

# New Perspectives in Modelling Heat Transfer and Multiphase Flow Work in Progress

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# Introduction

In this talk, we look at two separate problems in the modelling and simulation of both single-phase and multiphase flow involving heat transfer. We bring new methodologies to bear on these problems:

- Theoretical modelling of evaporating sessile droplets (**multiphase**)
- Numerical modelling of heat and momentum transfer in particle-laden channel flows (**single phase**)

# Evaporating Sessile Droplets – Context

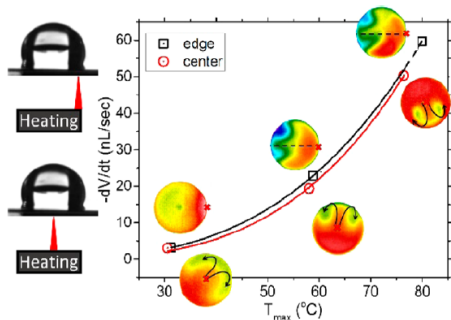


Figure: Askounis et al., Langmuir, 2017.

- Droplet Locally heated at hotspot;
- Evaporation into surrounding atmosphere;
- Marangoni effect induces vortices in droplet.
- Marangoni effect predicted in pure water but was only recently confirmed experimentally (contaminants).

# Evaporating Sessile Droplets – Modelling Problem

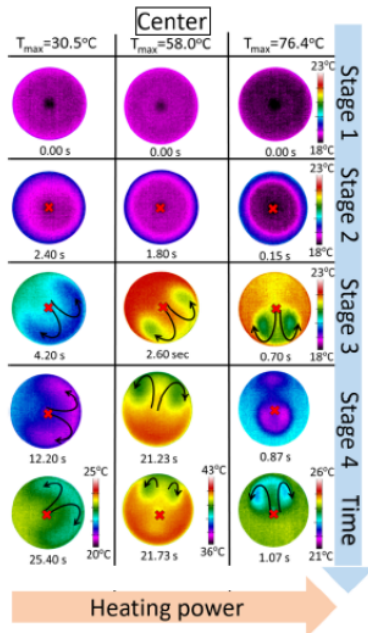


Figure from Askounis et al., Langmuir, 2017:

- Droplet heated at hotspot with laser – constant heat flux.
- **Symmetric** temperature distribution emerges.
- After some time, convection sets in.
- Convection happens fast, then evaporation on a much slower timescale.
- Vortices move around in the droplet in a dynamic fashion, suggesting non-linear behaviour.

# Modelling Assumptions

The aim of the research is to develop a theoretical model for predicting the onset of the convection. As such, the following simplifying assumptions can be made:

- Convection sets in long before evaporation starts – assume droplet keeps its shape in the model.
- Equilibrium contact angle  $\theta \approx 110^\circ$  – treat as hemispherical in the model.
- Idea – develop a temperature distribution for the case without convection – **base state**.
- Treat the onset of convection as a small-amplitude perturbation and develop a **linear stability analysis** of the system.
- Further assumptions are required for the boundary conditions.

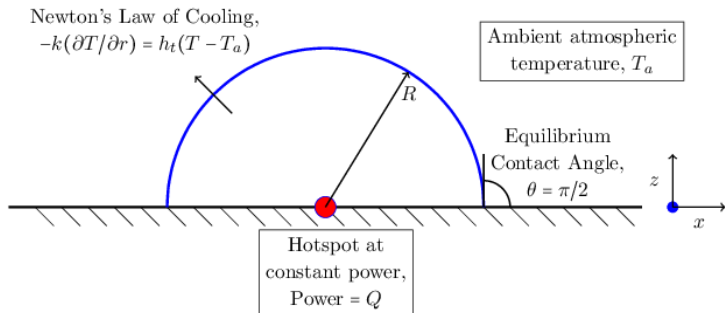
## Boundary Conditions

- One-sided model – treat only what happens inside liquid phase.
- Gas phase parametrized by Newton's Law of Cooling, and hence, a Robin boundary condition at  $r = R$ :

$$k(\partial T / \partial r) = h_t(T - T_a),$$

where  $T$  is the droplet temperature,  $k$  is the thermal conductivity,  $h_t$  is the coefficient in Newton's Law of Cooling, and  $T_a$  is the ambient gas temperature.

- Neumann / Dirichlet conditions are applied at  $z = 0$ , as appropriate.



## Base State

The base state describes what happens in the absence of flow. It should be the solution to the diffusion equation

$$\frac{\partial T_*}{\partial t} = \nabla^2 T_*, \quad \text{in the hemisphere,}$$

subject to the appropriate boundary conditions at the substrate. The choice of boundary conditions is crucial.

- Realistic boundary conditions at  $z = 0$ , e.g.  $k(\partial T/\partial z) = f(r)$ ;
- Here,  $f(r)$  is the source function which depends on the laser power (e.g. Gaussian)
- Then,  $T_*$  is not radially symmetric but instead depends on both  $r$  and  $z$ :  $T_* = T_*(r, z)$  – agrees with experimental observations.
- We have also investigated a radially symmetric solution with  $T_* \rightarrow T_*(r)$ .

For now we leave the  $T_*$  unspecified and outline the linear stability analysis in broad terms.

## Fluid Dynamics

Beyond the base state, we introduce the Navier–Stokes equations for viscous incompressible flow:

$$\rho_0 \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} - \rho_0 g [1 - \alpha(T - T_a)] \hat{\mathbf{z}},$$



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- Work in Boussinesq limit, where  $\rho_0$  denotes a constant reference density; also,  $\mu$  is the viscosity.
- We **locally** use  $\alpha$  to denote the coefficient of thermal expansion.
- Calculations suggest  $\text{Ma} \gg \text{Ra}$  (defined later); hence, buoyancy term can be dropped.

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Equations of motion simplify (and supplemented by incompressibility):

$$\begin{aligned} \rho_0 \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) &= -\nabla p + \mu \nabla^2 \mathbf{u} - \rho_0 g \hat{\mathbf{z}}, \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned}$$

(we henceforth drop the subscript on the density, for consistency). Finally, introduce advection-diffusion equation for the temperature:

$$\rho C_p \left( \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = k \nabla^2 T.$$

# Fluid Dynamics – Boundary Conditions

- No slip:  $\mathbf{u} = 0$  at  $z = 0$ .
- No mass flux at interface (evaporation suppressed at short times) – radial velocity condition:  $u_r = 0$  at  $r = R$ .
- Also, Marangoni stress condition at the interface, since the surface tension is a function of temperature:

$$\sigma = \sigma_0 - \gamma(T - T_a).$$

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Effective **vorticity source**:

$$\begin{aligned}\mu \hat{\mathbf{r}} \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \cdot \hat{\boldsymbol{\theta}} &= -\frac{\gamma}{R} \frac{\partial T}{\partial \theta}, \\ \mu \hat{\mathbf{r}} \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \cdot \hat{\boldsymbol{\varphi}} &= -\frac{\gamma}{R \sin \theta} \frac{\partial T}{\partial \varphi}.\end{aligned}$$

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With  $u_r = 0$  at  $r = R$ , these equations simplify:

$$\begin{aligned}\mu \frac{\partial}{\partial r} \left( \frac{u_\theta}{r} \right) \Big|_{r=R} &= -\frac{\gamma}{R^2} \frac{\partial T}{\partial \theta} \Big|_{r=R}, \\ \mu \frac{\partial}{\partial r} \left( \frac{u_\varphi}{r} \right) \Big|_{r=R} &= -\frac{\gamma}{R^2 \sin \theta} \frac{\partial T}{\partial \varphi}.\end{aligned}$$

# Linear Stability Analysis and Key Boundary Condition

- We introduce solutions of the Navier–Stokes equations which are a small perturbation around the base state.
- Fluid velocities are assumed to have a small amplitude;
- Temperature distribution given by

$$T = \underbrace{T_*(r, \theta, t)}_{\text{Base State}} + \delta T(r, \theta, \varphi, t).$$

If the model for  $T_*$  has a Neumann boundary condition at the substrate, (i.e.  $k\partial T_*/\partial z = f(r)$ ), then  $\delta T$  should also have a Neumann boundary condition at the substrate – a **homogeneous** one,  $\partial_z \delta T = 0$ .

# Linearized Equations of Motion

- In linear stability, the term  $\mathbf{u} \cdot \nabla \mathbf{u}$  is omitted from the equations of motion.
- We assume that  $T_*$  varies very slowly, such that  $\partial T_*/\partial t$  is ignored.
- By acting repeatedly on the resulting equations with the curl operator, we therefore obtain (following Ha and Lai, Proc. Lond. Roy. Soc. A, 2000):

$$\begin{aligned}\nabla^2 (\nu \nabla^2 - \partial_t) (r u_r) &= 0, \\ (\kappa \nabla^2 - \partial_t) \delta T &= u_r (\partial T_*/\partial z) + u_\theta (\partial T_*/\partial \theta),\end{aligned}$$

where  $\kappa = k/(\rho C_p)$  is the thermal diffusivity of the water.

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Boundary conditions at  $r = R$  simplify (Ha and Li):

$$\begin{aligned}\frac{\partial^2}{\partial r^2} (ru_r) - \frac{2 + \nabla_\Omega^2}{r^2} (ru_r) &= \frac{\gamma}{r} \nabla_\Omega^2 \delta T, \\ -k \partial_r \delta T &= h_t \delta T, \\ u_r &= 0.\end{aligned}$$

Here,  $\nabla_\Omega^2$  is the Laplace–Beltrami operator on the sphere.



## Linear Stability Analysis

We work at criticality such that  $\partial_t = 0$ . The aim of the remaining analysis (still to be done) is to solve

$$\begin{aligned}\nabla^4(ru_r) &= 0, \\ \nabla^2\delta T &= u_r(\partial T_*/\partial z) + u_\theta(\partial T_*/\partial\theta),\end{aligned}$$

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- By analogy to a prior study with  $T_*$  radially symmetric, we expect this to yield a solvability condition.
- Hence, we expect a consistent solution to these equations exist only for a critical value of  $\gamma$  dependent on the base-state temperature  $T_*$ :

$$\text{Ma} = \frac{\gamma R[Q/(2\pi k)]}{\kappa\mu} = \Phi(\langle T_* \rangle),$$

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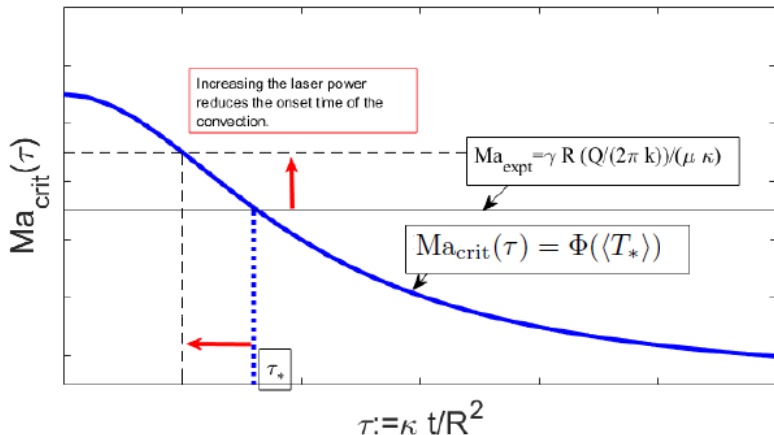
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- Here,  $\Phi(\langle T_* \rangle)$  is to be determined, and the angle brackets denote averaging over space.

We expect the time-dependence to enter via  $Ma_{\text{crit}} = \Phi(T_*)$ , where  $T_*$  depends weakly on time.

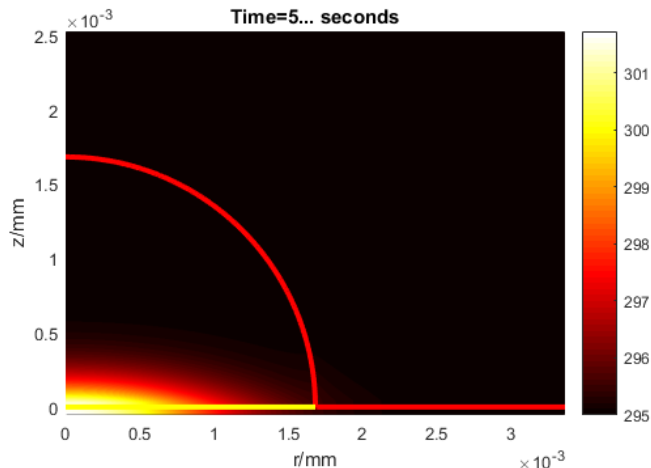
## Graphical representation of the criterion for onset of convection

The idea will be to solve the PDEs numerically and obtain  $Ma_{\text{crit}}(\tau) = \Phi(\langle T_* \rangle)$ , where the time dependence enters via  $\langle T_* \rangle$ , and where  $\tau = \kappa t/R^2$ .



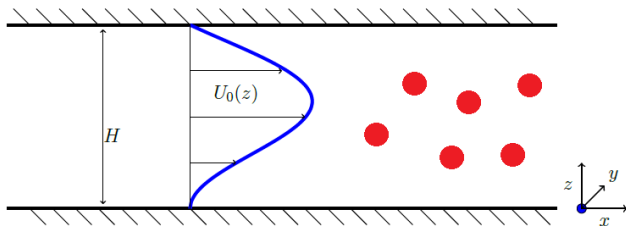
## Analytical progress

Analytical progress depends on finding a 'reasonable' shape for the base state  $T_*(z, r, t)$ . Simulation of  $\partial_t T_* = \nabla^2 T_*$  will help here, e.g.



## Part 2. Particle-laden channel flows

In this part of the talk we outline tentative work in the modelling and simulation of particles in channel flows:

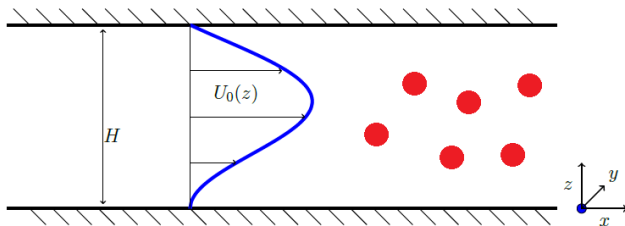


We take an existing parallel flow solver (S-TPLS) and we sequentially add:

- Immersed boundary capabilities to simulate particles (currently only stationary particles);
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We use ANSYS-Fluent for validation purposes; **using S-TPLS for modelling purposes** has advantages (e.g. scalability in future high-resolution studies).

## S-TPLS – overview

- S-TPLS is a stripped-down version of an in-house two-phase solver; S-TPLS is single-phase.
- S-TPLS solves the incompressible Navier–Stokes equation in a channel, using a finite-volume spatial discretization.



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- Projection method: Momenta are updated first, followed by a correction step involving a pressure update, thereby enforcing incompressibility.
- Code is written in Fortran90 and parallelized using MPI; parallelization scheme takes account of problem geometry (2D domain decomposition)

## Immersed boundary method

We use the method of Kajishima et al. (2001) to introduce the solid phase: a solid-body volume fraction  $\alpha$  is introduced, such that

$$\alpha(\mathbf{x}) = \begin{cases} 1, & \text{if } \mathbf{x} \text{ is in the solid phase,} \\ 0, & \text{if } \mathbf{x} \text{ is in the fluid phase,} \end{cases} \quad \text{note change in use of } \alpha !$$

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At the end of the pressure-correction step, the updated velocity is  $\mathbf{u}^{n+1}$ ; this updated velocity is modified further: to enforce  $\mathbf{u} = 0$  in the solid phase:

$$\mathbf{u}^{\text{modified}} = \mathbf{u}^{n+1} - \alpha \mathbf{u}^{n+1}$$

This is a simple and robust method and gives good results for **stationary** particles.

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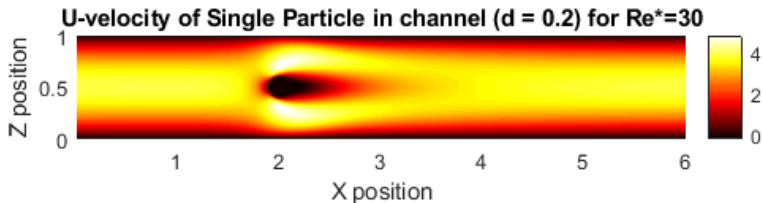
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## Validation I

We validate the method by computing the total drag past the cylinder, as a function of Reynolds number  $Re_*$ .

The drag coefficient  $C_D$  is computed from:

$$C_D = \frac{1}{\rho U^2} \int_{\Omega} (-pn_x) |\nabla\alpha| d^2x + \frac{1}{\rho U^2} \int_{\Omega} (\tau_{xx}n_x + \tau_{xz}n_z) |\nabla\alpha| d^2x,$$

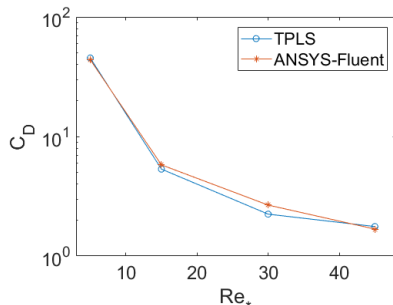
where

$$\tau_{ij} = \frac{1}{Re_*} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right).$$

Here,  $n_x$  and  $n_z$  are obtainable from the solid volume fraction:

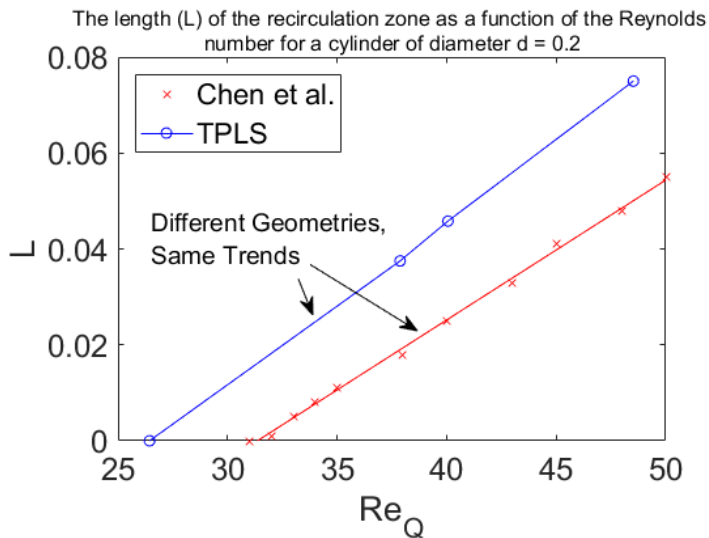
$$(n_x, n_z) = \nabla\alpha/|\nabla\alpha| \quad |\nabla\alpha| \text{ proportional to delta function};$$

also,  $U$  is the mean inlet velocity.



## Validation II

We also look at the critical Reynolds number for the onset of recirculation in the cylinder wake (classical problem; depends closely on inlet boundary conditions).





## With Advection-Diffusion

We also look at modelling heat transfer by adding the advection-diffusion equation to S-TPLS:

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \frac{1}{\text{Pe}} \nabla^2 T.$$

- Periodic boundary conditions in  $x$ -direction.
- Temperature gradient in wall-normal direction.
- Numerical solution via Crank–Nicolson method.
- Addition of particles: once  $T^{n+1}$  is obtained via Crank-Nicolson, temperature is modified to account for the fixed temperature in the particles:

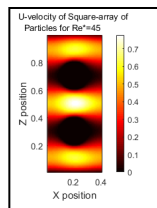
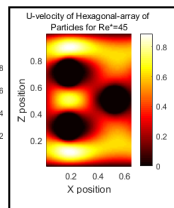
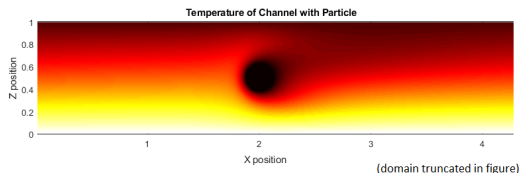
$$T^{\text{modified}} = T^{n+1} + \alpha (T_{\text{particle}} - T^{n+1}).$$

- Quantify enhancement to heat transfer from particles via Nusselt number:

$$\text{Nu} = \frac{L_x^{-1} \int_{\Omega} (1 - \alpha) (wT - \text{Pe}^{-1} \frac{\partial T}{\partial z}) d^2x}{\text{Pe}^{-1} (T_{\text{bottom}} - T_{\text{top}})}.$$

# Sample Results

- Quick check: S-TPLS preserves the constant stratification  $T = T_{\text{bottom}} + (T_{\text{top}} - T_{\text{bottom}})(z/L_z)$  in the absence of particles.
- Currently no buoyancy term in momentum equation; this will be added soon.
- We have also looked at one particle, with normalized temperature values  $T_{\text{bottom}} = 1$ ,  $T_{\text{top}} = 0.1$ , and  $T_{\text{particle}} = 0$ .
- We are also looking at flow / temperature distributions past arrays of particles.



# Conclusions

In **Part 1** we have:

- Looked at the problem of the onset of Marangoni convection in a locally heated sessile droplet.
- Formulated the linear stability analysis up to the point where the base state needs to be specified in concrete terms.
- Outlined how this approach can predict the critical **time** for the onset of Marangoni convection.

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- Formulated the linear stability analysis up to the point where the base state needs to be specified in concrete terms.
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In **Part 2** we have:

- Added solid bodies to the S-TPLS highly parallelized single-phase channel-flow solver.
- Added a temperature equation to model heat transfer
- Outlined how enhancement to heat transfer can be quantified via the **Nusselt number**
- Invite suggestions for which systems to look at next.