Effect of surface contamination on isotropic-turbulence-driven interfacial gas transfer

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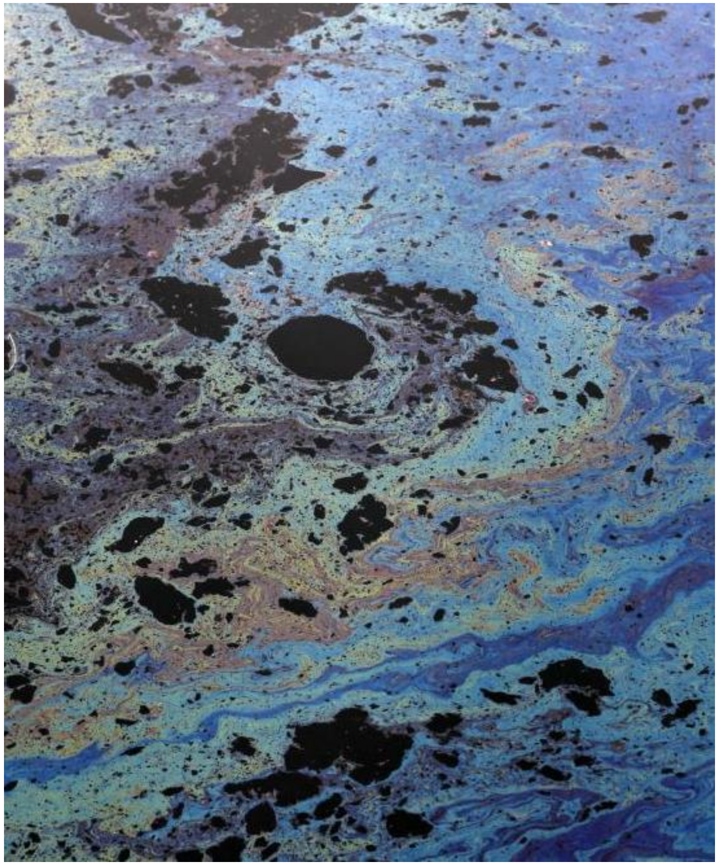

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Background

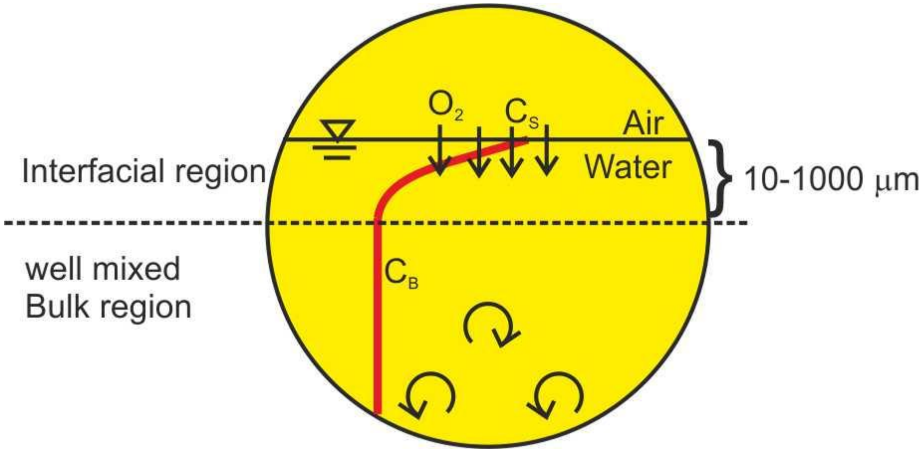
Interfacial Mass Transfer

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



Pollution

Focus is on interfacial pollution by surfactants

Surfactants reduce the surface stress of water

Surface divergence typically leads to non-uniform surfactant concentrations

Which is counteracted by the Marangoni effect trying to force surface divergence to zero.

Modelling Pollution Effects

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

$$\boldsymbol{\sigma = \sigma(\gamma)}$$

After normalization define the Marangoni number by

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

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

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

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

u: *x*-velocity
v: *y*-velocity
Re: Reynolds number
We: Weber number
γ: surfactant concentr.

Aim

To determine a parametrization of the effect of pollution on the interfacial gas transfer velocity 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 $\frac{Ma\,Re}{We}$

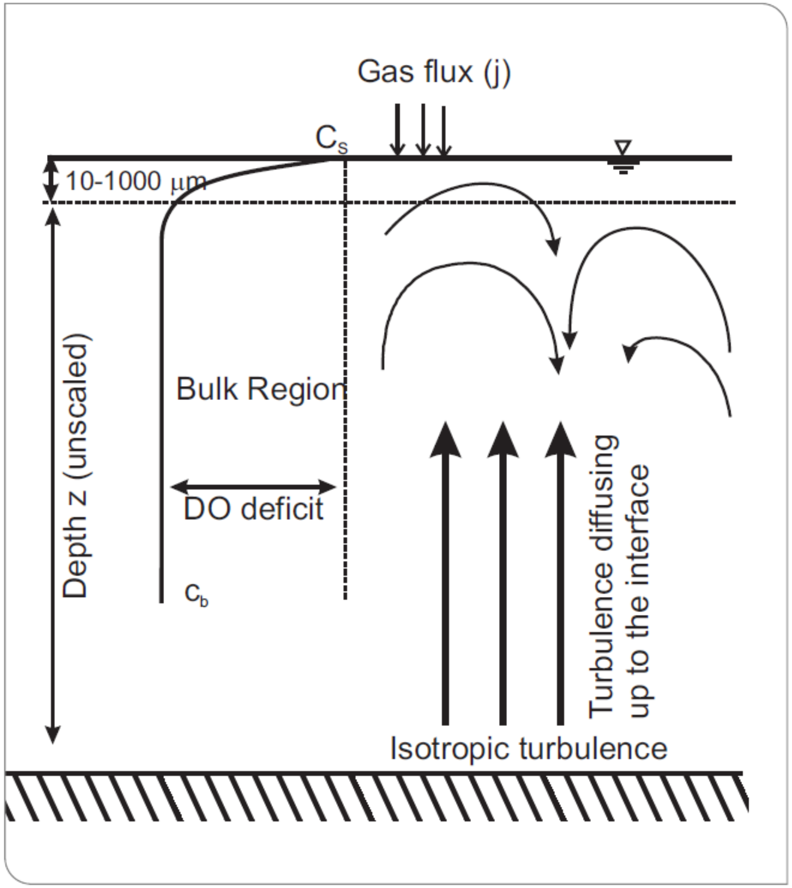
Problem Investigated

Physical Problem

Grid-stirred-driven gas transfer

Convenient analogy to bottom shear induced turbulence

www.xs4all/rdemming/travel/Indonesia



Computational Setup

Boundary conditions

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

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

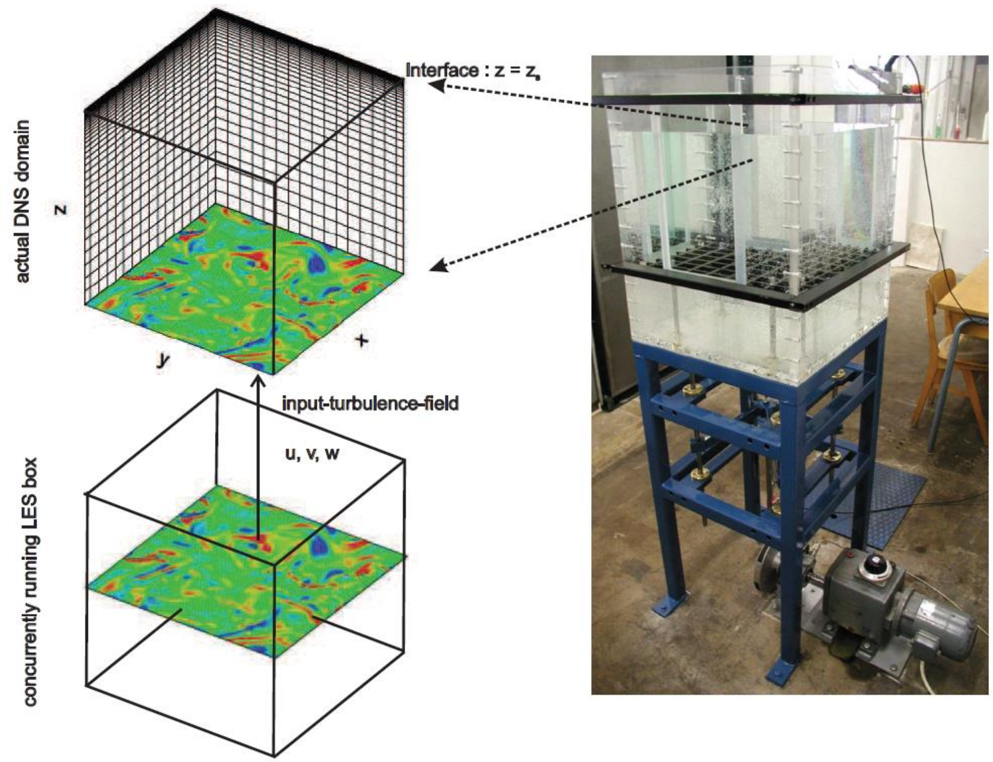
various levels of contamination

Sides: periodic

Bottom: flow-field copied from isobox

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

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



Simulations performed

Simulation	Re Ma/We
S30p0	30
S6p0	6
S1p2	1.2
S0p6	0.6
S0p12	0.12

For all DNS simulations:

128 x 128 x 212 mesh for the box of size 5L x 5L x 3L

Mesh is refined in the z-direction towards the surface

Surfactant Schmidt number = 2

Turbulent flow with Tu = 40% introduced at the bottom

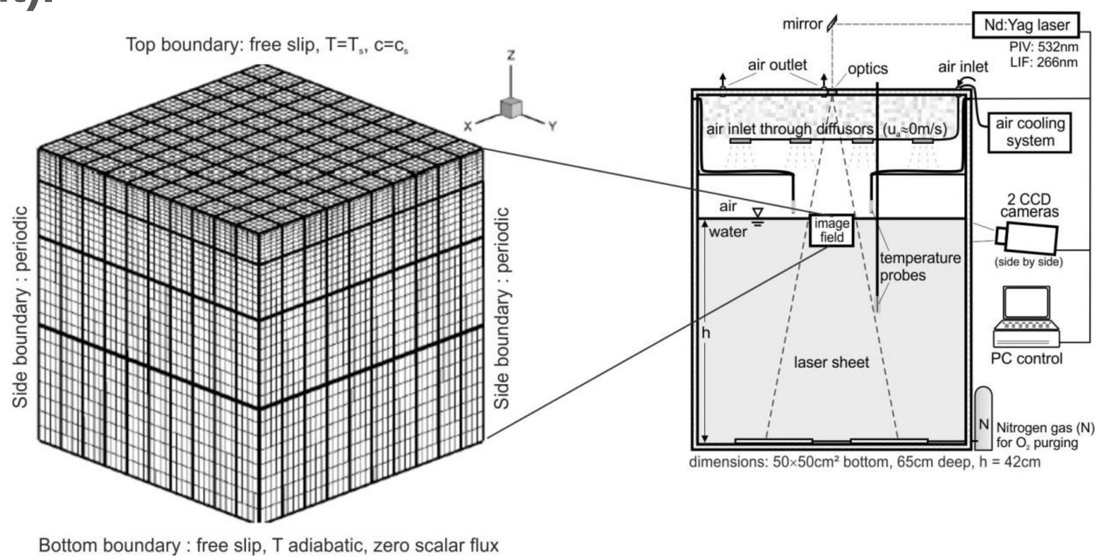
Numerical Method

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).

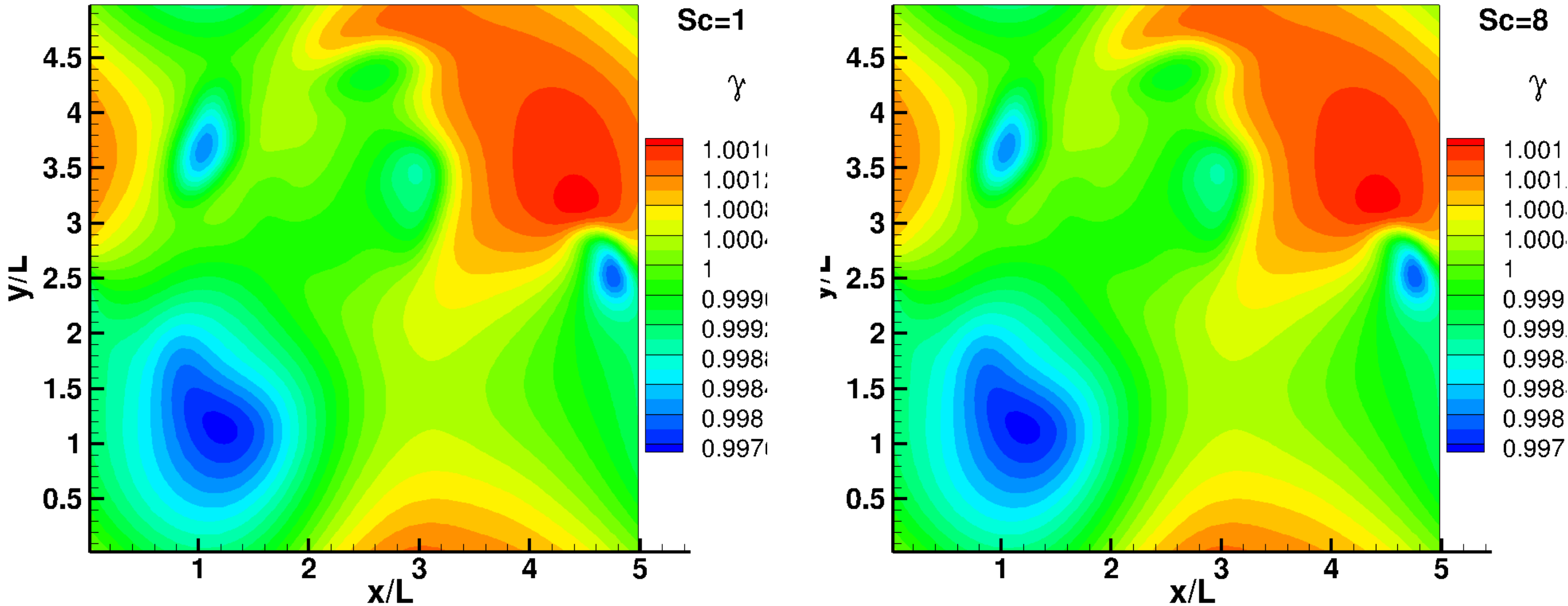
Standard Message passing interface (MPI) is applied for communication between blocks.



Surfactant Diffusivity

How important is Surfactant Diffusivity?

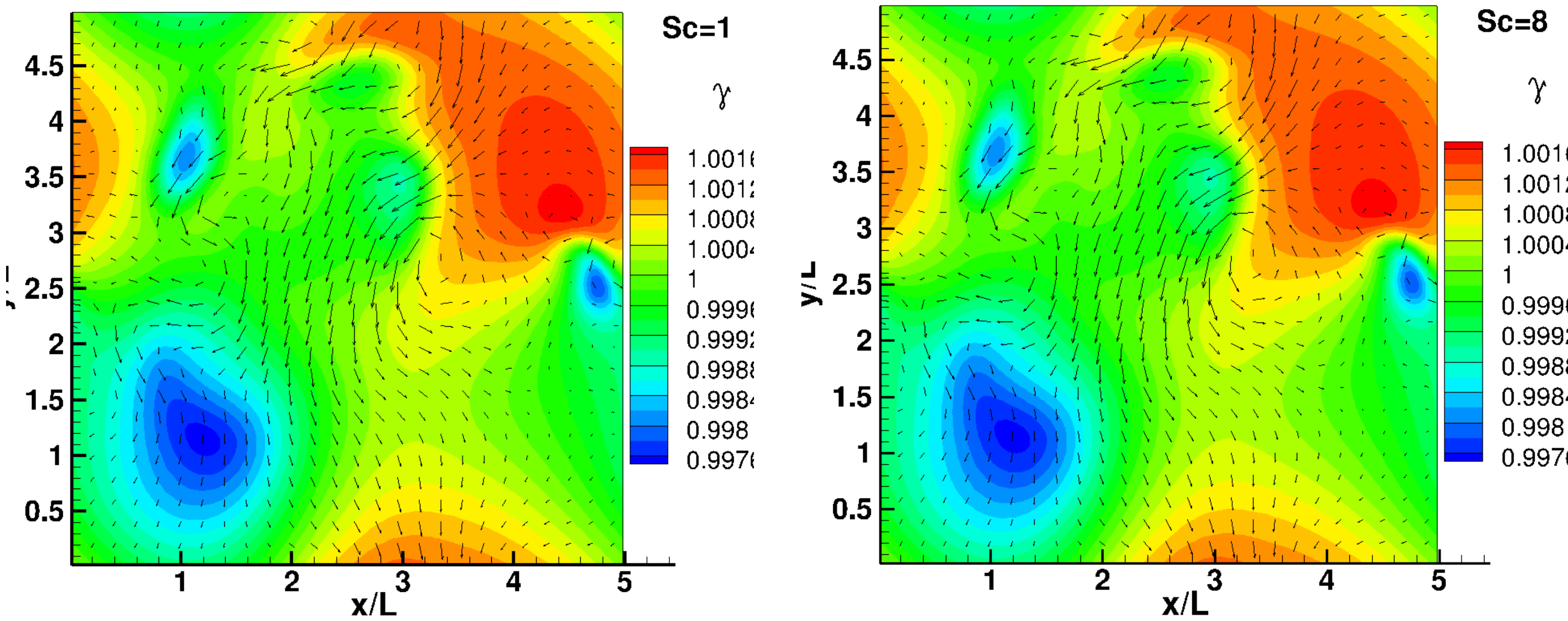
Surfactant distribution for various $Sc = \frac{\nu}{D_{surf}}$



Snapshots of γ at t = 100 L/U

How important is Surfactant Diffusivity?

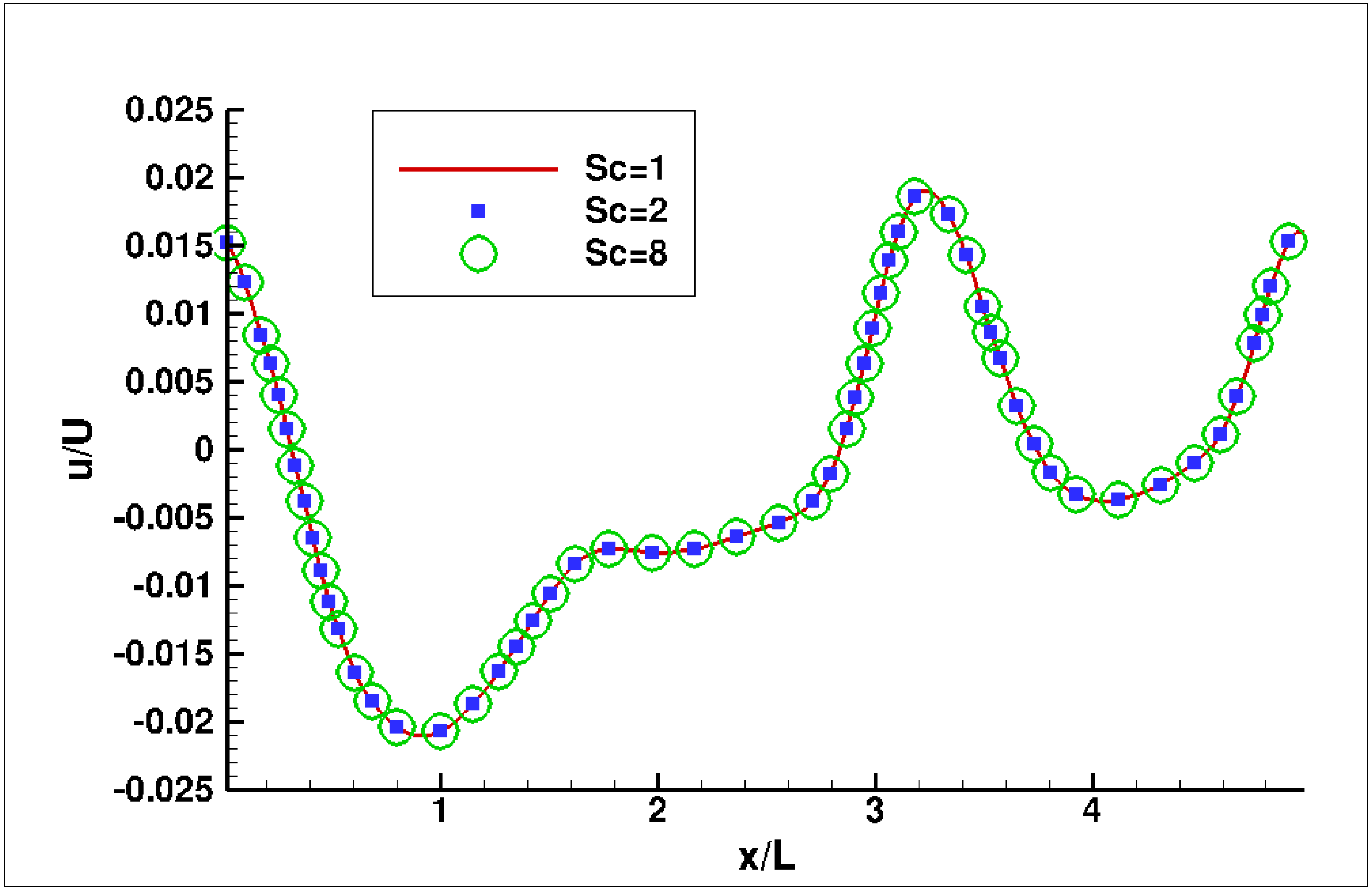
Surfactant distribution for various $Sc = \frac{\nu}{D_{surf}}$



Snapshots of γ at t = 100 L/U

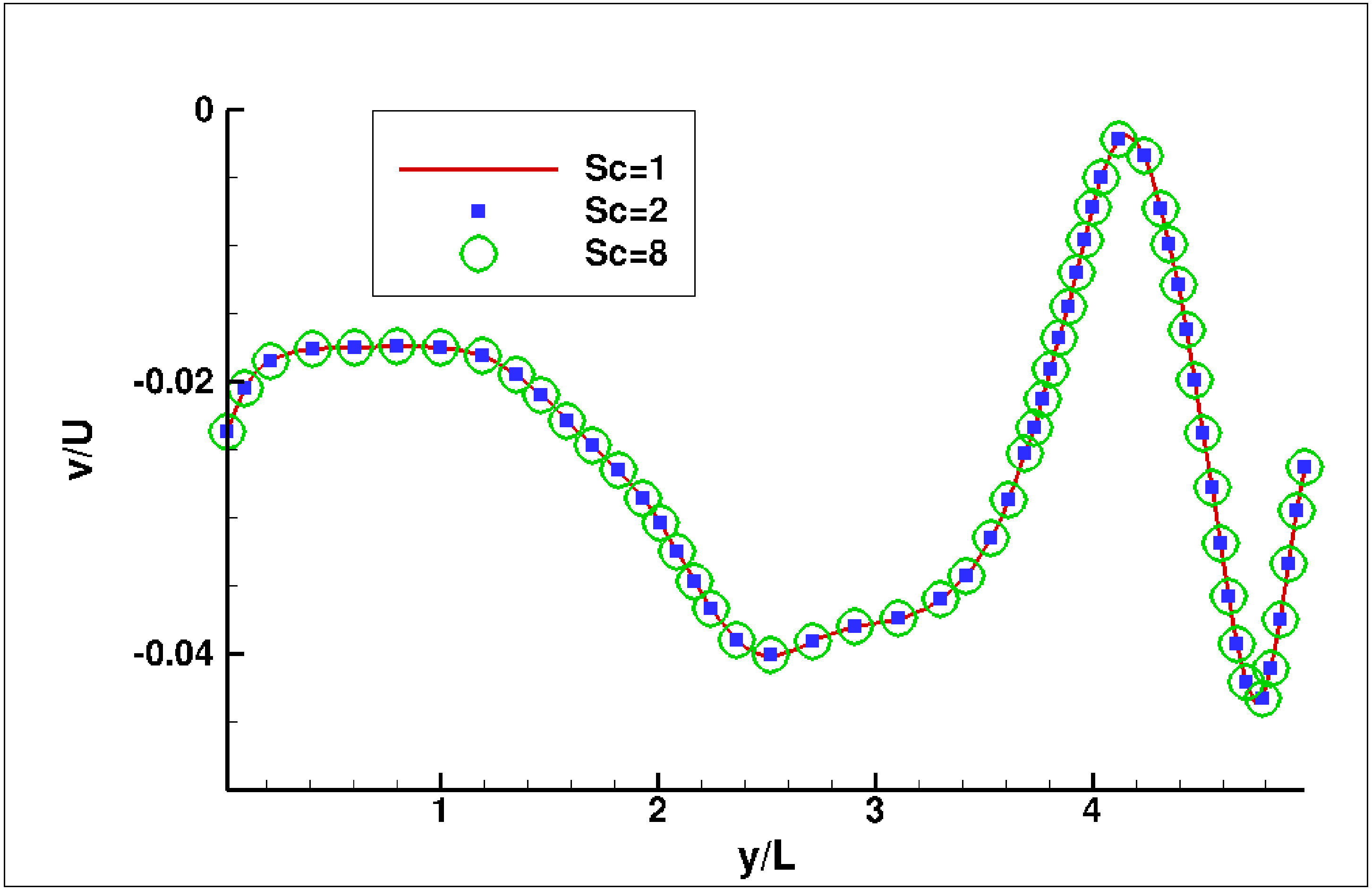
How important is Surfactant Diffusivity?

Effect on interfacial u-velocity at y/L = 2.5



How important is Surfactant Diffusivity?

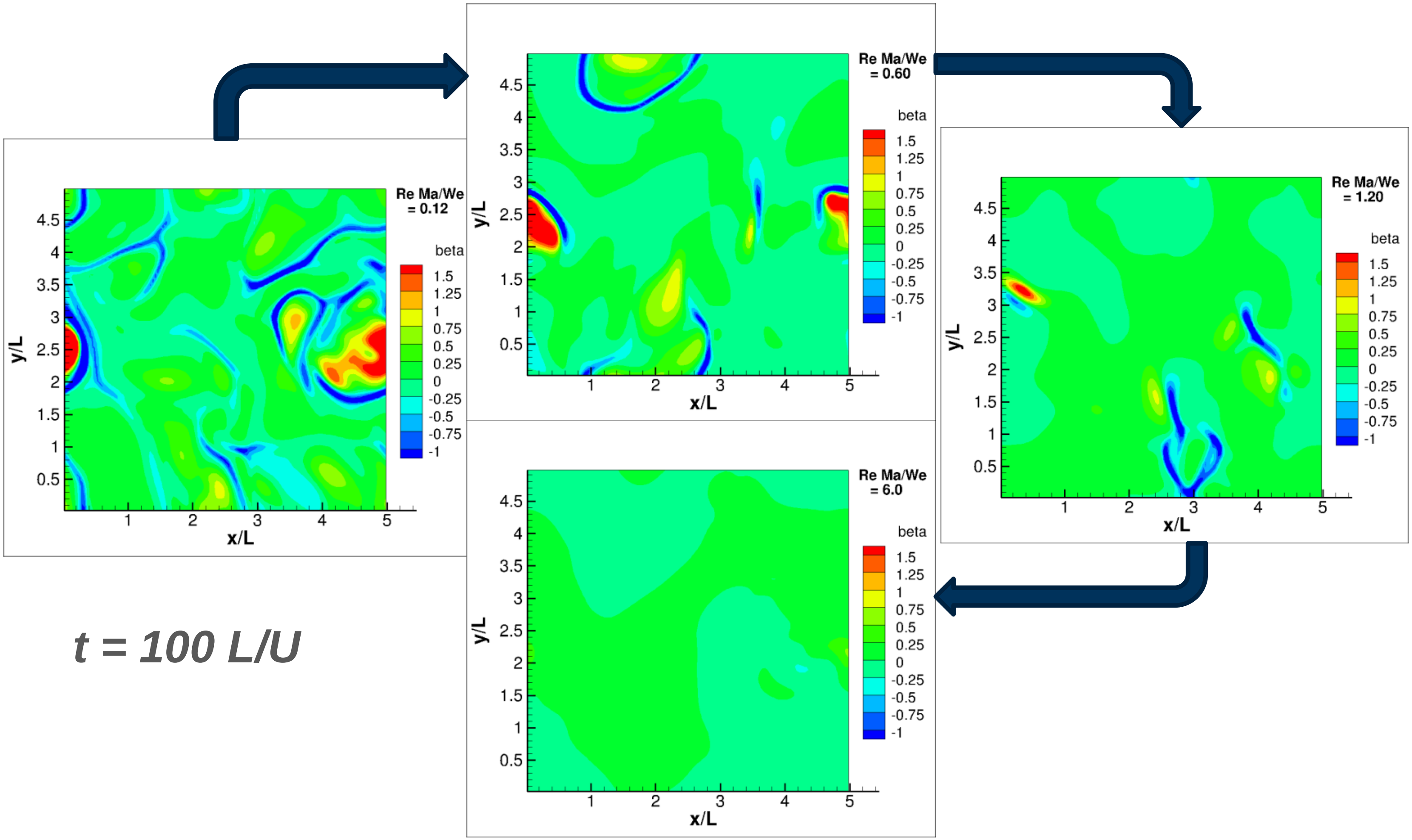
Effect on interfacial v-velocity at x/L = 2.5



Preliminary Results

Surface Divergence β

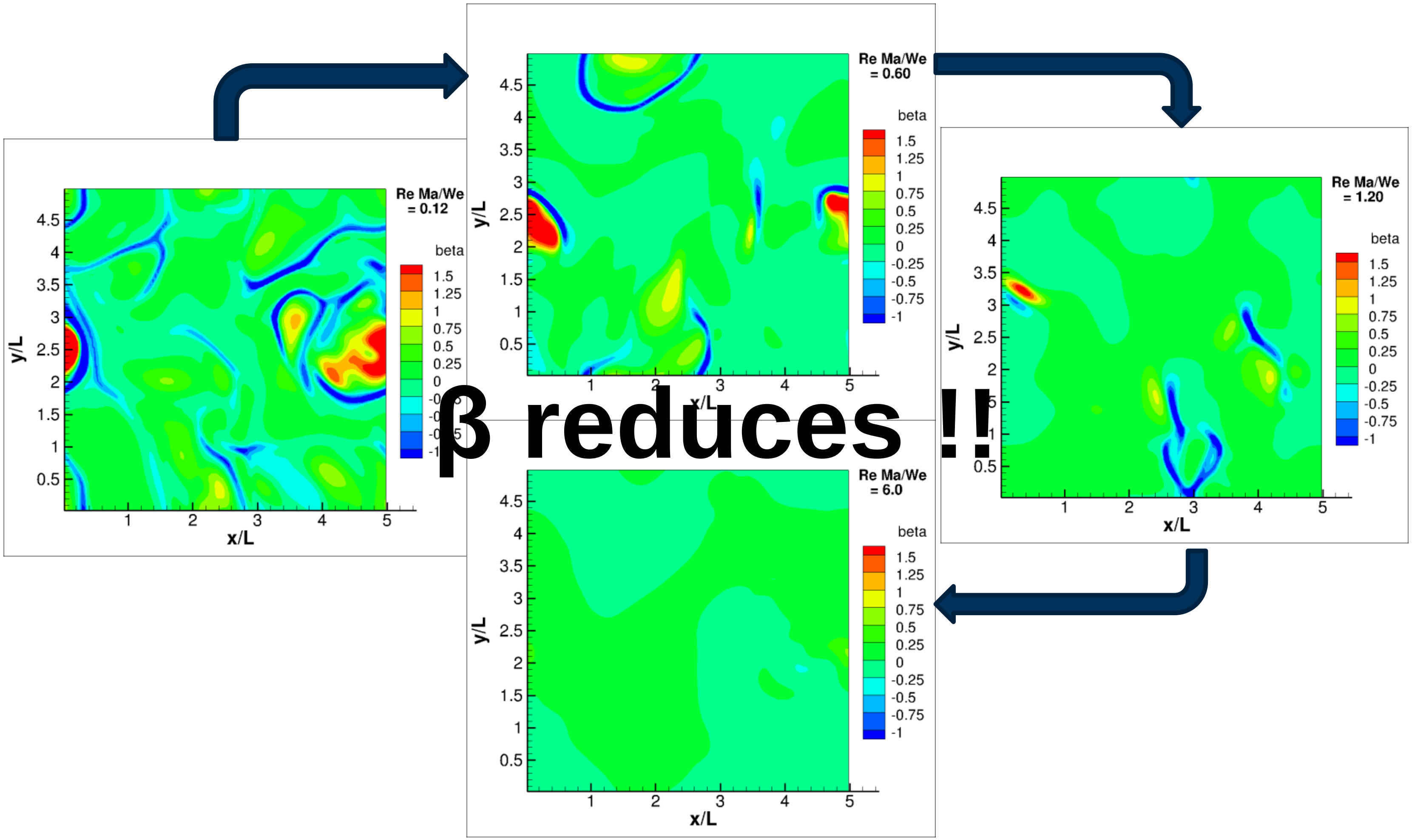
Effect of increasing $Re\,Ma/We$



t = 100 L/U

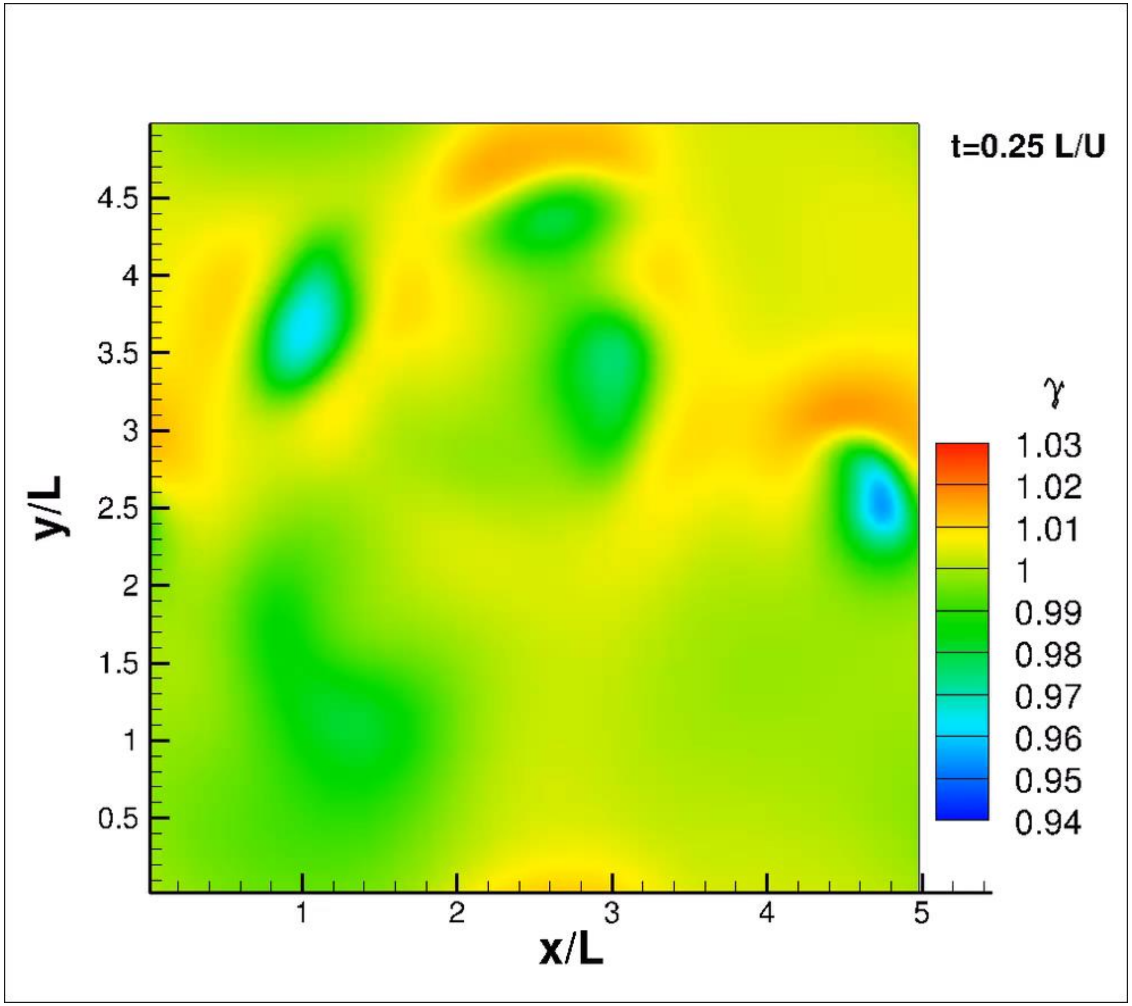
Surface Divergence β

Effect of increasing $Re\,Ma/We$



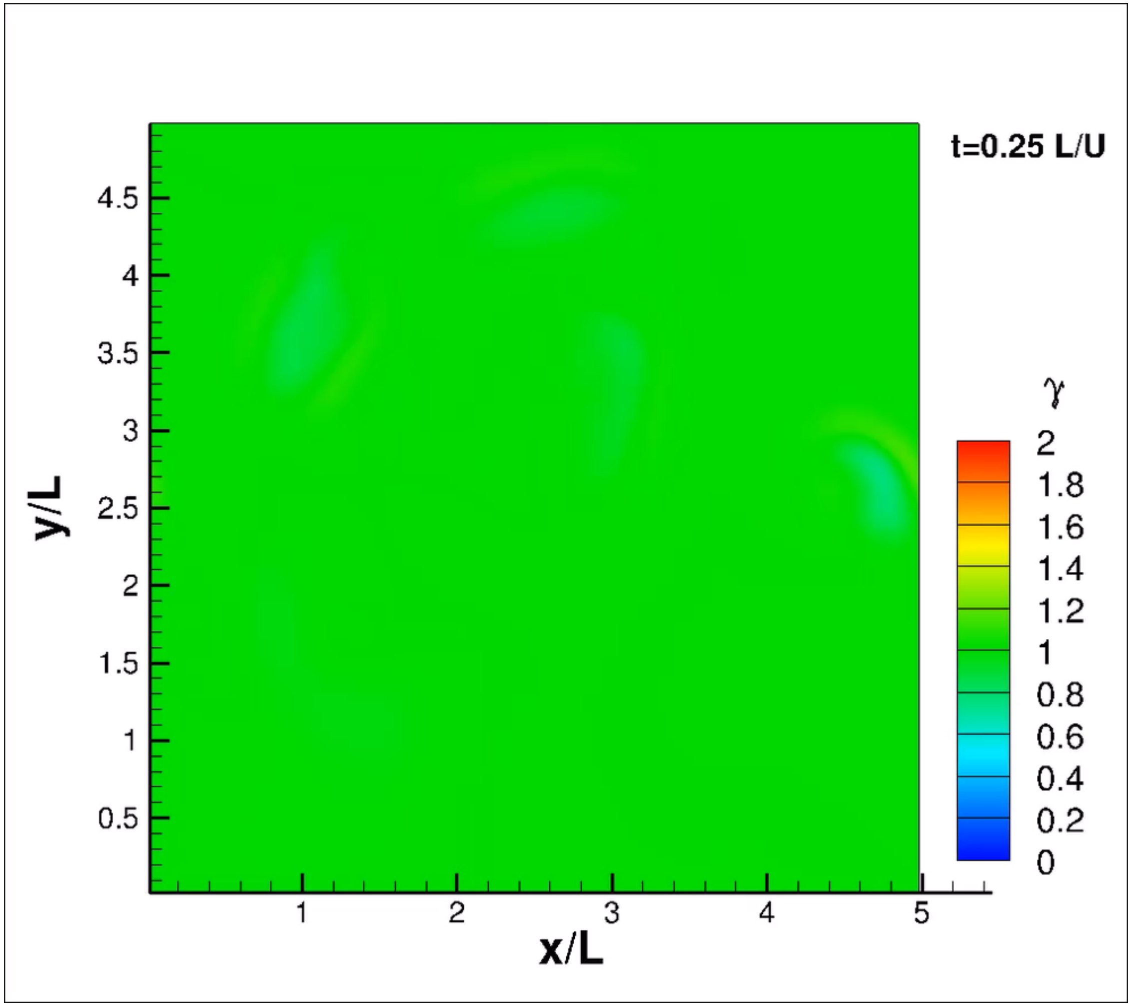
Surfactant Concentration Distribution

$Re\ Ma/We$ = 30.0



Surfactant Concentration Distribution

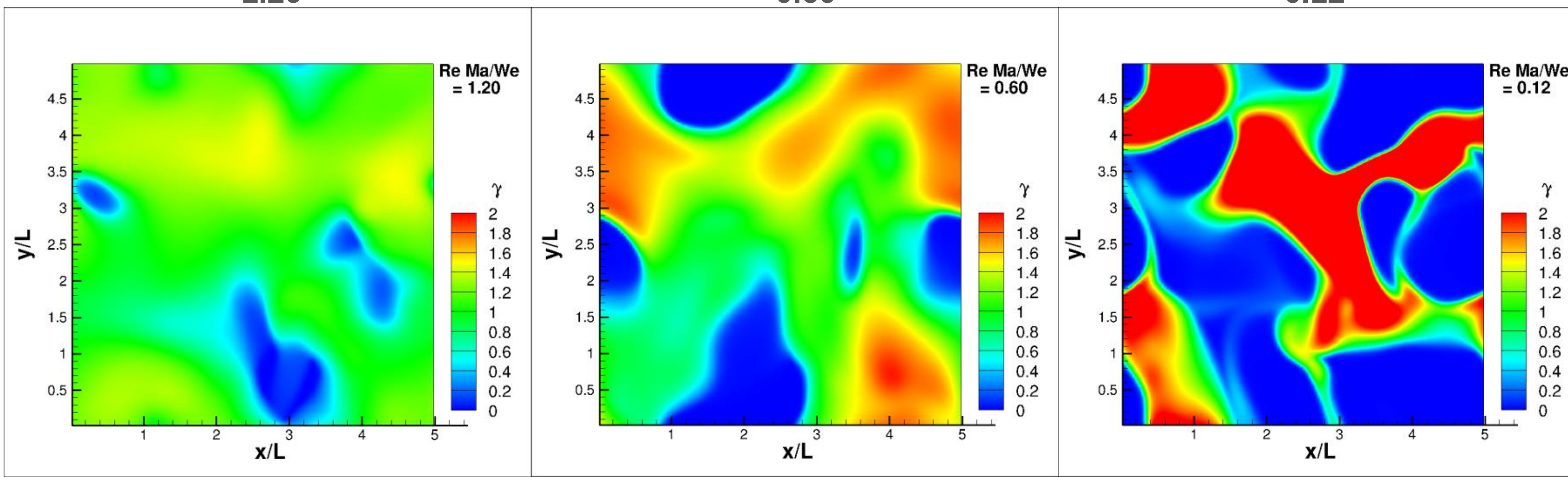
$Re\ Ma/We = 0.12$



Surfactant Concentration Distribution

Effect of decreasing $Re\ Ma/We$

1.20 0.60 0.12



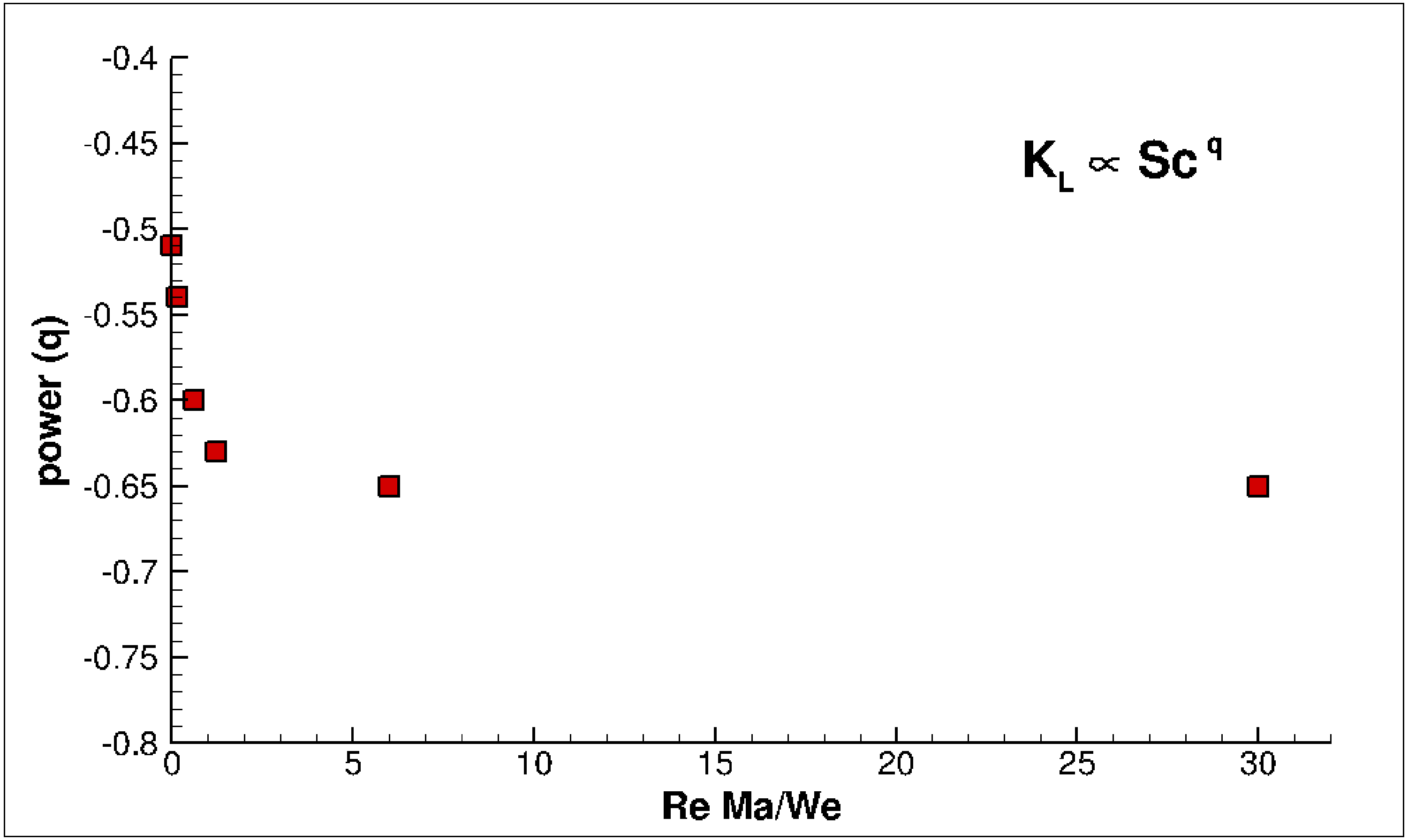
With decreasing *Re Ma/We* clean surface regions grow in size

In these regions K_L will scale with $Sc^{-1/2}$

In the remaining regions K_L may scale with $Sc^{-2/3}$???

Transfer Velocity Scaling

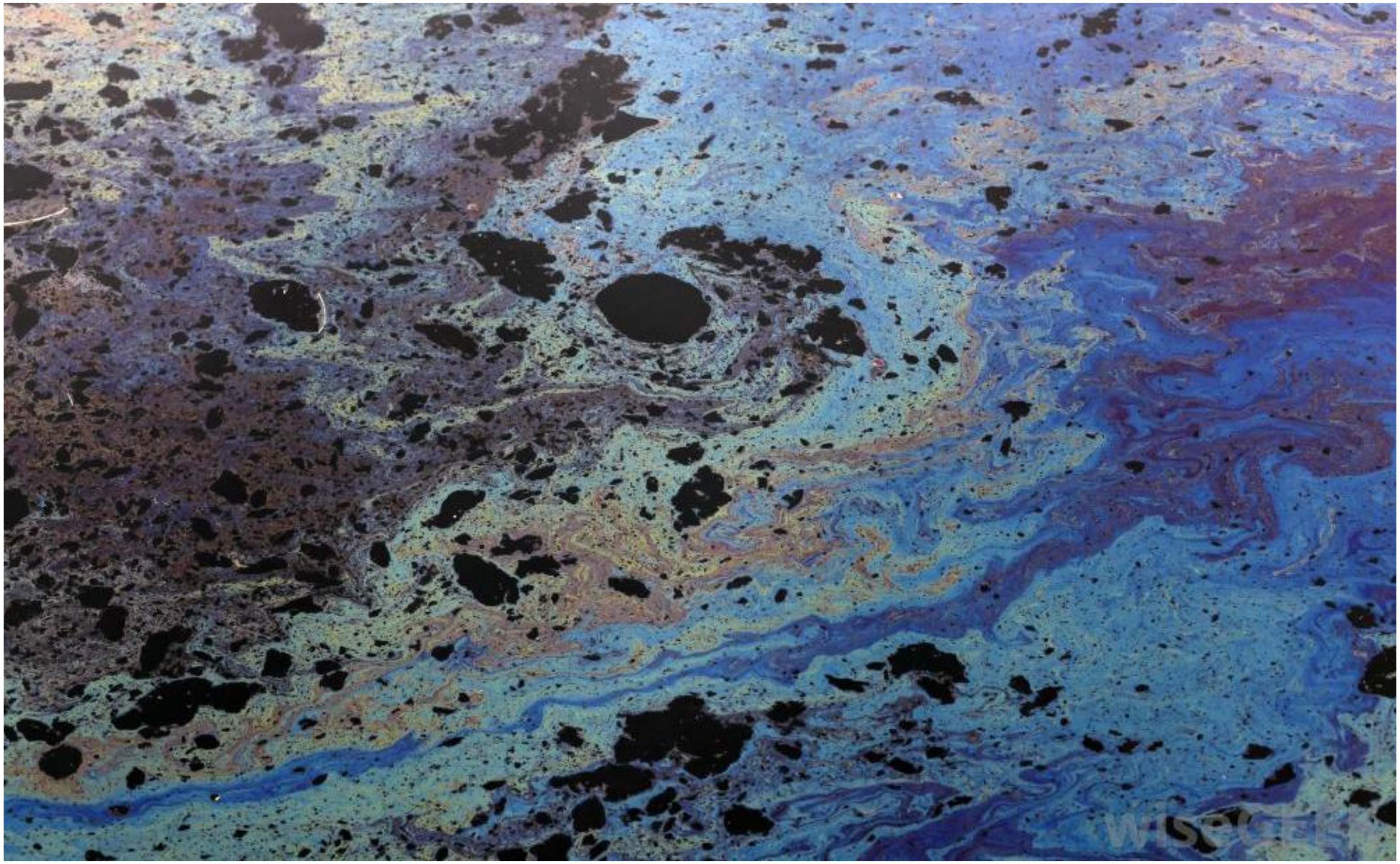
Effect of increasing $Re\ Ma/We$



Conclusions

- It was confirmed that the surfactant transport is largely unaffected by the amount of diffusivity
- Even low levels of contaminations can have a large effect on interfacial gas flux
- With increasing Re Ma/We, 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 (shear!!)
- At lower Re Ma/We areas on the surface will develop with a zero surfactant concentration

The end



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