

High Meadows
Environmental
Institute



PRINCETON
UNIVERSITY

Surfactant effects on parasitic capillary wave dynamics

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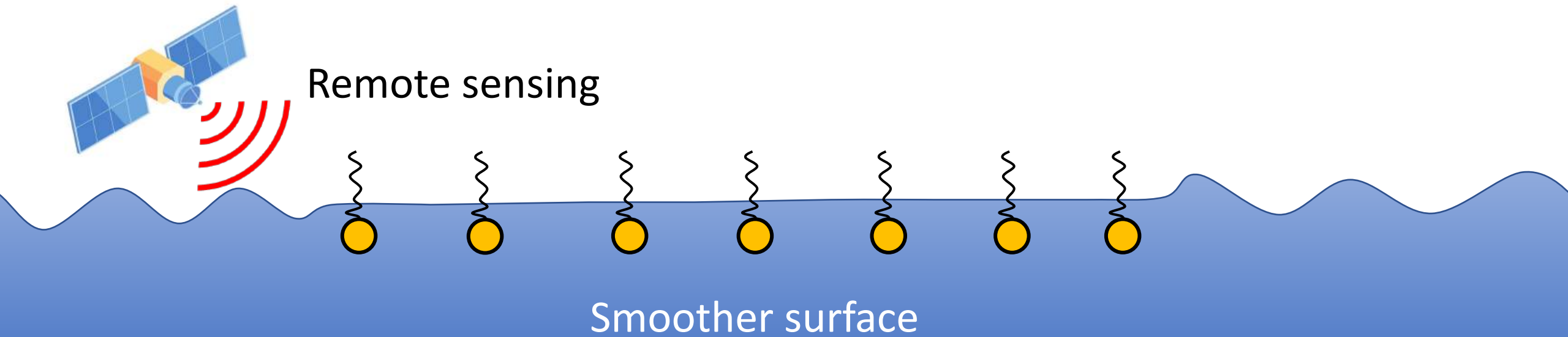
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Motivation

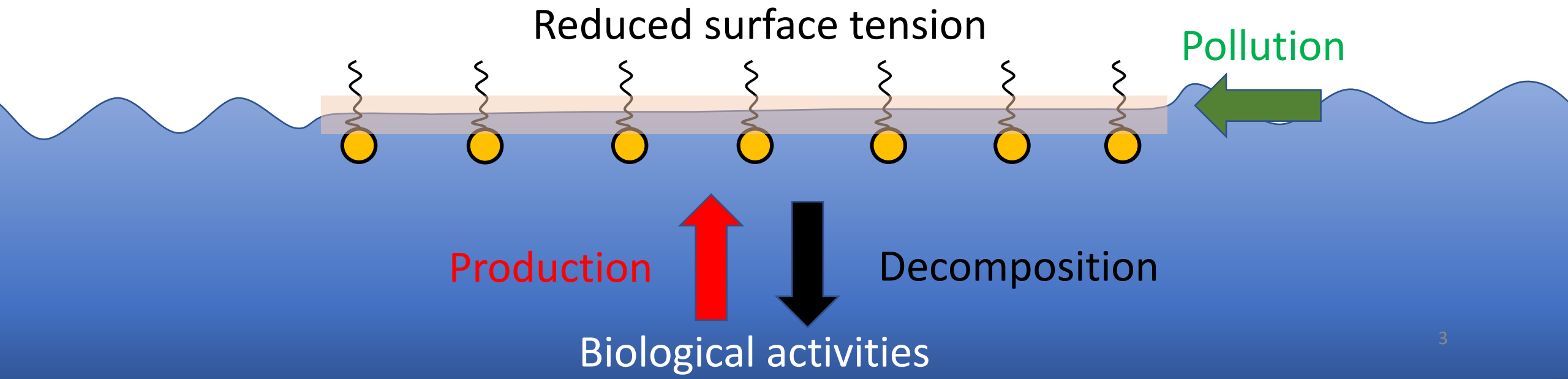
Kurata, N., Vella, K., Hamilton, B., Shivji, M., Soloviev, A., Matt, S., Tartar, A., & Perrie, W. (2016). Surfactant-associated bacteria in the near-surface layer of the ocean. *Scientific Reports*, 6.

- Sea surface is smoother in surfactant-concentrated area
- Surfactants influence the data collected by a scatterometer and its interpretation
- Goal: understand how surfactants influence the small-scale waves



What are surfactants?

- Compounds that lower the surface tension between two substances
- Unique molecular structures with hydrophilic head and hydrophobic tail
- Surfactants come from
 - active biological production in the sea surface microlayer
 - human-made pollution



Dynamic effects of surfactants

- Tears of wine

- Marangoni flow

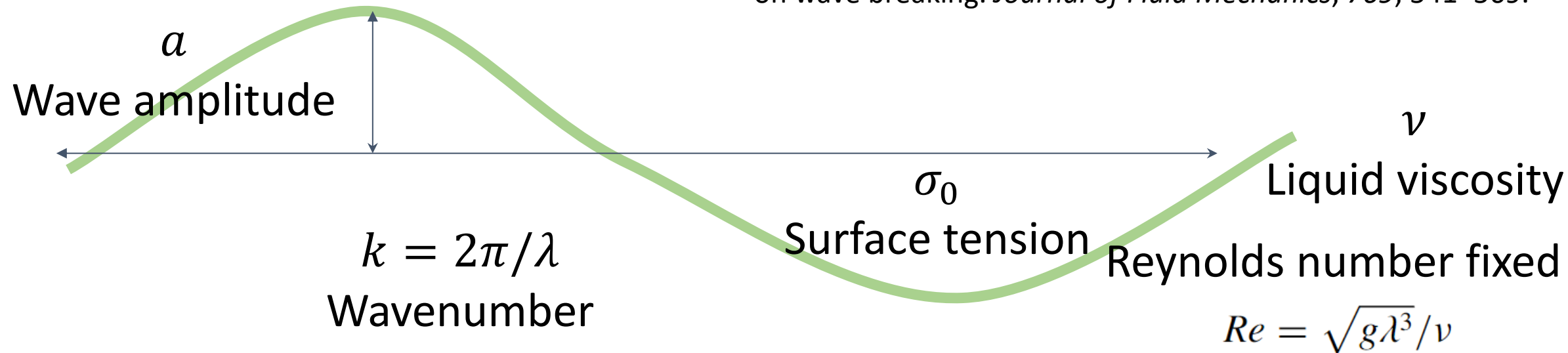
Surfactants distribution
cause gradients in surface
tension along the interface



Marangoni stresses that move fluids
from area of many surfactants to
fewer surfactants

Problem set-up: first without the surfactant

Deike, L., Popinet, S., & Melville, W. K. (2015). Capillary effects on wave breaking. *Journal of Fluid Mechanics*, 769, 541–569.



Initial condition:

- 3rd order stokes wave

Controlling parameters:

Wave steepness $\epsilon = ak$

Bond number $Bo = \Delta\rho g / (\sigma_0 k^2)$

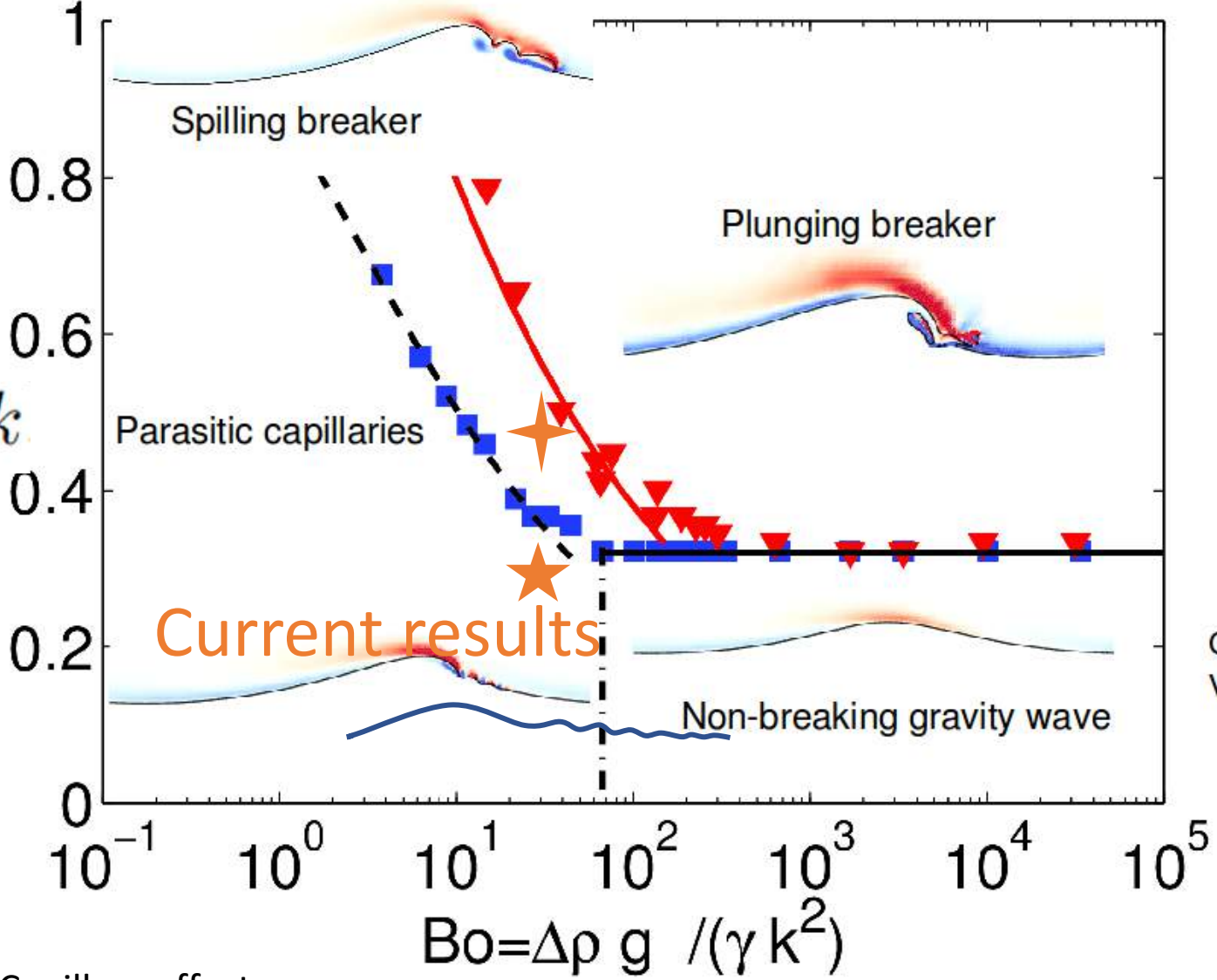
Slope and Bond number control the wave shape

$$\text{Wave slope} = \frac{\text{Wave amplitude}}{\text{Wavelength}}$$

$$\epsilon = ak$$

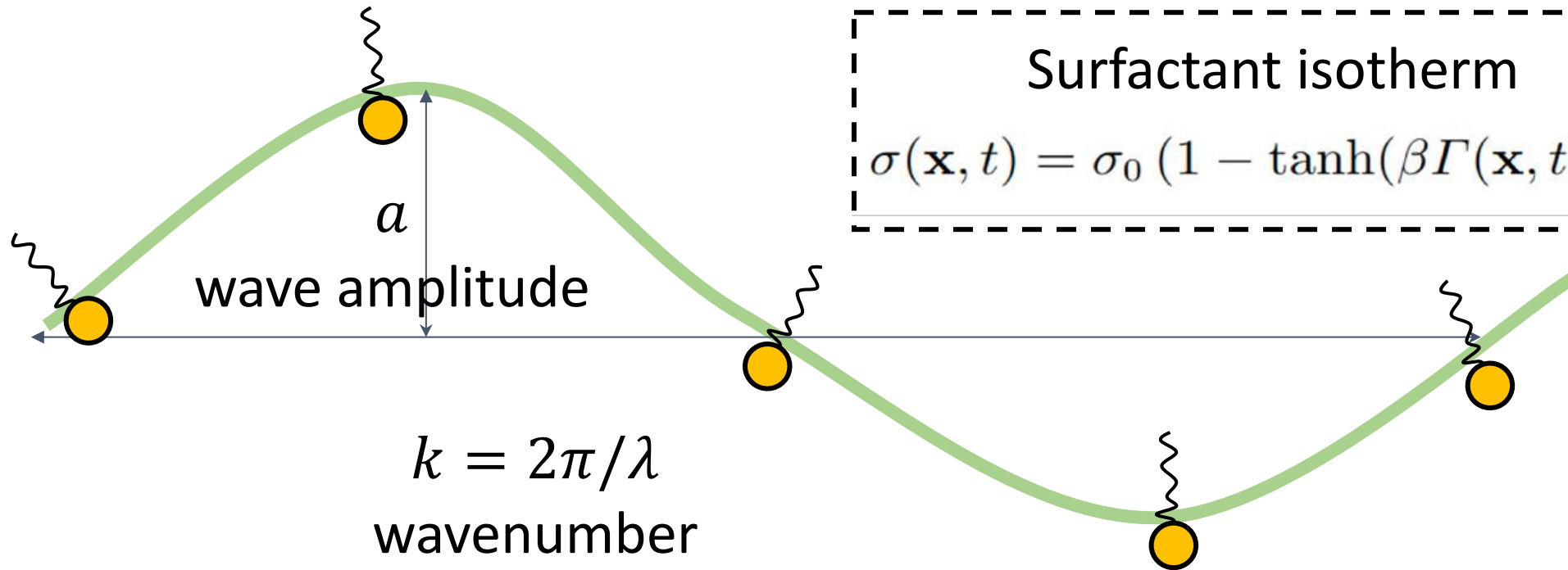
Modification of wave patterns by surfactant?

main wave is O(0.1-0.5m)
capillaries are mm-cm



Deike, L., Popinet, S., & Melville, W. K. (2015). Capillary effects on wave breaking. *Journal of Fluid Mechanics*, 769, 541–569.

Problem set-up: with surfactant



Surfactant isotherm

$$\sigma(\mathbf{x}, t) = \sigma_0 (1 - \tanh(\beta\Gamma(\mathbf{x}, t)/\Gamma_0))$$

Initial condition:

- Uniform distribution of surfactants $\Gamma(\mathbf{x}, t) = \Gamma_0$

Controlling parameters:

Wave steepness $\epsilon = ak$

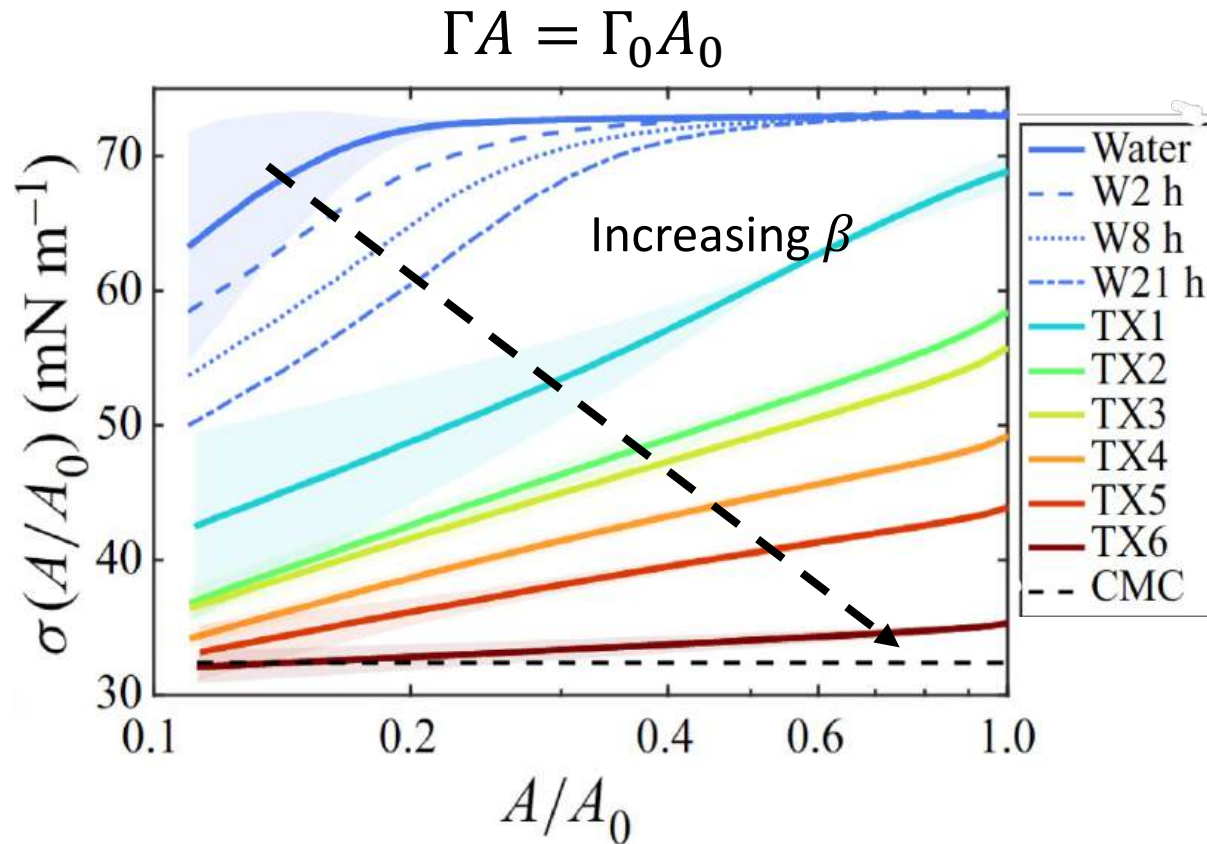
Bond number $Bo = \Delta\rho g / (\sigma_0 k^2)$

β reflects how surfactants change surface tension

$$\sigma(\mathbf{x}, t) = \sigma_0 (1 - \tanh(\beta\Gamma(\mathbf{x}, t)/\Gamma_0))$$

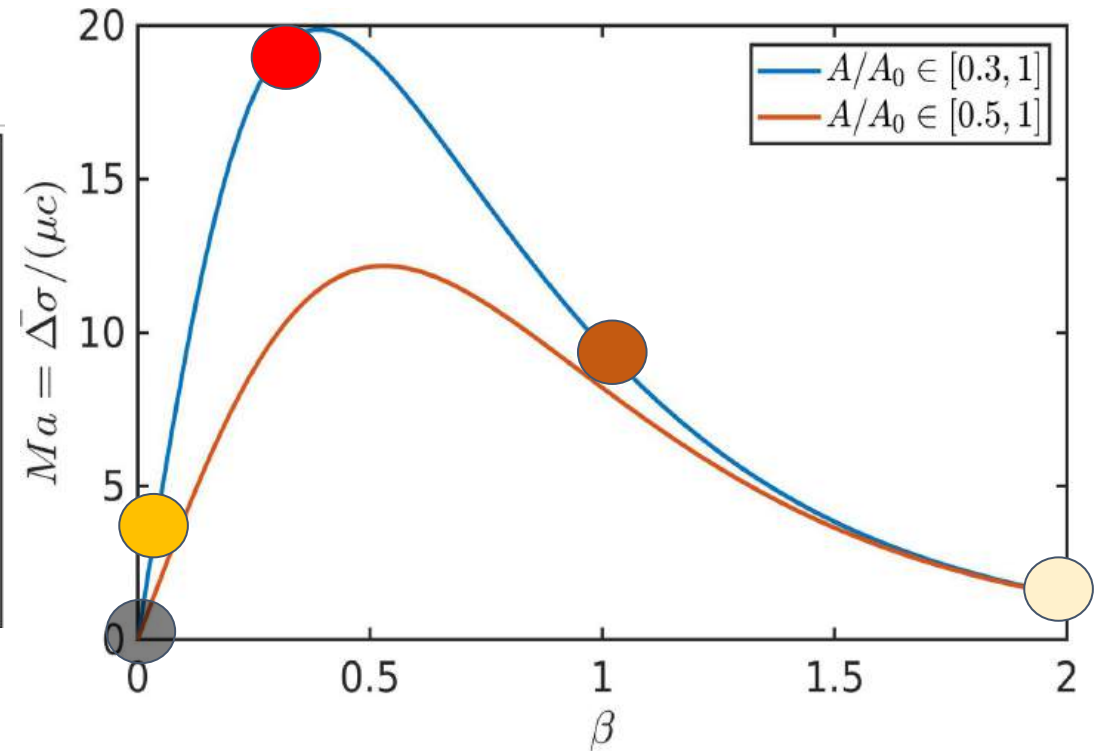
Erinin, M. A., Liu, C., Liu, X., Mostert, W., Deike, L., & Duncan, J. H. (2023). The effects of surfactants on plunging breakers. *Journal of Fluid Mechanics*, 972.

Surface tension change when compress interface



TX: Triton X (one type of surfactant used in the lab)

Effective Marangoni stress due to the surface tension gradient



Small $\beta \sim 0.01$: clean water, small Marangoni stresses

Intermediate $\beta \sim 0.3$: TX1, maximal Marangoni stresses

Large $\beta \sim 2$: TX6, small Marangoni stresses

Approach: direct numerical simulations

Two phase Navier-Stokes equation:

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) = \frac{1}{\rho} [-\nabla p + \nabla \cdot (\mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T))] + \boxed{\frac{\gamma}{\rho} \kappa \mathbf{n} \delta_s} + \boxed{\delta_s \nabla_s \gamma} \quad \text{Marangoni stresses}$$
$$\nabla \cdot \mathbf{u} = 0,$$

Surface tension

Volume of fluid method to resolve interface:

$$\frac{\partial \mathcal{T}}{\partial t} + \mathbf{u} \cdot \nabla \mathcal{T} = 0.$$

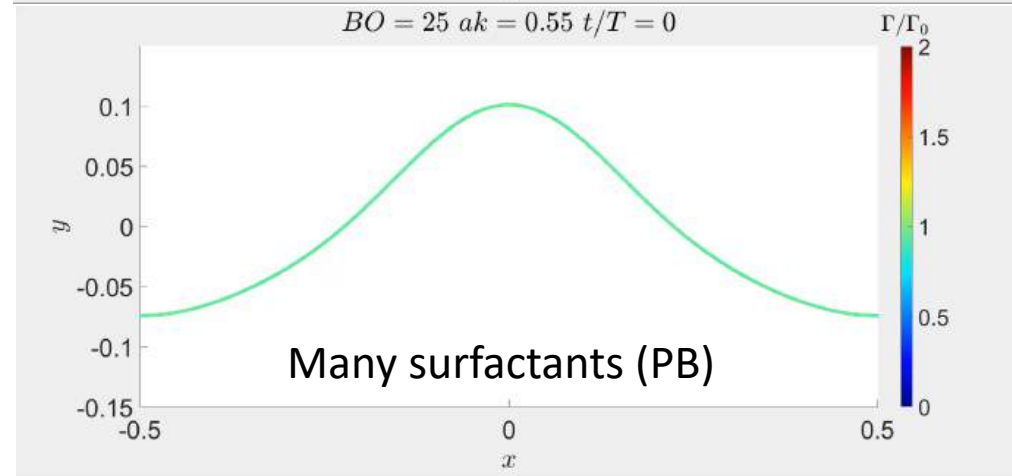
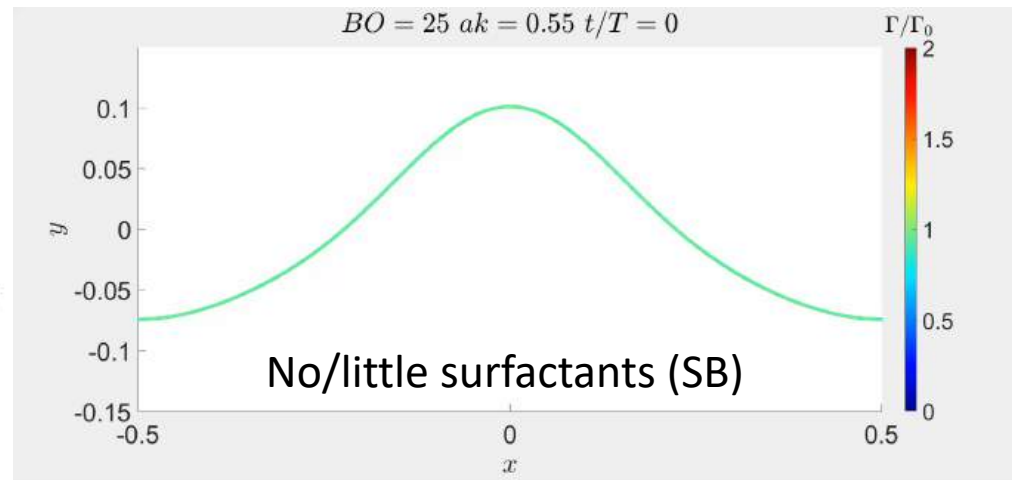
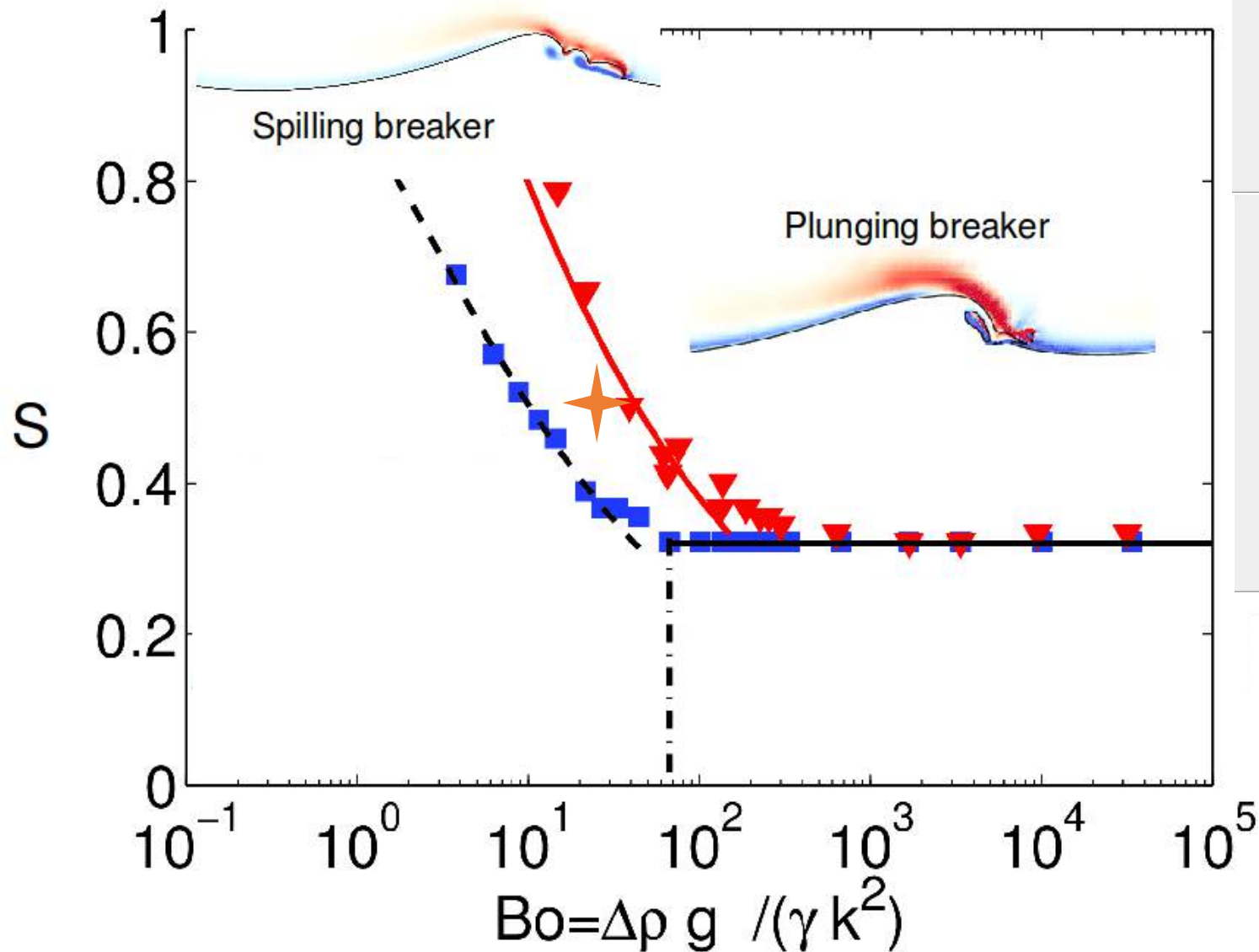
Advection-diffusion equation for surfactant transport:

$$\frac{\partial \Gamma}{\partial t} + \nabla_s \cdot (\Gamma \mathbf{u}_s) + \Gamma (\nabla_s \cdot \mathbf{n})(\mathbf{u} \cdot \mathbf{n}) = D_s \nabla_s^2 \Gamma \quad (\text{Advection dominated})$$



Basilisk, Partial
Differential
Equations solver

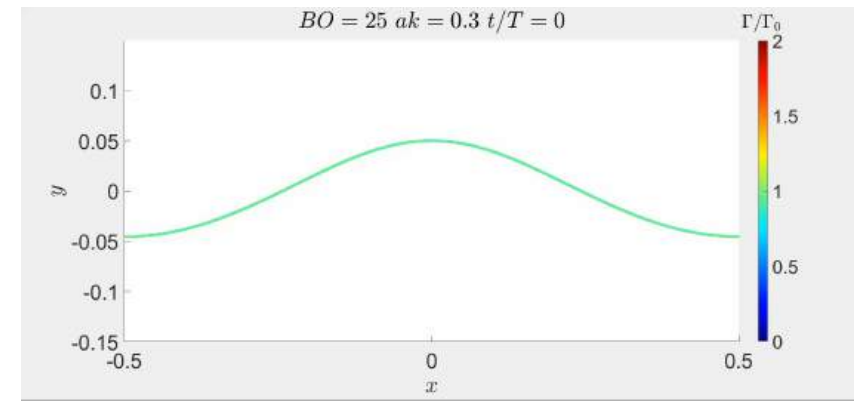
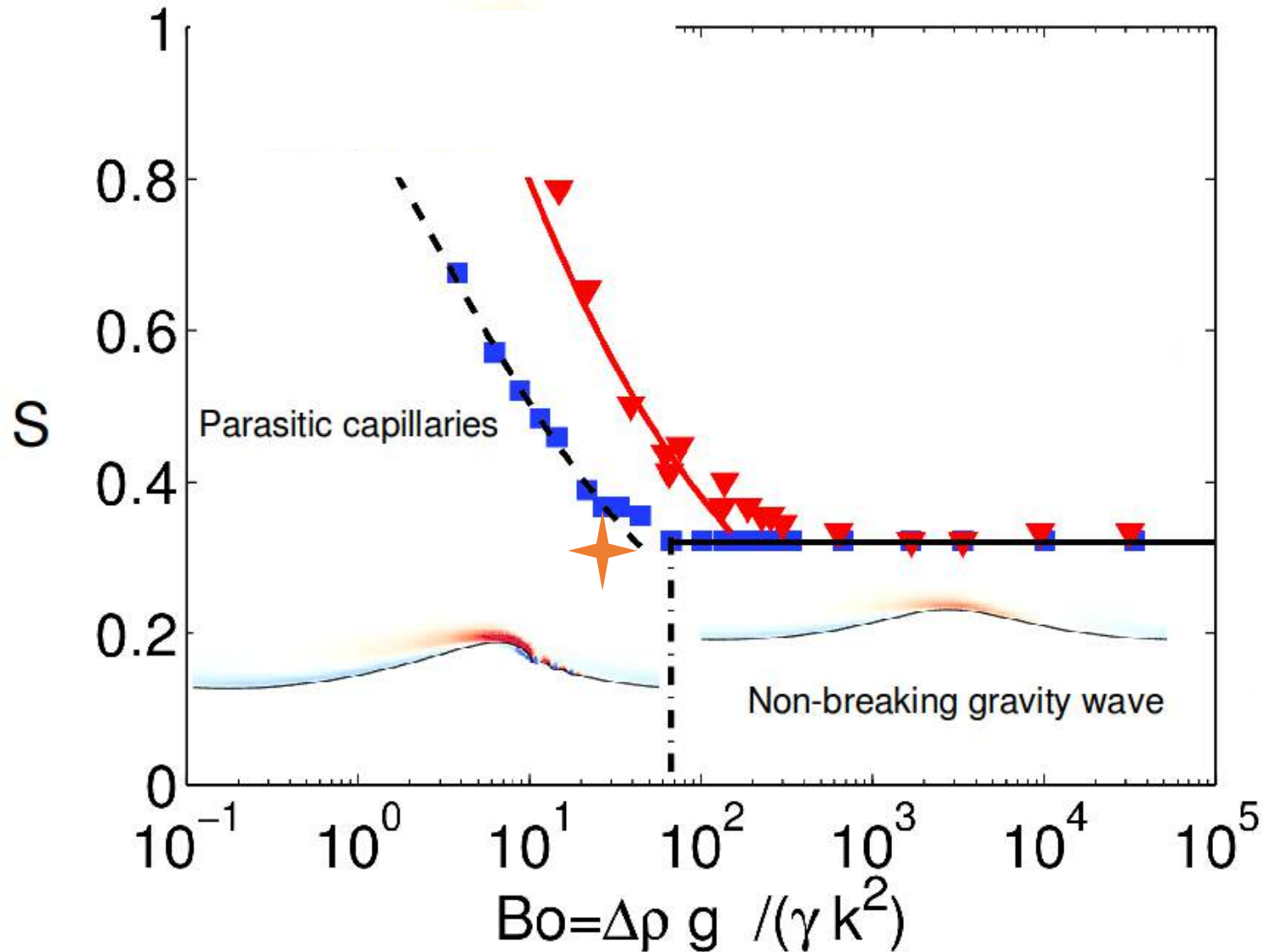
Results



Surfactant concentration color-coded

Surfactants shift SB to PB

Results



No/little surfactants (PCW)

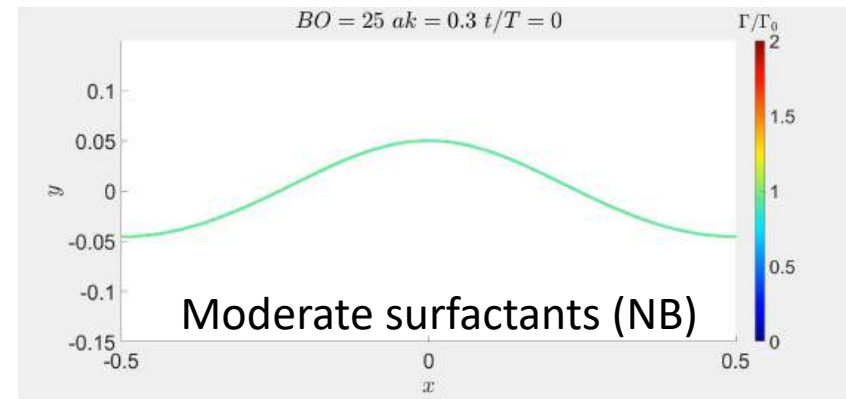
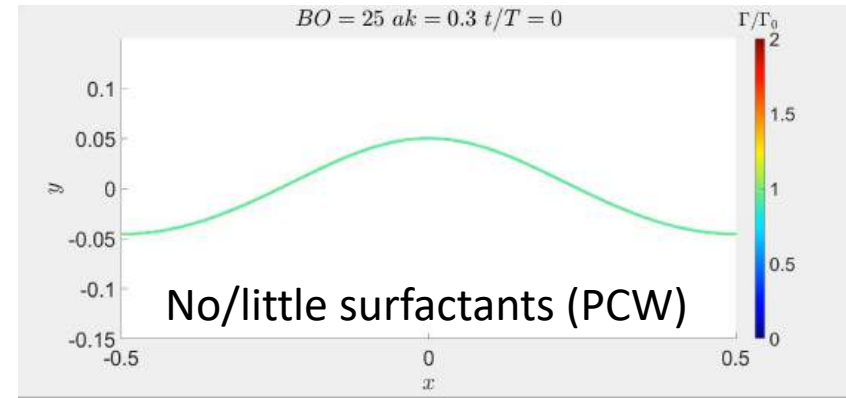
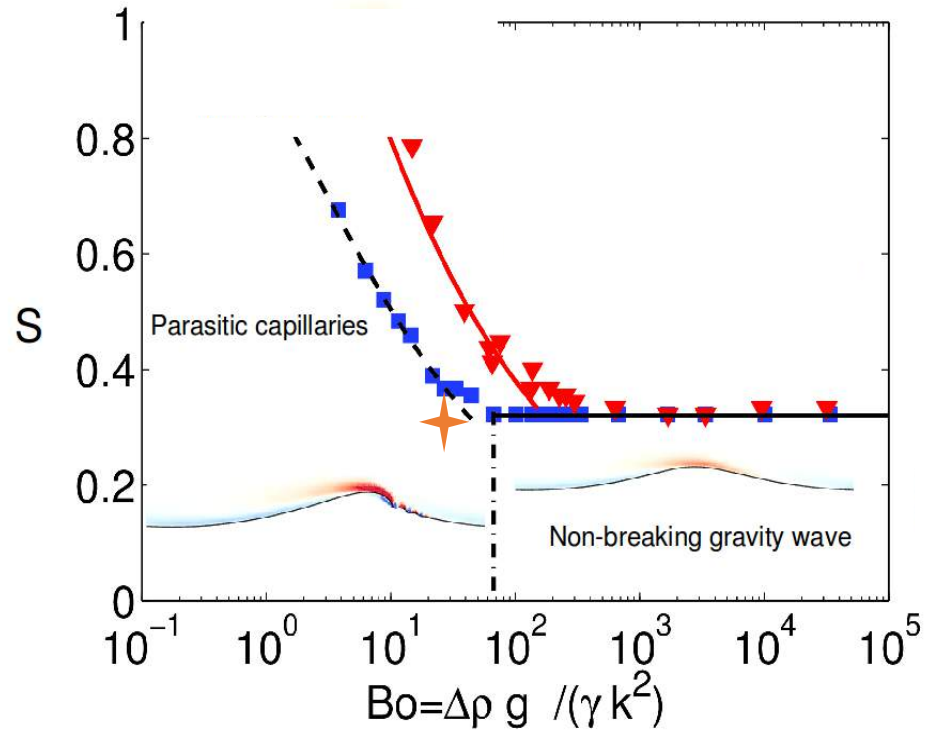
No Marangoni stresses

Color-coded the
surfactant concentration

Surfactants transported purely by
waves (surface compression)

Surfactants concentrated on wave crest
Small-scale capillary waves

Results

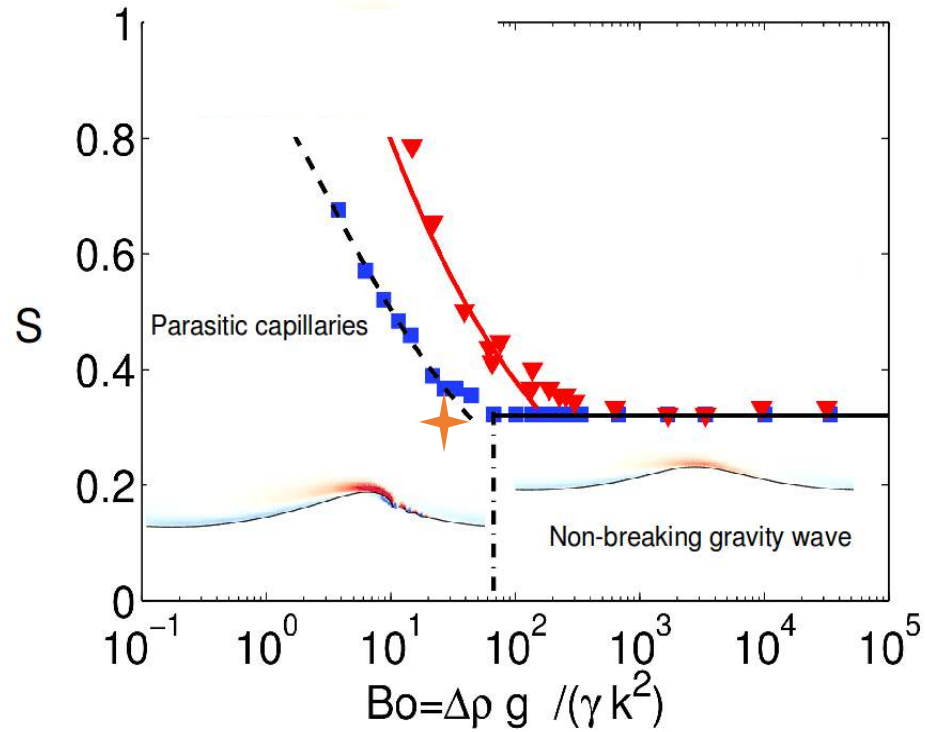


Surfactants transported

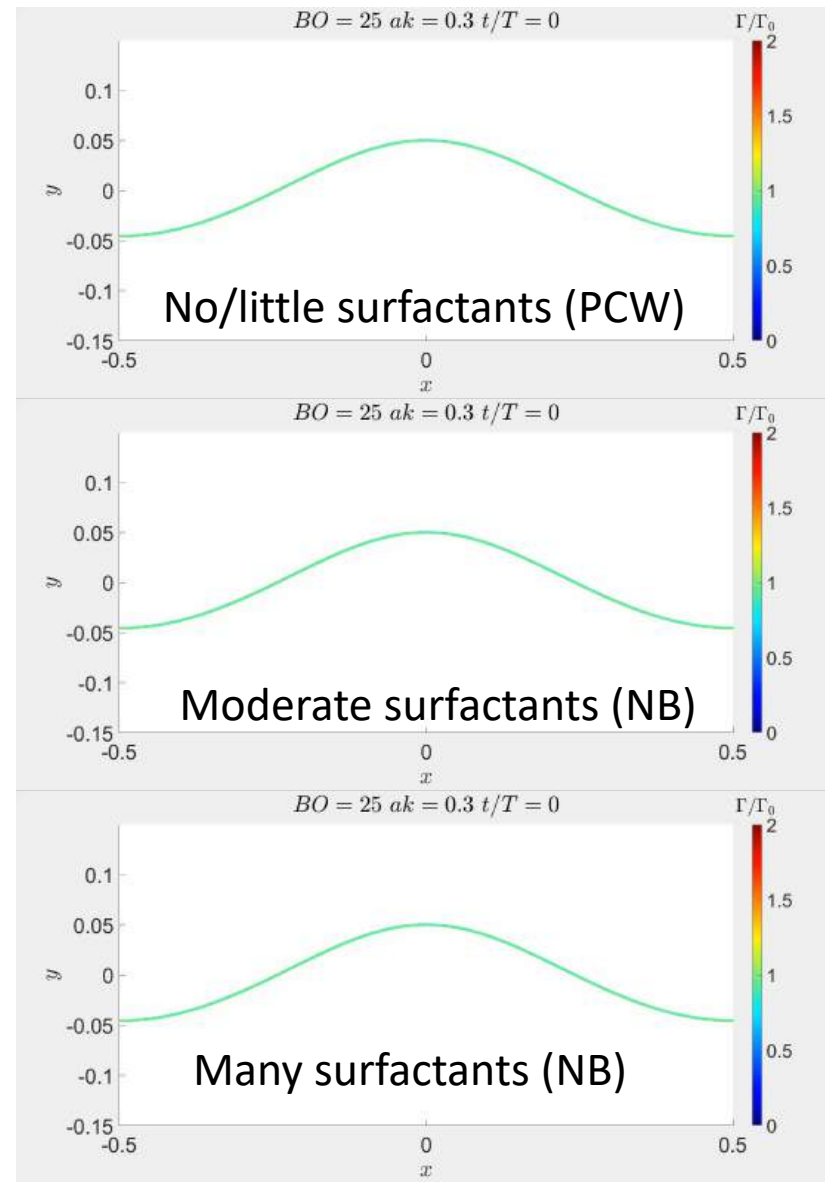
- By waves (more concentrated)
- By Marangoni-induced flow (more even)

High Marangoni stresses distribute surfactants more evenly
 Marangoni stress damp capillary waves

Results



Surfactants damp PCW



Low Marangoni stresses

High Marangoni stresses

Low Marangoni stresses

Conclusions

- Surfactants change the wave shape: shift SB to PB and damp parasitic capillary waves
- Surfactants influence wave dynamics through Marangoni stresses (surface tension variation) and reduced surface tension
- Understand how surfactant influence the surface profile will help interpret the scatterometer data

