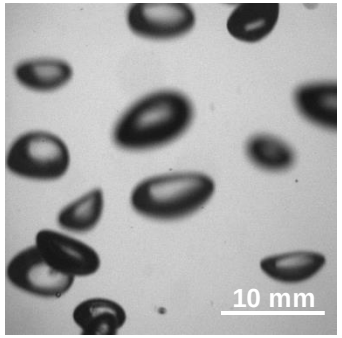
Several industrial processes involves transfer and/or reaction of components from a gaseous phase and dissolution into the liquid phase.

Gas-liquid contacting is very inefficient; bubbles have very short residence times, and easily coalesce, meaning only a small fraction of components in the gas phase are utilised.

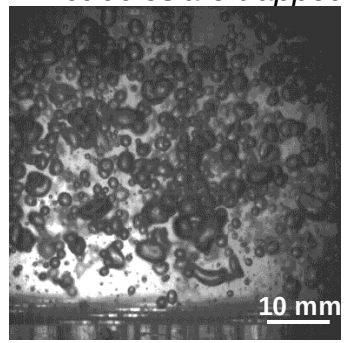
We have developed a novel gas-liquid contacting system that uses tube baffles and gentle pulsations of the fluid to achieve 100% efficiency in utilisation of components in the gas-phase, which is relevant e.g. for ozonation or syngas bioconversion – where the cost is related to the efficiency of the process. Also, as the mass transfer is enhanced, the technology is more compact and safer.

Our research would benefit with the development of CFD models capable of capturing gas-liquid flow characteristics in the pulsating column, something never reported to date.

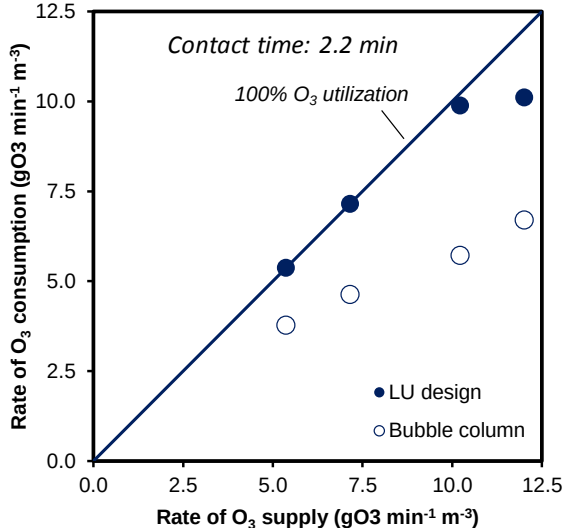
Conventional gas-liquid contactors produce large bubbles with short contact time



'Super-Ozonation' technology generates very large surface area and bubbles are trapped



Pereira et al. 2015, I&ECR



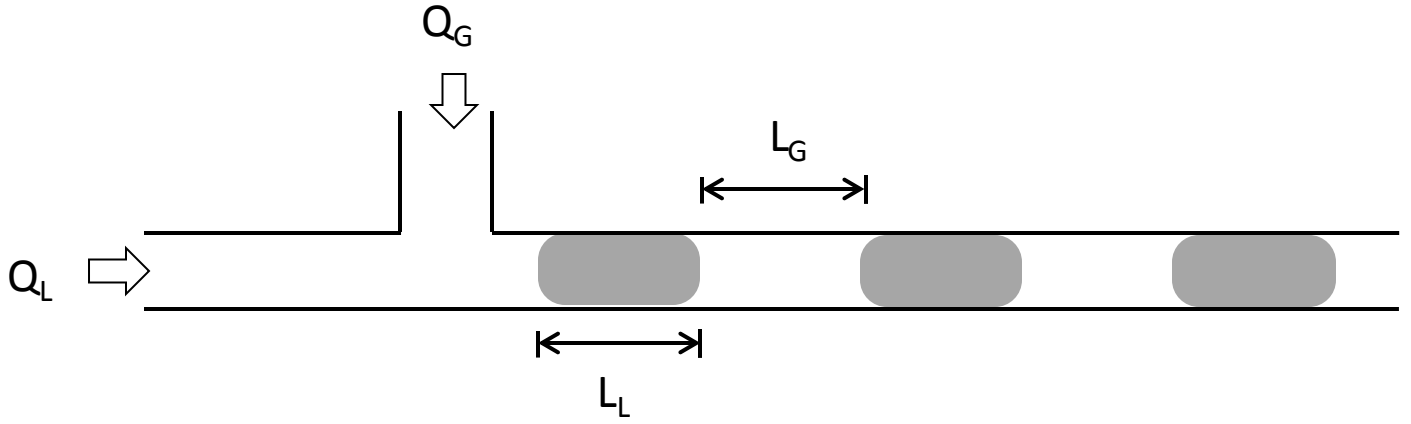
Reis and Li Puma, GB patent application 1412749.2
Lucas, Reis and Li Puma, Chem Eng J, 296: 335–339 (2016)

2. CFD modelling of gas-liquid slug formation in microfluidic T-junctions

There are a number of analytical and processing situations where gas-liquid flow is utilised in miniaturised devices, benefiting from the enhanced mass transfer.

CFD simulation of gas-liquid in microfluidics channels is challenging, with commercial CFD software that use e.g. VOF model struggling to match experiments with realistic surface tension values.

Also, could a CFD model capture the fluid dynamics within the droplets/slugs, as they can inform about mass transfer characteristics between the gas and liquid phases in the system.



3. Modelling of diffusion and antigen-antibody binding effects in microfluidic diagnostics tests

Can we model interference of biological sample (often called 'matrix effect') in performance of diagnostic test, which remains poorly understood?

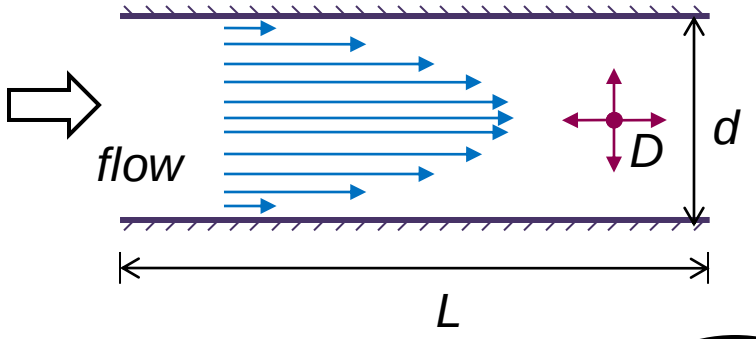
This is related to effect of viscosity on diffusion, but also to adsorption/binding effects

This is extremely important for development of miniaturised point-of-care diagnostic tests (market estimated worth >US$13Bn).

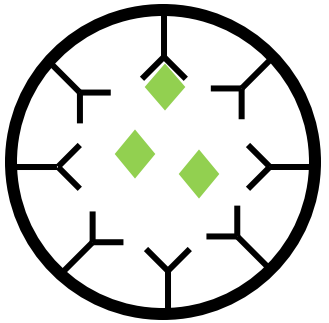
We have 'discovered' that is it possible to carry out quantitation of protein biomarkers from whole blood with sample preparation, by simply extending the incubation time of the sample (Barbosa et al., Lab Chip, 2014, 14, 2918).

This is a game changer in development of modern point-of-care diagnostic tests, yet we would like to understand at fundamental level how the 'matrix' effect works in microfluidic systems. We noticed experimentally there is a tight window at which 'matrix effect' is minimised in microfluidic systems, however this has stopped development of robust, portable test for several decades.

$$x = (2*D*t)^{1/2}$$



$$A/V = 4/D$$



$$B/F = k_a(\text{N-B})$$