Theoretical and numerical modelling of three-phase dynamic contact line and atomisation

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1. Summary for the General Public

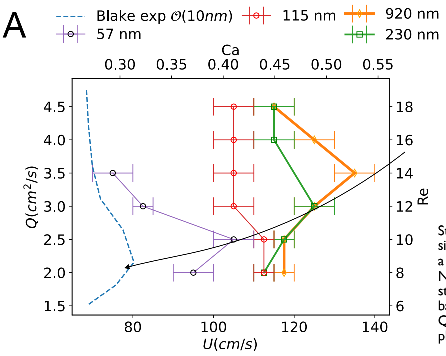
My PhD thesis combines computational and analytical approaches to study the dynamics of (A) the moving three-phase contact line and (B) atomization processes. The interface between a liquid droplet, a solid surface, and air is an example of a three-phase contact line. Studying moving contact line is astoundingly challenging, because of the no-slip force singularity. Simply said, continuum mechanics with no-slip boundary condition makes it mathematically impossible to sink a solid. My research implemented and even proposed some thermodynamically consistent models to resolve force singularities at the moving contact line. Together with High Performance Computing, these models enabled industrial-scale simulations for coating processes. In coating processes, we want to coat a substrate as fast as possible, however, there exists a critical speed, beyond which air-entrainment will occur, leaving air bubbles and air films on the coated substrate thus degrading the final product. Our computations enabled us to predict the optimum wetting point and flow physics up to the experimental resolution. My second main work, atomisation, where a fluid breaks into fine droplets, spans a wide range of scales and is computationally intensive. We performed computations on the national supercomputers in France using up to 50,000 cores in parallel with a total compute time of 50 million CPU hours. With the highest-ever resolution [1], we revealed a rich variety of drop formation mechanisms including compound droplets (drop with a bubble inside!). We showed why existing breakup models fail to predict spray droplet sizes. Our novel model with breakup timescales inspired from Kibble-Zurick theory in astrophysics applied on the Manifold Death perfortions, we achieved statistically converged droplet distributions for the first time. I also applied my expertise in atomisation and moving contact lines to study fragmentation of droplets sitting on the leaf with tracer particles inside them (mimicking pathogens) informing us widely about the spread of diseases in crops and plants. My research has applications in disease transmission, pharmaceutical (respiratory drug delivery through nebuliser), fuel sprays (atomising of fuels), industrial scale coating processes, space and defence sector (protective coating of satellite parts and equipments). I also carried out two internships to study coalescence of compound drops and cooling in Supercritical fluids.

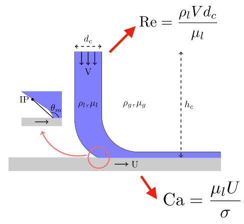
2. Scientific Summary

A three phase contact line is the common line formed at the intersection of fluid interface with the solid. While the static contact line in equilibrium is well understood by the Young's law based on energetics argument, the moving contact line however, results in a non-integrable stress singularity at the contact line assuming the no-slip boundary condition. This singularity can be regularised by violating the no-slip boundary condition below a cut-off length scale, often of the order of nanometers. My thesis starts by analytically solving the flow field for three such boundary conditions, the Navier-slip, super-slip and the generalised Navier boundary condition (GNBC). These three boundary conditions can be justified from

[1] an effective 35 trillion grid points in the computational domain - highest to the best of our knowledge in this type of flow

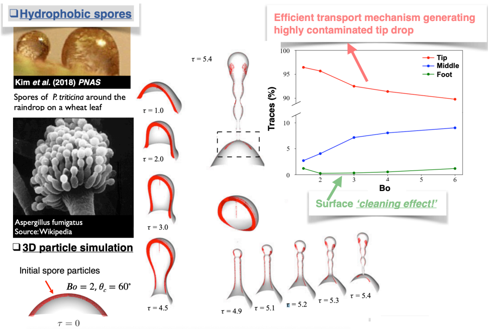
A





Stability window for the curtain coating simulations. Simulations are performed with a fixed microscopic contact angle θ_m and Navier-slip boundary condition. Parametric study is done by varying Reynolds number, based on feed flow velocity V (or flow rate Q) and a capillary number based on solid plate speed U.

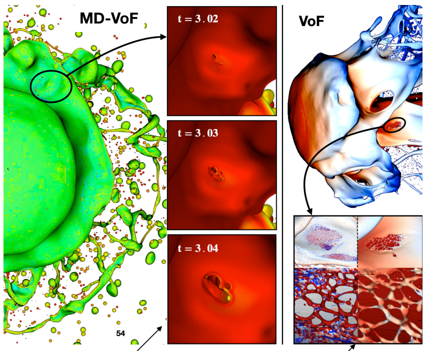
Non-monotonic stability window on Q-U plane is obtained and shown to move towards experiments of Blake et al. as the slip length is decreased. All the points on the right of the stability window are where wetting failure is seen, while the points on the left are those where stable steady state solution is obtained. Solid black arrow shows the movement of optimum wetting point and legends indicate the slip length.



C

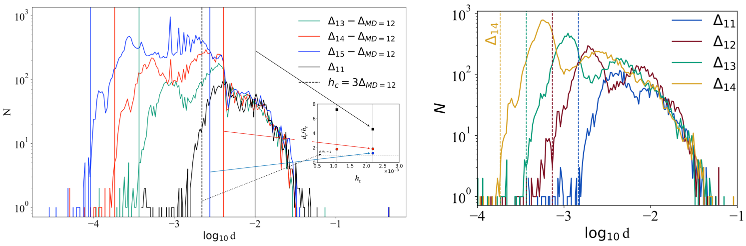
DNS for a droplet on a leaf subject to impulsive impact. Tracer particles are put on the drop-air interface to mimic hydrophobic pathogens like spores. The fragmentation results in a highly contaminated tip droplet while a clean leaf surface.

B



Holes with controlled perforation

Uncontrolled perforation resulting in curvature ripples and grid dependent droplets



The drop size distribution as a function of grid refinement with (left) and without Manifold Death (right). One can see that for usual VoF breakup without Manifold Death (right), the distribution is bimodal and there is no convergence in the drop size distribution. Δ_{LEVEL} denotes the resolution implying there are $2^{LEVEL} \times 2^{LEVEL} \times 2^{LEVEL}$ effective grid points in the cube. This is the highest ever resolution to the best of our knowledge. On the left, we show drop size distribution with the Manifold Death method, where h_c is the critical sheet thickness at which we punch the holes. **When we increase the resolution, we see that we do attain a statistical convergence in the drop sizes greater than our critical sheet thickness.** The inset shows the shifting of the converged region d_c towards the critical sheet thickness h_c as the resolution is increased.

molecular kinetics and entropy considerations. The solutions informed us about the flow regularisation characteristics for these three boundary conditions [1]. We then integrated these numerically in Basilisk flow solver to study the industrial scale coating process where we aim for a rapidly advancing contact line. In coating processes, we want contact line to move as fast as possible, but, there exists a critical speed, beyond which air-entrainment will occur, leaving air bubbles and air films on the coated substrate thus degrading the final product. This transition to wetting failure originates from the instability of the contact line. For a rapidly advancing contact coupling of macroscopic and microscopic length scales was notoriously complicated enabling determination of the optimum wetting speed only experimentally. Our computations spanning length scale of six orders of magnitude shed light on the coupling of various length scales and with improved modelling of the contact line dynamics, we did predict a non-monotonic stability window shown in Fig. A and an onset of wetting failure with correct flow physics up to experimental resolution.

My research on atomisation focused on the Direct Numerical Simulation (DNS) of a pulsed round liquid jet injected into a stagnant gas, under high Reynolds and Weber numbers. We used up to 50,000 cores on national supercomputers in France, amounting to 50 million CPU hours, to achieve an unprecedented resolution of 35 trillion effective grid points. Despite advances in computation, accurate prediction of drop size distributions in such jets remains poor. We showed that standard Volume of Fluid (VoF) methods suffer from a *numerical sheet breakup*, where curvature oscillations at high wavenumbers prevent statistical convergence. To overcome this, we introduced a “manifold death” procedure, piercing thin sheets before they reach a critical thickness $h_c > 6\Delta$, enabling convergence of the droplet size distribution above a diameter $d_c \sim h_c$. The resulting distribution is unimodal in converged range (see Fig. B) [2]. We use the Kibble-Zurek theory to predict the number of holes and associated timescale on heuristic physical grounds. We then studied inertial fragmentation of droplet with pathogens on a leaf under an impulse impact. The impulsive acceleration, quatified by Bond number, cause the drop to retract on the leaf while at the same time elongate and atomise into satelite droplets, hence involves both moving contact lines and atomisation. A seamless integration of theory, numerics and experiments, explained the physics of impulse-driven fragmentation, providing insights into how the wetting properties of pathogens would impact their transmission [Fig. C] emitted from fragmenting jets [3].

My research has implications across a range of engineering and industrial applications. In coating processes, our predictive models can inform the optimum speeds for processes such as glass coating, inkjet printing, and photographic film production. The atomization studies, traditionally applied in combustion and spray engineering, are now also proving essential in disease transmission via respiratory droplets and the precision delivery of medication through nebulizers. Combined knowledge of contact lines and atomisation impacts studying plant health, spray coating applications in numerous sectors like agriculture sector (enabling smarter fertiliser spreading, smart drones, and seed coating), pharmaceuticals (coating of tablets and capsules for ease of swallowing and controlled drug delivery), and the aerospace and defense sectors (spray-coating of protective layers on satellite components).

I also carried out two research internships one on studying partial coalescence in compound droplets during my BTech project [4] and another in France awarded by the Charpak Lab scholarship wherin, I used matched asymptotic analysis to theoretically explain anomalous cooling in super-critical fluids (SCF) [5]. SCFs widely used as coolant in space technology, this work was selected for presentation at French Space agency CNES.

Selected Publications

1. **Kulkarni, Y.**, Fullana, T., & Zaleski, S. (2023). *Stream function solutions for some contact line boundary conditions: Navier slip, super slip and the generalized Navier boundary condition.* ***Proceedings of the Royal Society A***. `http://doi.org/10.1098/rspa.2023.0141`

2. **Kulkarni, Y.**, Pairetti, C., Villiers, R., Popinet, S., & Zaleski, S. (2025). *The atomizing pulsed jet.* ***Journal of Fluid Mechanics***. `https://doi.org/10.1017/jfm.2025.218`

3. Naijian, S., **Kulkarni, Y.**, Popinet, S., Zaleski, S., & Bourouiba, L. (2024). *Fragmentation from inertial detachment of a sessile droplet: implications for pathogen transport.* ***Journal of Fluid Mechanics***. `https://doi.org/10.1017/jfm.2024.874`

4. Deka, H., Biswas, G., Sahu, K. C., **Kulkarni, Y.**, & Dalal, A. (2019). *Coalescence dynamics of a compound drop on a deep liquid pool.* ***Journal of Fluid Mechanics***. `https://doi.org/10.1017/jfm.2019.137`

5. **Kulkarni, Y.**, Khayat, R., & Amiroudine, S. (2021). *On the long-time transient formation of sink zones in near-critical fluids. A theoretical perspective.* ***Journal of Fluid Mechanics***. `https://doi.org/10.1017/jfm.2021.134`

Total publication output: In addition to the above published journal papers, I am the lead author on three more manuscripts on contact lines: one under revision (J. Fluid Mech.), one submitted (J. Fluid Mech.), and one in preparation on curtain coating. I also co-authored a paper on vibrating droplets submitted to *Phys. Rev. Fluids.* During my PhD Sept 2021 to Jan 2025, I have participated in 10 plus international conferences and won first prize at student poster competition at APS-DFD 2021 for atomisation.