James Weir Fluids Laboratory

University of Strathclyde Engineering

Implementation of a Volume of Fluid-based Solver for Multiphase Thermocapillary Flows

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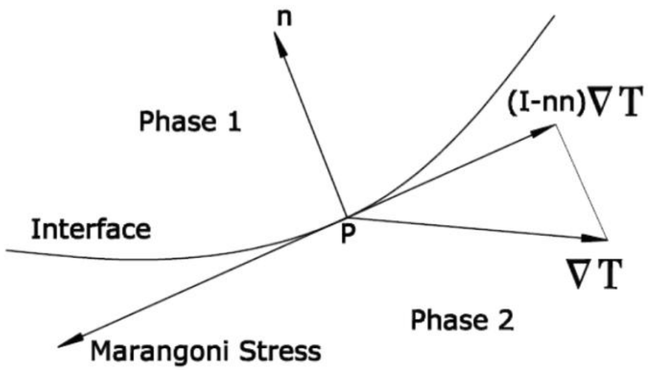
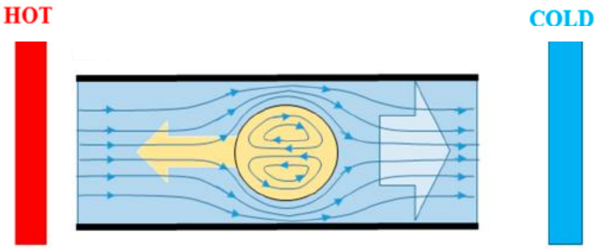
Thermocapillary Flows

Marangoni stresses at the interface

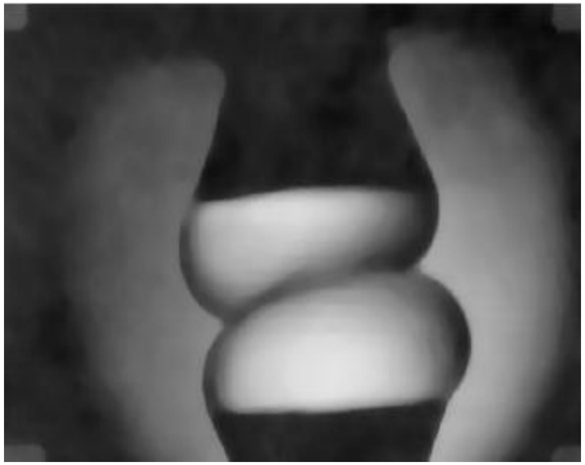


Droplet migration in a bulk fluid



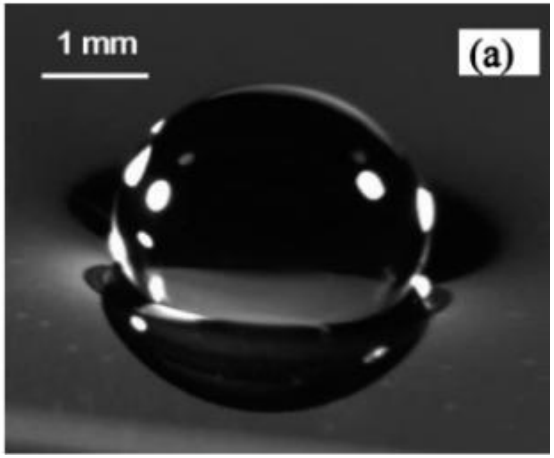
A. Karbaley, R. Kumar, H. Jin Ho, Michromachines, 2016

Non coalescence of two silicone oil drops



M. Lappa,, FDMP, vol 1, pp 201-211, 2005

Levitating aqueous drop in a fluorocarbon pool



E. Yakhshi-Tafti, H. J. Cho, R. Kumar, Appl. Phys. Lett, 2010

Thermocapillary Flows

Conservation of Mass:

$$\nabla \cdot \mathbf{U} = 0$$

Conservation of Momentum ("single fluid" approach):

$$\rho_{\mathrm{r}}\left(\frac{\partial \mathbf{U}}{\partial \mathrm{t}} + \mathbf{U}\cdot\nabla\mathbf{U}\right) = -\nabla \mathrm{p} + \frac{1}{\mathrm{Re}}\nabla\cdot\left[\mu_{\mathrm{r}}\cdot\left(\nabla\mathbf{U} + \nabla\mathbf{U}^{\mathbf{T}}\right)\right] + \frac{1}{\mathrm{ReCa}}\left(\sigma^{*}(\bar{\mathrm{T}})\mathrm{k}\delta\mathbf{n} + \nabla_{\|}\sigma^{*}(\mathrm{T})\delta\right)$$

Dimensionless interfacial tension

"Additional term" due to the presence of the interface (modeled as a body force)

Additional force due to the presence of the interface tension gradients

Reference fluid property

$\Phi_r = \Phi_1 \;\; or \;\; \Phi_2$

Conservation of Energy:

$$\rho_{\mathrm{r}}\mathrm{c}_{\mathrm{p,r}}\left(\frac{\partial \mathrm{T}}{\partial \mathrm{t}} + \mathbf{U}\cdot\nabla\mathrm{T}\right) = \frac{1}{\mathrm{Ma}}\nabla\cdot\mathrm{k}_{\mathrm{r}}\nabla\mathrm{T}$$

The Marangoni number is defined as:

$$\mathrm{Ma} \equiv \frac{\sigma_T G_T L}{\mu D} = \frac{Thermal\ convection}{Thermal\ diffusion}$$

where

$\sigma_T = -\partial\sigma / \partial T$

$G_T = temperature\ difference$

$L = characteristic\ length$

$D = thermal\ diffusivity$

'MarangoniFoam': Code Implementation

We implemented our code starting from InterFoam (OF-2.1.x). The main modifications are:

- the inclusion of the thermocapillary stresses in the momentum equation,
- the addition of the energy transport equation

We need to model the Marangoni stresses

$$F_{Ma} = \nabla_{\parallel}\sigma(T)\delta$$

Using the CSF (Continuum Surface Force) model, in the VOF approach we have the following expression:

$$F_{Ma} = \left[\sigma_T\left(\mathbf{I} - \mathbf{nn}\right)\cdot\nabla T\right]\|\nabla\alpha\|$$

UEqn.H

```
fvVectorMatrix UEqn
(
    fvm::ddt(rho, U)
  + fvm::div(rhoPhi, U)
  + turbulence->divDevRhoReff(rho, U)
  + ddTSigma*gradTParallel * mag(fvc::grad(alpha1))
 ==
    sources(rho, U)
);
```

The temperature field is obtained solving the energy equation

$$\frac{\partial T}{\partial t} + \mathbf{U}\cdot\nabla T = \frac{1}{\rho c_p}\nabla\cdot k\nabla T$$

After few manipulations* we get the following equivalent formulation

$$\frac{\partial T}{\partial t} + \mathbf{U}\cdot\nabla T = \nabla\cdot D\nabla T - \frac{1}{\rho c_p}\nabla k\cdot\nabla T + \nabla D\cdot\nabla T$$

TEqn.H

```
fvScalarMatrix TEqn
 (
      fvm::ddt(T)
    + fvm::div(phi,T)
    - fvm::laplacian(D,T)
    - 1.0/(rho*cp)*(fvc::grad(kappa) & fvc::grad(T))
    + (fvc::grad(D) & fvc::grad(T))
 );

 TEqn.solve();
```

*Density and specific heat may vary at the interface

Code Implementation

In the VOF approach for the generic fluid property Φ is written as a linear combination of the volume fraction α:

$$\Phi = \alpha \ \Phi_1 + (1-\alpha)\Phi_2$$

with Φ_1 and Φ_2 being the properties of the two "pure" phases far from the interface

$$\rho = \alpha \ \rho_1 + (1-\alpha)\rho_2$$

$$c_p = \alpha \ c_{p1} + (1-\alpha)c_{p2}$$

$$k = \alpha \ k_1 + (1-\alpha)k_2$$

$$D = \alpha \frac{k_1}{\rho_1 c_{p1}} + (1-\alpha)\frac{k_2}{\rho_2 c_{p2}}$$

TEqn.H

```
rho =
(
    alpha*rho1 + (1.0 - alpha)*rho2
);

cp =
(
    alpha*cp1 + (1.0 - alpha)*cp2
);

kappa =
(
   alpha*kappa1 + (1.0 - alpha)*kappa2
);

D =
 (
   alpha*kappa1/(rho1*cp1) + (1.0 - alpha)*kappa2/(rho2*cp2)
);
```

Code Validation

"Asymptotic velocity" test at vanishing Ma and Re

The code was tested by simulating the migration of a spherical drop of radius R in the limiting case studied by Young *et al.* [1]

Theory

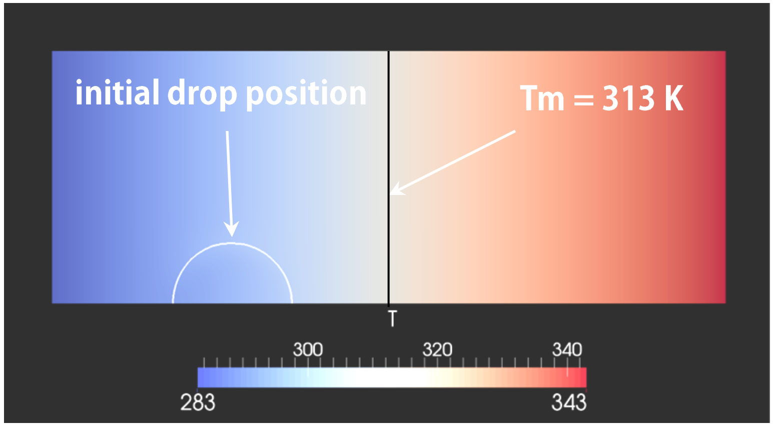
- Perfectly spherical drop
- Absence of confinement
- Ma = 0 and Re = 0

$$U_{\mathbf{YGB}} = \frac{2v_0}{\left(2+3\frac{\mu_d}{\mu_m}\right)\left(2+\frac{k_d}{k_m}\right)}$$

where $v_0 = \dfrac{\sigma_T G_T R}{\mu_m}$

Simulation Setup

- Axisymmetric Domain
- Constant Fluid Properties: ρ and μ evaluated for the temperature at the middle of the domain :



$$\rho = \alpha + \beta / T_m$$

$$\ln \mu = \gamma + \delta / T_m$$

$\alpha,\ \beta,\ \gamma,\ \delta$ ***are constants***

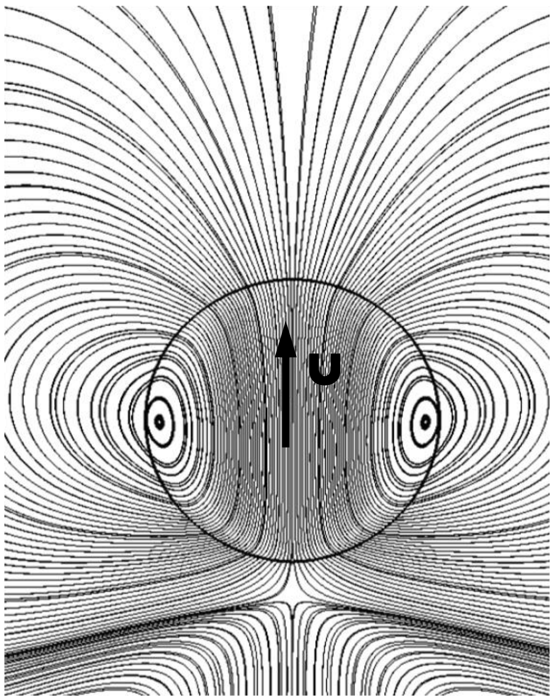
- k and cp are also constant and selected from tabulated values

[1] N. O. Young, J. S. Goldstein, M. J. Block, "*The Motion of Bubbles ina Vertical Temperature Gradient*", J. of Fluid Mech. 6, 350-356, 1959

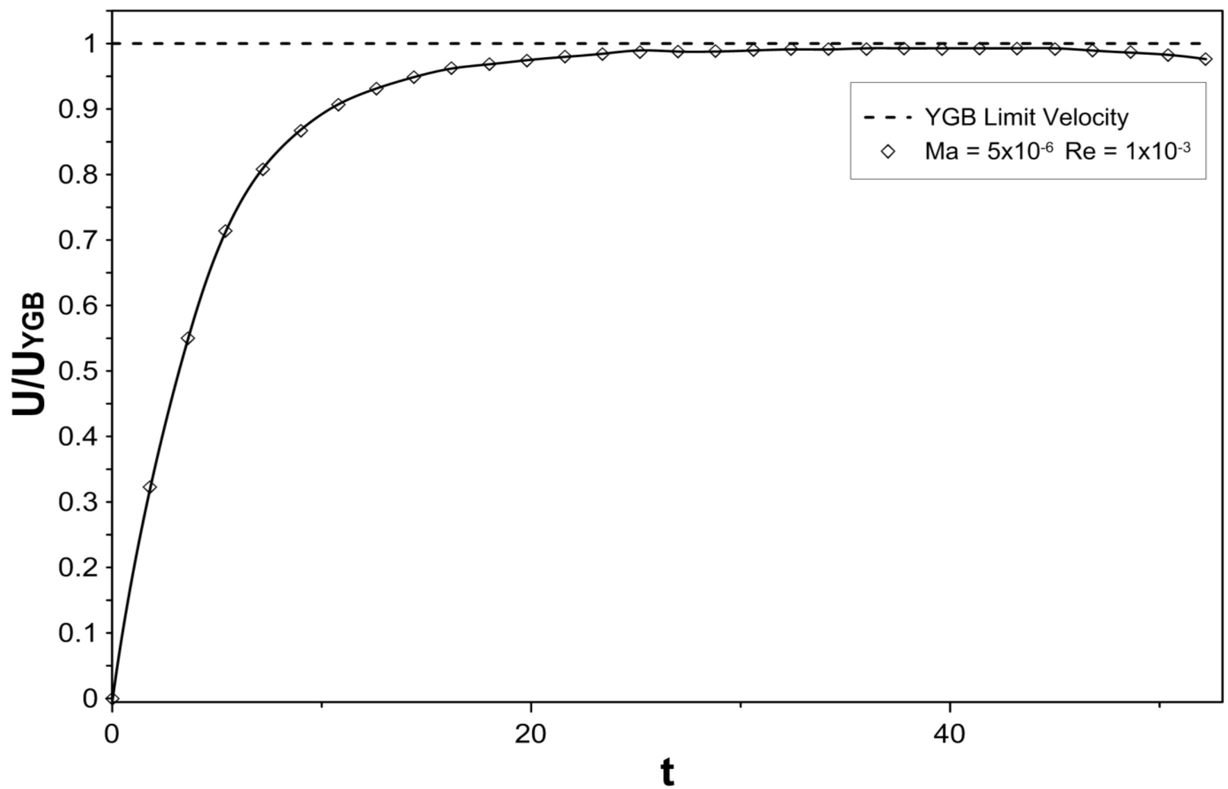
Code Validation

"Asymptotic velocity" test at vanishing Ma and Re

Streamlines and shape of the drop



Droplet normalised velocity: comparison between the analytical solution of Young et al. (1959) and our simulations

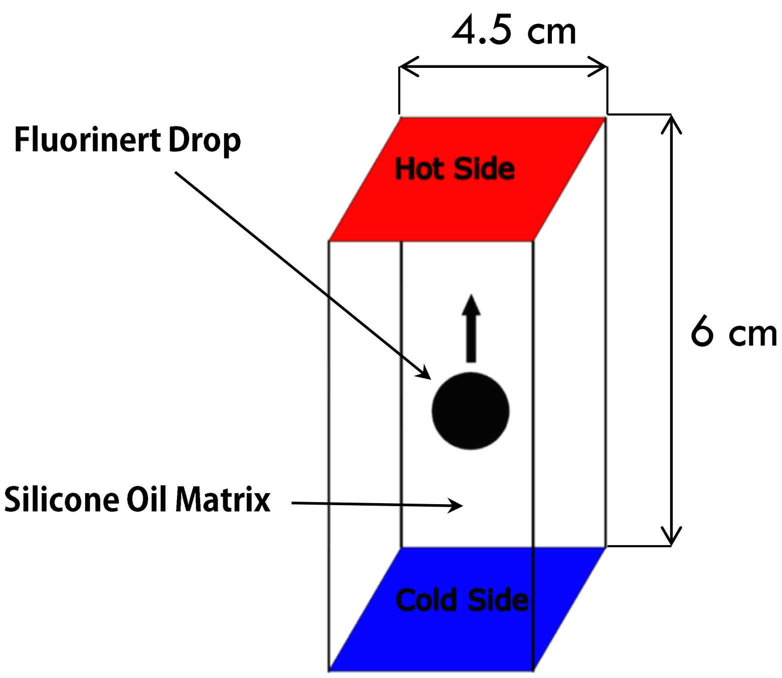


Case of Study

Comparison with the experiment of Hadland *et al.* (1999)

- We tested the code by simulating the migration of a drop in a reduced gravity environment
- We compared our results with the experiments of Hadland *et al.* [2] performed in a space shuttle

Schematic of the experiment



Simulation set-up

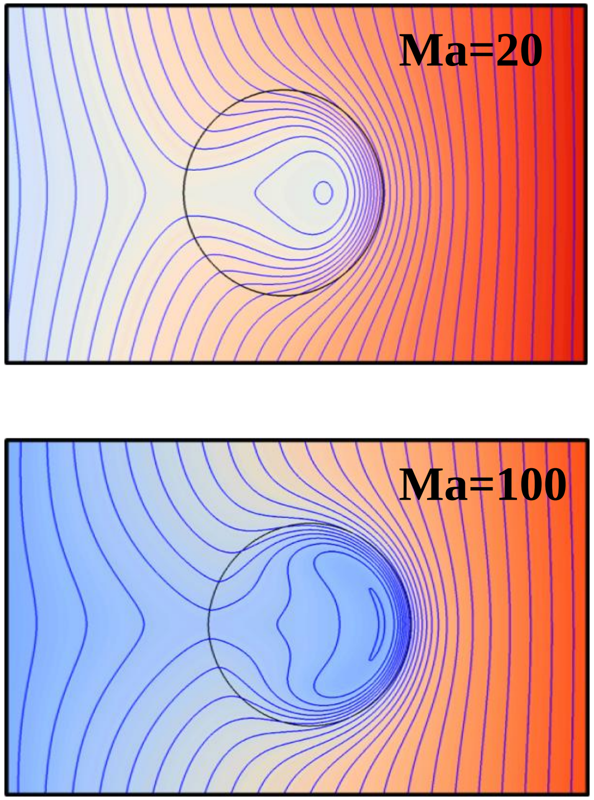
- Geometry and assumptions as the previous case
- Ma = 2 - 500
- Constant radius R = 5.35 mm
- σ_T varied to change Ma
- Constant Ca=0.3
- The "limiting" velocity has been evaluated at steady state or after ¾ of the geometry [2]

[2] P. H Hadland, R. Balasubramanian, G. Wozniac, R. S. Subramanian, *"Thermocapillary Migration of bubbles and drops at moderate to large Reynolds Numbers in Reduced Gravity"*, Exp. Fluids, 26, 240 (1999)

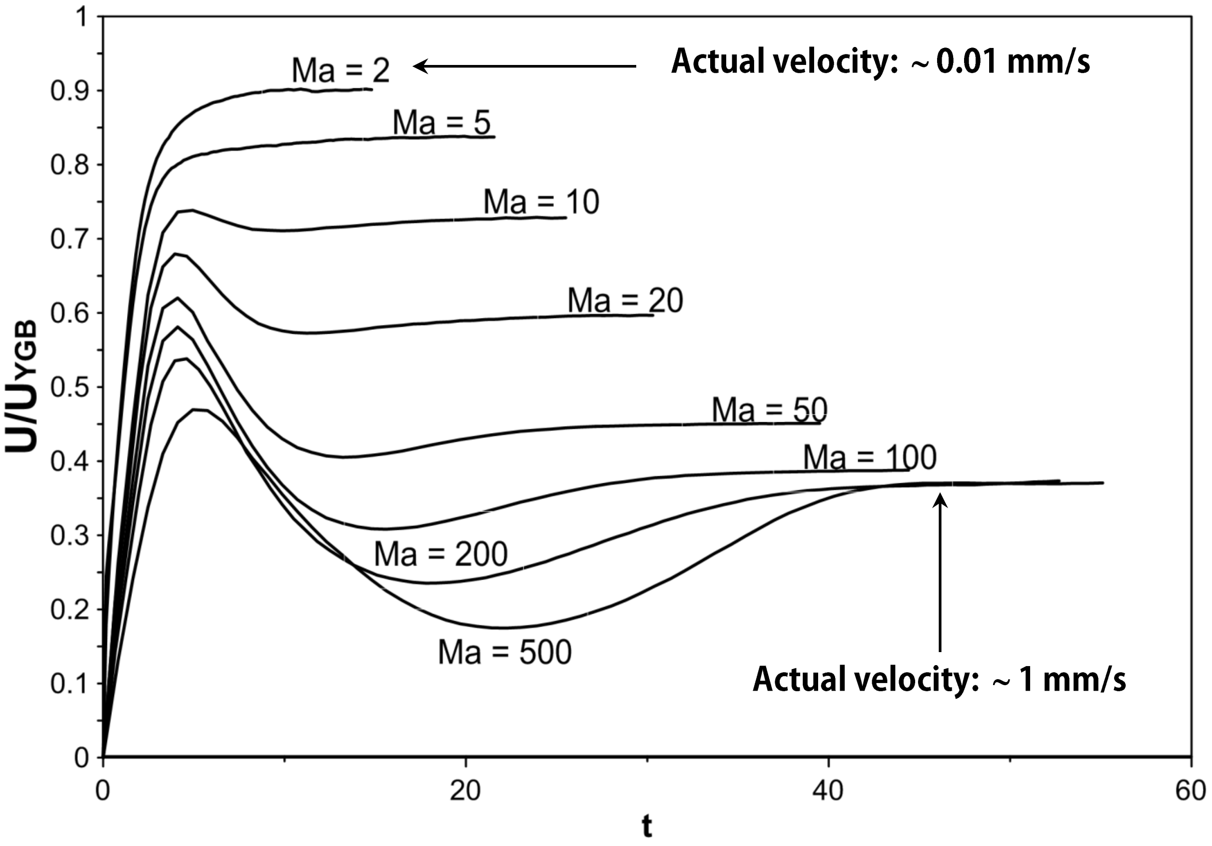
Case of Study

Comparison with the experiment of Hadland

Isotherms for different Marangoni numbers



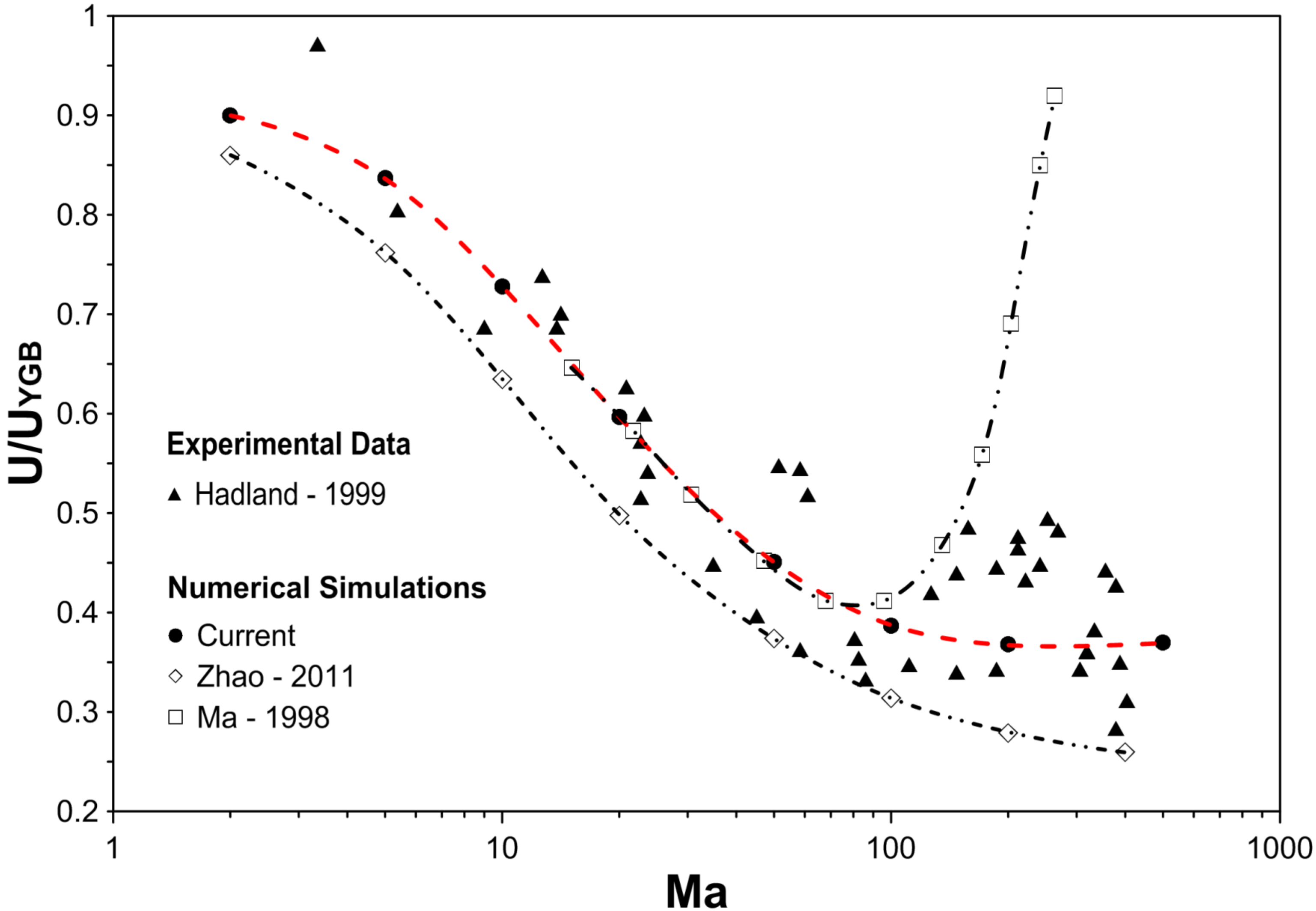
Normalized droplet velocity for different regimes



Case of Study

Comparison with the experiment of Hadland

Effect of Marangoni number on the asymptotic droplet velocity: comparison between experiments and simulations



Conclusions and Future Work

- The Solver has been implemented and tested for a wide range of Marangoni numbers

- The results in the case of vanishing Marangoni and Reynolds number successfully matched the analytic solution of Young with an error $< 1\%$

- Our predictions are in excellent agreement with the experimental measurements of Hadland

- Next, we aim to investigate the effect of elasticity and shear dependent viscosity on thermocapillary convection

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Thanks very much for your Attention...

...Any Question?

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Stratified Flow