Fluid and porous particles settling in a stratified ambient

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in collaboration with

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Why study particles and stratification?

- Particles are present in the atmosphere, oceans, magma (i.e. pretty much everywhere). Where they end up has environmental and geological consequences.

- The fluids surrounding the droplets are rarely of a uniform density: temperature, salinity and composition all vary.

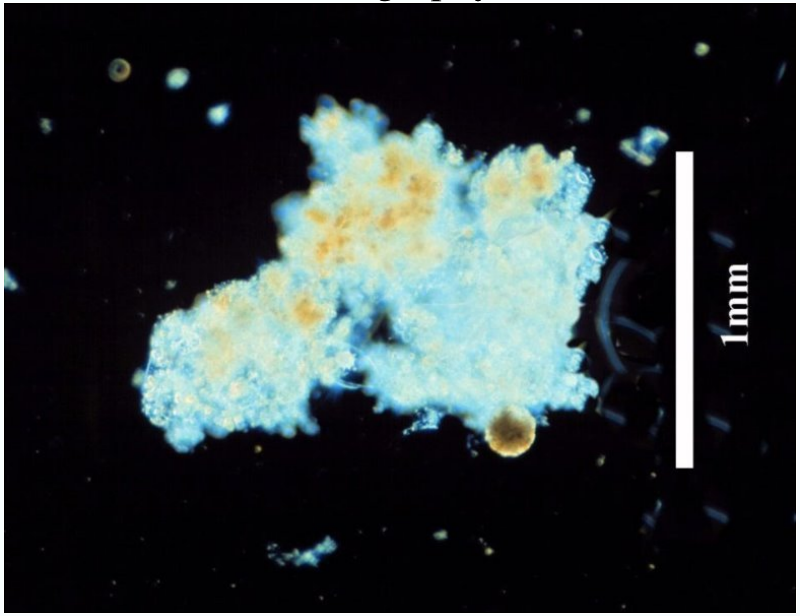
- We could consider and contrast 3 main types of particles:
  - Solid
  - Liquid (today)
  - Porous (today)

- These processes can also be studied in the lab, but they are difficult to control. They are also difficult to study accurately in the field.

- Simulations are an excellent tool to use, in conjunction with experiments and field observations.

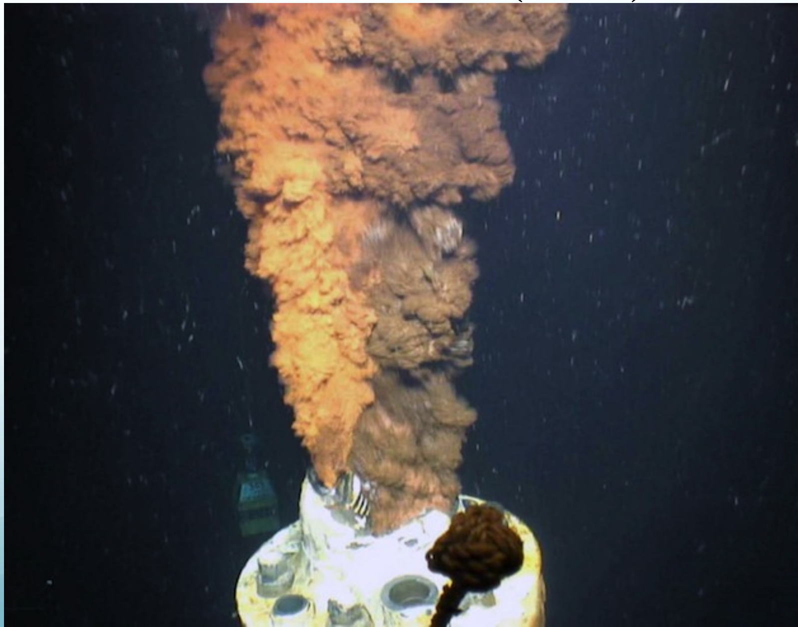
Sample Applications:

- Storms, wildfire ash.
- Oil spills.
- Oceanic carbon cycle.



Phoenix, Az (2011)

Gulf of Mexico (2010)



Contents of this presentation

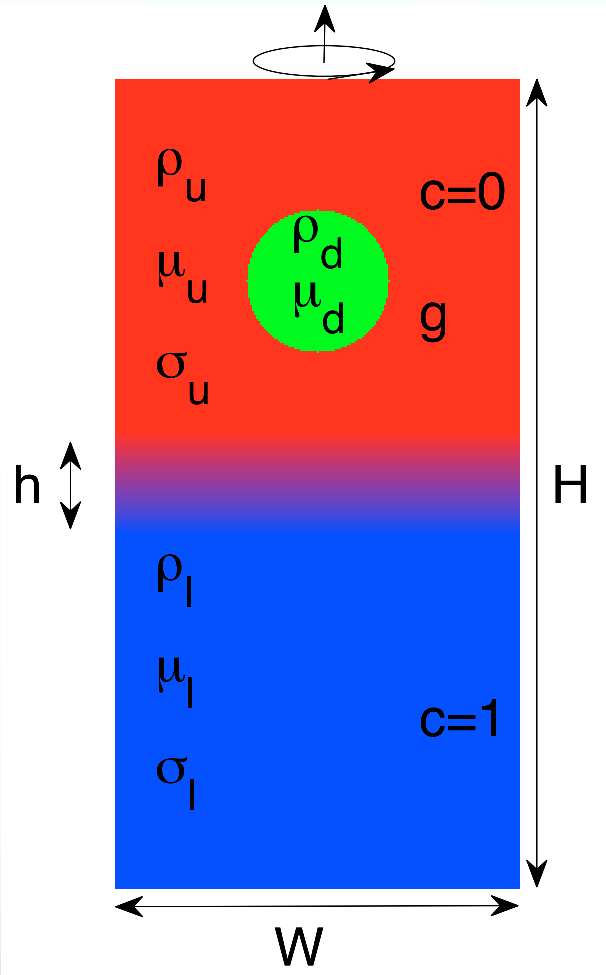
- Drops settling in stratification
  - Without Marangoni effects
  - With Marangoni effects
- Porous particles in stratification
  - How to model the porosity
  - Resulting delays
  - Capturing complicated shapes

Drops settling in a sharp stratification

- We study drops settling in sharply stratified liquids.
- We use $\rho_d \geq \rho_l \geq \rho_u$ (stable, drops fall).
- The upper and lower layers are miscible.
- The surface tension of the two layers with the drop may or may not be the same.
- We focus on density and surface tension effects

This is applicable to oil drops settling in the ocean.

- temperature variations (1° C => $|\sigma_u - \sigma_l|/\sigma_u = 0.3\%$)
- salinity variations (10g/kg => $|\sigma_u - \sigma_l|/\sigma_u = 0.3\%$)

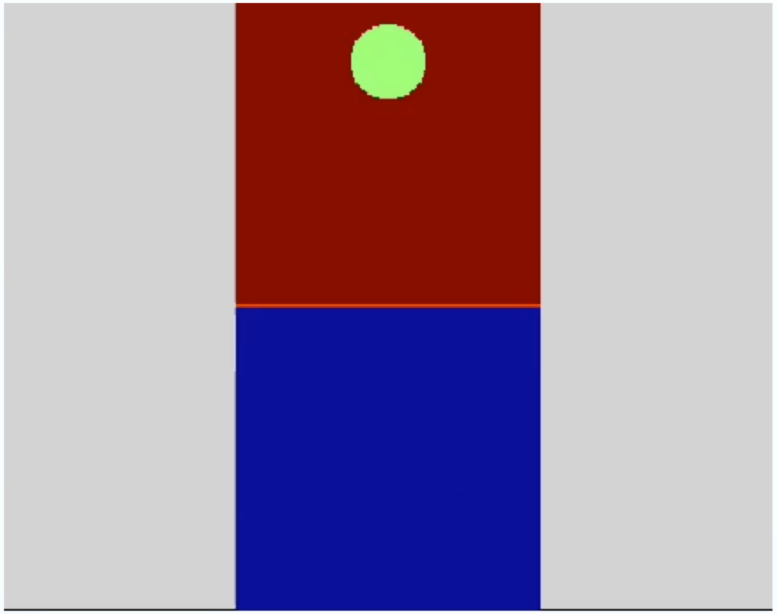


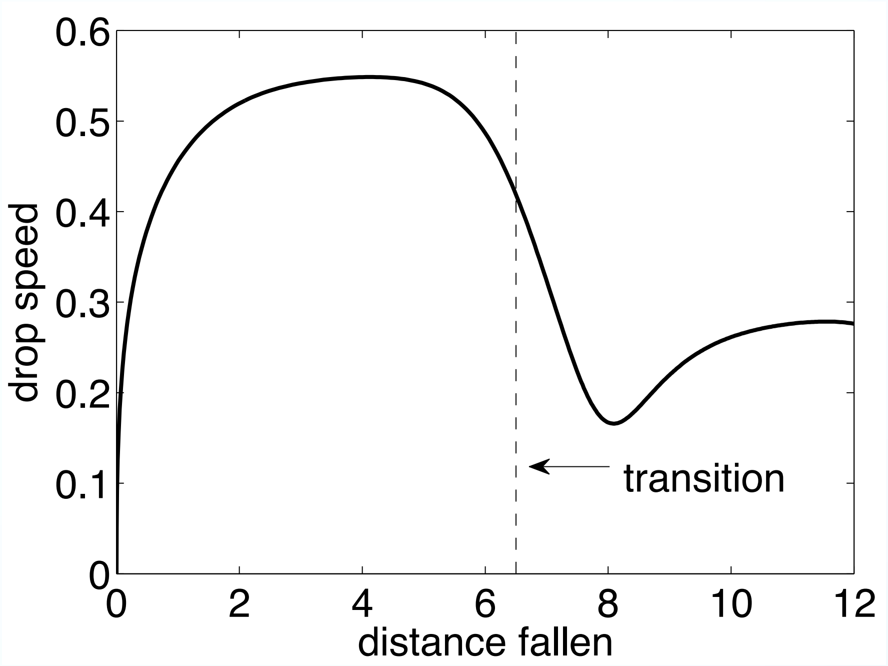
$\rho_d \geq \rho_l \geq \rho_u$

$\sigma_u \neq \sigma_l$ or $\sigma_u = \sigma_l$

$R \sim h$

Constant Surface Tension Ambient Results





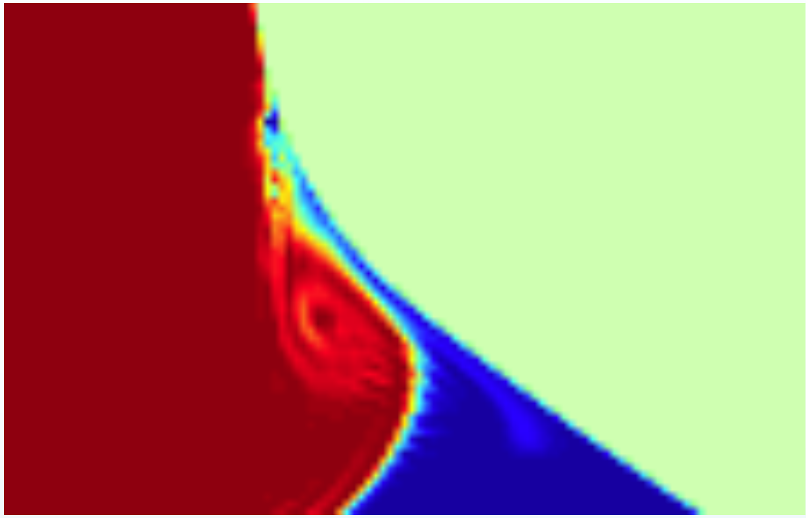
- The drop first accelerates.
- As it settles, the drop entrains surrounding fluid.
- At the transition, light upper fluid is drawn into denser lower fluid.
- The drop slows down significantly (can even stop).
- In the lower layer, the drop reaches its new terminal velocity.

Similar to a solid sphere, but less entrainment (slip instead of no-slip)

Comparable solid spheres results: Srdic-Mitrovic *et al*. (1999), Abaid *et al*. 2004
Camassa *et al*. (2009)

Surface tension variations => Marangoni Effects

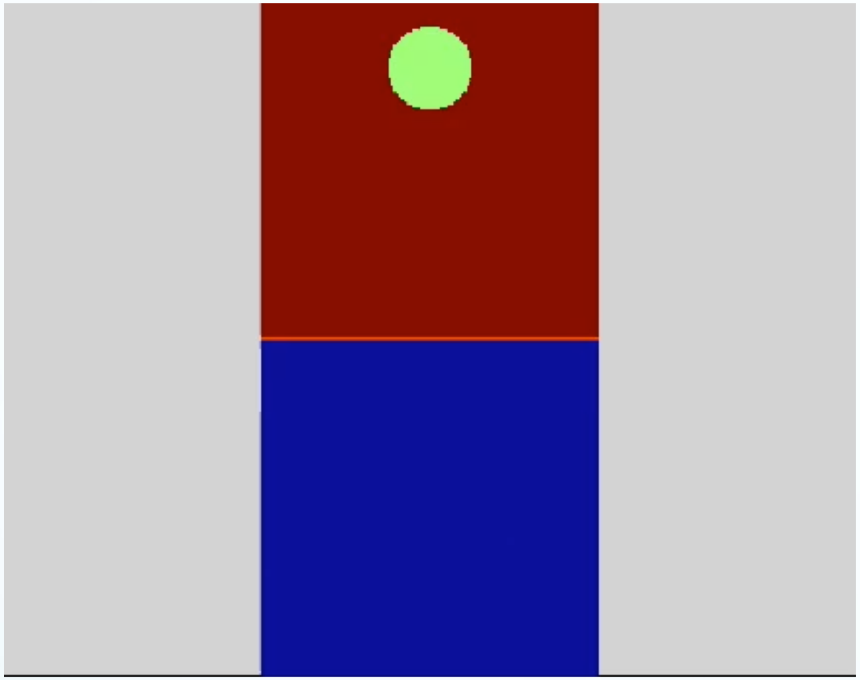
- Surface tension gradient => tangential motion.
- Larger surface tension pulls on smaller surface tension (hot liquid spreads on cold liquid).



Blue has small surface tension
Red has large surface tension

How does this affect the settling process?

Results for $\sigma_l < \sigma_u$

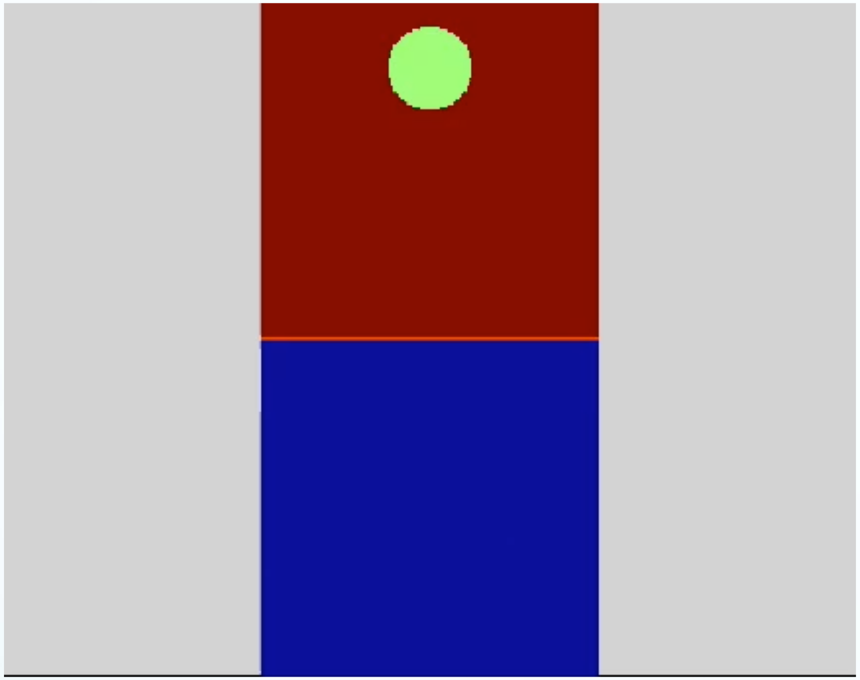


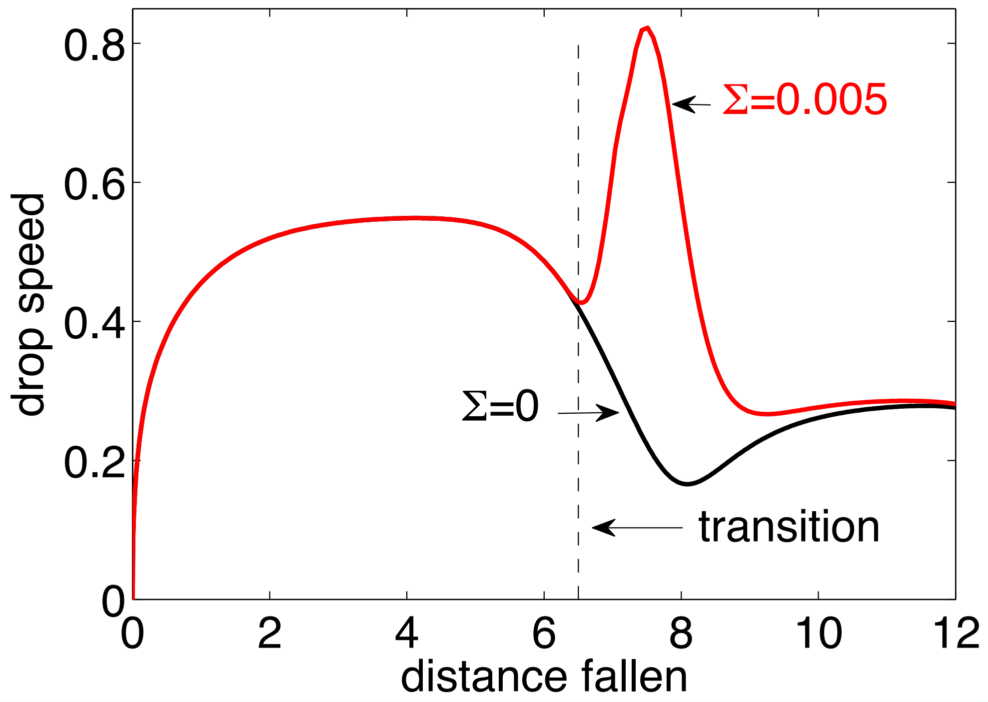
Here $\sigma_u = 30 g/s^2$ and $\sigma_l = 29.85 g/s^2$, $\Sigma = 0.005$
Re = 4.1 and D = 2

- Upper fluid is still entrained downward.

- Tangential flows are dominant and “suck” the drop in the lower layer.

Results for $\sigma_l < \sigma_u$



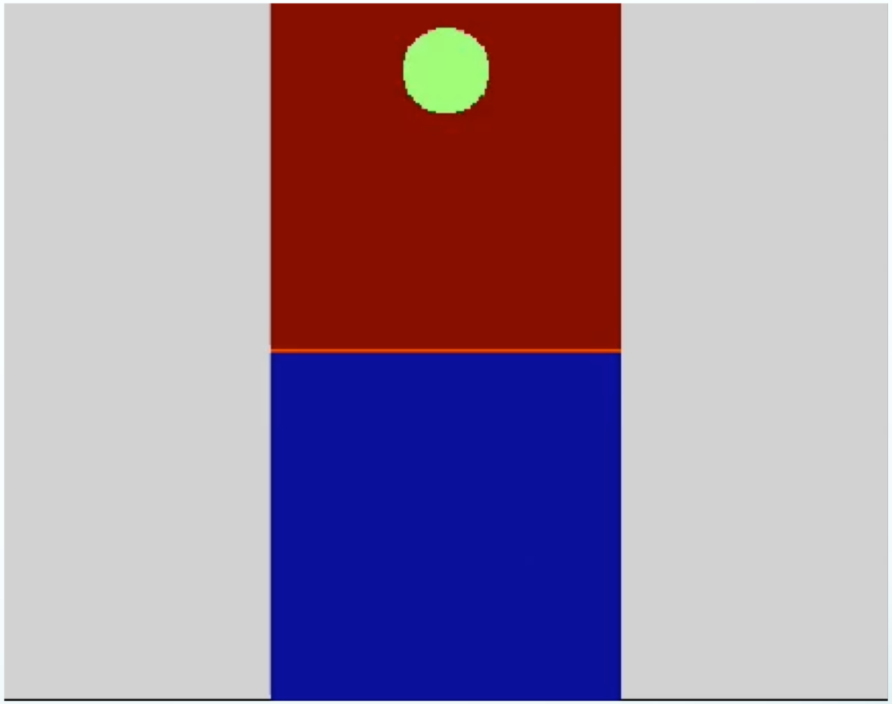


Here $\sigma_u = 30 g/s^2$ and $\sigma_l = 29.85 g/s^2$, $\Sigma = 0.005$
Re = 4.1 and D = 2

- Upper fluid is still entrained downward.
- Tangential flows are dominant and "suck" the drop in the lower layer.

Numerical Results for $\sigma_l > \sigma_u$

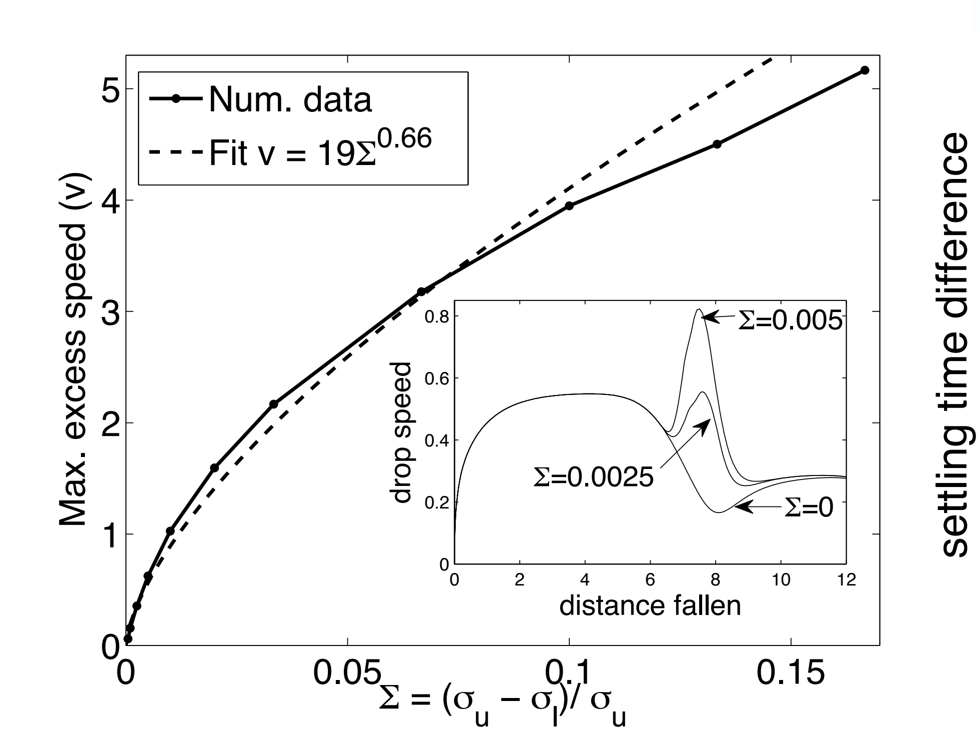
$\sigma_u = 30.075\ g/s^2$
$\sigma_l = 30.0\ g/s^2$

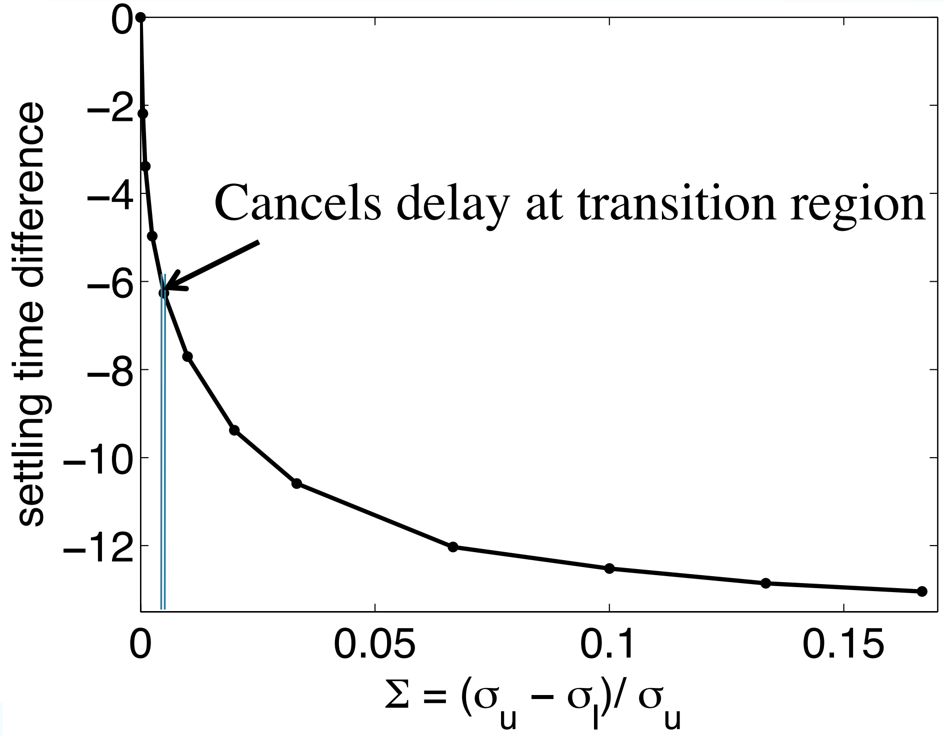


$\sigma_u = 30.15\ g/s^2$
$\sigma_l = 30.0\ g/s^2$

- Lower fluid is entrained upward
- Marangoni effects compete against gravity, even for Σ close to 0

Numerical Results for $\sigma_l < \sigma_u$

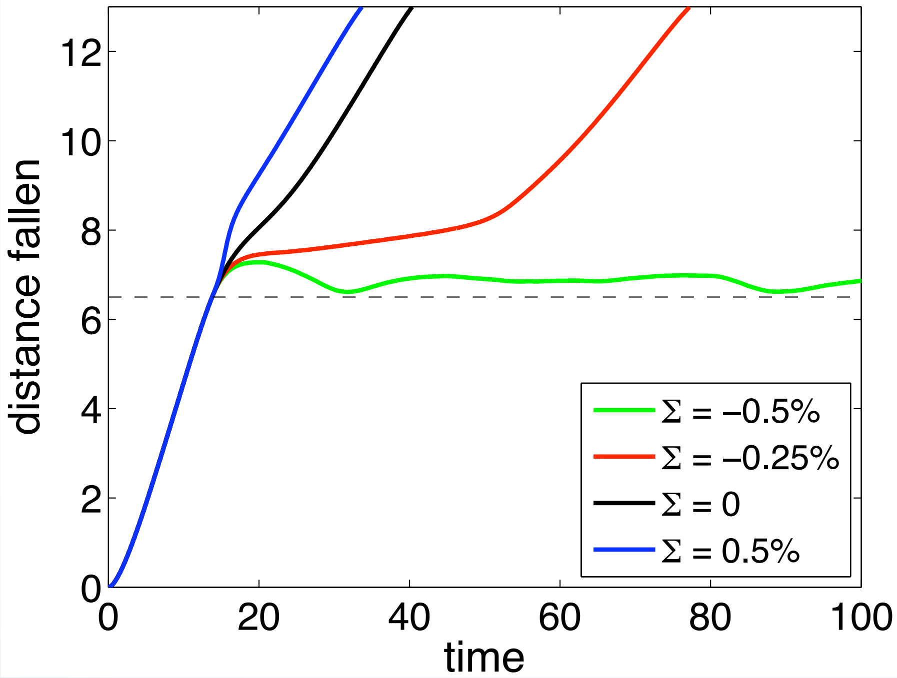


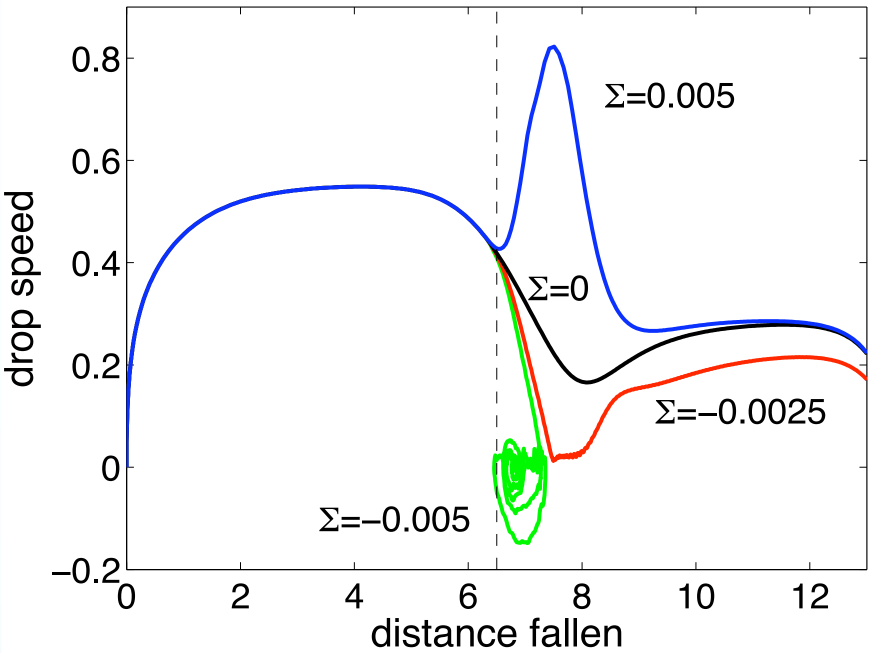


$v \sim \Sigma$ in the viscous regime,
$v \sim \Sigma^{1/2}$ in the inertial regime

- We are in the transition regime with $\Sigma^{0.66}$.
- Even for small Σ (~0.5%) the acceleration more than overcomes the delay due to entrained fluid.

Long-term behavior



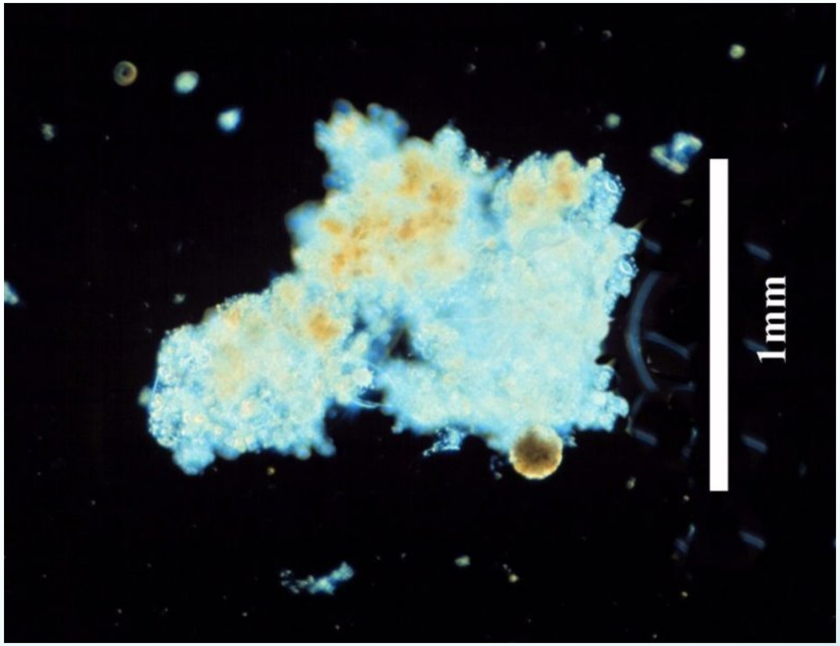


Over the time scale of settling, drops may either be:

- accelerated if $\Sigma > 0$
- decelerated if $\Sigma_{cr} < \Sigma < 0$.
- stuck if $\Sigma < \Sigma_{cr}$

Porous particles: Aggregates, marine snow, and carbon cycle

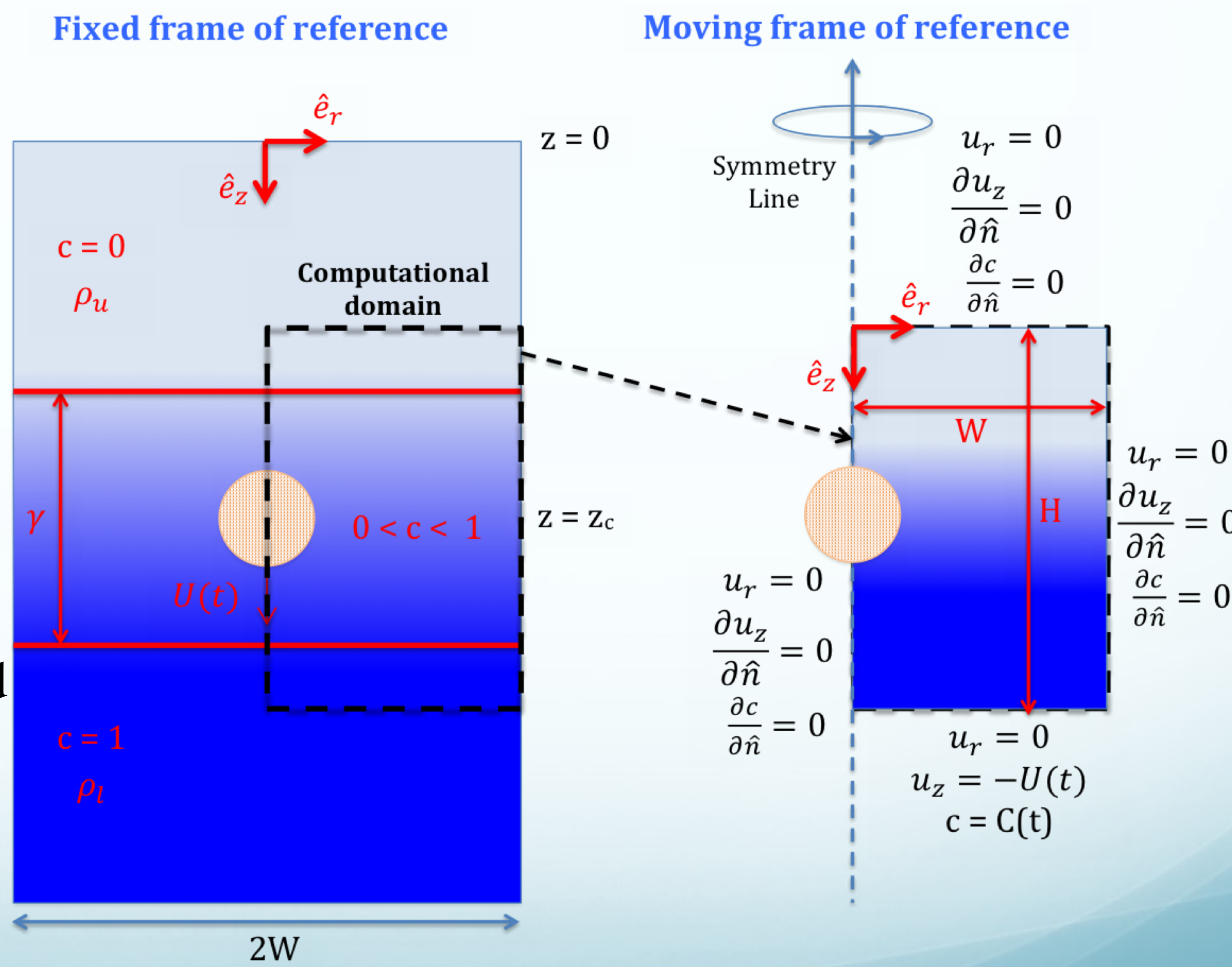
- Micro-organisms form aggregates in the oceans.
- Large aggregates are called marine snow.
- These porous particles are slightly denser than water and settle slowly.
- They effectively stop in stratified ambients.
- These particles account for a large fraction of the carbon flux from surface to depth.



We want to characterize the settling dynamics of porous particles.

Simulations of settling porous spheres

- Dense, highly porous particle settle in a stratification.
- Light fluid is entrained within the particle.
- Salt diffuses in, slowly.
- Particle velocity computed using a force balance.
- Use axisymmetric simulations, with penalty term in the porous region.



Non-Dimensional parameters and equations

Parameters

$$Re = \frac{\rho U L}{\mu} \qquad \xi = \frac{\rho_l - \rho_u}{(\rho_s - \rho_u)(1-\phi)}$$

$$Da = \frac{\kappa}{L^2} \qquad \eta = \frac{\rho_l - \rho_u}{\rho_u}$$

$$Pe = \frac{UL}{D} \qquad \gamma = \frac{\text{thickness of the transition layer}}{L}$$

l = lower
u = upper
s = solid
Φ = porosity

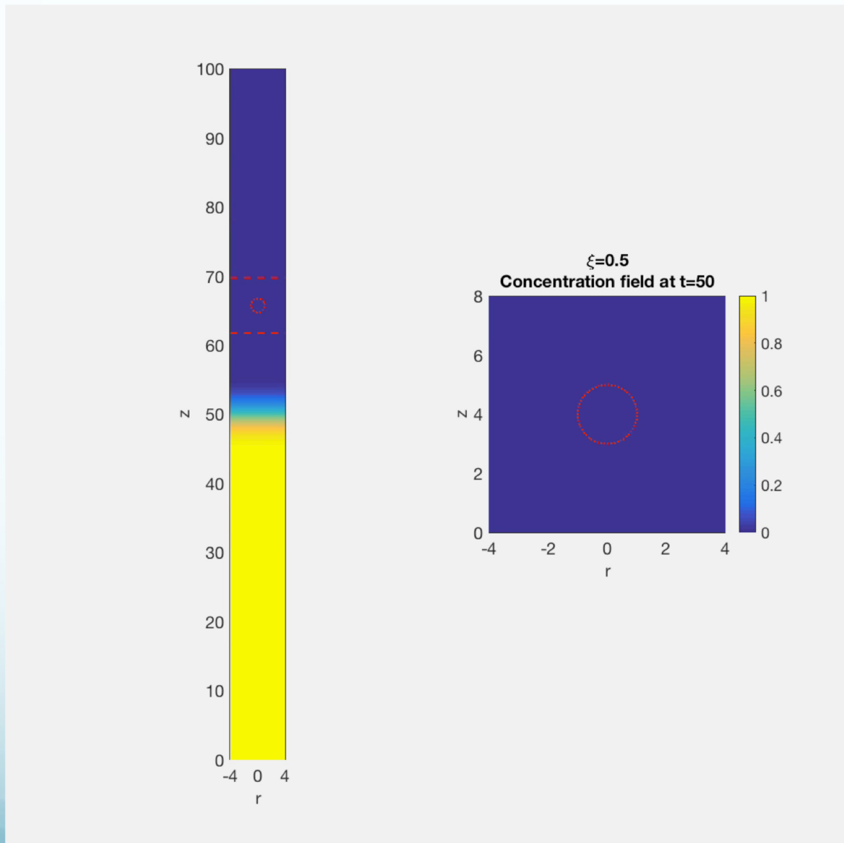
Here the dominant parameters are Pe and ξ.

- Pe captures the (inverse of) the diffusive effects
  small Pe means diffusion is fast
  large Pe means diffusion is slow
- ξ is an unusual ratio that measures how much the external density changes, relative to the excess density of the solid part of the particle.
  small ξ means the external density can be treated as constant
  large ξ means the external density dominates the dynamics

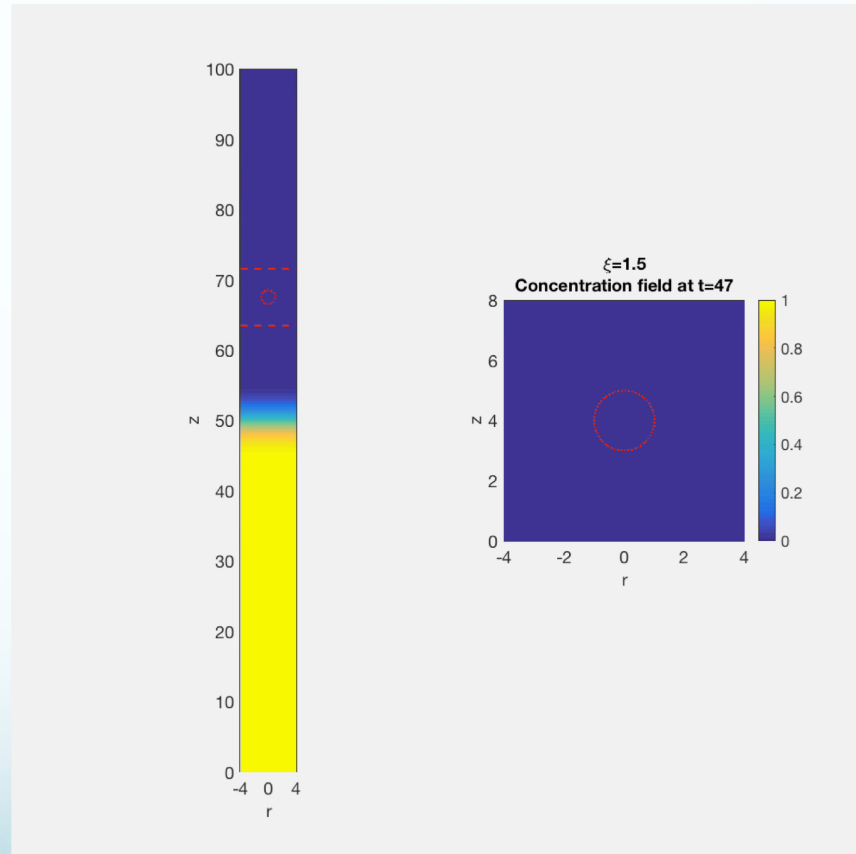
Sample simulations, two different ξ values

$$\xi = \frac{\rho_l - \rho_u}{(\rho_s - \rho_u)(1-\phi)}$$

ξ = 0.5



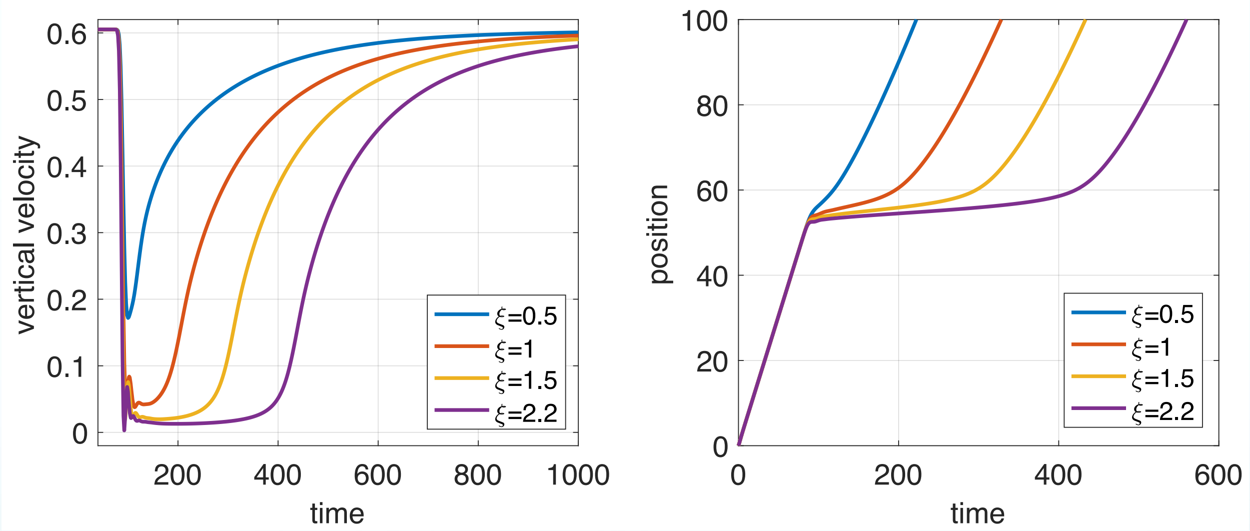
ξ = 1.5



Fitting formula for the delay: $t_{sim}(\xi) \approx t_{ref}(\xi) + 185\xi$

Effect of ξ on settling delay

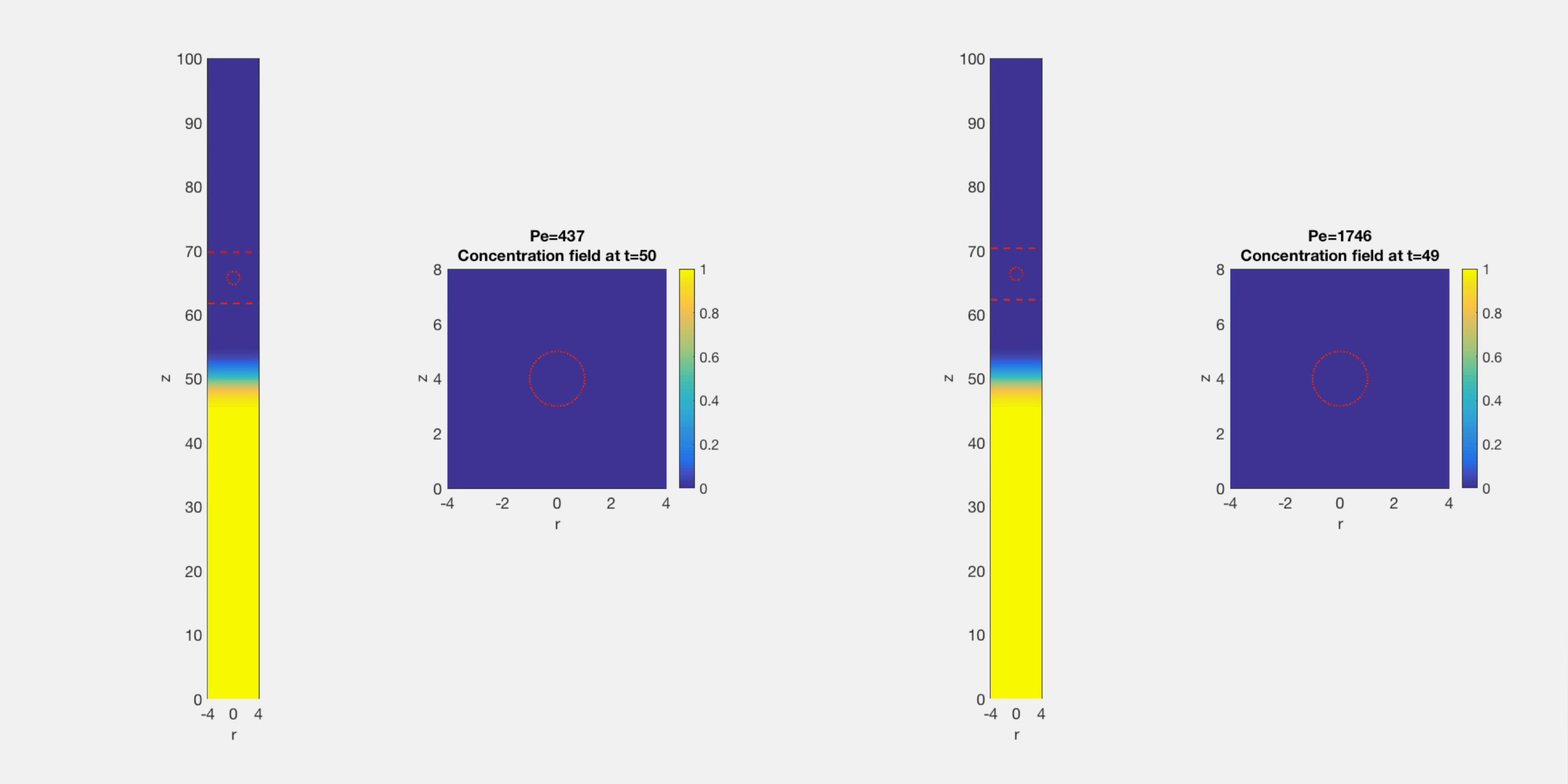
$$\xi = \frac{\rho_l - \rho_u}{(\rho_s - \rho_u)(1-\phi)}$$



Fitting formula: $t_{sim}(\xi) \approx t_{ref}(\xi) + 185\xi$

Sample simulations, two different *Pe*

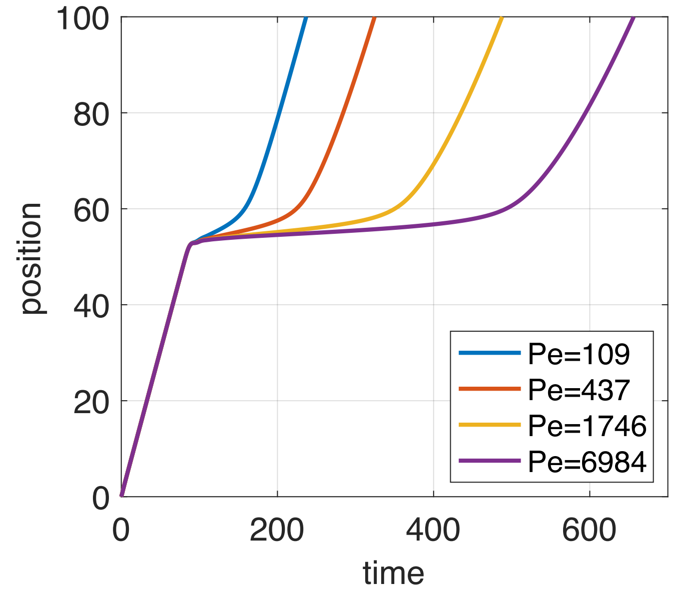
$Pe = 440$ $Pe = 1700$



Higher Pe implies slower diffusion, longer retention

Effect of *Pe* on retention time

Settling position vs time
for various *Pe*.



Larger *Pe* implies longer delays

Dependence on *Pe* is weaker than anticipated because of entrainment

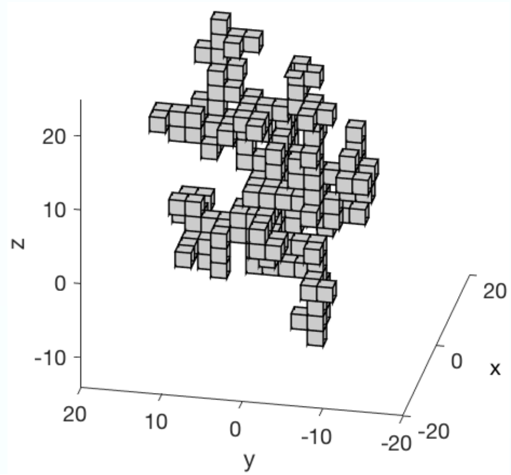
Fitting formula: $$t_{sim}(\mathrm{Pe}) \approx t_{ref}(\mathrm{Pe}) + 120\log(1+\frac{\mathrm{Pe}}{100})$$

We also quantified the effects of Re, Da, and transition thickness γ.
Varying one parameter at a time only, we find:

$$t_{sim} \approx t_{ref} + 125\xi\left[\log(1+Pe/100)\left(\frac{1}{1+0.024Re^{1/2}}\right)\left(\frac{1+0.042Re^{1.18}}{1+1700(ReDa)^{1.18}}\right)\left(1-\frac{0.225}{1+0.016\gamma^2}\right)\right]$$

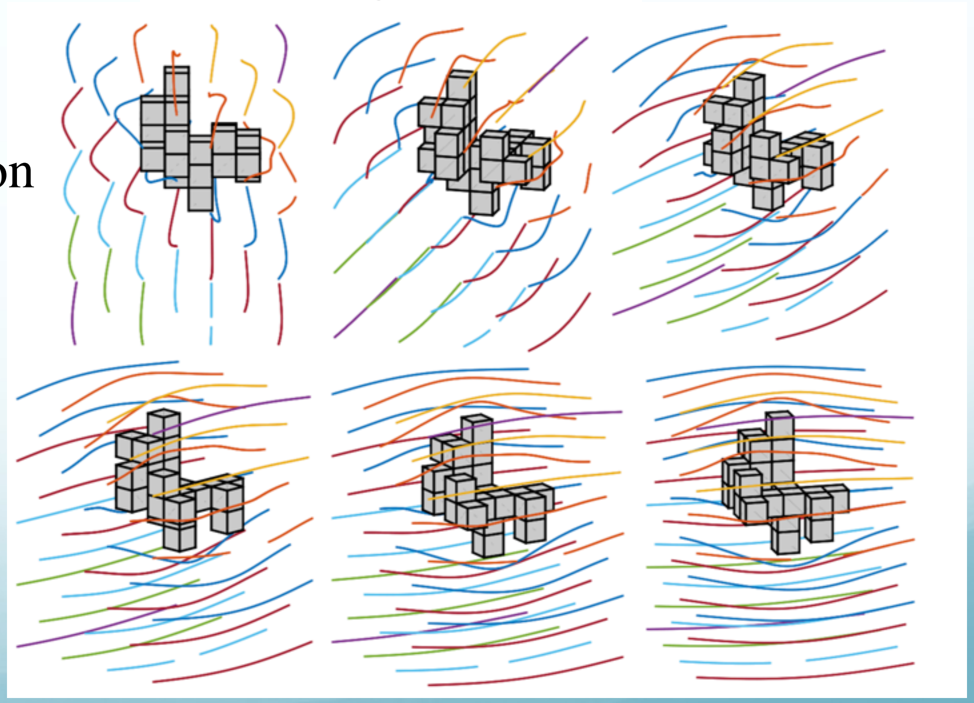
This remains to be verified when several parameters varied simultaneously.

Ongoing work: irregular objects



Fractal-shaped aggregate

- In reality, aggregates are far from spheres
- For small objects, we can compute flow around aggregated cubes
- We form aggregates as a collection of randomly moving cubes.
- We solve for the flow using a boundary integral methods
- One goal is to determine the equivalent sphere, to use our previous results.

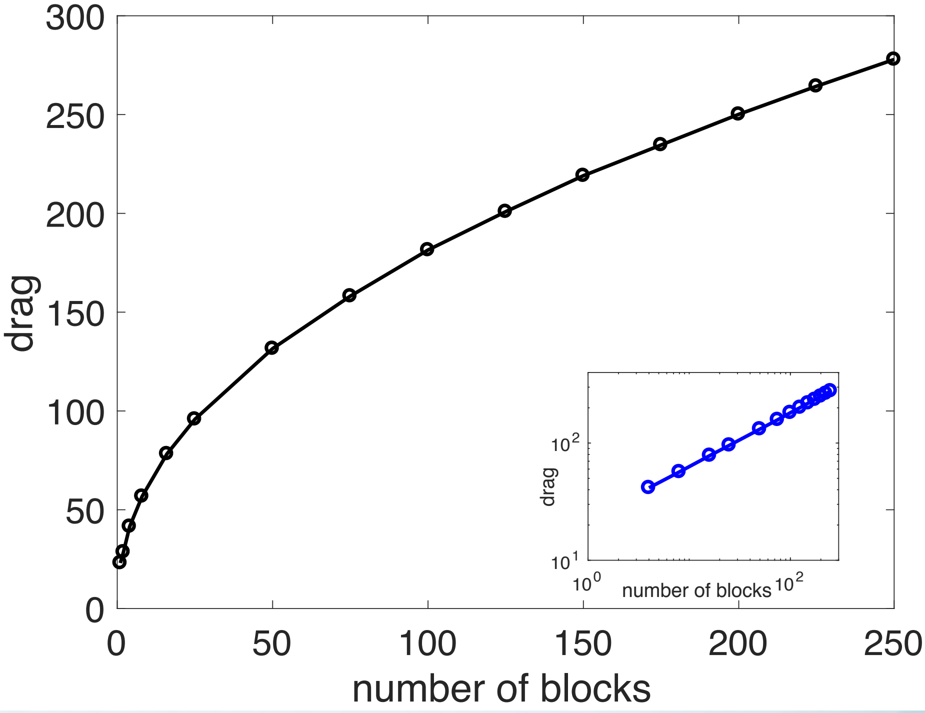


Flow past complex shape

Drag vs Mass relation

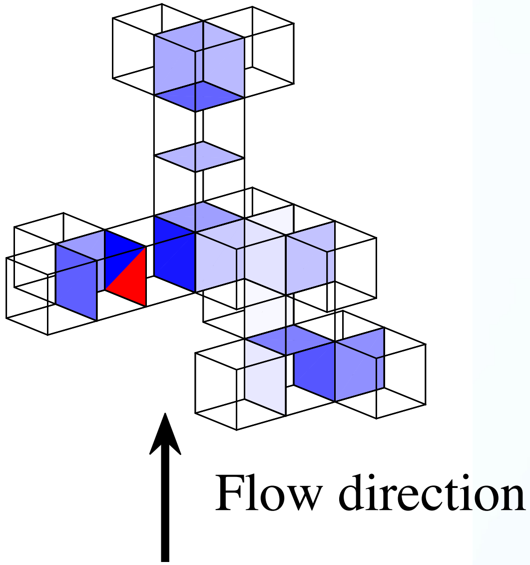
- A critical question is how fast do such particles settle.
- We compute the drag as a function of size of the aggregate
- We find Drag ~ $N^{0.46}$
- For a solid, we have Drag ~ $N^{1/3}$
- The drag will also depend on the exact aggregation mechanism,

Drag as a function of aggregate mass

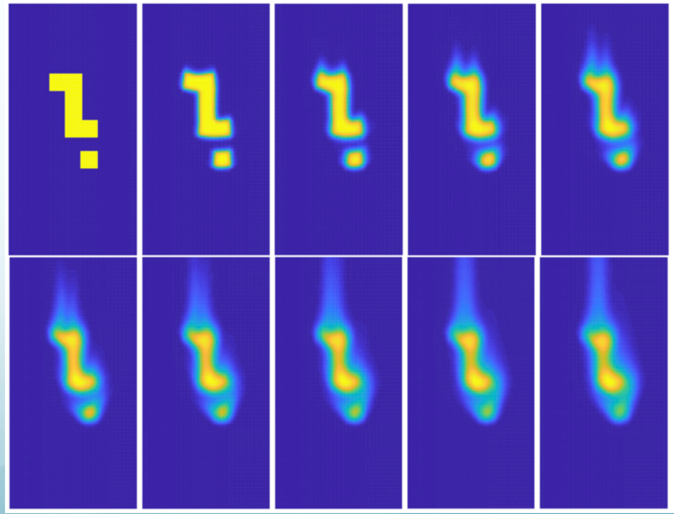


Aggregate dynamics

- We can now compute the evolution of aggregates
- What are the stresses on them? Do they break up?
- How are solutes diffusing in and out of them?
- The goal is to describe the entire formation process, more realistically than ever!



Internal stresses during settling



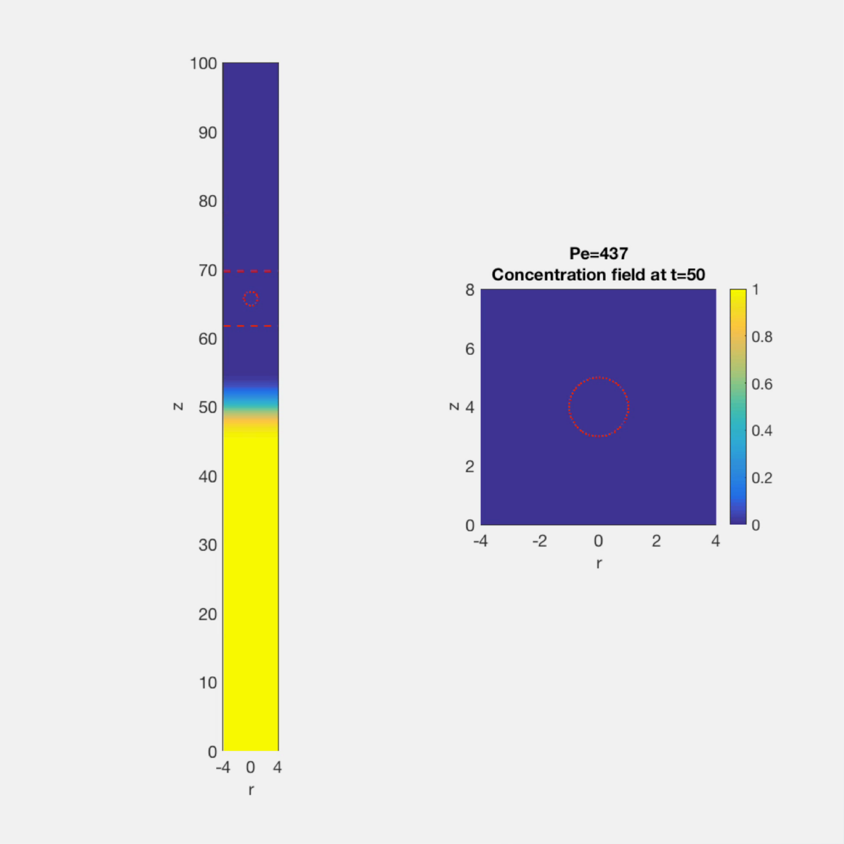
Evolution of a solute

Conclusions

When settling:

- Drops are subject to Marangoni effects, which can have a significant influence even when small

- Porous particles are influenced by diffusion of temperature/salt, which can result in lengthy stagnation.



Future/ongoing work:

- Incorporate stratification in aggregate simulations
- Use point-particles model that allow capture collective effects.

Conclusions

- We quantified the dominant dependencies of marine snow retention time:
  Linear in ξ, $\xi = \dfrac{\rho_l - \rho_u}{(\rho_s - \rho_u)(1-\phi)}$, Logarithmic in *Pe*.
- We quantified the effects of Re, Da, and transition thickness γ.

Varying one parameter at a time only, we find:

$$t_{sim} \approx t_{ref} + 125\xi \left[\log(1 + Pe/100)\left(\frac{1}{1+0.024Re^{1/2}}\right)\left(\frac{1+0.042Re^{1.18}}{1+1700(ReDa)^{1.18}}\right)\left(1 - \frac{0.225}{1+0.016\gamma^2}\right)\right]$$

This remains to be verified when several parameters varied simultaneously.

Our results have appeared in PRF.

Next steps

- Develop a more realistic model by
  - tracking individual point-particles position, velocity, density.
  - tracking the flow field around them
- Validate the model using detailed simulations
- Study fractal-like particles
- Use the model to characterize retention time more completely

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Continuum governing equations

T_f is a fluid temperature (defined everywhere)
T_s is a particle temperature (also defined everywhere)
All exchanges between solid and fluid are treated as sources/sinks.
Nu = Nusselt number = $\dfrac{\text{total heat flux}}{\text{unperturbed diffusive heat flux}}$

$$\frac{\partial T_f}{\partial t} + (\vec{u}_f \cdot \nabla) T_f = \alpha_f \nabla^2 T_f + \phi \frac{3\alpha_f Nu}{R^2}(T_s - T_f)$$

$$\frac{\partial T_s}{\partial t} + (\vec{u}_s \cdot \nabla) T_s = \frac{(\rho C_p)_f}{(\rho C_p)_s} \frac{3\alpha_f Nu}{R^2}(T_f - T_s)$$

Mean temperature (if $\phi \ll 1$, $Pe_s \ll 1$, $Re_p \ll 1$): $T = \frac{(\rho C_p)_s}{(\rho C_p)_f} \phi T_s + T_f$

$$\boxed{\frac{\partial T}{\partial t} + (\vec{u}_f \cdot \nabla) T + \frac{(\rho C_p)_s}{(\rho C_p)_f} \phi (U_s \hat{k} \cdot \nabla) T = \alpha_f \nabla^2 T}$$

Governing equations

- **Incompressible Navier-Stokes** in the fluid domain

$$\begin{aligned} \nabla \cdot \vec{u} &= 0 \\ \rho\Big(\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u}\Big) &= \nabla \cdot (-P\bar{\bar{I}} + \mu(\nabla \vec{u} + (\nabla \vec{u})^T)) + \vec{f} \end{aligned}$$

- **Brinkman** equation in the porous domain

$$\frac{\mu}{\kappa}\vec{u} = \nabla \cdot (-P\bar{\bar{I}} + \mu[\nabla \vec{u} + (\nabla \vec{u})^T]) + \vec{f}$$

- **Advection-Diffusion** for the soluble agent in the fluid

$$\frac{\partial c}{\partial t} + \vec{u} \cdot \nabla c = D\nabla^2 c$$

Natural applications

Sediments in the oceans

$\phi \approx 0.02$

$\varkappa_s / \varkappa_f \approx 1.5$

$U_s \approx 0.001$ m/s

$L \approx 100$ m

$\alpha_s \approx 4 \times 10^{-7}$ m^2/s

$Pe \approx 10^4$

Fly-ash in the atmosphere

$\phi \approx 10^{-6}$

$\varkappa_s / \varkappa_f \approx 30$

$U_s \approx 0.001$ m/s

$L \approx 1000$ m

$\alpha_s \approx 10^{-7}$ m^2/s

$Pe \approx 10^2$

Crystals in magma chambers

$\phi \approx 0.1$

$\varkappa_s / \varkappa_f \approx O(1)$

$U_s \approx 5 \times 10^{-7}$ m/s

$L \approx 1000$ m

$\alpha_s \approx 4 \times 10^{-7}$ m^2/s

$Pe \approx 10^2$

In all 3 systems, in the absence of convection, settling particles can be the dominant mode of heat transport.

$$Pe = \phi \frac{\kappa_s}{\kappa_f} \left(\frac{L}{R} \right) Pe_s = \phi \frac{\kappa_s}{\kappa_f} \left(\frac{L}{R} \right) \frac{U_s R}{\alpha_s}$$

Tracking individual particles

We now track individual particles to allow:

- Inertial effects (history dependent settling speed)
- Temperature differences between particles and fluid

We want to know:

- Do settling particles erode temperature gradients as they settle?
- Can larger particles heat a gradient from below?

Non-dim. #	Definition	Range
Re_p	$U_s R \rho_0/\mu$	$0.4 - 400$
Re	$U_s H \rho_0/\mu$	$1000 - 40,000$
Pe	$U_s H/\alpha$	$1000 - 40{,}000$
Fr^2	$U_s^2/Hg\frac{\Delta\rho}{\rho_0}$	$0.01 - \infty$
P	$\frac{\rho_p (C_p)_p}{\rho_0 C_p}\frac{Pe}{3Nu}(\frac{R}{H})^2$	$0.05 - 20$
A	$\frac{\rho_p (C_p)_p}{\rho_0 C_p}$	$0.05 - 1000$
Nu	total heat flux/ conductive heat flux	$6 - 14$
C_D	Drag coefficient	$2 - 32$
B	$\frac{\rho_p - \rho_0}{\Delta\rho}$	$200 - \infty$

Numerical Simulations

- Incompressible Navier-Stokes (NS) for all three fluids.

- Drop interface moves with the fluid.

- Advection-diffusion for the temperature.

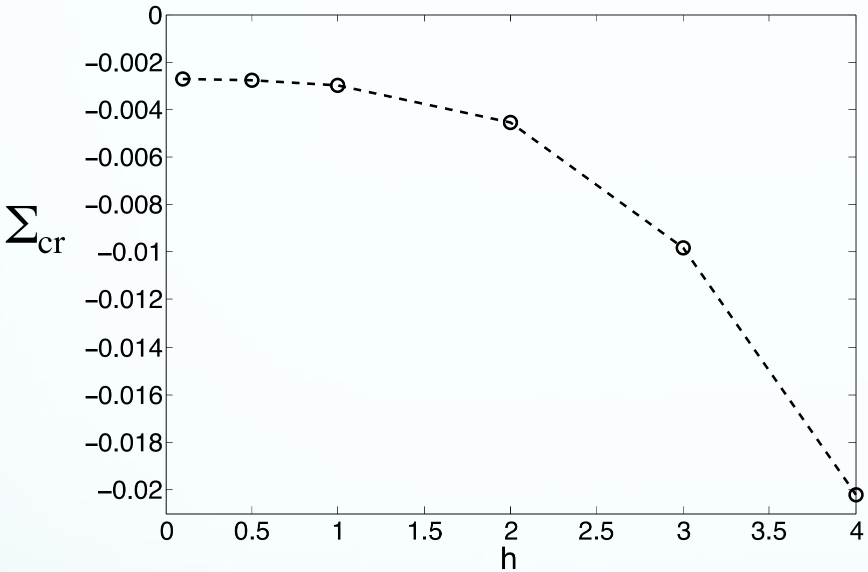
- We non-dimensionalize using: ρ of the drop,
  U_s the Hadamard-Rybczinskii settling speed
  R the drop radius.

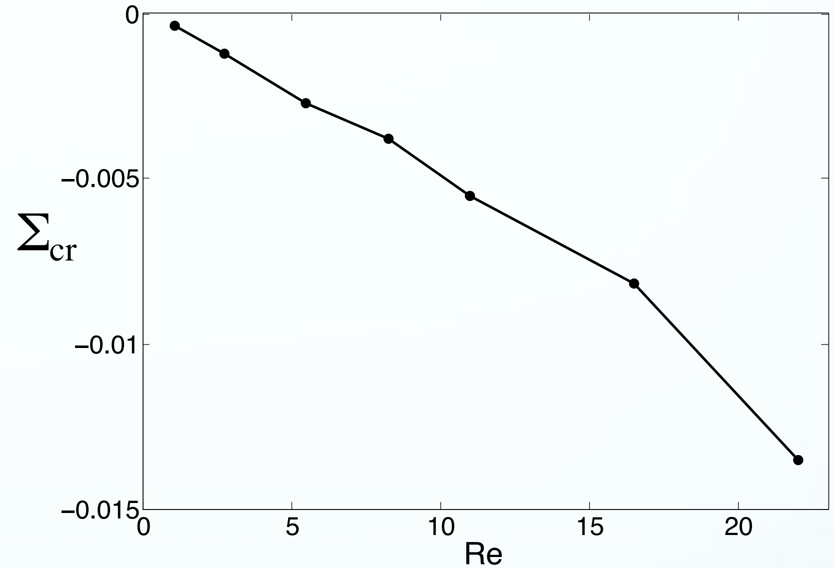
- Solve NS over the whole domain, supplemented of a forcing term on the interface

- We use an axisymmetric domain, with walls far enough away that they do not influence the dynamics.

Our numerical method is based on that of Popinet & Zaleski (1999)

How does Σ_{cr} depend on flow conditions?



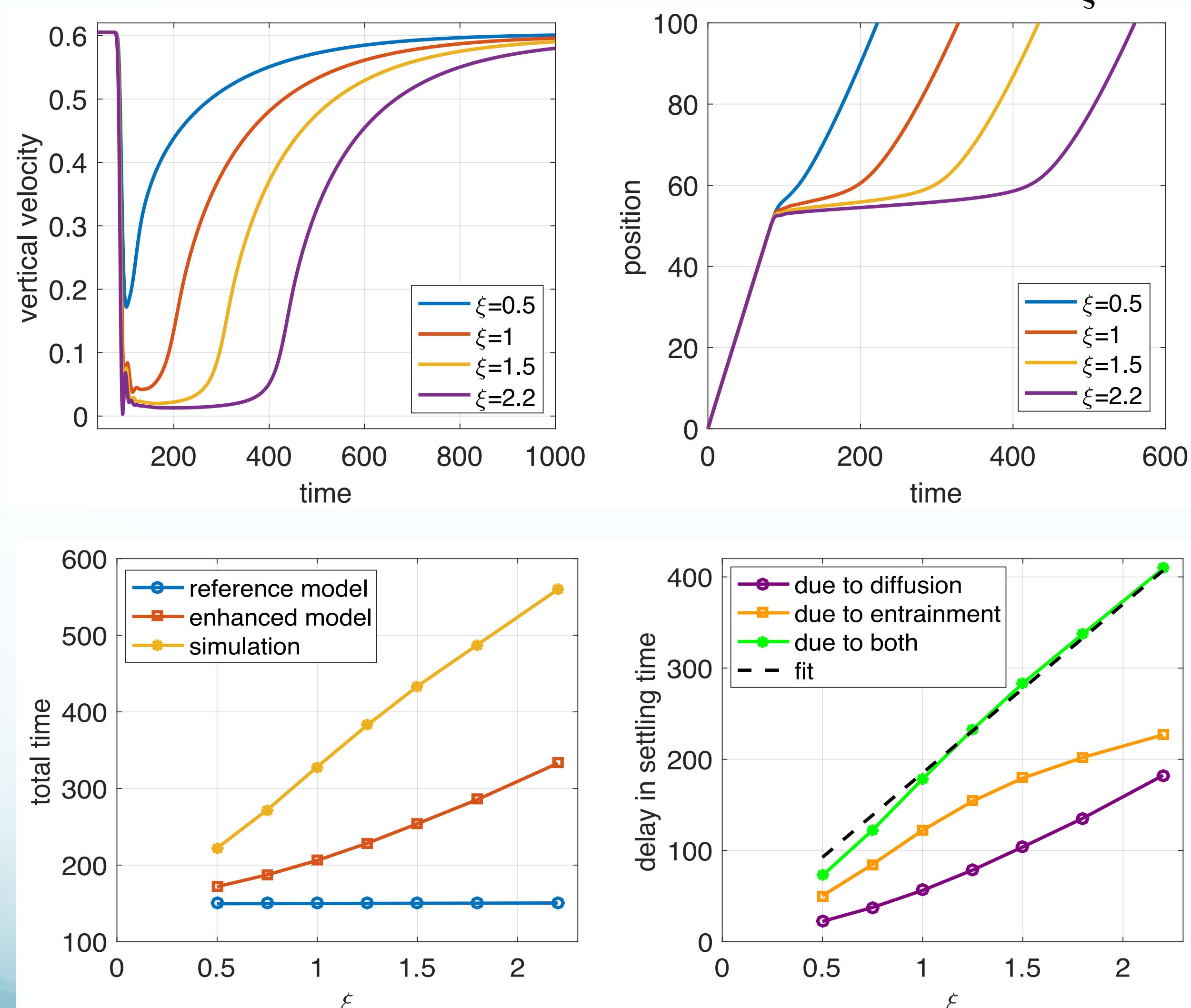


- The dependence on transition thickness h is (still) weak if $h \leq 2$

- The dependence on settling Reynolds number is nearly linear.
  this confirms the direct competition between gravity and Marangoni effects

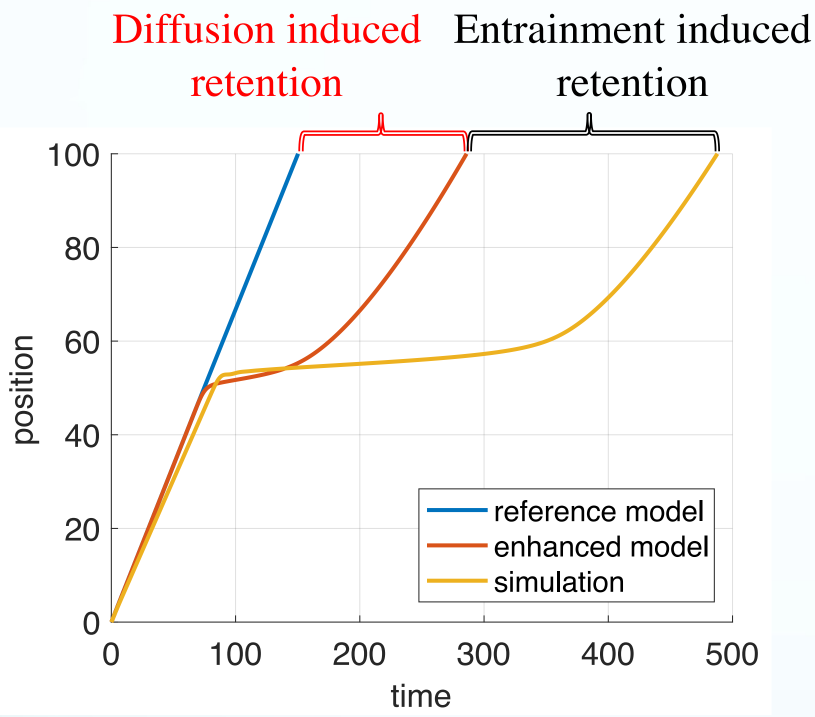
Effect of ξ on settling delay

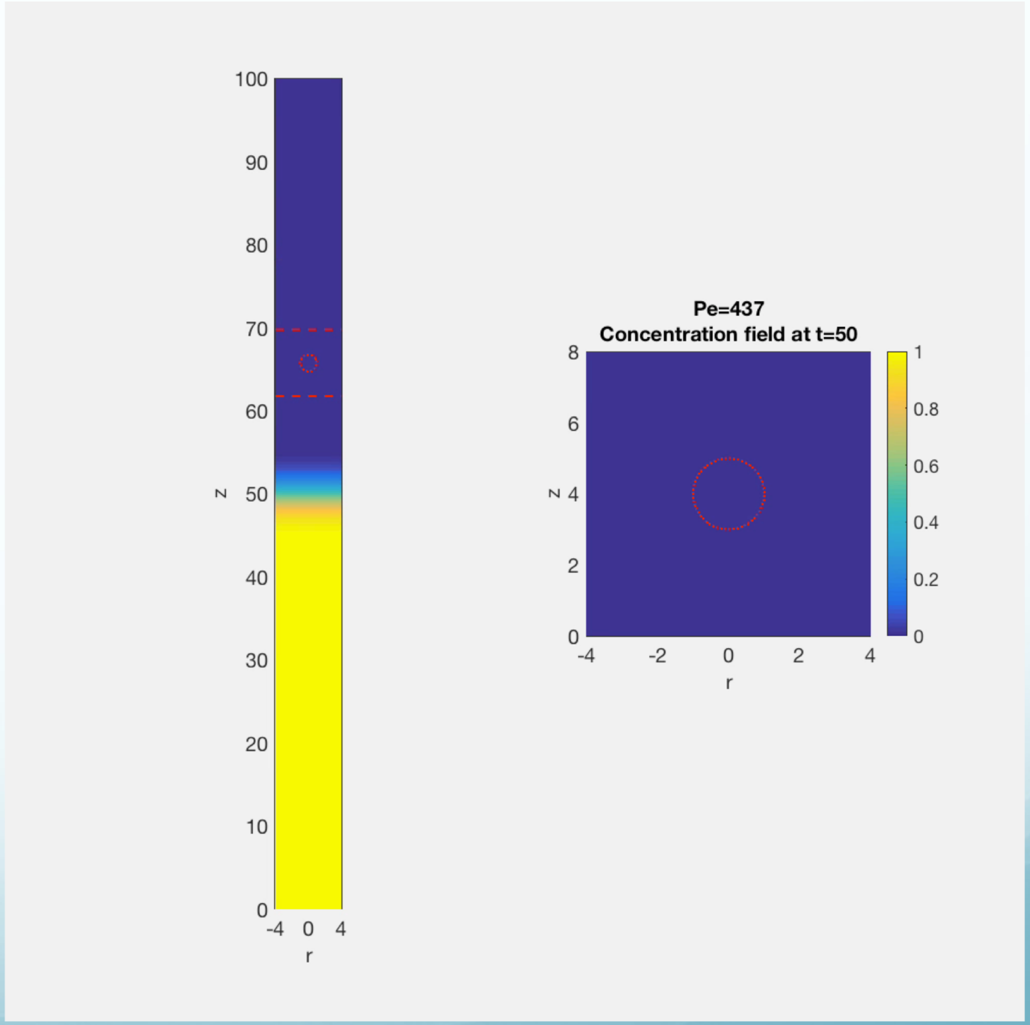
$$\xi = \frac{\rho_l - \rho_u}{(\rho_s - \rho_u)(1 - \phi)}$$



Fitting formula: $t_{sim}(\xi) \approx t_{ref}(\xi) + 185\xi$

Quantifying retention





Reference parameters

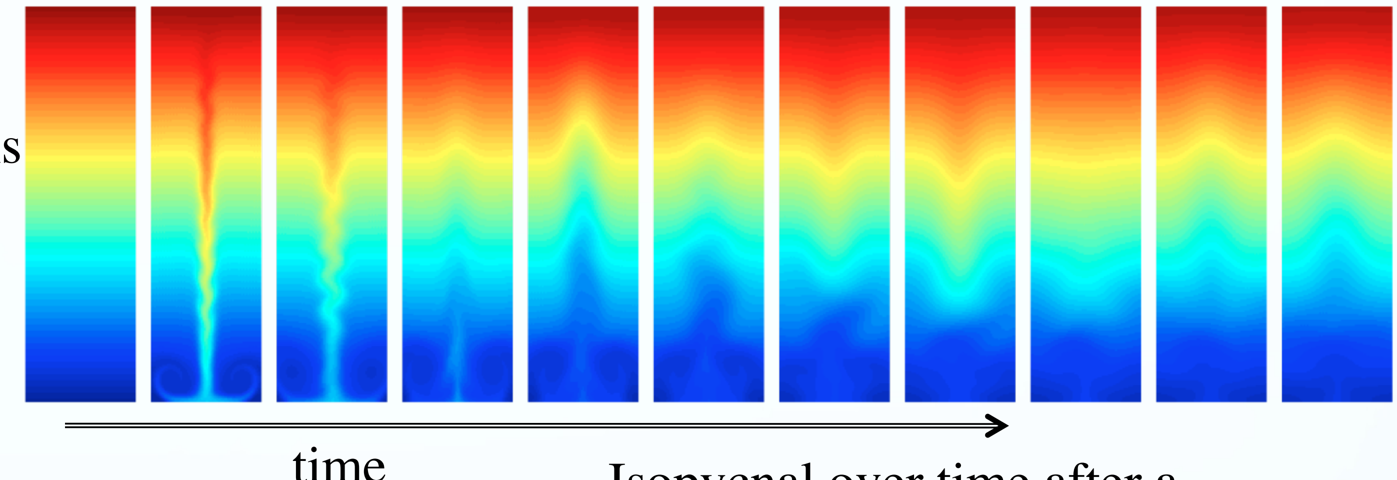
$$
\begin{aligned}
Re &= 4 \\
Pe &= 440 \\
Da &= 5 \times 10^{-4} \\
\xi &= 1.8 \\
\gamma &= 11.6
\end{aligned}
$$

Effect of a single particle

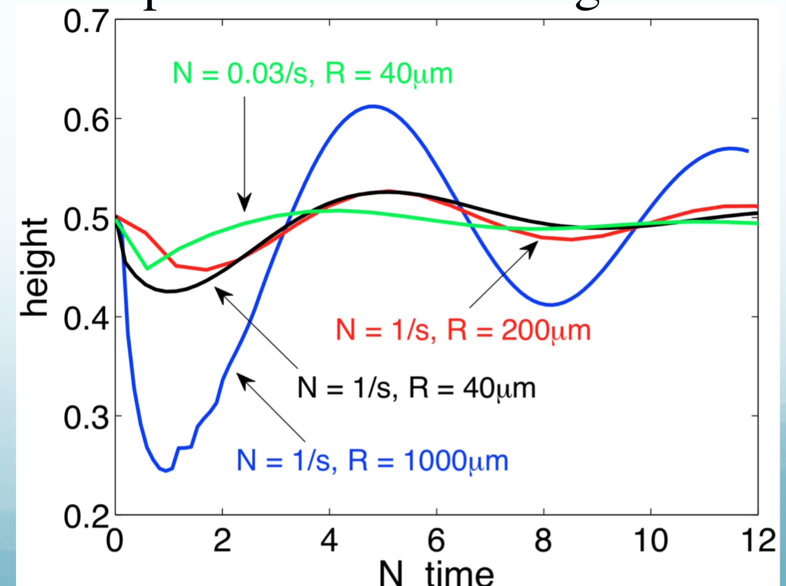
A single particle triggers oscillations of frequency

$$N = \left(\frac{g\Delta\rho}{H\rho_0} \right)^{1/2}$$

Temperature profile



Isopycnal over time after a particle settles through



The frequency is independent of size.

The amplitude increases with size.

Summary

• Drops settling in a sharp stratification are dramatically slowed by lighter fluid entrained into denser fluid.

•This phenomena is remarkably robust to variations in transition thickness.

• A lower layer with smaller surface tension significantly accelerates a settling drop.

• A lower layer of larger surface tension can stop settling drops.

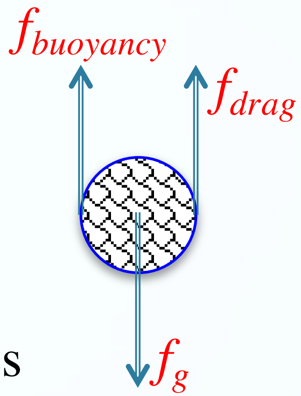
• We can find a critical surface tension variation for hovering.

• Σ_{cr} varies linearly with drop Reynolds number

• Drops eventually fall through once the transition ceases to be sharp.

• Small variations in surface tension matter.

Mathematical models



1) Reference model

Assumes: - Empirical drag, based on Reynolds number
- Constant excess density of the particle
- No perturbations to the initial density profile
- Instantaneous diffusion: inner fluid density always matches outer fluid density

2) Enhanced model

Assumes: - Empirical drag, based on Reynolds number
- No perturbations to the initial density profile
- Inner fluid density changes as salt diffuses in from initial profile

Enhanced Model from:
R. Camassa , S. Khatri , R. M. McLaughlin , J. C. Prairie , B. L. White, Phys. Fluids 25, 081701 (2013)

Only simulations account for the entrained fluid, which affects

Buoyancy

Diffusion time