

Thermal Science meets Mathematical Modelling - opportunities for Applied Mathematics Work in Progress

Lennon Ó Náraigh¹, Daniel R. Jansen van Vuuren^{1,2}, Miguel Bustamante¹

¹School of Mathematics and Statistics, University College Dublin, Belfield, Dublin 4, Ireland

¹School of Engineering, University of Pretoria, cnr Lynnwood Road and Roper Street, Hatfield, Pretoria
South Africa

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Introduction

In this talk, we look at three 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:

- 1 Fundamental theoretical description of evaporating sessile droplets (multiphase, theory)
- 2 Fundamental numerical modelling of heat and momentum transfer in particle-laden channel flows (single-phase, numerics)
- 3 Mathematical modelling of industrial drying (multiphase, correlation-based)

Plan of talk:

- Present the three problems separately
- Talk about their complementarity
- Talk about how solving these problems can help the Europe's goal of net-zero-emissions by 2050.

Evaporating Sessile Droplets – Context

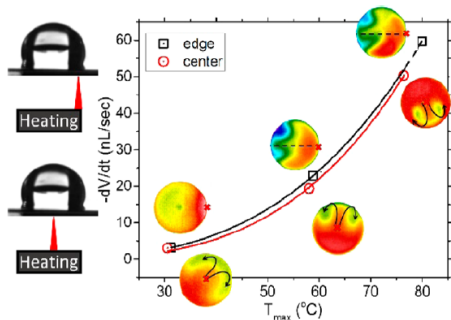


Figure: Askounis et al., Langmuir, 2017.

- 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

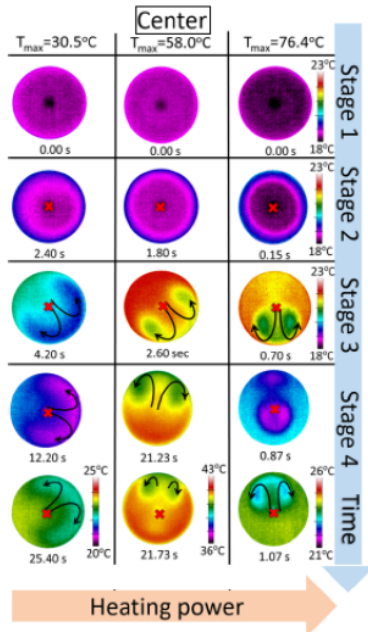


Figure from Askounis et al., Langmuir, 2017:

- 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.

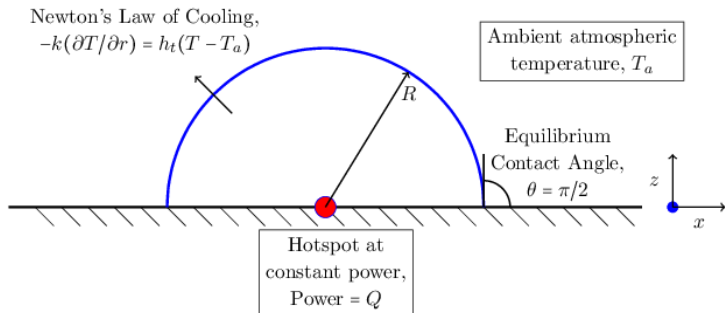
Boundary Conditions

- 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 ρ_0 denotes a constant reference density; also, μ is the viscosity.
- We **locally** use α 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 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 $\mathbf{u} \cdot \nabla \mathbf{u}$ 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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where $\kappa = k/(\rho C_p)$ is the thermal diffusivity of the water.

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_* :

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

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

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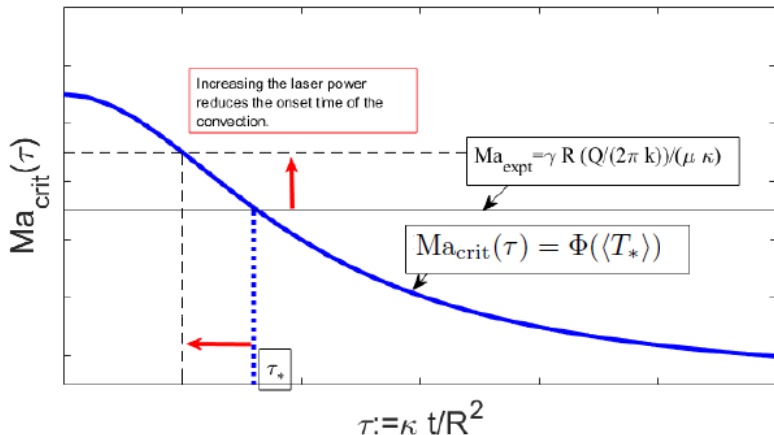
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We expect the time-dependence to enter via $Ma_{\text{crit}} = \Phi(\langle T_* \rangle)$, where T_* depends weakly on time.

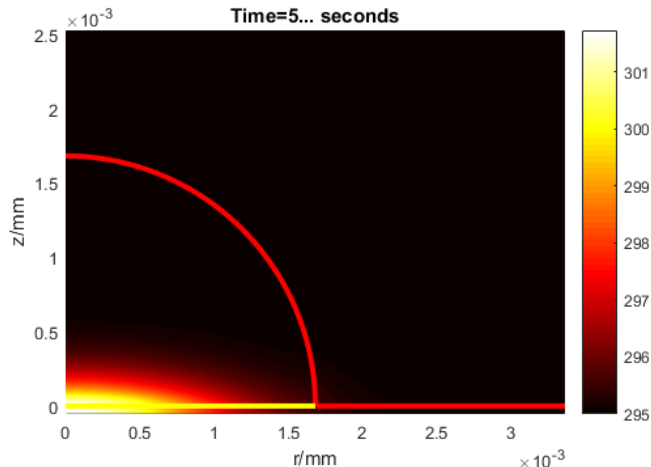
Graphical representation of the criterion for onset of convection

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



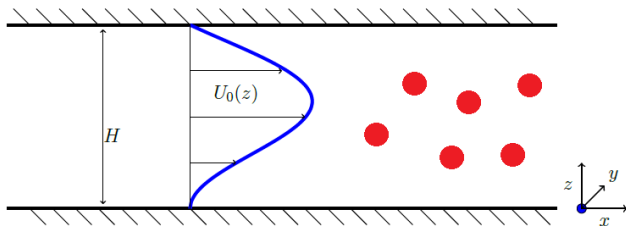
Analytical progress

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:

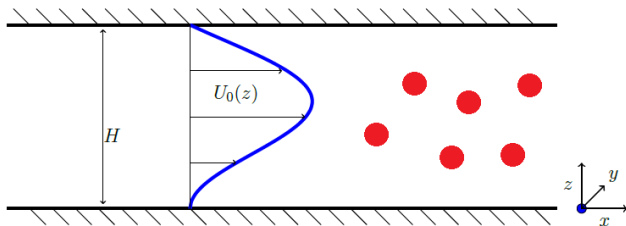


We take an existing parallel flow solver (S-TPLS) and we sequentially add:

- 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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- Momentum step: centred differences for the convective derivative, Crank–Nicolson treatment for the diffusion, third-order Adams–Bashforth for the time evolution.
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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 α 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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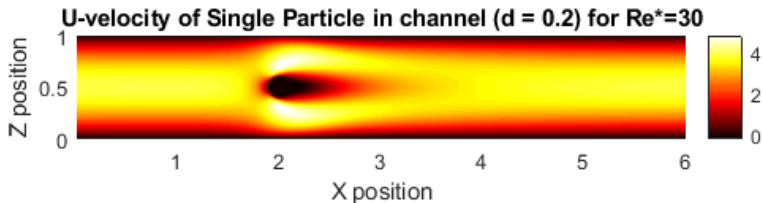
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Validation I

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:

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

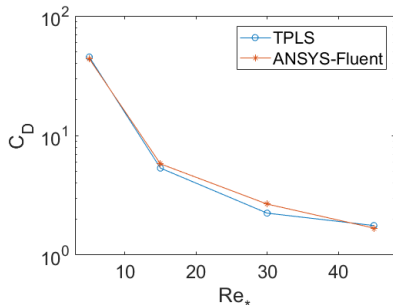
where

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

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

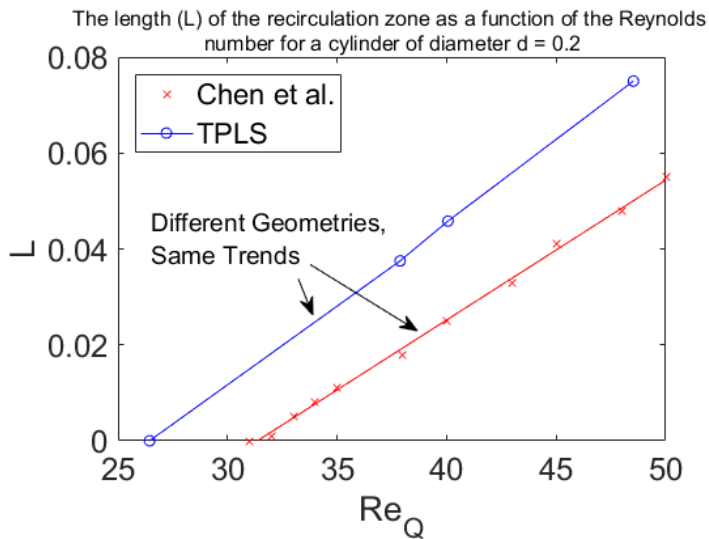
$$(n_x, n_z) = \nabla\alpha / |\nabla\alpha| \quad |\nabla\alpha| \text{ proportional to delta function};$$

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:

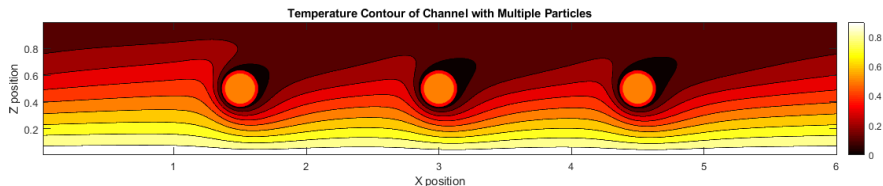
$$T^{\text{modified}} = T^{n+1} + \alpha (T_{\text{particle}} - T^{n+1}).$$

- 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.



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Don't blame me: <https://thoughtcatalog.com>

Industrial Drying – Context

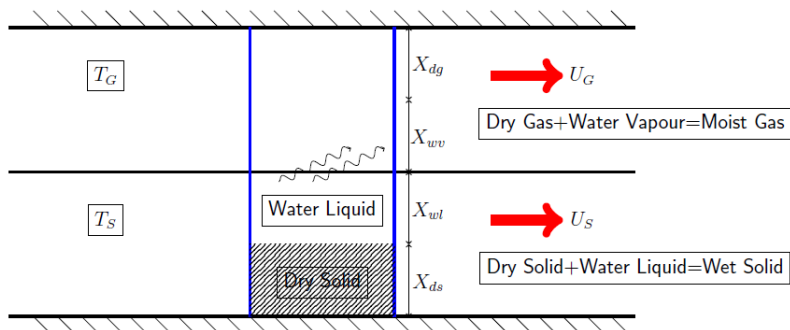
- In Process Engineering, many products need to have moisture removed ('drying') – foodstuffs, food waste, textiles, etc. The drying is done in a machine on a large scale – industrial drying.
- The product is heated and the moisture is evaporated.
- Heating the product is expensive. Large amounts of energy are required to overcome the latent heat of the water and to produce evaporation – **energy intensive**.
- The dried product has to meet certain constraints on the moisture content for quality control.
- The drying must therefore be **controlled** to minimize energy consumption while at the same time maximizing product quality.
- This is a complicated problem in control theory – understanding the drying process is the first step in achieving such control.

Generic Process Calculations

We begin by writing down the generic process calculations relevant for all industrial dryers.

- We assume a one-dimensional model where x is a coordinate along the length of the dryer (inlet \rightarrow outlet).
- Hence, averages are taken over the cross-sectional-area S of the dryer.
- We break the dryer up into a series of infinitesimal control volumes. We perform mass, momentum, and energy balances across each control volume.
- We introduce four phases – dry solid, liquid water, dry gas, and water vapour. Mass, momentum, and energy are transferred between the liquid water and water vapour phases (first-order phase transition).

Schematic Description



We introduce a test volume $V = \Delta V = \Delta x S$, where S is the area of the dryer orthogonal to the plane of the page. The control volume is the blue section in the figure. We therefore introduce volume fractions,

$$X_{ds} = \frac{V_{ds}}{V}, \quad X_{wl} = \frac{V_{wl}}{V}, \quad X_{wv} = \frac{V_{wv}}{V}, \quad X_{dg} = \frac{V_{dg}}{V},$$

where the subscripts stand for 'dry solid', 'water liquid', 'water vapour', and 'dry gas', respectively. The volume fractions evidently sum to one: we use the subscript $i \in \{ds, wl, wv, dg\}$. Hence, we have

$$\sum_i X_i = 1.$$

Mass Balance

We look at Δm_i – this is the mass of the i^{th} phase inside the test volume ΔV .
We have:

$$\Delta m_i = \rho_i X_i \Delta V.$$

For the test volume, we have the following mass-conservation law:

$$\frac{d}{dt} \int_{\Delta V} \rho_i X_i dV = - \left[\rho_i X_i U_i \Big|_{x+\Delta x} - \rho_i X_i U_i \Big|_x \right] + \dot{m}_i \Delta V. \quad (1)$$

Here, \dot{m}_i is the mass loss of the i^{th} phase, in units of $\text{kg}/[\text{m}^3 \text{s}]$.

Evaporation Rate

We have:

$$\dot{m}_i = \begin{cases} 0, & \text{if } i = ds, \\ \dot{m}_{wl \rightarrow wv} & \text{if } i = wl, \\ -\dot{m}_{wl \rightarrow wv} & \text{if } i = wv, \\ 0, & \text{if } i = dg. \end{cases} \quad (2)$$

The functional form of the **evaporation rate** $\dot{m}_{wl \rightarrow wv}$ will be discussed in what follows. Notice that $\dot{m}_{wl \rightarrow wv}$ is either negative or zero, corresponding to a mass loss due to evaporation of the liquid water into the vapour phase. We take the limit as $\Delta x \rightarrow 0$ on Equation (1) to obtain the following continuity equations:

$$\frac{\partial}{\partial t}(\rho_i X_i) + \frac{\partial}{\partial x}(\rho_i X_i U_i) = \dot{m}_i. \quad (3)$$

Mass Balance – Results

If we wish, we can write these out explicitly for the phases as follows ('continuity equation'):

$$\begin{aligned}\frac{\partial}{\partial t}(\rho_{ds}X_{ds}) + \frac{\partial}{\partial x}(\rho_{ds}X_{ds}U_{ds}) &= 0, \\ \frac{\partial}{\partial t}(\rho_{wl}X_{wl}) + \frac{\partial}{\partial x}(\rho_{wl}X_{wl}U_{wl}) &= \dot{m}_{wl \rightarrow wv}, \\ \frac{\partial}{\partial t}(\rho_{wv}X_{wv}) + \frac{\partial}{\partial x}(\rho_{wv}X_{wv}U_{wv}) &= -\dot{m}_{wl \rightarrow wv}, \\ \frac{\partial}{\partial t}(\rho_{dg}X_{dg}) + \frac{\partial}{\partial x}(\rho_{dg}X_{dg}U_{dg}) &= 0,\end{aligned}$$

Notice that

$$\frac{\partial}{\partial t} \left(\sum_i \rho_i X_i \right) + \frac{\partial}{\partial x} \left(\sum_i \rho_i X_i U_i \right) = 0,$$

which is the principle of global conservation of mass.

Momentum Balance

We look at the quantity of momentum in the i^{th} phase inside the control volume $\Delta V - \rho_i U_i X_i \Delta V$. Newton's Law:

$$\begin{aligned} \frac{d}{dt} \int_{\Delta V} \rho_i U_i X_i dV &= - \left[\rho_i X_i U_i^2 \Big|_{x+\Delta x} - \rho_i X_i U_i^2 \Big|_x \right] S \\ &+ \left[(-p_i) X_i S \Big|_{x+\Delta x} - (-p_i) X_i S \Big|_x \right] \\ &+ \int_{\Delta V} \rho_i X_i f_i dV + (\tau_{i+1,i} + \tau_{i-1,i}) [\Delta x \times (\text{Width})], \quad (4) \end{aligned}$$

where

- $p_i|_x$ is the pressure on the i^{th} phase at the control-volume face at location x ,
- f_i is an acceleration corresponding to a body force (dimensions m/s^2),
- $\tau_{i+1,i}$ is the shear stress exerted by the neighbouring $i + 1$ phase on phase i , with dimensions of Force/Area. Similarly for $\tau_{i-1,i}$.
- 'Width' means a characteristic width of the dryer into the plane of the page (sketch).

Momentum Balance – Equations

Performing the usual manipulations on the momentum balance (4) gives the following partial differential equation:

$$\frac{\partial}{\partial t}(\rho_i X_i U_i) + \frac{\partial}{\partial x}(\rho_i X_i U_i^2) = -\frac{\partial}{\partial x}(X_i p_i) + \rho_i X_i f_i (\tau_{i+1,i} + \tau_{i-1,i}) (\text{Width}/S).$$

We use $S = \text{Width} \times H$, where H means the characteristic height of the dryer, to re-write the momentum balance as follows:

$$\frac{\partial}{\partial t}(\rho_i X_i U_i) + \frac{\partial}{\partial x}(\rho_i X_i U_i^2) = -\frac{\partial}{\partial x}(X_i p_i) + \rho_i X_i f_i + \frac{\tau_{i+1,i} + \tau_{i-1,i}}{H}.$$

We group several of the terms on the right-hand side together as follows:

$$\rho_i X_i f_i + \frac{\tau_{i+1,i} + \tau_{i-1,i}}{H} = \rho_i X_i F_i.$$

Hence, the momentum balance for the i^{th} phase becomes:

$$\frac{\partial}{\partial t}(\rho_i X_i U_i) + \frac{\partial}{\partial x}(\rho_i X_i U_i^2) = -\frac{\partial}{\partial x}(X_i p_i) + \rho_i X_i F_i. \quad (5)$$

Energy Balance

We look at the total energy of the i^{th} component on a per-unit mass basis, i.e.

$$\frac{\text{Energy}}{\text{Volume}} = \frac{1}{2}\rho_i U_i^2 + \rho_i e_i,$$

where

- $(1/2)\rho_i U_i^2$ is the kinetic energy (per unit mass),
- e_i is the thermodynamic (internal) energy, per unit mass.

We formulate the energy-balance principle for the control volume ΔV :

$$\frac{d}{dt} \int_{\Delta V} \left(\frac{\text{Energy}}{\text{Volume}} \right) dV = \text{Energy flux out of the control volume} +$$

Rate at which work is done by the external forces on the fluid parcel +

Rate at which work is done by the internal fluid forces on the fluid particle +

Dissipation of energy by heat flux +

Heat transfer between phases

Energy Balance – Equations

Mathematical form of energy balance:

$$\begin{aligned} \frac{d}{dt} \int_{\Delta V} [\frac{1}{2}\rho_i U_i^2 + \rho_i e_i] X_i dV \\ = - [(\frac{1}{2}\rho U_i^2 + \rho_i e_i) X_i U_i|_{x+\Delta x} - (\frac{1}{2}\rho U_i^2 + \rho_i e_i) X_i U_i|_x] S \\ + \int_{\Delta V} \rho_i X_i F_i U_i dV + \int_{\Delta V} \left[-\frac{\partial}{\partial x} (X_i p_i) \right] U_i dV \\ + \left[\left(k_i \frac{\partial T_i}{\partial x} \right) X_i|_{x+\Delta x} - \left(k_i \frac{\partial T}{\partial x} \right) X_i|_x \right] S + \dot{Q}_i \Delta V \end{aligned}$$

- Heat flux given by Fourier's law, Heat Flux = $k_i(\partial T/\partial x)$, k_i = thermal conductivity.
- \dot{Q}_i is the heat transfer from phase i to the other phases, with units of $J/[m^3 s]$.

The kinetic terms drop out of the energy equation

Take limits:

$$\begin{aligned} \frac{\partial}{\partial t} \left(\frac{1}{2} \rho_i X_i U_i^2 + \rho_i X_i e_i \right) + \frac{\partial}{\partial x} \left[\left(\frac{1}{2} \rho_i X_i U_i^2 + \rho_i X_i e_i \right) U_i \right] \\ = -U_i \frac{\partial}{\partial x} (X_i p_i) + \rho_i X_i F_i U_i + \frac{\partial}{\partial x} \left(k_i X_i \frac{\partial T_i}{\partial x} \right) + \dot{Q}_i. \end{aligned}$$

After many algebraic manipulations, the kinetic terms can be eliminated from the energy equation altogether, leaving an energy balance in terms of thermodynamic quantities only:

$$\frac{\partial}{\partial t} (\rho_i X_i e_i) + \frac{\partial}{\partial x} (\rho_i X_i e_i U_i) = \frac{\partial}{\partial x} \left(k_i X_i \frac{\partial T_i}{\partial x} \right) + \dot{Q}_i + \dot{m}_i \left(\frac{1}{2} U_i^2 \right) \quad (6)$$

In some sense, this decouples the energy and momentum balances...

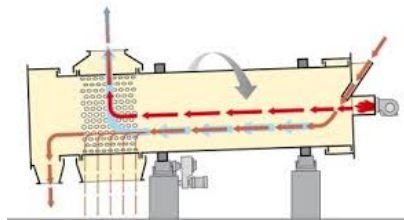
The Momentum Balance is Redundant

- In some application (e.g. oil-gas transport), the averaged mass-balance equations are important to obtain a closed set of equations.
- In industrial drying, this approach is unnecessarily complicated. Instead, it is assumed that the gas and solid streams each have a constant velocity U_G and U_S respectively, that are modelled via algebraic closure relations.

For instance, in a rotary drum dryer, it is assumed that

- $U_G = L\dot{m}_{dg,inlet}/m_{dg}$,
- $U_S = L/T_R$,
- T_R is the residence time of a parcel of product in the drum, obtained via a correlation, e.g.

$$T_R(\text{minutes}) = \frac{0.23kL}{\tan\theta(\text{r.p.m.})^{0.9}D}$$



<https://www.powderbulksolids.com>

Simplifying the Energy Balances I

Taking U_S and U_G simplifies the energy balances. We make further simplifying assumptions:

- Heat fluxes unimportant.
- Kinetic energy transfer terms $\dot{m}_i \left(\frac{1}{2}U_i^2\right)$ unimportant.
- No compressibility effects: $\rho_i e_i = c_{p,i} T_i$ (reference temperature at 0° C).

Energy balances simplify:

$$\frac{\partial}{\partial t}(\rho_i X_i e_i) + \frac{\partial}{\partial x}(\rho_i X_i e_i U_i) = \dot{Q}_i. \quad (7)$$

Simplifying the Energy Balances II

We simplify the energy balances further:

- The solid stream has a single temperature T_S
- The gas stream has a single solid temperature T_G .
- We then take two independent sums over i in the energy equation:
 $i \in \{ds, wl\}$ (solid stream), and $i \in dg, wv$ (as stream)

Simplifying the Energy Balances III

Hence:

$$\begin{aligned} \frac{\partial}{\partial t} [(\rho_{ds} X_{ds} c_{p,ds} + \rho_{wl} X_{wl} c_{p,wl}) T_S] \\ + \frac{\partial}{\partial x} [(\rho_{ds} X_{ds} c_{p,ds} + \rho_{wl} X_{wl} c_{p,wl}) U_S T_S] = \dot{Q}_{wl}, \end{aligned}$$

and

$$\begin{aligned} \frac{\partial}{\partial t} [(\rho_{dg} X_{dg} c_{p,dg} + \rho_{wv} X_{wv} c_{p,wv}) T_G] \\ + \frac{\partial}{\partial x} [(\rho_{dg} X_{dg} c_{p,dg} + \rho_{wv} X_{wv} c_{p,wv}) U_S T_G] = -\dot{Q}_{wl}. \end{aligned}$$

Also,

$$\dot{Q}_{wl} = \dot{m}_{wl \rightarrow wv} [c_{p,wv}(T_S - 0^\circ\text{C}) + \Delta q(0^\circ\text{C})].$$

Here, Δq is the **latent heat of vapourization** of the water.

Summary of the model so far

- Six variables – $\rho_i X_i$ and T_L and T_G . Six PDEs in the same variables – **hyperbolic conservation laws**
- Closures for U_L and U_G - also for \dot{m}_{wl} .
- Closure for the **drying rate** from the literature:

$$\dot{m}_{wl} = -\rho_{dg} X_{dg} K(X - X_*), \quad X = \frac{\rho_{wl} X_{wl}}{\rho_{ds} X_{ds}}.$$

Here, $X = \rho_{wl} X_{wl} / \rho_{dg} X_{dg}$ is the moisture content of the solid phase and X_* is the equilibrium moisture content. The coefficients K and X_* are obtained from thermodynamics and depend on the gas-stream temperature T_G .

Hyperbolic Conservation Laws

Summarize by looking at $X = \rho_{wl}X_{wl}/\rho_{dg}X_{dg}$, with $U_S = \text{Const.}$:

$$\frac{\partial X}{\partial t} + U_S \frac{\partial X}{\partial x} = -R_X, \quad R_X = k(X - X_*).$$

Discretize in space k and time n using backward Euler (time) and upwind differentiation (space):

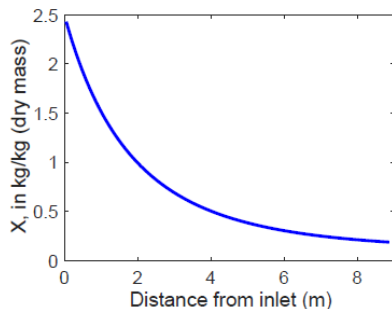
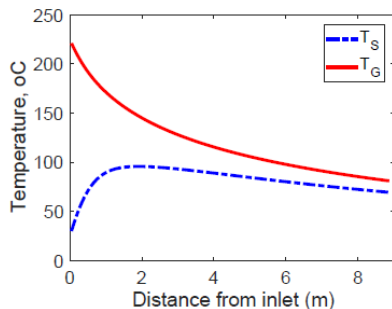
$$\frac{X_k^{n+1} - X_n^k}{\Delta t} + U_S \frac{X_k^{n+1} - X_{k-1}^{n+1}}{\Delta x} = -R_{X,k}^n$$

Re-arrange:

$$X_k^{n+1} = \frac{X_n^k + U_S(\Delta t/\Delta x)X_{k-1}^{n+1} - \Delta t R_{X,k}^n}{1 + U_S(\Delta t/\Delta x)}, \quad k = 2, 3, \dots$$

- Implicit method – unconditionally stable (no CFL condition on $U_S \Delta t/\Delta x$).
- Can be used to ‘sweep’ updated information from the inlet towards the outlet – hyperbolic system.
- Update at $k = 1$ supplied by Dirichlet condition $X_{k=1} = X_{inlet}$.
- Shows insight that Mathematics can bring to bear on engineering problems.

Sample Results for an Industrial Rotary Dryer



Length (m)	9
Diameter (m)	0.9
Slope (deg)	0.63
Rotational speed (rev min ⁻¹)	3.3
Volumetric air flow rate (m ³ s ⁻²)	1.2
Dry solid intrinsic density (kg m ⁻³)	630

Summary I

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.

Summary I

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- Outlined how this approach can predict the critical **time** for the onset of Marangoni convection.

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.

Summary II

In **Part 3** we have:

- Formulated a model of an industrial dryer using mass- and energy-balances.
- Shown how the model needs algebraic correlation to close the system of differential equations.
- Solved the model for a typical rotary dryer.

Complementarities – beyond ‘all heat transfer’

- In Part I we have looked at a theoretical problem in Hydrodynamics
- In Part II we have looked at using large-scale numerical simulations to obtain a correlation relation (‘Nusselt number’)
- In Part III we have solved a simple mass/energy balance model to characterize an industrial dryer:
 - ▶ Velocities modelled using algebraic closures (solution: theoretical Hydrodynamics)
 - ▶ Heat-transfer coefficients (effectively, the Nusselt number) modelled using correlations from the literature (solution: DNS)

Suggests a way forward for a unified research programme in Thermal Science:

- Formulate simple models and apply them to real industrial systems;
- Obtain closures from theoretical / numerical modelling.

Opportunities

- Carbon taxes are increasing. Businesses need to get more energy-efficient.
- The European Commission wants Europe to produce no net CO₂ emissions by 2050.
- There are big opportunities to apply fundamental mathematical modelling techniques to industrial problems and hence, to promote energy efficiency.
- Case studies here – evaporating droplets (H2020 project ThermaSMART); industrial dryers (joint research project with industry).

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