

Moving from batch to continuous processes

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Numerical Investigation of Laminar Liquid-Mixing Efficiency for Nanoparticle Synthesis

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PI Institute for Energy
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EM PARTICLE SCIENCE AND
TECHNOLOGY
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From a turbulent gas-phase CFD perspective (e.g. c

- The scalar spectrum extends to the **Batchelor length**
- At high Sc , Batchelor scales can be **far smaller than**

$$\eta_B \propto \eta_K Sc^{-1/2} \quad (\text{Similar for Prandtl-Number})$$

- Mixing layers are thin, but **not interfaces!** (no VOF,
- Direct Numerical Simulation (DNS) gets extremely e

	Sc
Liquid	600-3000
Particles	10^2 - 10^6

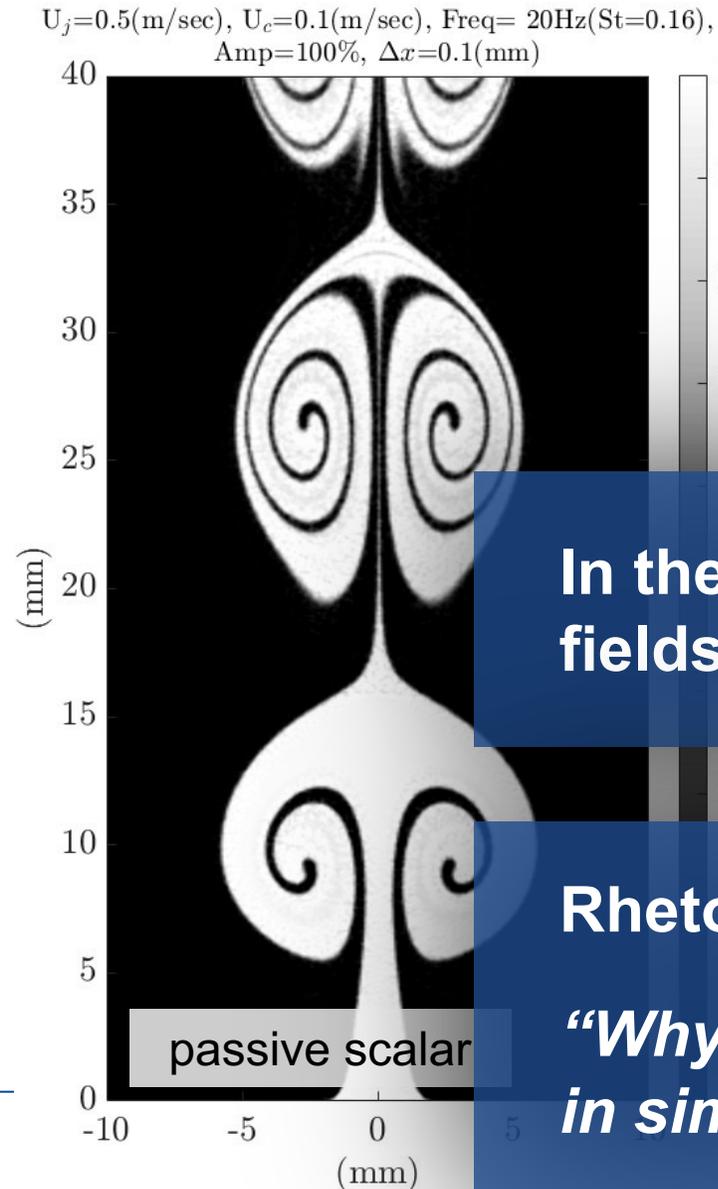


Example: Pulsed Laminar Jet ($Sc = 1000, Re < 50$)

Here (2D):

The computational cost is increased by **~30.000** due to the high Schmidt number.

In 3D, the cost would even increase by **~1.000.000** due to the Schmidt number.



$U_j=0.5(\text{m/sec}), U_c=0.1(\text{m/sec}),$
 $\text{Amp}=100\%, \Delta x=0.1(\text{mm})$



High resolution is needed only locally!

→ New approach!

In the gas phase, velocity and scalar fields would be similar...

Rhetorical question:

“Why does CFD appear far more developed in simulations of gas phase combustion?!”

Inspiration: Reynolds-Decomposition $u = \bar{u} + u'$

The scalar field Φ and the equation are decomposed: $\Phi = \Phi_L + \Phi_H$

$$\frac{\partial \Phi}{\partial t} + \frac{\partial \Phi u_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\nu}{Sc} \frac{\partial \Phi}{\partial x_i} \right) \rightarrow \frac{\partial(\Phi_L + \Phi_H)}{\partial t} + \frac{\partial(\Phi_L u_i + \Phi_H u_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\nu}{Sc} \frac{\partial(\Phi_L + \Phi_H)}{\partial x_i} \right) \rightarrow \quad (1)$$

$$\frac{\partial \Phi_L}{\partial t} + \frac{\partial \Phi_H}{\partial t} + \frac{\partial \Phi_L u_i}{\partial x_i} + \frac{\partial \Phi_H u_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\nu}{Sc} \frac{\partial \Phi_L}{\partial x_i} \right) + \frac{\partial}{\partial x_i} \left(\frac{\nu}{Sc} \frac{\partial \Phi_H}{\partial x_i} \right) \quad (2)$$

$$\frac{\partial \Phi_L}{\partial t} + \frac{\partial \Phi_L u_i}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\frac{\nu}{Sc} \frac{\partial \Phi_L}{\partial x_i} \right) = \frac{\partial \Phi_H}{\partial t} + \frac{\partial \Phi_H u_i}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\frac{\nu}{Sc} \frac{\partial \Phi_H}{\partial x_i} \right) := 0 \quad (3)$$

$$\Phi = \Phi_L + \Phi_H$$

This can be satisfied by any Φ_L and Φ_H \longrightarrow

$$\begin{cases} \frac{\partial \Phi_L}{\partial t} + \frac{\partial \Phi_L u_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\nu}{Sc} \frac{\partial \Phi_L}{\partial x_i} \right) \\ \frac{\partial \Phi_H}{\partial t} + \frac{\partial \Phi_H u_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\nu}{Sc} \frac{\partial \Phi_H}{\partial x_i} \right) \end{cases}$$

- **Low-wave-number** part is transported in the **Eulerian** framework using conventional FVM.
- **High-wave-number** part is transported in the **Lagrangian** framework using particles.

$$\Phi = \Phi_L + \Phi_H$$

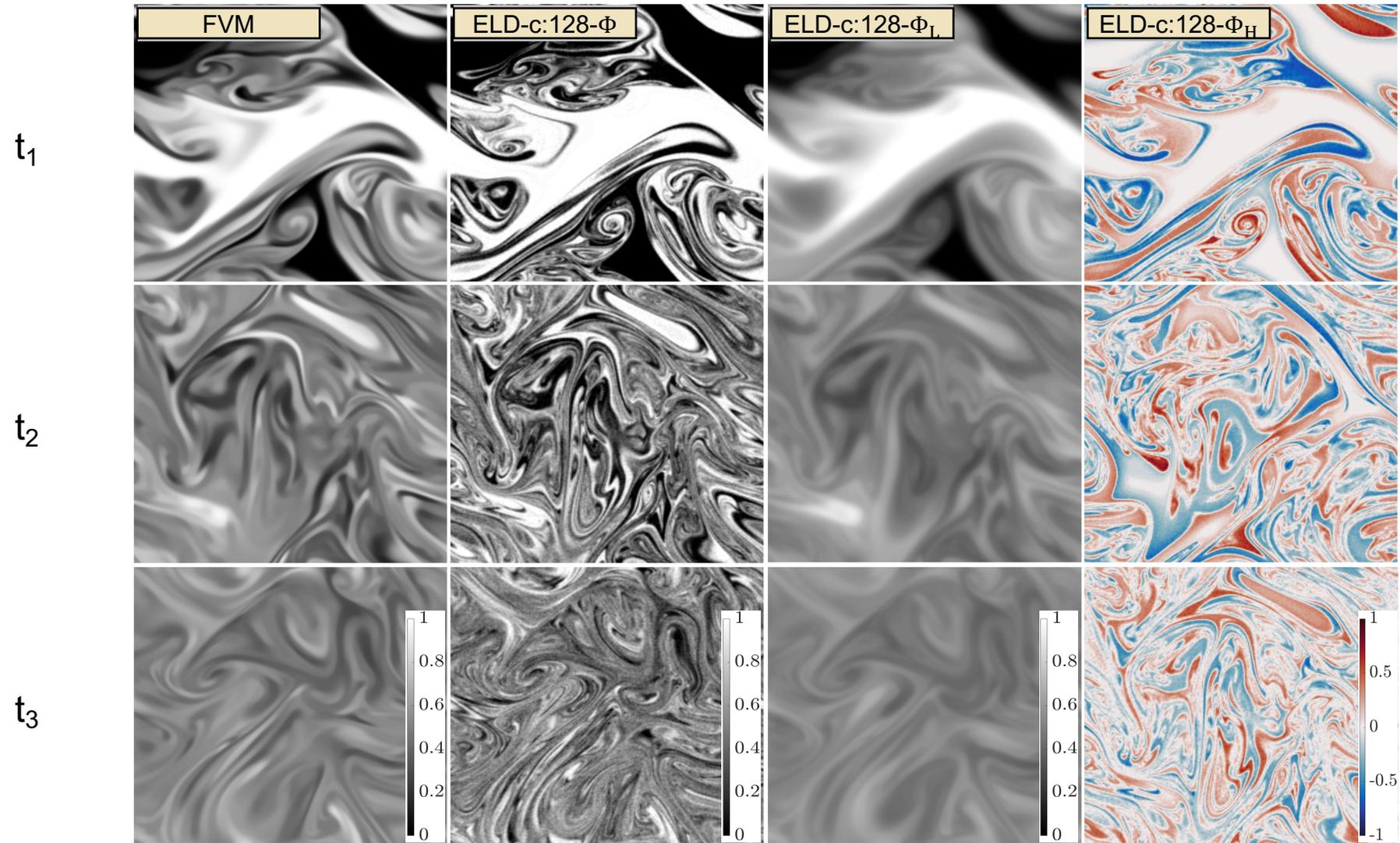
→
$$\frac{\partial \Phi_L}{\partial t} + \frac{\partial \Phi_L u_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\nu}{Sc} \frac{\partial \Phi_L}{\partial x_i} \right)$$

→
$$x_{p,i}(t + \delta t) = x_{p,i}(t) + u_i(t)\delta t + W_{p,i} \sqrt{\frac{2\nu}{Sc}} \delta t$$

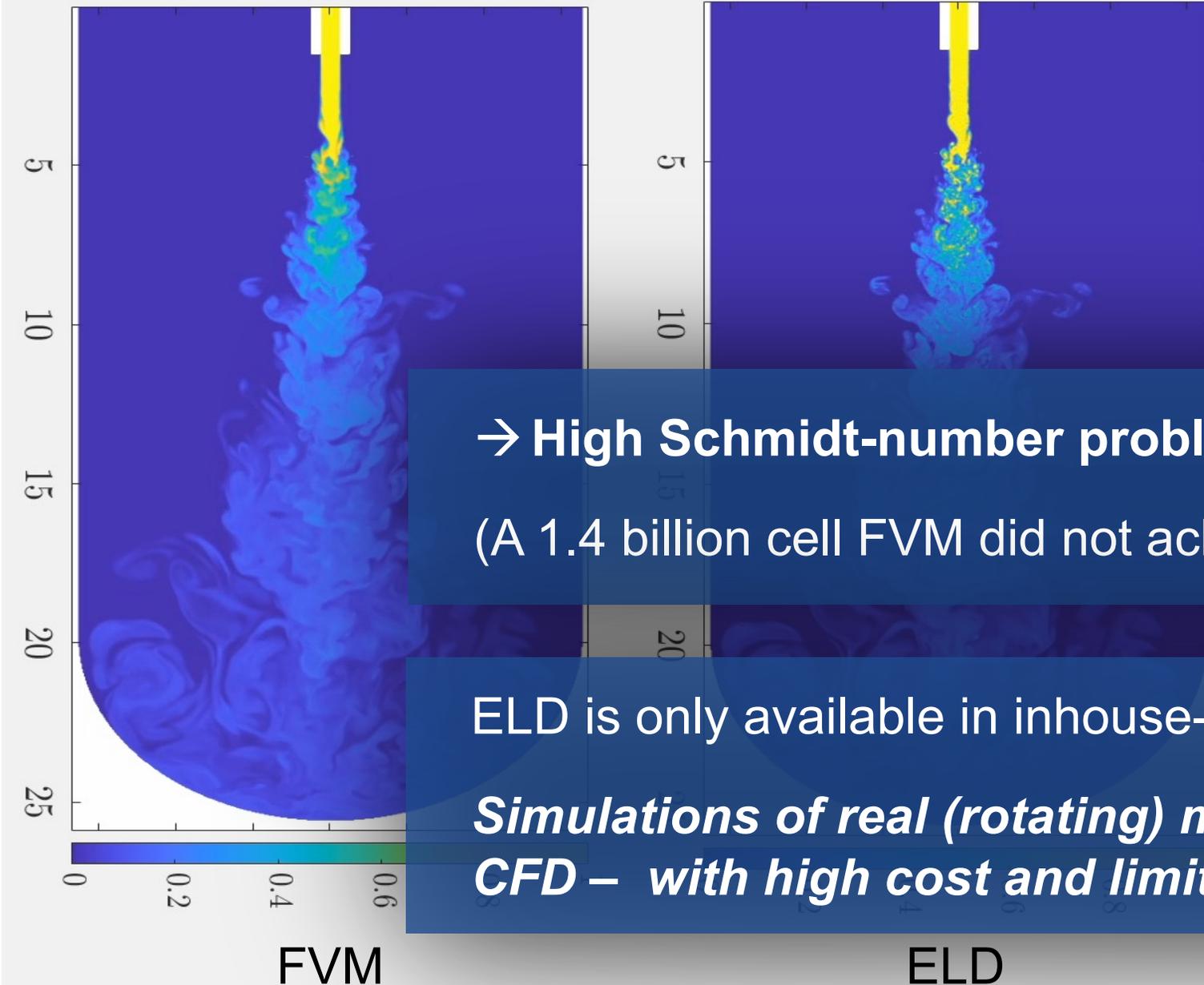
Important:

We resolve small scales — no turbulence closure here!

One way for dealing with high Schmidt numbers (3)



Example: Injection in test-tube (3D, ~170M cells)



→ High Schmidt-number problems are **REALLY** hard!
(A 1.4 billion cell FVM did not achieve similar resolution.)

Note: The timestep-width depends on CFL.

The timestep-width

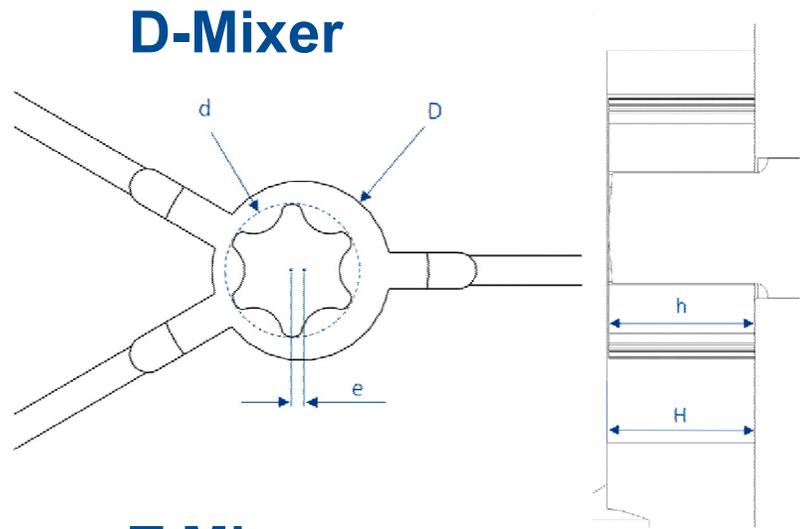
ELD is only available in inhouse-code PsiPhi yet

Simulations of real (rotating) mixers still require conventional CFD – with high cost and limited resolution.



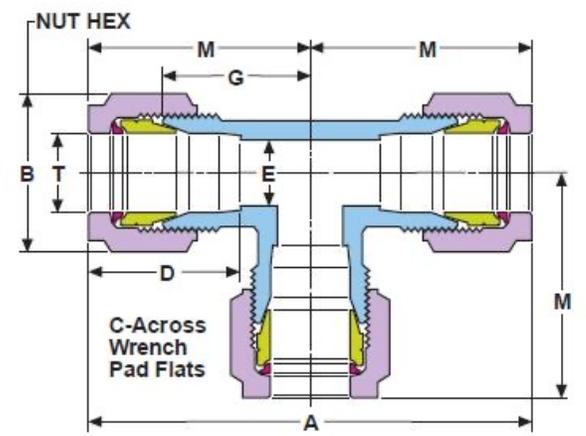
- The mixing of two liquids to synthesize nanoparticles
 - solution 1: indium chloride (InCl_3) and oleylamine
 - solution 2: zinc chloride (ZnCl_2), tris(dimethylamino)phosphine ($\text{P}(\text{Net}_2)_3$), and oleylamine
- At **low Reynolds** number (laminar regime) and **high Schmidt** number
- Heat the mixture up to about 200 °C to form quantum dots (InP)

Goal of mixing:
A homogeneous mixture for (InP) quantum dot formation



D	3.4 mm	H	1.25 mm
d	2.512 mm	h	1.245 mm
e	≈ 0.2 mm		

T-Mixer



A	39.624 mm	D	10.414 mm
B	7.9375 mm	E	1.27 mm
C	11.1125 mm	G	14.224
M	19.812 mm		

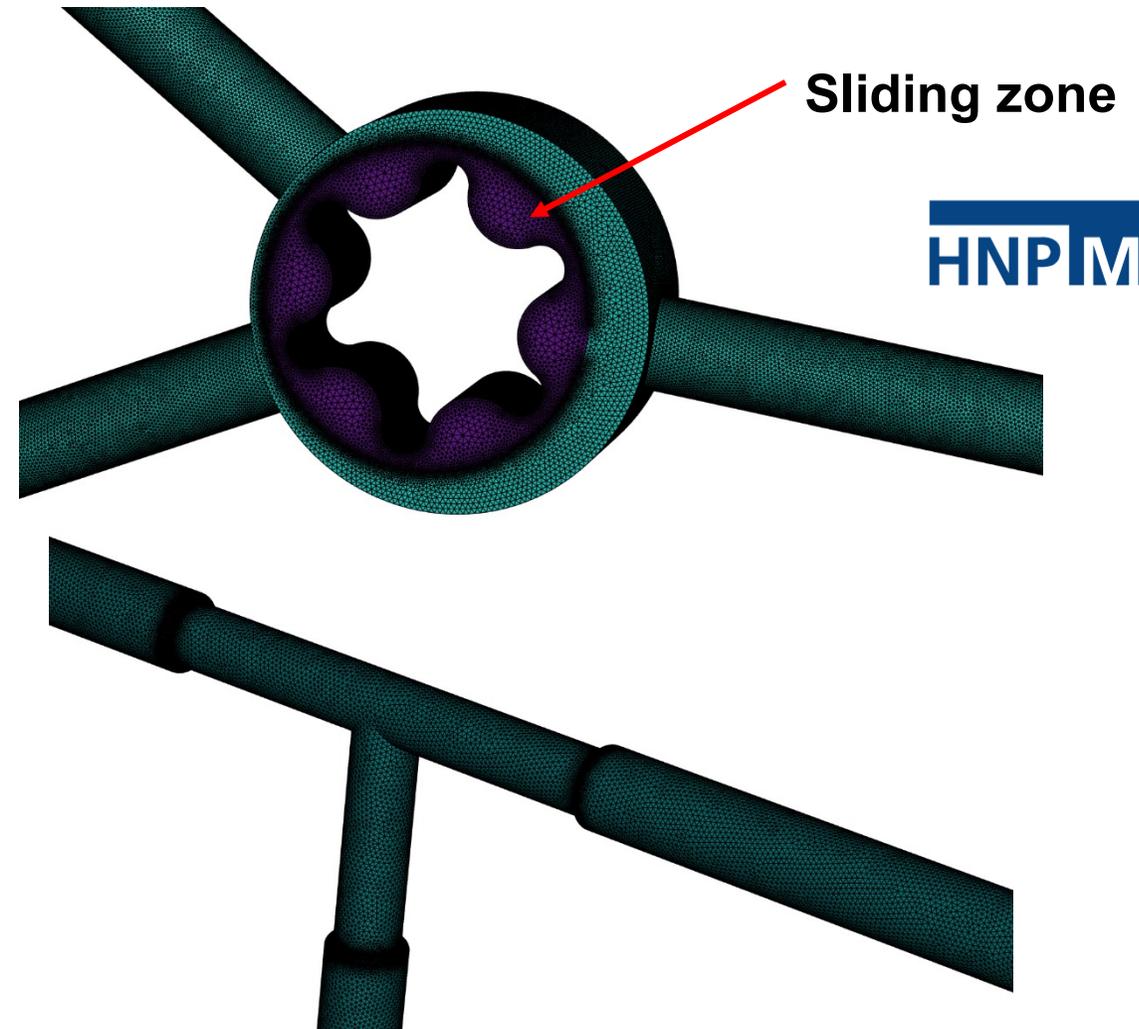
Ansys Fluent

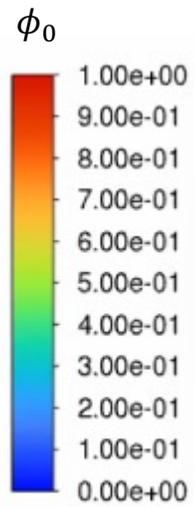
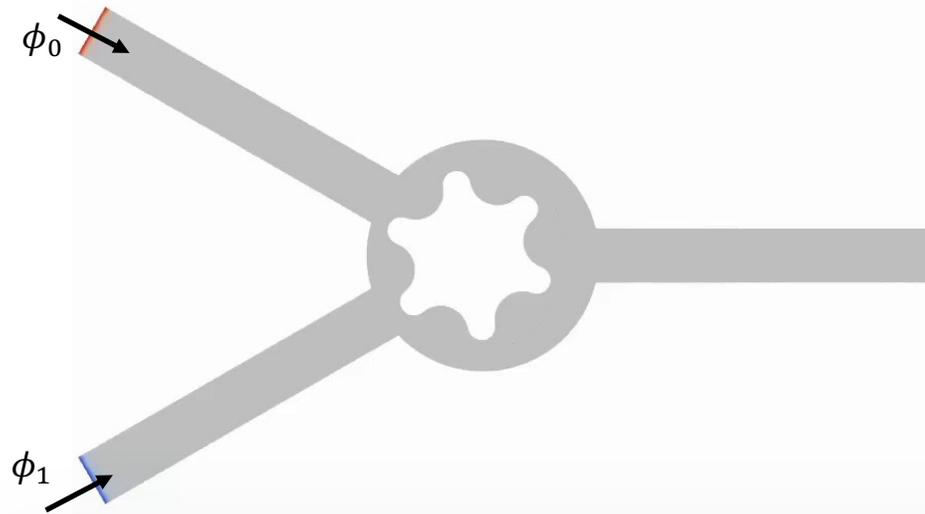
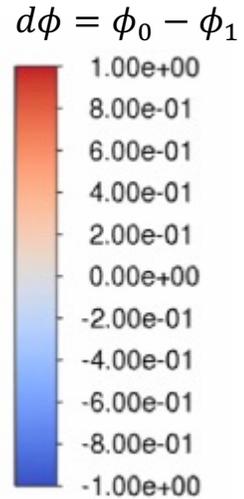
$$\frac{\partial \rho \phi_k}{\partial t} + \frac{\partial}{\partial x_i} \left(\rho u_i \phi_k - \Gamma_k \frac{\partial \phi_k}{\partial x_i} \right) = S_{\phi_k}, k = 1 \dots N$$

$\Gamma = \frac{\mu}{\rho D}$: Diffusion coefficient

S_{ϕ_k} : Source term

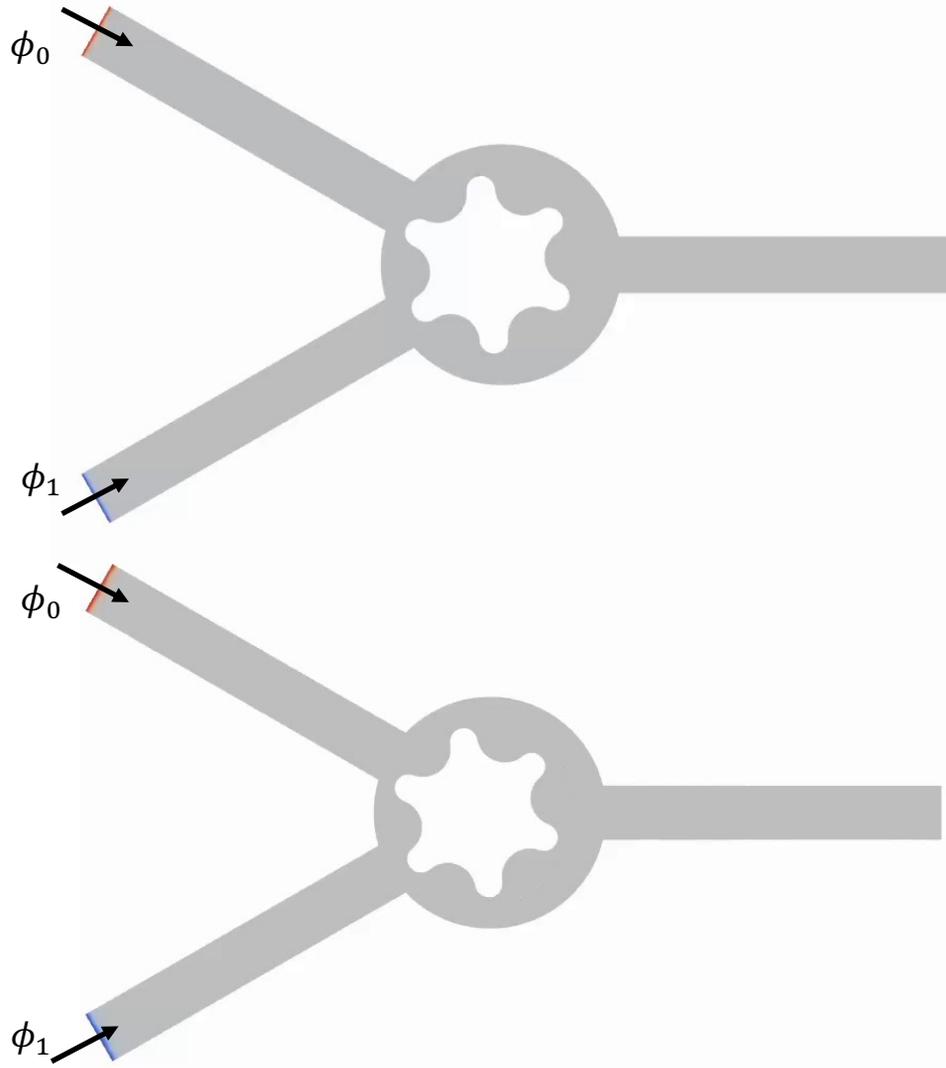
Test cases	Mesh size
D-mixer, Coarse	0.24 mcells
D-mixer, Fine	2.6 mcells
T-mixer	1.14 mcells



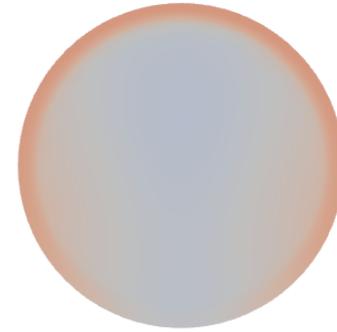
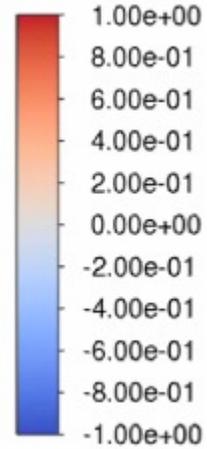


- „Fairly good“ mixing →
- Near wall region „less critical“ due to low velocity

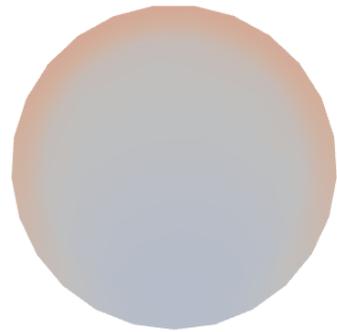
Grid Refinement (~ factor 11)



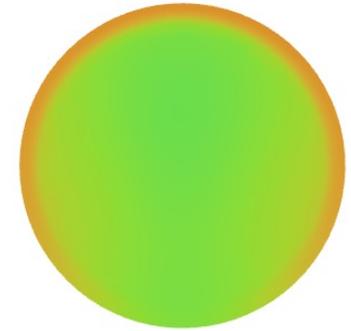
$$d\phi = \phi_0 - \phi_1$$



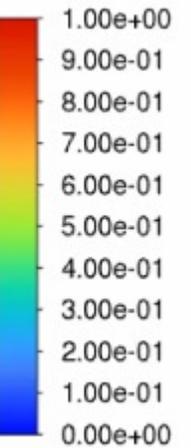
Fine



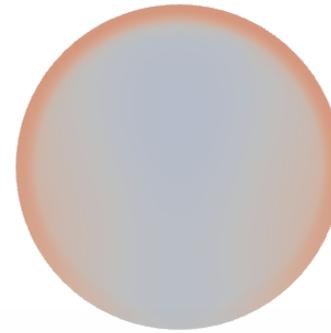
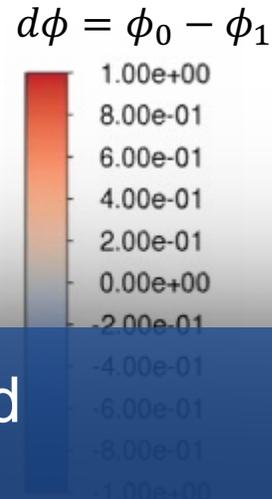
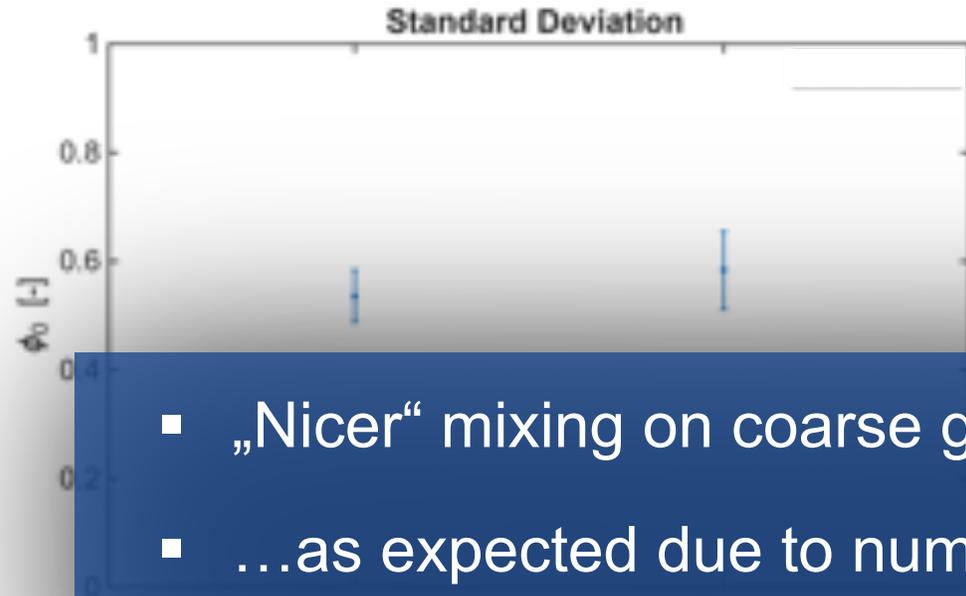
Coarse



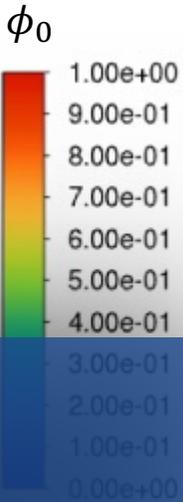
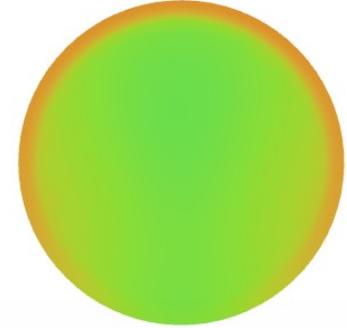
$$\phi_0$$



10000 rpm, $\dot{V}_{\phi_0} = \dot{V}_{\phi_1} = 0.2 \text{ mL/s}$



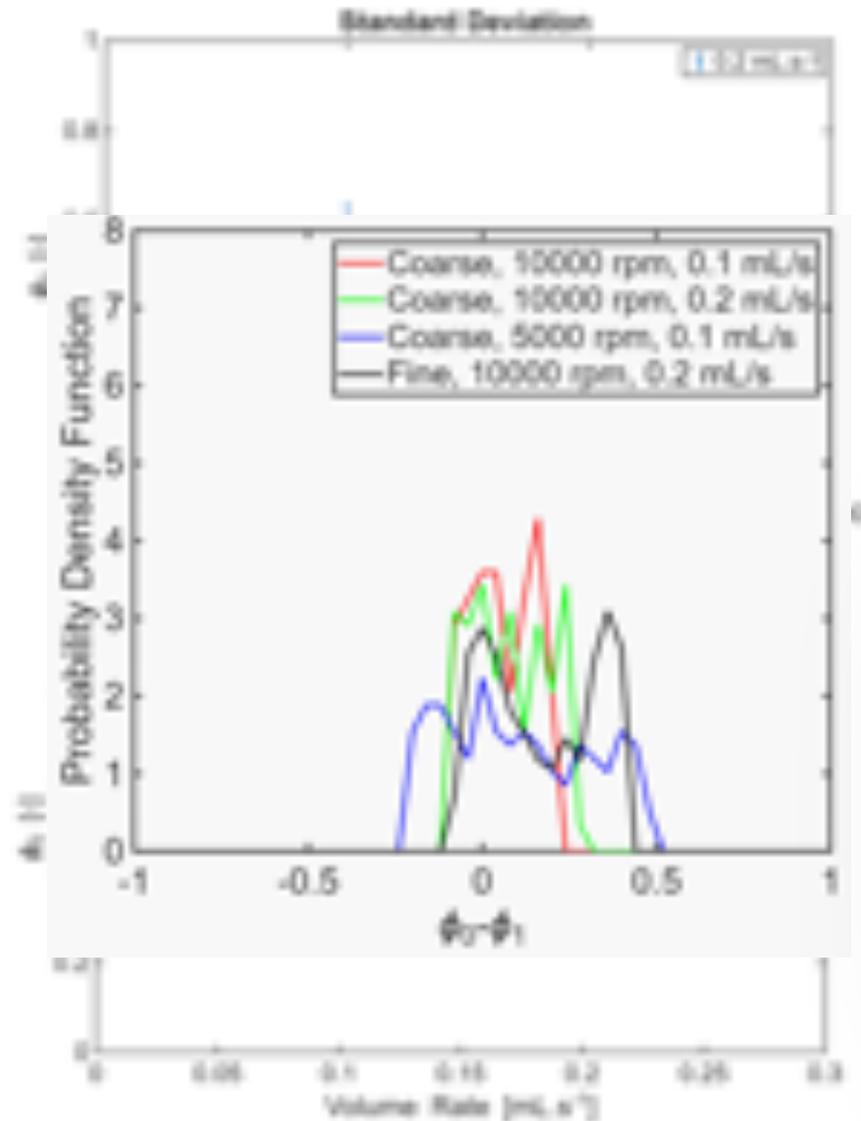
Fine



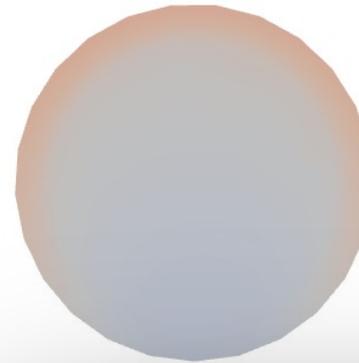
- „Nicer“ mixing on coarse grid
- ...as expected due to numerical diffusion at high Sc

Caveat: Simulation results should be considered „best case scenario“

Coarse



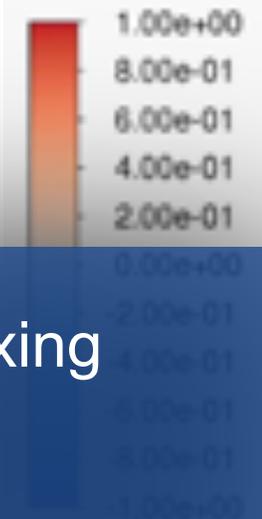
10000 rpm, 0.2 mL/s



5000 rpm, 0.2 mL/s

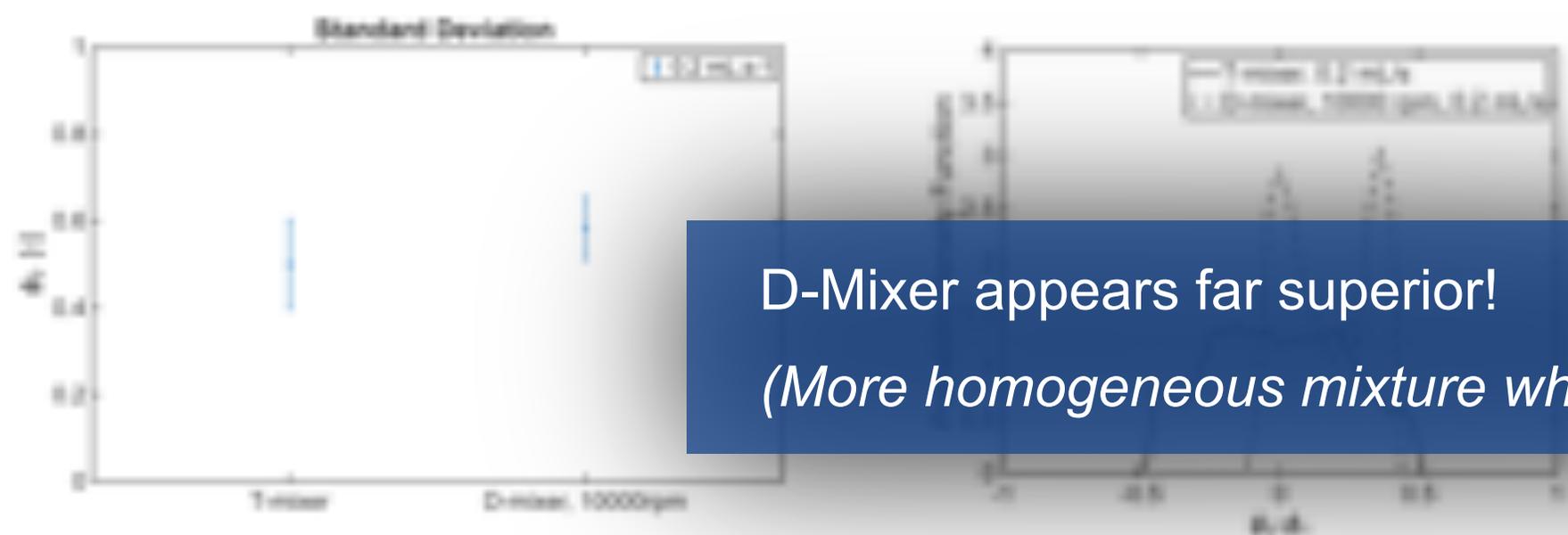
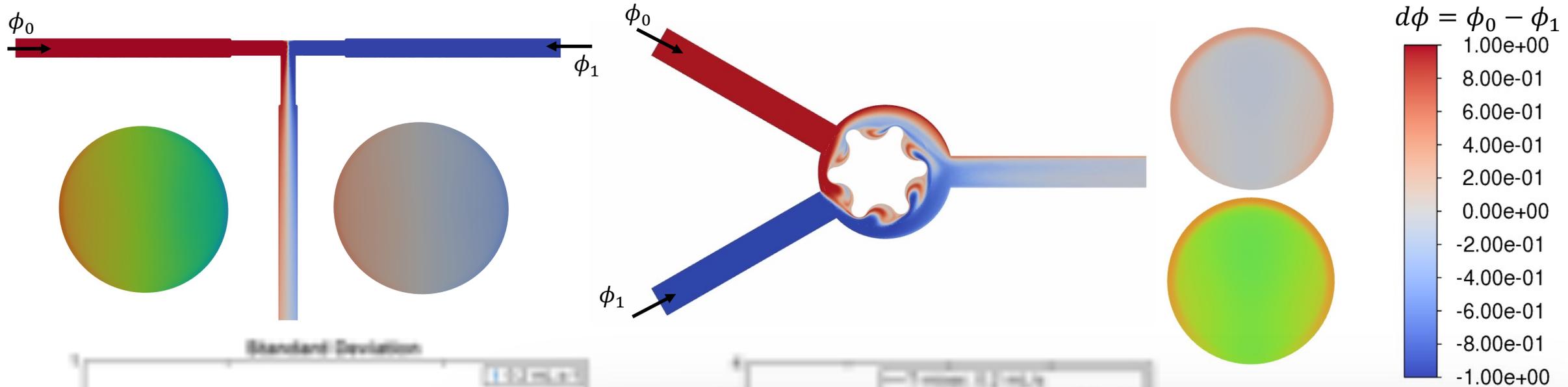


$$d\phi = \phi_0 - \phi_1$$



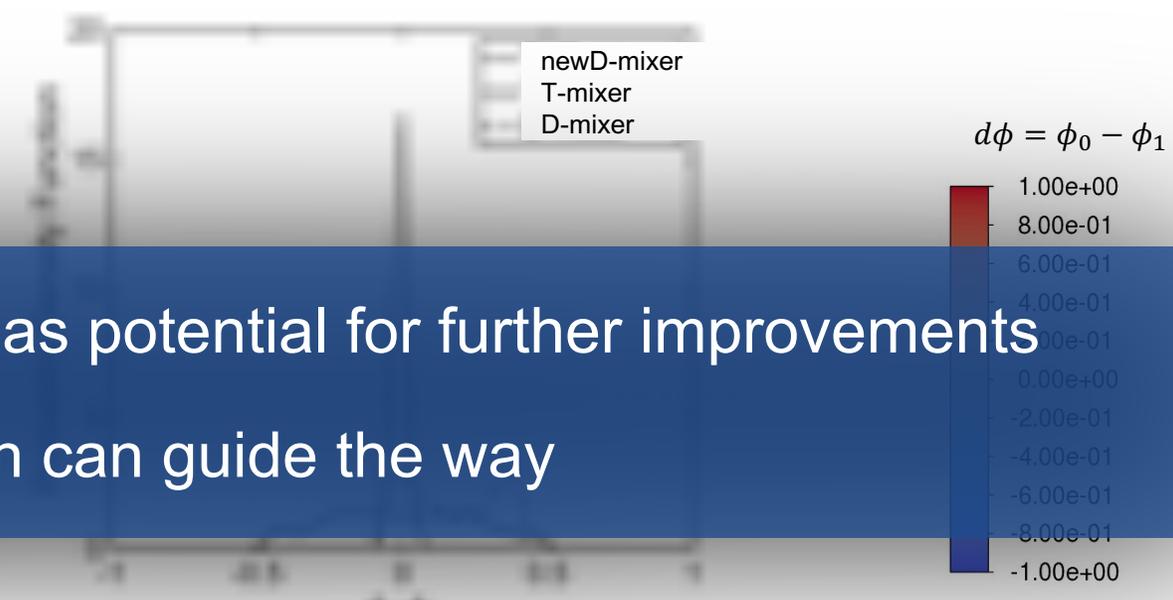
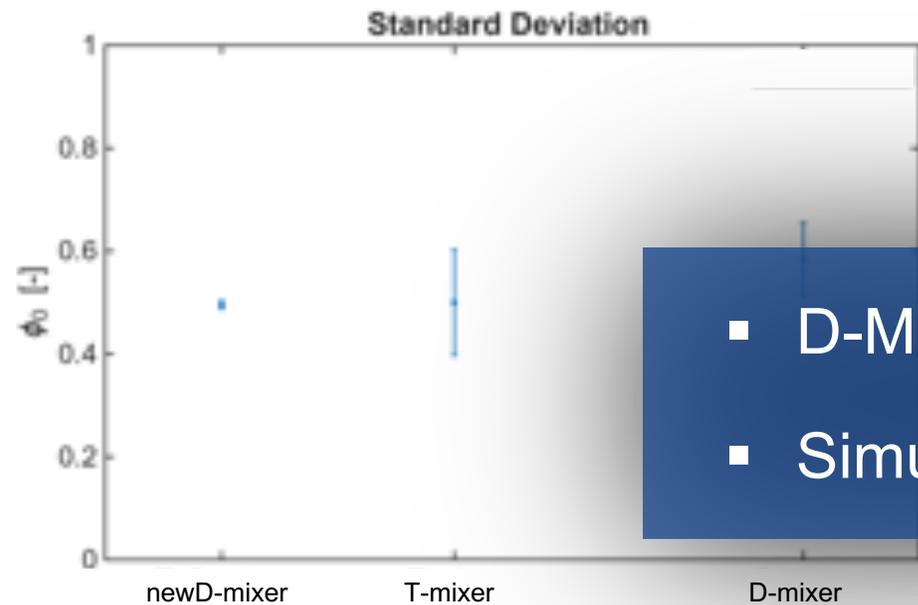
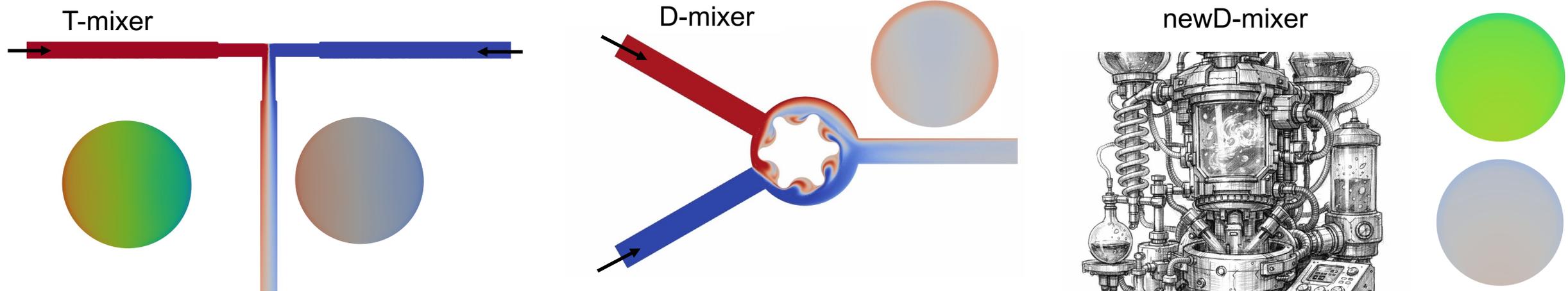
- Rotational speed enhances mixing
 - Flow rate worsens mixing
- ...as expected*

Comparison: T-mixer vs. D-mixer



D-Mixer appears far superior!
(More homogeneous mixture where flow is fast)

Results: CFD-based improved design



- D-Mixer has potential for further improvements
- Simulation can guide the way

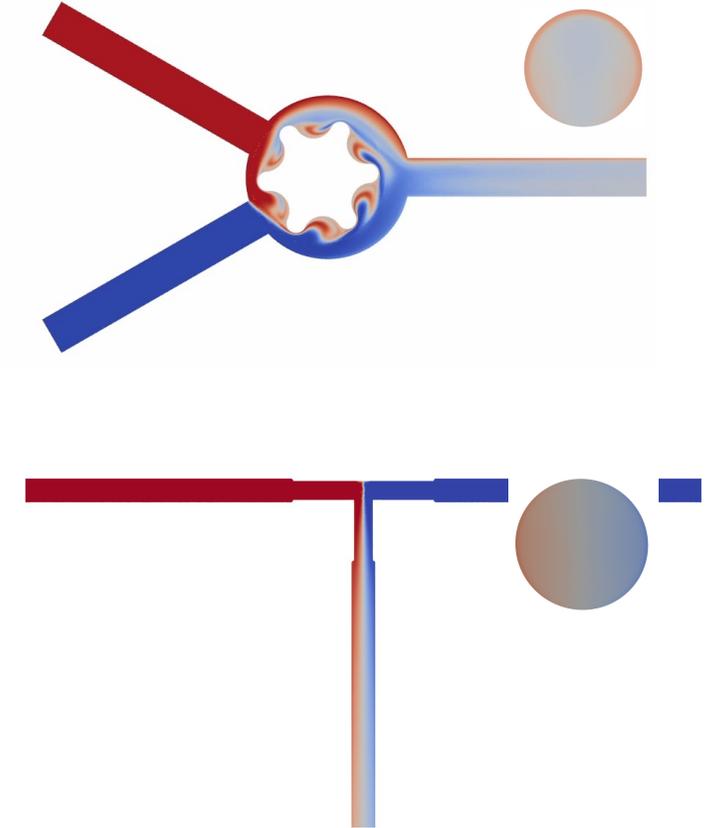
- Mixing simulations at high Schmidt-number are challenging
- The effect of Schmidt number has been illustrated
- The mixing of two liquids to form InP quantum dots has been numerically studied
- **The (rotating) D-mixer is superior**, improved designs are in work

Future work:

- Evaluate residence time distribution and mixing time.
- Move from qualitative to quantitative validation against experiments
- Simulate the nanoparticle formation by PBE

Caveat:

At high Schmidt number, simulations will show best-case scenarios for mixing! → Research!



Thank you for your attention



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