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

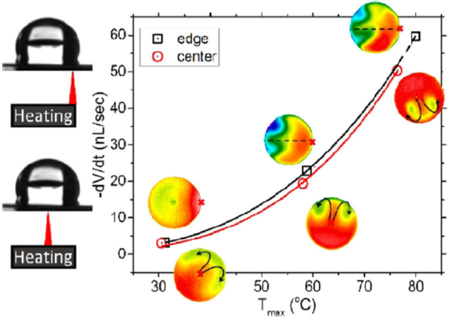


Figure: Askounis et al., Langmuir, 2017.

- 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

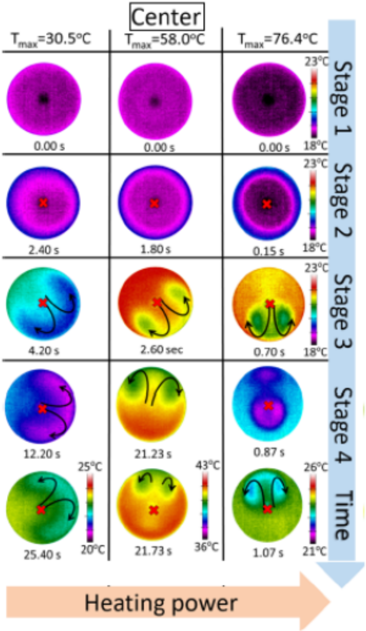


Figure from Askounis et al., Langumuir, 2017:

- Droplet heated at hotspot with laser – constant heat fluix.
- **Symmetric** temperature distribution emerges.
- After some time, convection sets in.
- Convection happens fast, then evaporation n 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:

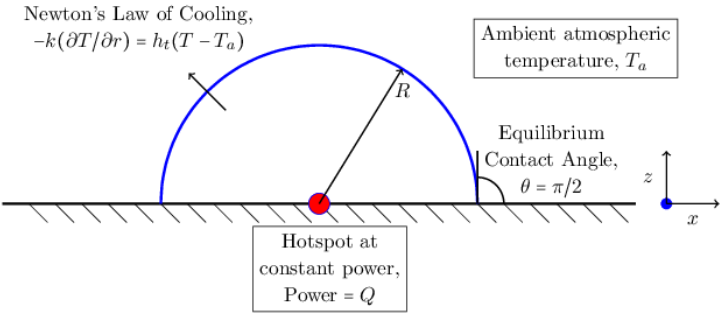
- Convection sets in long before evaporation starts – assume droplet keeps its shape in the model.
- Equilibrium contact angle $\theta \approx 110^\circ$ – treat as hemispherical in the model.
- Idea – develop a temperature distribution for the case without convection – **base state**.
- Treat the onset 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 $r = R$:

$$k(\partial T/\partial r) = h_t(T - T_{\mathrm{a}}),$$

  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

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

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 $T_* \to T_*(r)$.

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:

$$\rho_0 \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \right) = -\nabla p + \mu \nabla^2 \boldsymbol{u} - \rho_0 g \left[1 - \alpha (T - T_{\mathrm{a}}) \right] \widehat{\boldsymbol{z}},$$

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- Work in Bousinesseq limit, where ρ_0 denotes a constant reference density; also, μ is the viscosity.
- We **locally** use α to denote the coeffcient of thermal expansion.
- Calculations suggest $\mathrm{Ma} \gg \mathrm{Ra}$ (defined later); hence, buoyancy term can be dropped.

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Equations of motion simplify (and supplemented by incompressibility):

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

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

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

Fluid Dynamics – Boundary Conditions

- No slip: $\boldsymbol{u} = 0$ 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:

$$\sigma = \sigma_0 - \gamma \left(T - T_{\mathrm{a}} \right).$$

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Effective **vorticity source**:

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

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

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

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 δT 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 $\boldsymbol{u}\cdot\nabla\boldsymbol{u}$ 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):

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

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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, ∇_Ω^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 γ dependent on the base-state temperature T_*:

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

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

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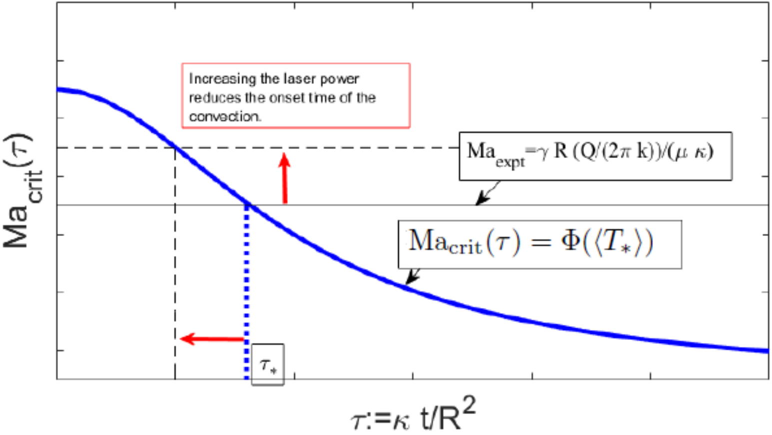
We expect the time-dependence to enter via $Ma_{\mathrm{crit}} = \Phi(\langle T_* \rangle)$, where T_* depends weakly on time.

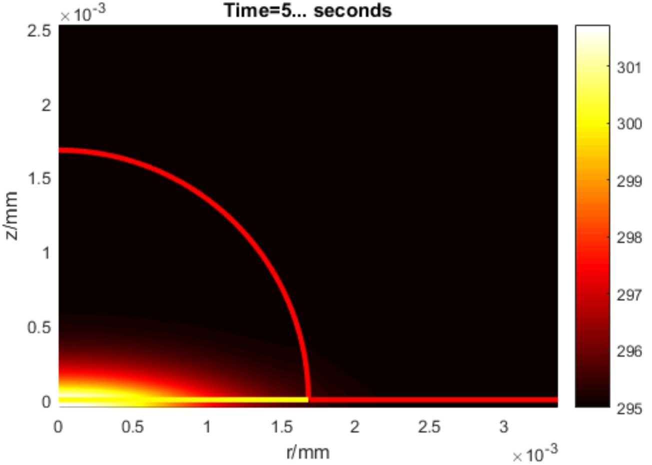
Graphical representation of the criterion for onset of convection

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



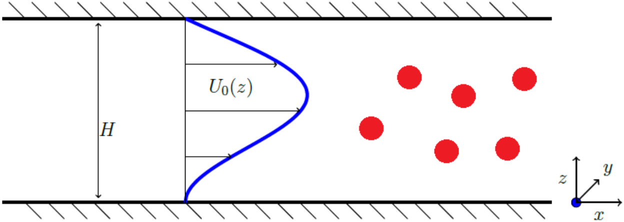
Analytical progress

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:



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- Immersed boundary capabilities to simulate particles (currently only stationary particles);
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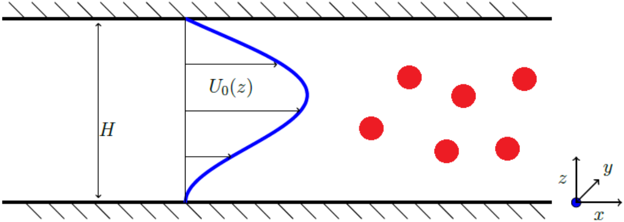

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We use ANSYS-Fluent for validation purposes; **using S-TPLS for modelling purposes** has advantages (e.g. scalability in future high-resolution studies).

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 is α is introduced, such that

$$\alpha(\boldsymbol{x}) = \begin{cases} 1, \text{if } \boldsymbol{x} \text{ is in the solid phase,} \\ 0, \text{if } \boldsymbol{x} \text{ is in the fluid phase,} \end{cases}$$

note change in use of α !

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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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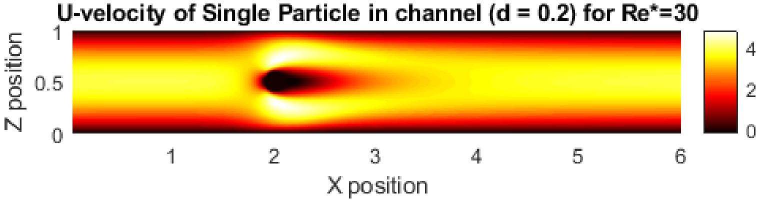


Validation I

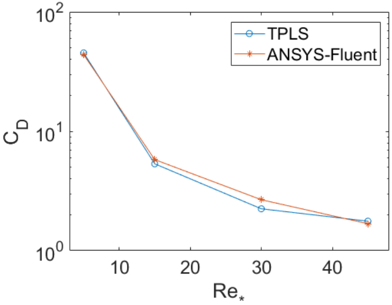
We validate the method by computing the total drag past the cylinder, as a function of Reynolds number Re_*.

The drag coefficient C_D is computed from:

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

where

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



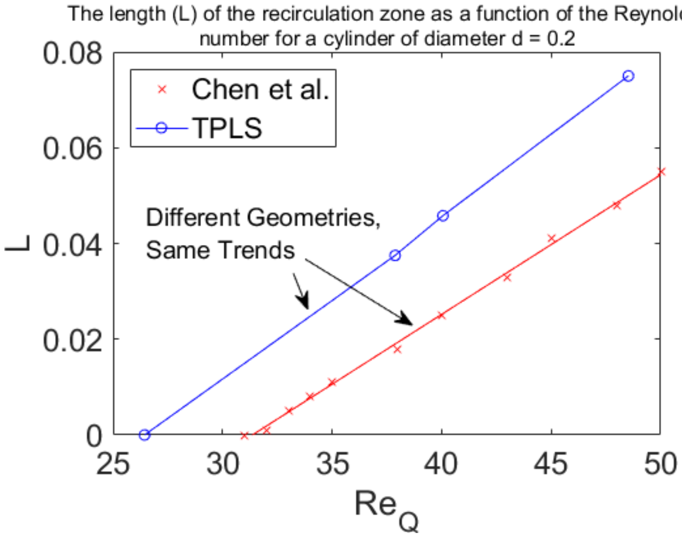
Here, n_x and n_z are obtainable from the solid volume fraction:

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

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:

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

- 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:

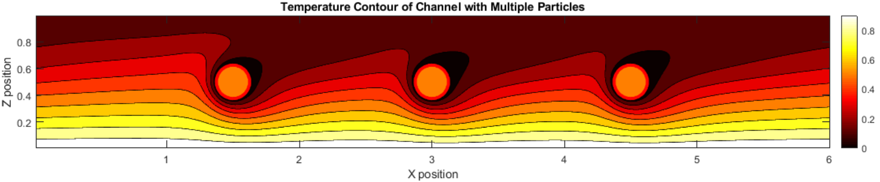
$$T^{\mathsf{modified}} = T^{n+1} + \alpha \left(T_{\mathsf{particle}} - T^{n+1} \right).$$

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

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

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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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.