Effect of Marangoni Forces on Interfacial Heat and Mass Transfer

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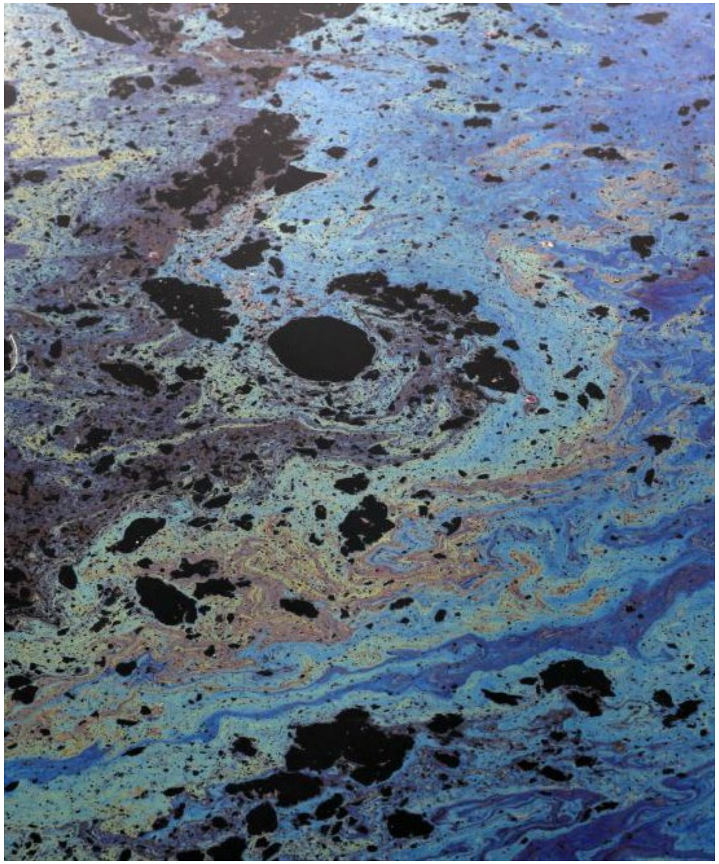

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Background

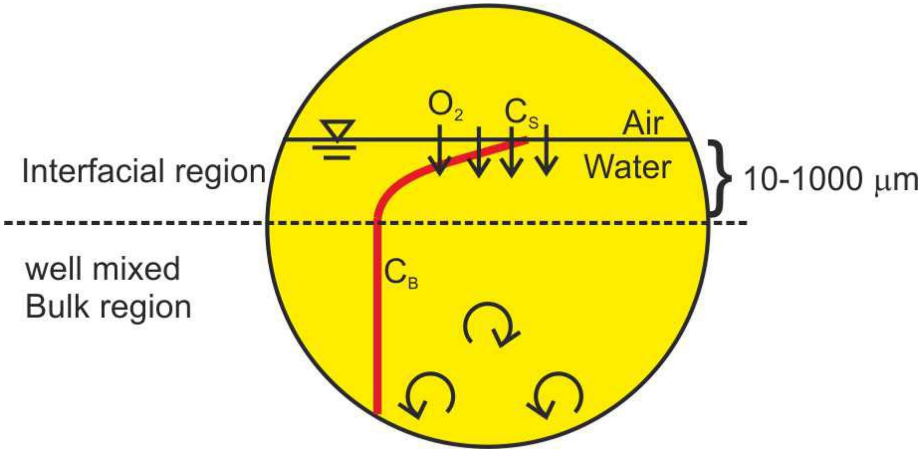
Interfacial Mass Transfer

Gas transfer ; molecular diffusion ⟺ turbulence in the water phase

Advective-diffusive : $\langle j_z \rangle = -\left[D \frac{\partial \langle c \rangle}{\partial z} - \langle w' c' \rangle \right]$

j: gas flux
D: molecular diffusion
c: concentration
w: vertical velocity

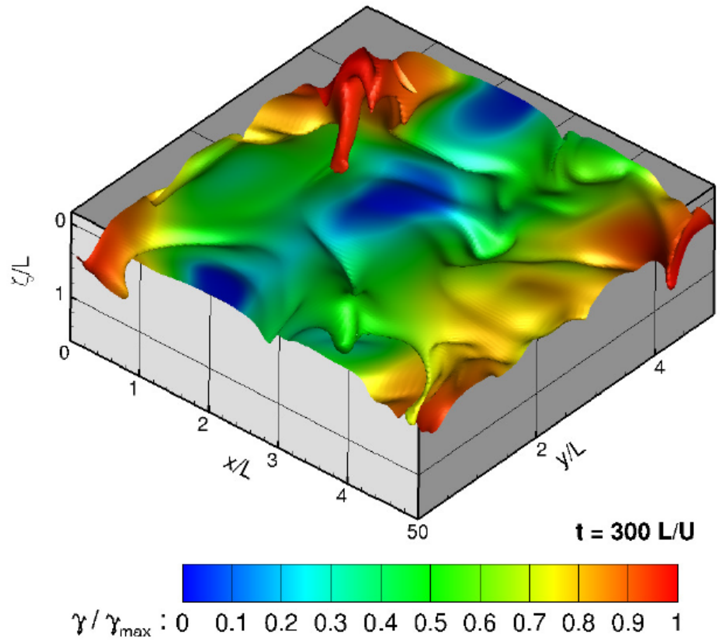
Gas transfer of low-diffusive gases (O_2, CO_2) is marked by a very thin concentration boundary layer at the water side



Surface contamination

Focus is on interfacial pollution by (insoluble) surfactants

- Surfactants reduce the surface stress of water
- Upwelling and downwelling motions typically lead to non-uniform surfactant concentrations and non-uniform surface stresses
- Resulting in Marangoni forces that counteract surface divergence.



Isosurface at 50% C_{sat} coloured by the surface divergence

Aim

To determine a parametrization of the effect of surface contamination on the transfer function K_L

For a clean (no pollution) interface K_L scales as

$$K_L \propto Sc^{-1/2}$$

where Sc is the Schmidt number.

For a very dirty interface

$$K_L \propto Sc^{-2/3}$$

What happens at (very) moderate levels of pollution?

$$K_L \propto Sc^{-q}$$

The power q will likely depend on $\frac{Ma}{Ca}$

Modelling Pollution Effects

Surface tension, σ, depends on the pollutant concentration, γ.

$$\sigma = \sigma(\gamma)$$

After normalization define the Marangoni number by

$$Ma = -\frac{d\sigma}{d\gamma}$$

which we assume to be constant. From the model presented in Shen *et al.,* (2004) JFM, Vol. 506, after some algebra, we obtain:

$$\left.\frac{\partial u}{\partial z}\right|_{interface} = -\frac{Ma}{Ca}\frac{\partial \gamma}{\partial x}$$

$$\left.\frac{\partial v}{\partial z}\right|_{interface} = -\frac{Ma}{Ca}\frac{\partial \gamma}{\partial y}$$

u: *x*-velocity
v: *y*-velocity
Re: Reynolds number
Ca: Capillary number
γ: surfactant concentr.

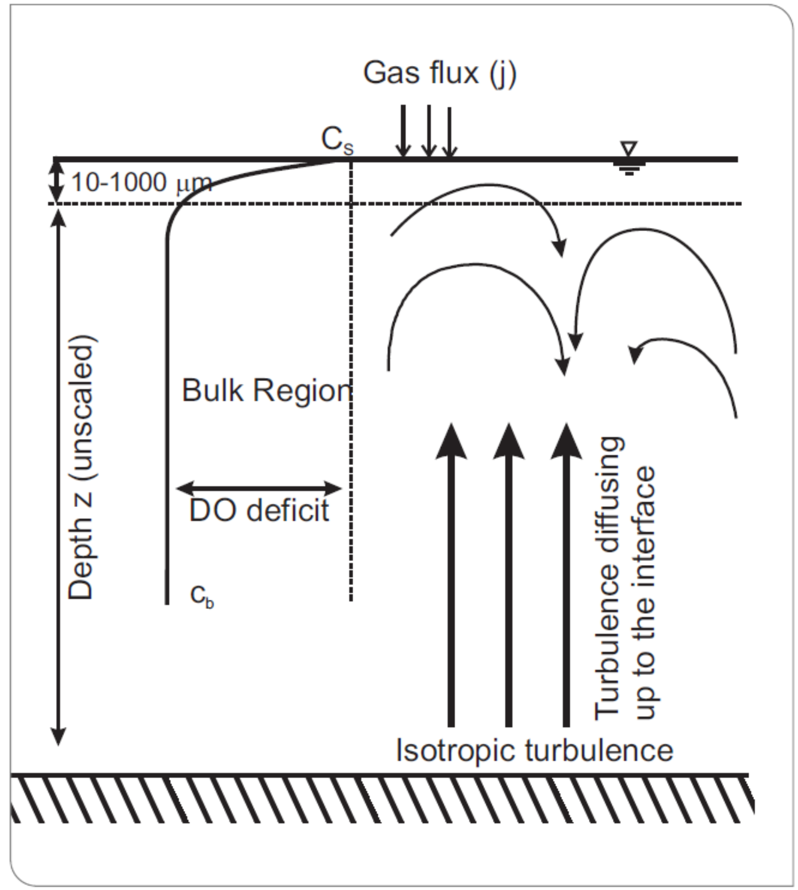
Problem Investigated

Physical Problem

Grid-stirred-driven gas transfer

Convenient analogy to bottom shear induced turbulence

www.xs4all/rdemming/travel/Indonesia



Computational Setup

Boundary conditions

Top: $\left.\frac{\partial u_i}{\partial z}\right|_{top} = -\frac{Ma}{Ca}\frac{\partial \gamma}{\partial x_i}$, ***i* = 1, 2**

x_1, u_1 : *x*, *x*-velocity
x_2, u_2 : *y*, *y*-velocity

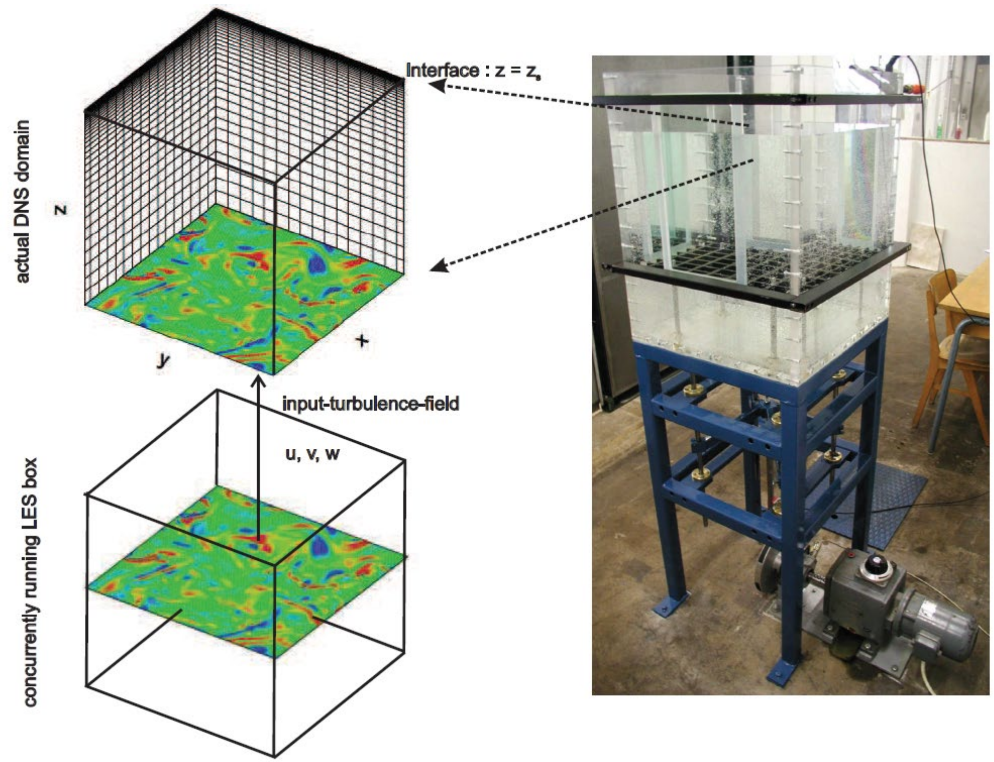
various levels of contaminations

Sides: periodic

Bottom: flow-field copied
from LES of isotropic turbulence

$c_{top} = 1$
(saturated at all times)

$c_{bottom} \rightarrow \frac{\partial c}{\partial z} = 0$



Simulations performed

Case	U_∞	L_∞	R_T	Ma/Ca_T
S0	0.113	1.033	141	0
S1	0.112	0.958	128	1
S2	0.117	0.994	139	5
S3	0.109	0.984	131	11
S4	0.110	0.927	125	54
S5	0.111	1.021	138	269
SN	0.107	0.898	117	no-slip

Ma is Marangoni number; $Ca_T = \mu U_\infty / \sigma$ is turb. capillary number

All simulations: 128 x 128 x 212 mesh for 5L x 5L x 3L box
Mesh is refined in z-direction towards surface
Schmidt numbers Sc = 2….32; Surfactant: Sc = 2
Turbulent flow with Tu = 40% introduced at bottom

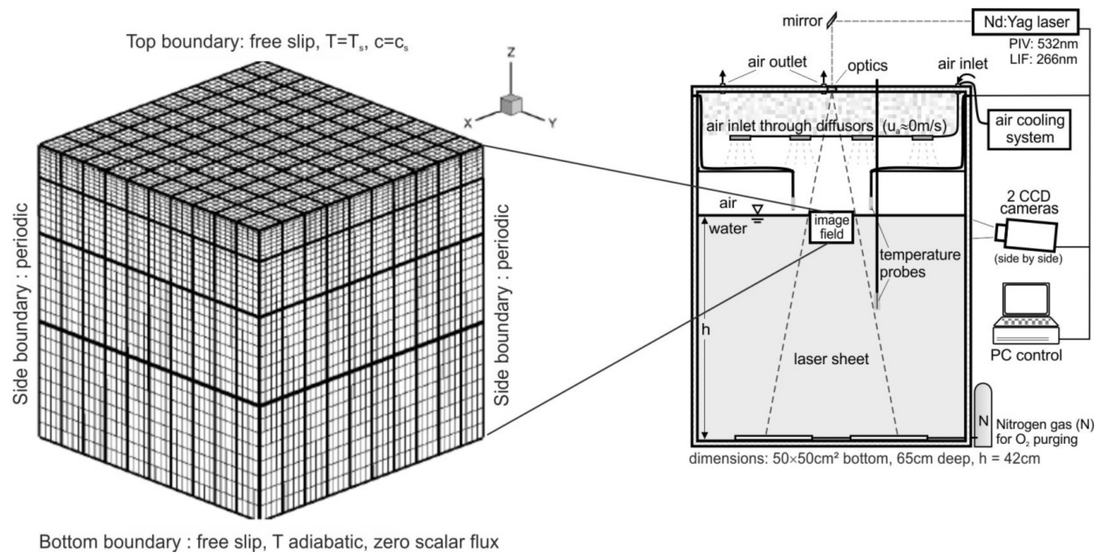
Numerical Method

Flow fields in main DNS and LES isobox are solved using fourth-order discretisations of convection and diffusion.

A dual mesh strategy is used where up to five scalars can be solved simultaneously on a refined mesh

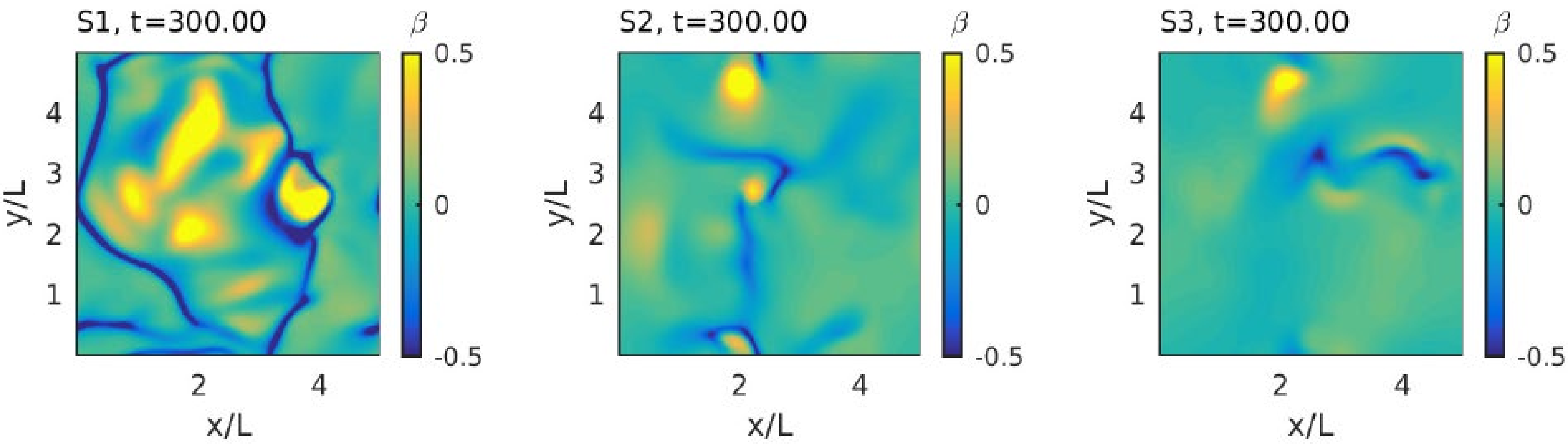
A fifth-order-accurate WENO scheme is used for scalar convection, combined with a fourth order central discretisation for scalar diffusion (same in 2D for surfactant).

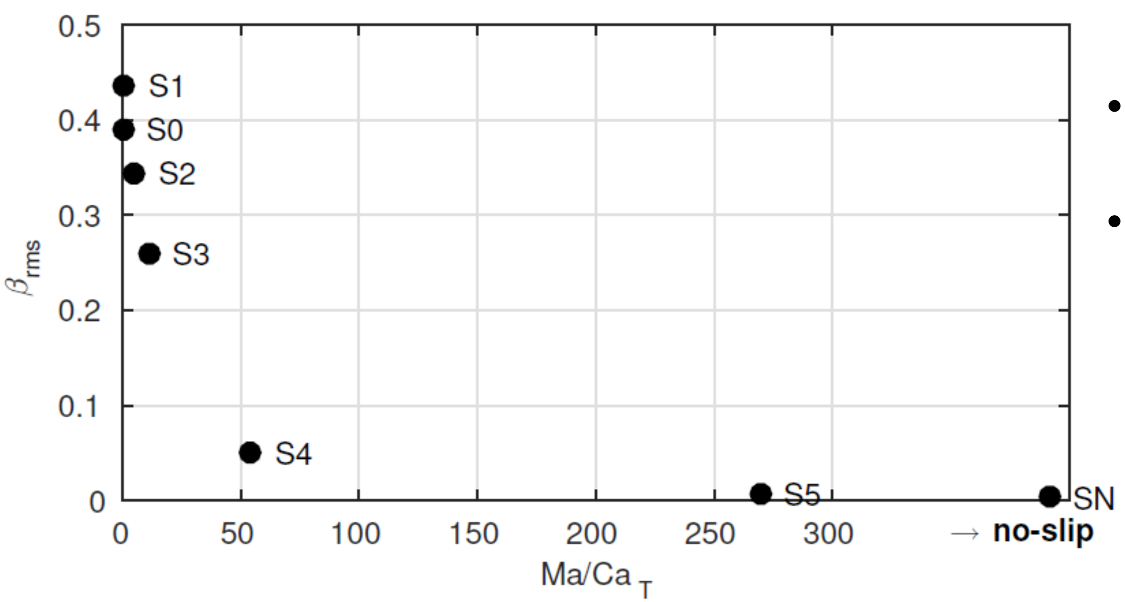
Standard Message passing interface (MPI) is applied for communication between blocks.



Effect on near-surface hydrodynamics

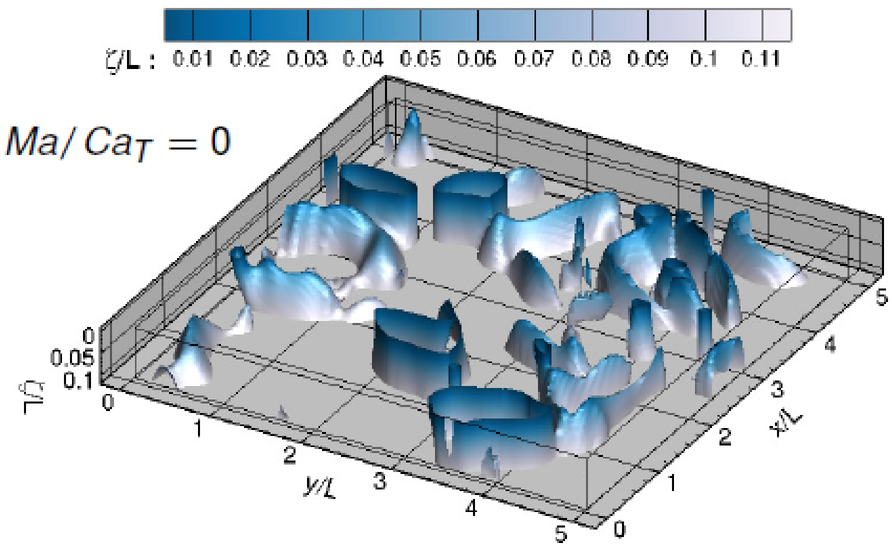
Surface Divergence (β)

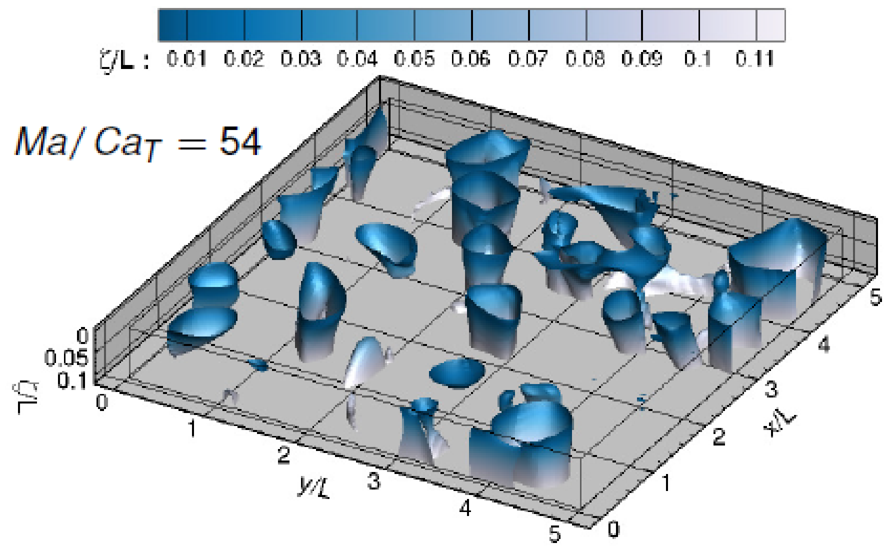


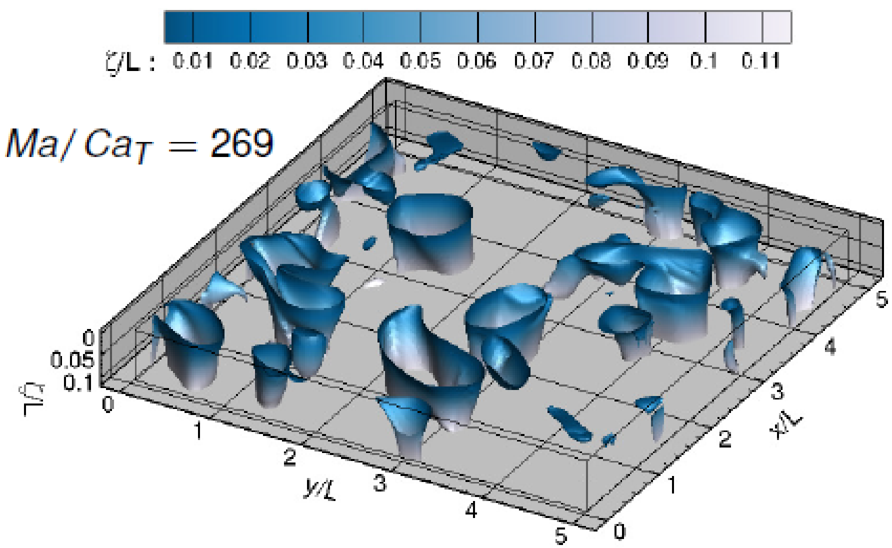


- β reduces sharply
- Surface divergence model $\left(K_L \propto \sqrt{D\beta_{rms}}\right)$ only works for a small range of Ma/Ca_T

Instantaneous shear



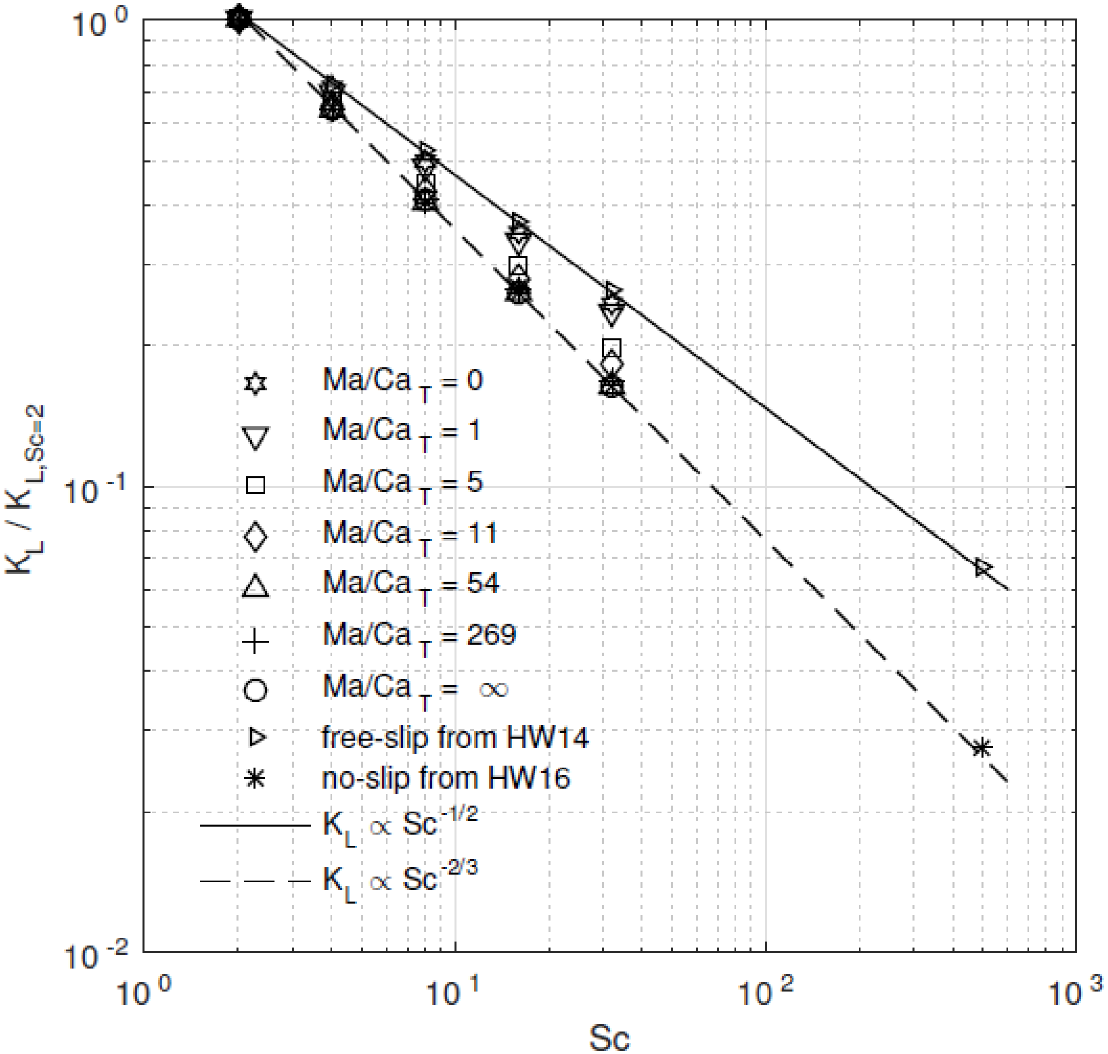




- orientation and cross-sectional area become different
- explain the apparent increase in the integral length scale
- strong correlation between low concentration regions and strong positive surface divergence is lost

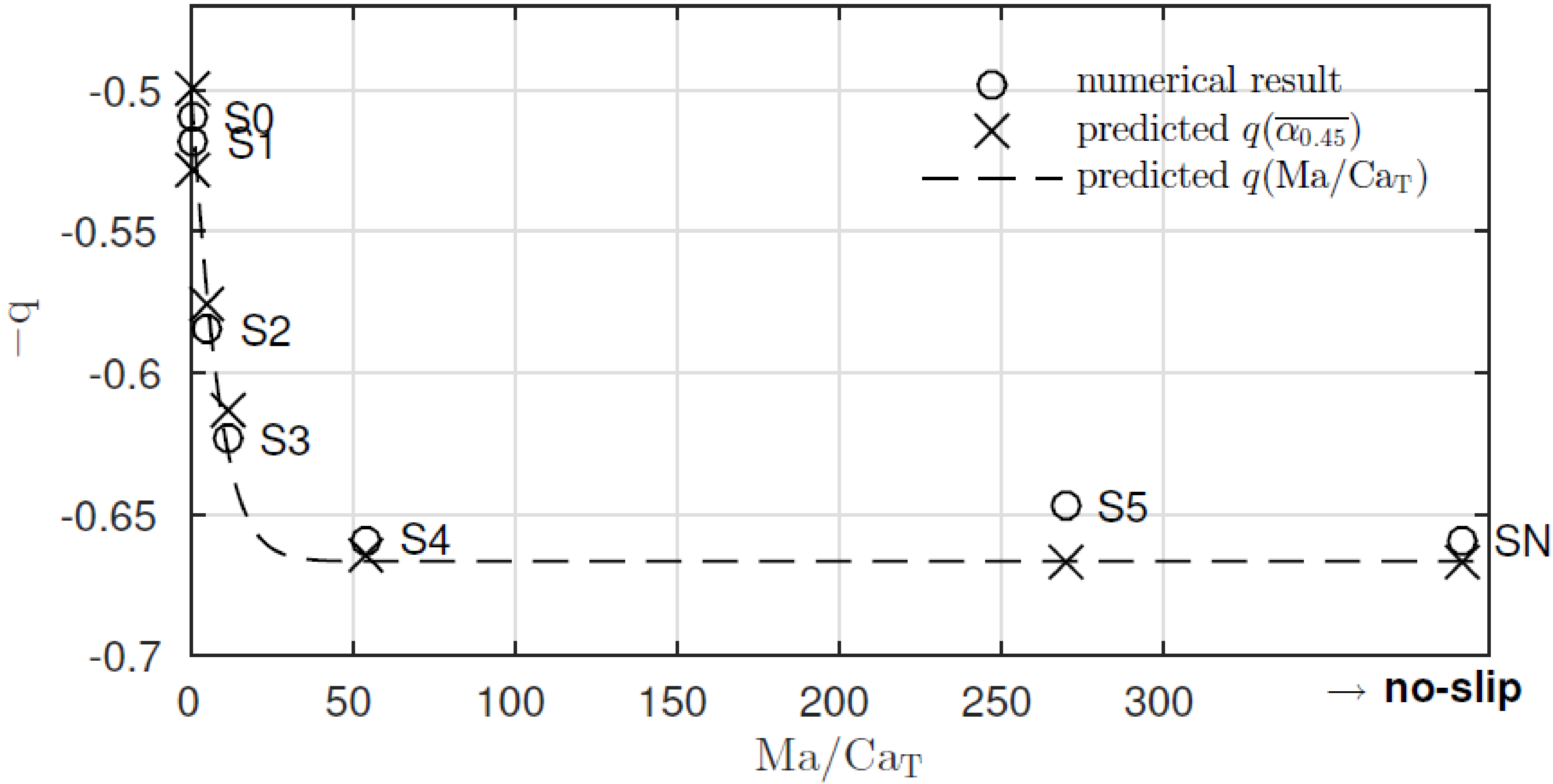
Consequences on interfacial mass transfer

K_L reduction



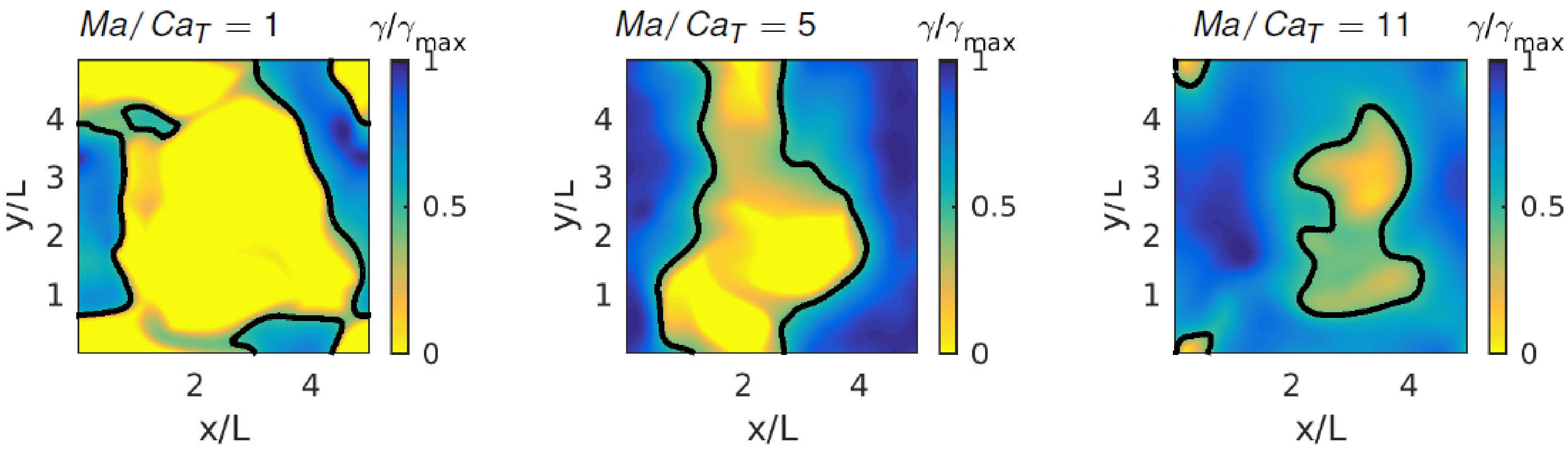
- Reduction of K_L
- For each Ma/Ca_T : $K_L \propto Sc^{-q}$

Transition of q



Steep transition of q from $\frac{1}{2}$ (clean) to $\frac{2}{3}$ (very dirty)

Clean surface fraction



A good correlation was found between the Schmidt exponent q and clean surface fraction.

Model

First we assume that for any surface condition

$$K_L = cSc^{-q}R_T^{-r}$$

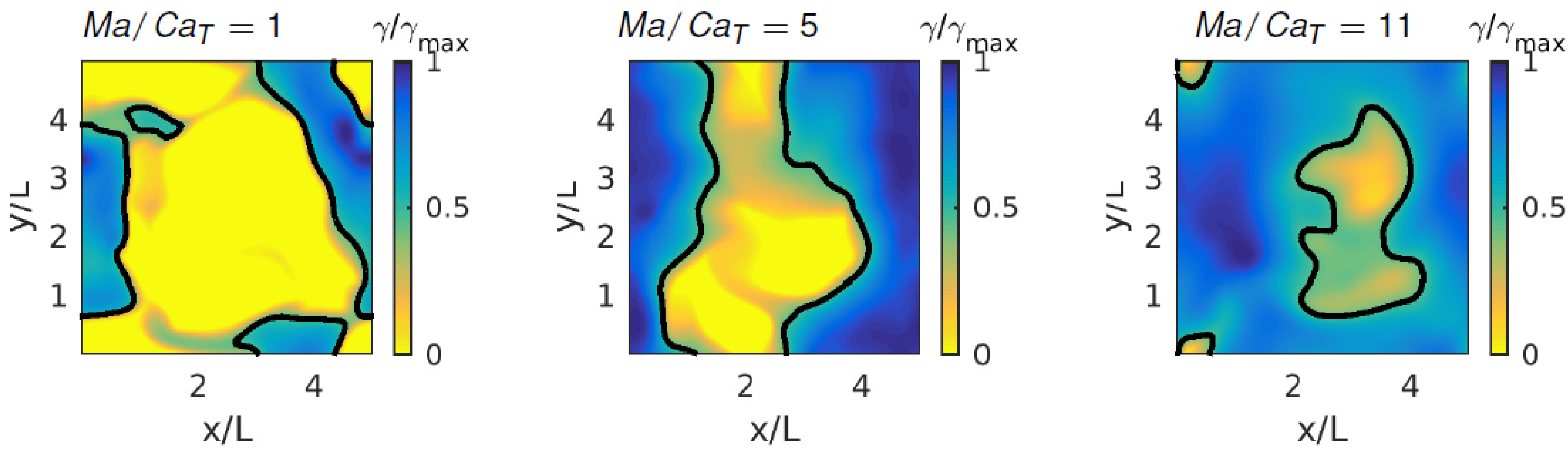
Clean regions behave as a free-slip boundary $(q = 1/2)$, while “dirty” regions behave as a no-slip boundary $(q = 2/3)$

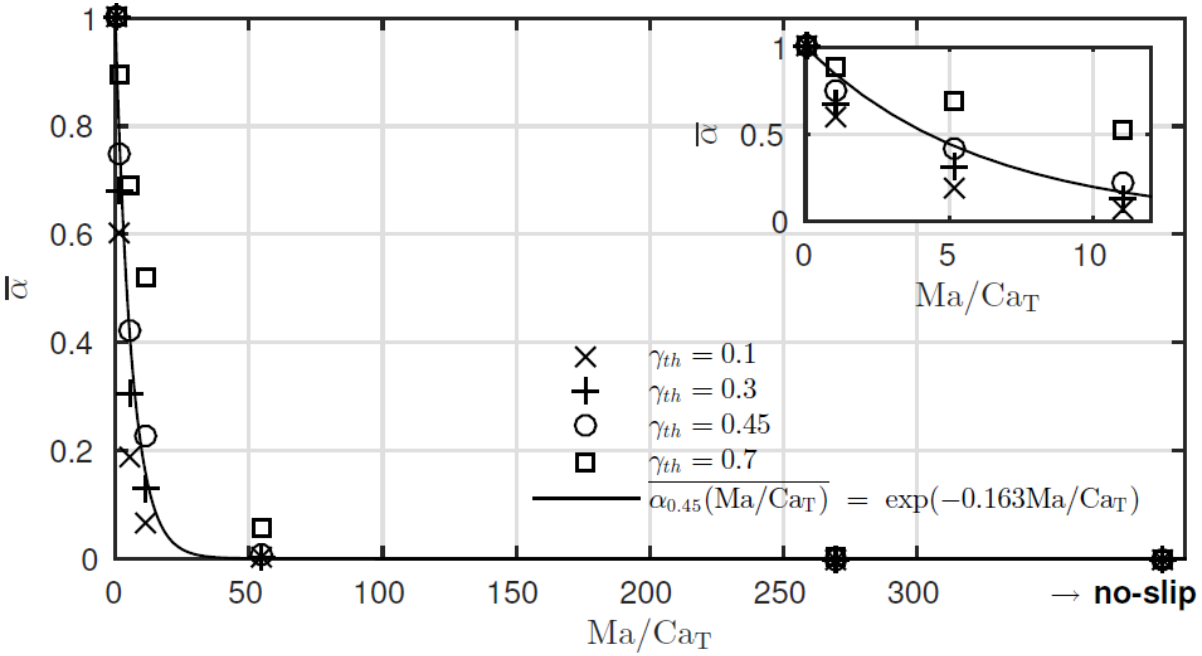
$$cSc^{-q} = \bar{\alpha}c_f Sc^{-1/2} + (1-\bar{\alpha})c_n Sc^{-2/3}$$

Use Taylor series expansions to obtain first order appr. of *c* and *q* that are independent of *Sc*

$$c = \bar{\alpha}c_f + (1-\bar{\alpha})c_n$$
$$q = \frac{2}{3} - \frac{\bar{\alpha}c_f}{6c}$$

Definition of clean



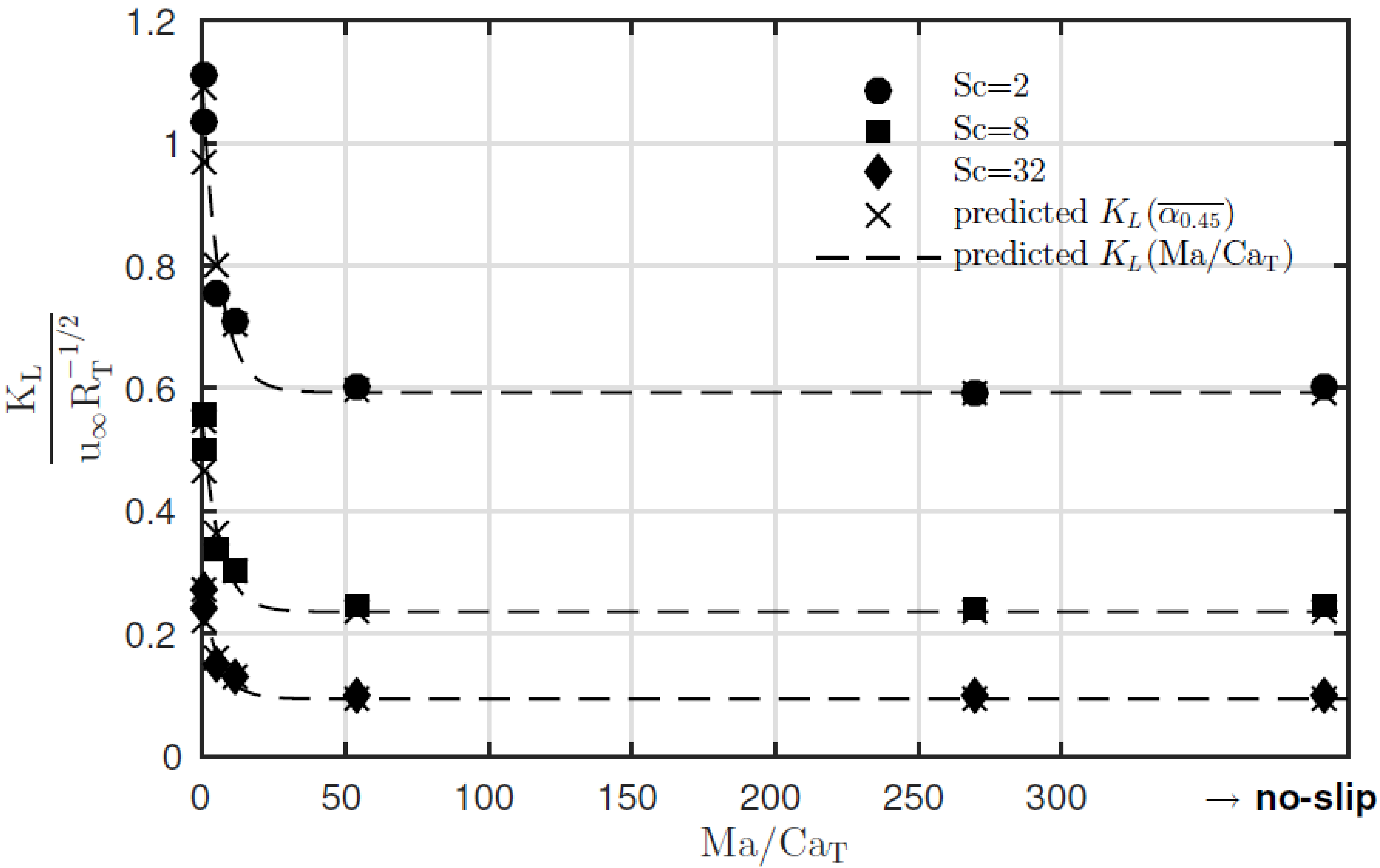


γ : surfactant concentr.

α : clean surface fraction

$\gamma_{th} = \gamma/\gamma_{max}$ is threshold

Evaluation of model



Conclusions

- It was confirmed that the even small levels of surfactant contamination have a large effect on heat and gas transfer
- With increasing Ma/Ca_T, the surface divergence, β, becomes progressively damped
- Resulting in a quick transition to a $K_L \propto Sc^{-2/3}$ scaling which is typical for a no-slip surface
- The transition can be linked to the mean clean surface fraction which is a relatively easily observable parameter.

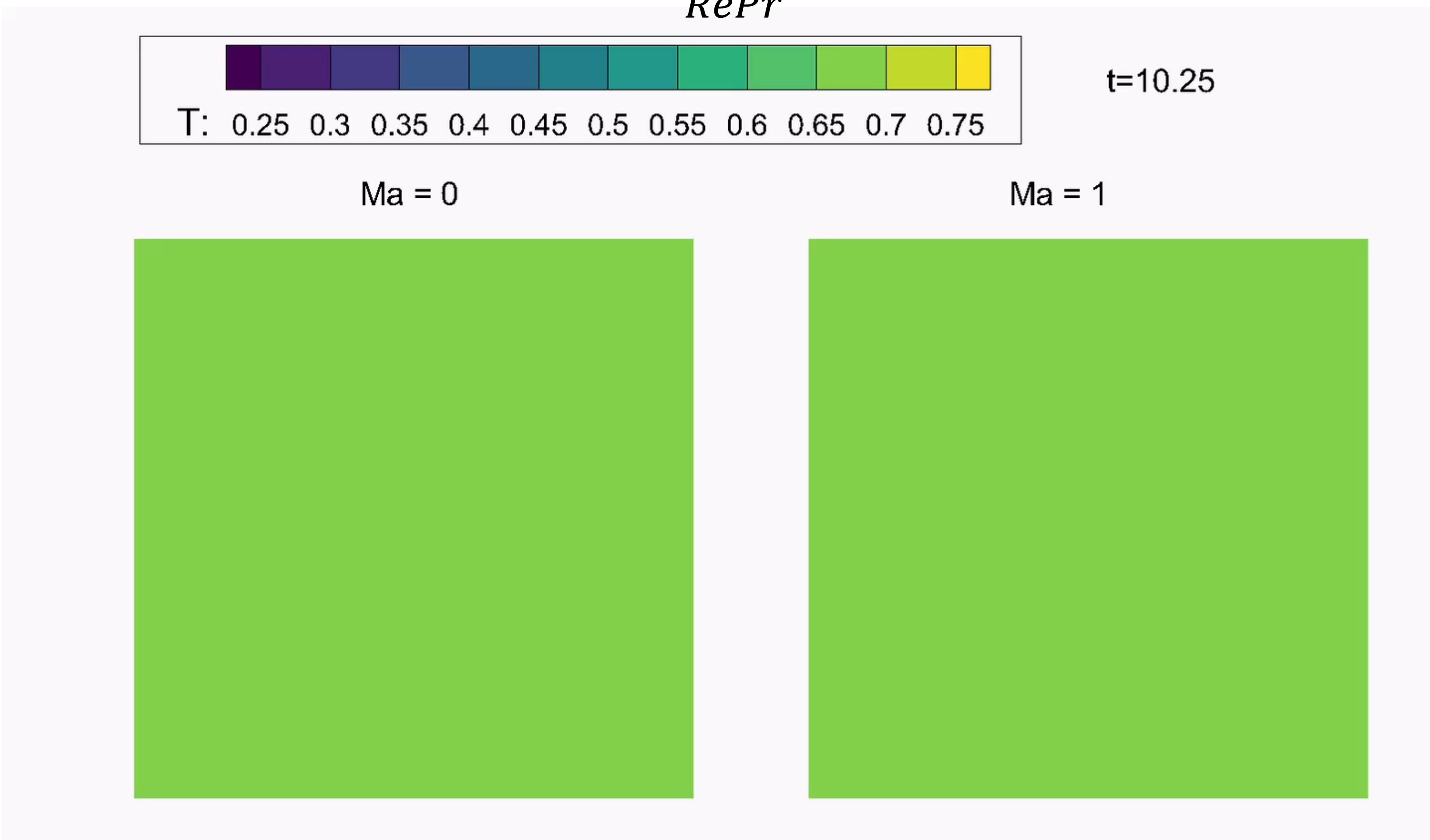
Future work

Marangoni Forces promoting Buoyant Instability

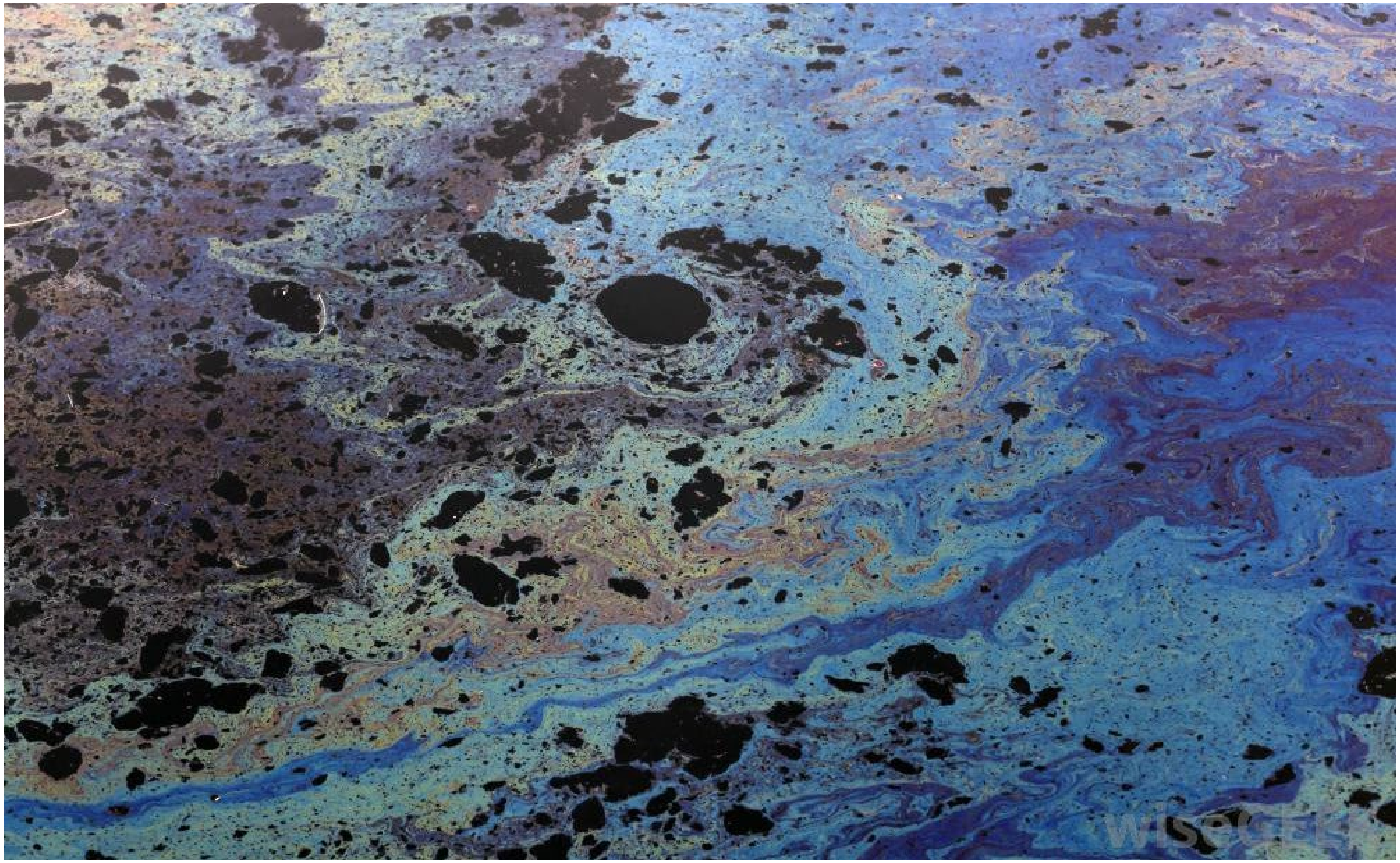
- Surface cooling due to evaporation can be modelled by applying a constant heat flux at the surface.
- A buoyant instability results from this unstable layering of the water as cold water is heavier than warm water.
- The developing buoyant instability results in horizontal gradients in the surface temperature
- As surface tension reduces with increasing temperature, Marangoni forces are generated that act to promote the buoyant instability

Marangoni Forces promoting Buoyant Instability

Top plane view, heat flux = $-\frac{2.33}{RePr}, Re = 100, Pr = 7$



The end



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