Numerical Simulation of a Solubility Process in a Stirred Tank Reactor

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Computational Fluid Dynamics in Chemical Reaction Engineering IV, Barga, Italy
August 8, 2005

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Outline

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- industrial mixing
- objective

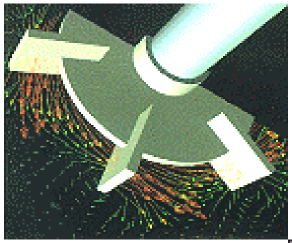
Simulation approach

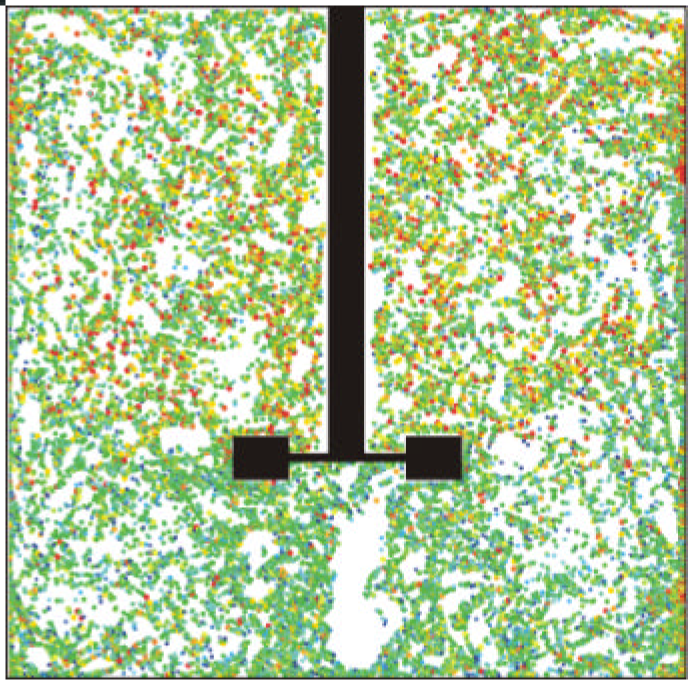
- LES (lattice-Boltzmann)
- scalar mixing (finite volume)
- particle transport
- flow system & settings

Results

- solids and scalar distributions
- particle size distribution
- solubility time

Conclusions and perspectives





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Introduction

Industrial mixing

Multi-phase mixing

Products

- competitiveness
- product quality
- process optimization, etc

Lack of insight in hydrodynamic phenomena → Need for information on ...

Turbulence

heat & mass transfer

break-up/coalescence

chemistry

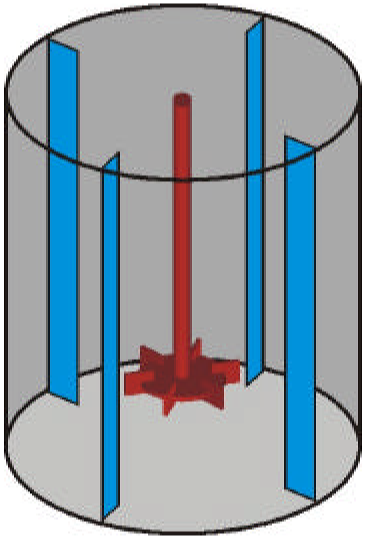
particle/bubble/droplet motion

agglomeration/attrition

collisions

Introduction
Scalar mixing; objectives

- Contribute to reliable numerical predictions of complex, multi-phase processes



- Focus: solid-liquid mixing including mass transfer
- Complex geometry: Rushton turbine stirred tank
- Applications: crystallization, solubility processes, ...
- Tools: - LES flow solver (lattice-Boltzmann)
  - Scalar transport solver (finite volume)
  - Particle transport solver (extension of the work of Derksen[1])

[1] Derksen (2003)

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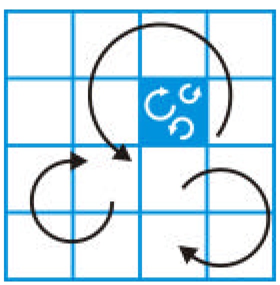
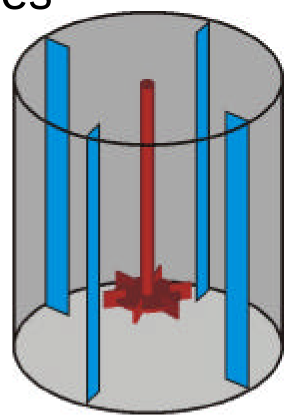
Simulation approach

Large Eddy Simulation (LES)

- Realistic description of multi-phase/ chemical reacting processes

  - Small scale mixing
  - Time dependency flow

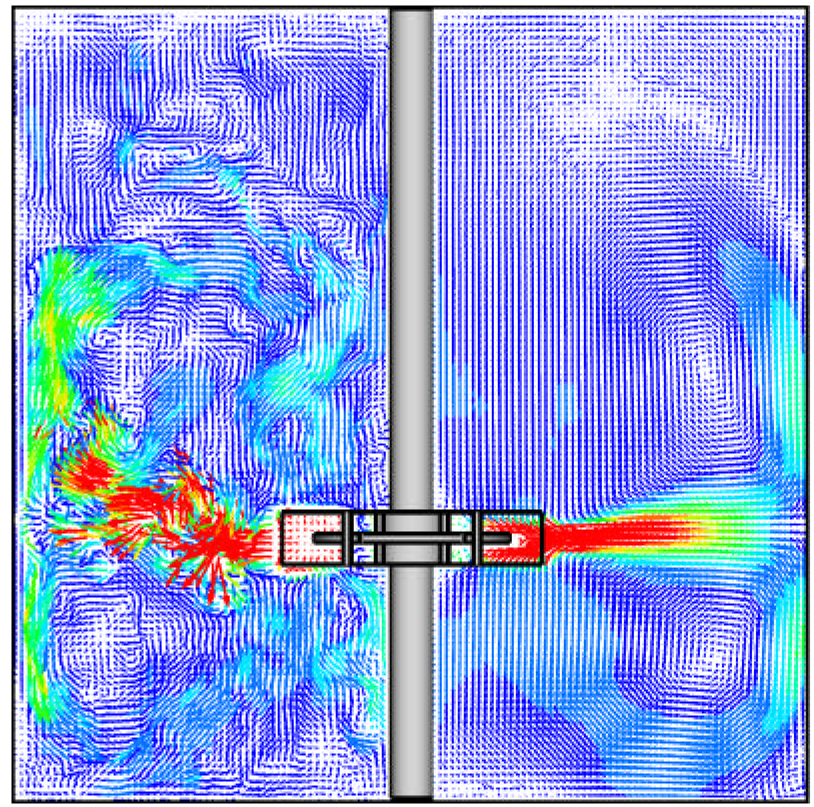




- Large Eddy Simulation

- Smagorinsky SGS model[1]
- Lattice Boltzmann discretization[2]

Instantaneous Time-averaged



Colors: kinetic energy

[1] Smagorinsky (1963)
[2] Somers (1993)

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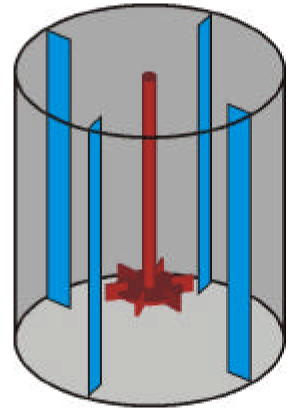
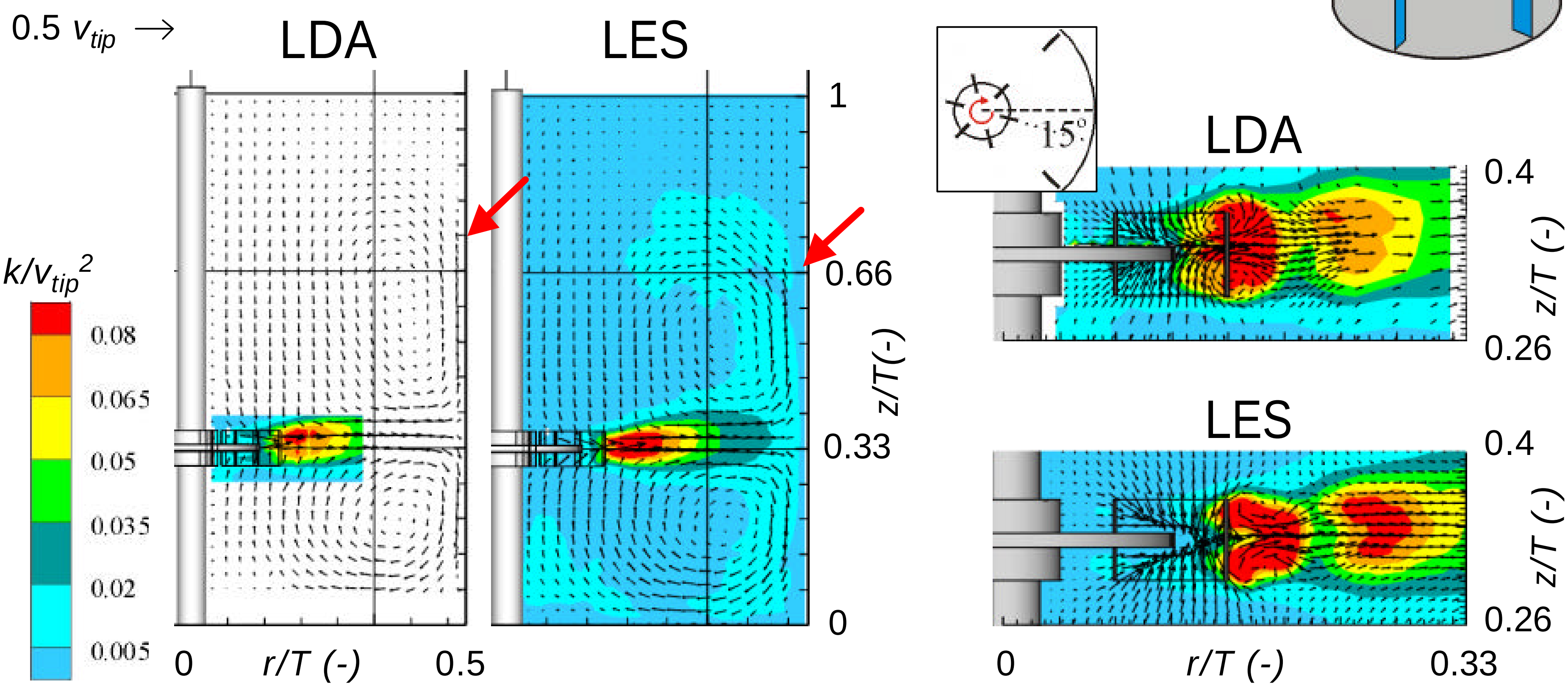
Simulation approach, cont'd

Assessment stirred tank flow (LES), Re = ND^2/n = 7,300[1]





[1] Hartmann et al (2004)

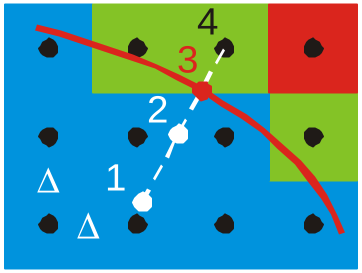
Simulation approach, cont'd

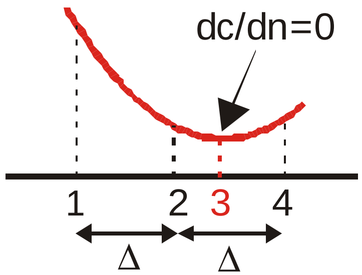
Scalar mixing

- Explicit finite volume scheme (LES; small time steps)
- Cartesian grid of the flow
- Coupled to LES

- Flux-limited convection scheme (TVD)

- Staircase-shaped walls inaccurate wall representation (impeller!)
- Impose dc/dn = 0 by means of ghost cells (2nd order)





- No cut cells; no stability problems
- Scalar mass conservation not guaranteed

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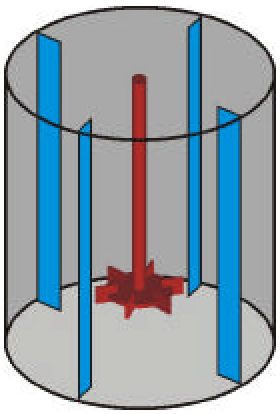
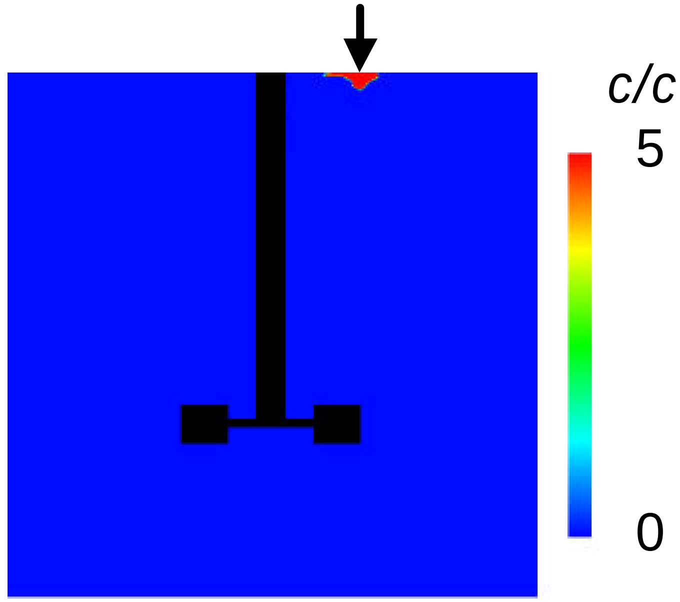
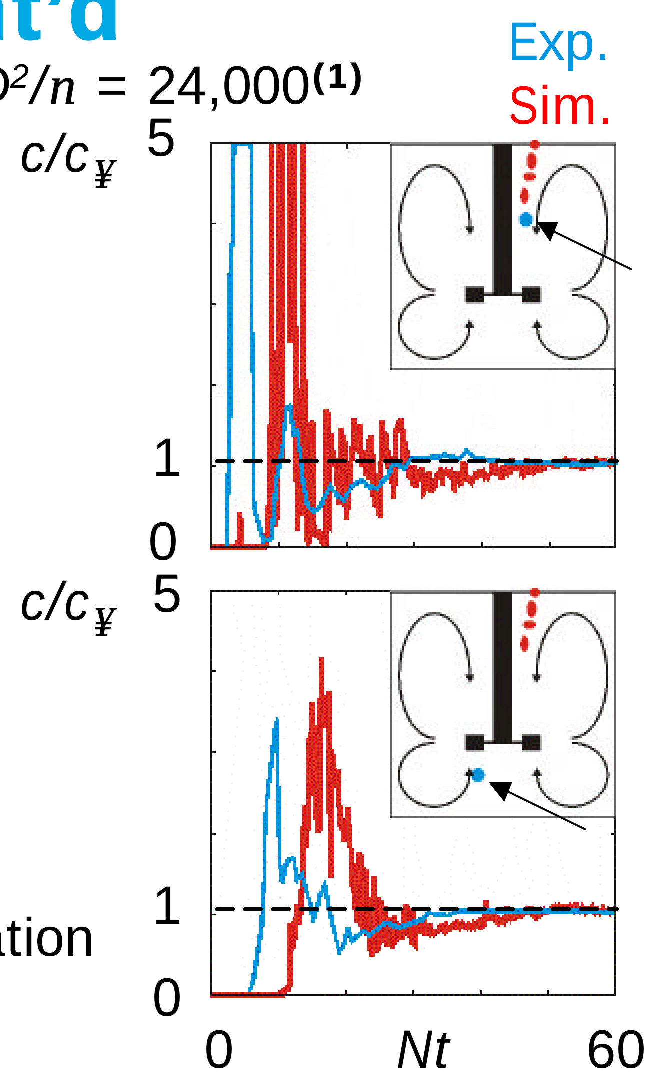
Simulation approach, cont'd

Assessment mixing time experiment, Re = ND^2/n = 24,000[1]







- <u>99% Mixing time:</u>
  concentration fluctuations < 1% final concentration

$$Nq_{m,99\%} = 73 \text{ (26\% overprediction)}$$

(1) Distelhoff et al (1997)

Simulation approach, cont'd

Particle transport[(1)]

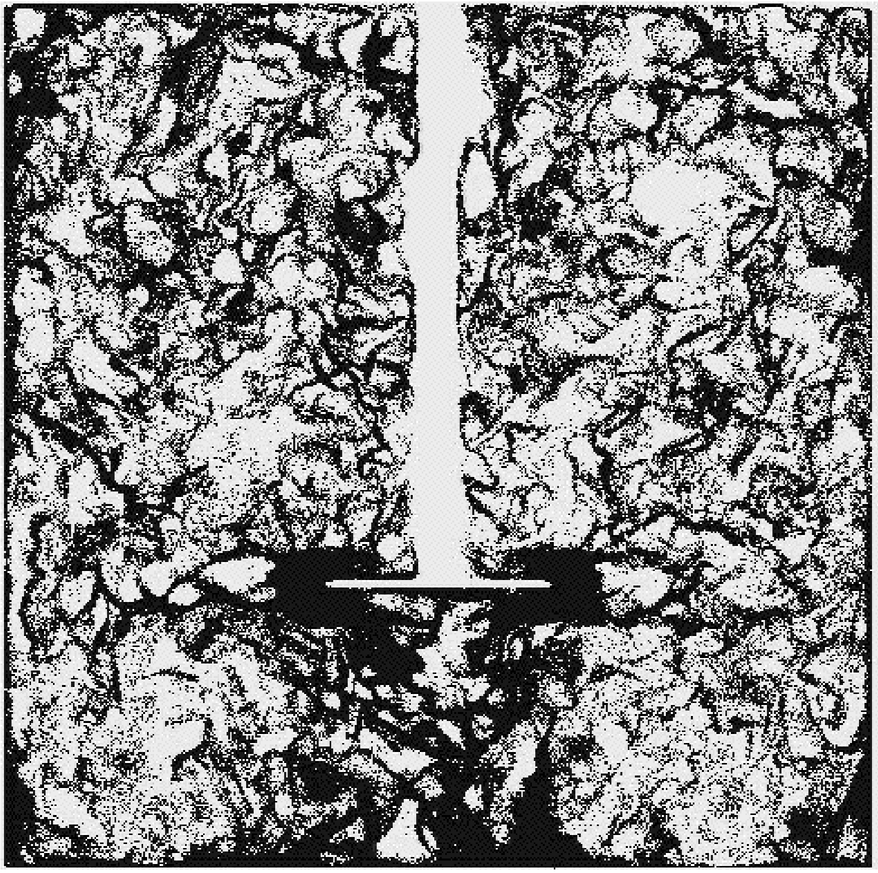
- Euler-Lagrange approach
- 'Point' particles; $d_p < \Delta$

- Particle dynamics
  - forces from *single*-particle correlations (drag, lift, ...)
  - collisions
  - simple two-way coupling

↓

limits the applicability to "low" f_V

- Particle-impeller and particle wall collisions: fully elastic



Re = 10^5

(1) Derksen (2003)

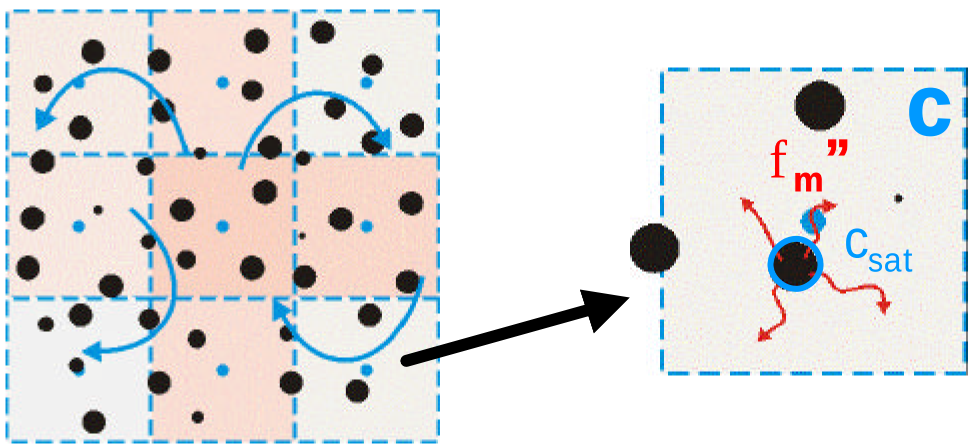
Simulation approach, cont'd

Solid-liquid mixing including mass transfer

- Single-phase LES solver
- Scalar mixing solver
- Particle transport solver

} → mass transport → crystallization process, solubility process, ...

- Focus on solubility process



- source term FV code:

$$S = \Sigma_p \, \phi_m$$

- mass flux:

$$\phi_m'' = Sh \rho_p (\Gamma / d_p)(c_{sat} - c)$$

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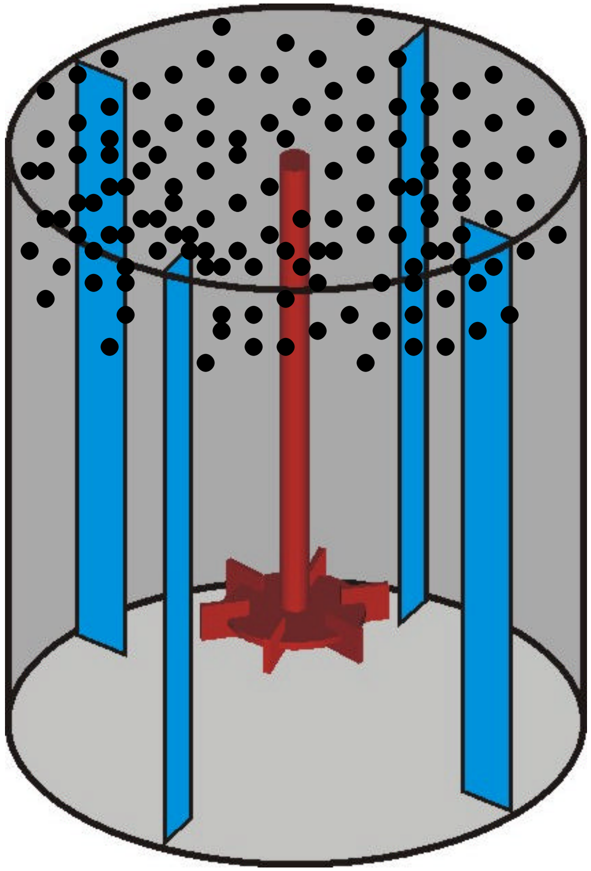
Simulation approach, cont'd

Flow system, settings



Physical case

- T = 0.23 m (10 liter vessel)
- working fluid: water
- $Re = 10^5 \rightarrow N$ = 16.5 rev/s
- $7{\cdot}10^6$ calcium-chloride beads
- c_{sat} = *600 kg/m³*
- $\Gamma_{mol} = 0.7{\cdot}10^{-9}$ m²/s (calcium ions)
- beads released in upper part (0.9T-T)
- d_p = 0.3 mm; ρ_p/ρ_{liq} = 2.15
- ϕ_V = 10% (average 1%)
- N_{js} = 11.4 rev/s

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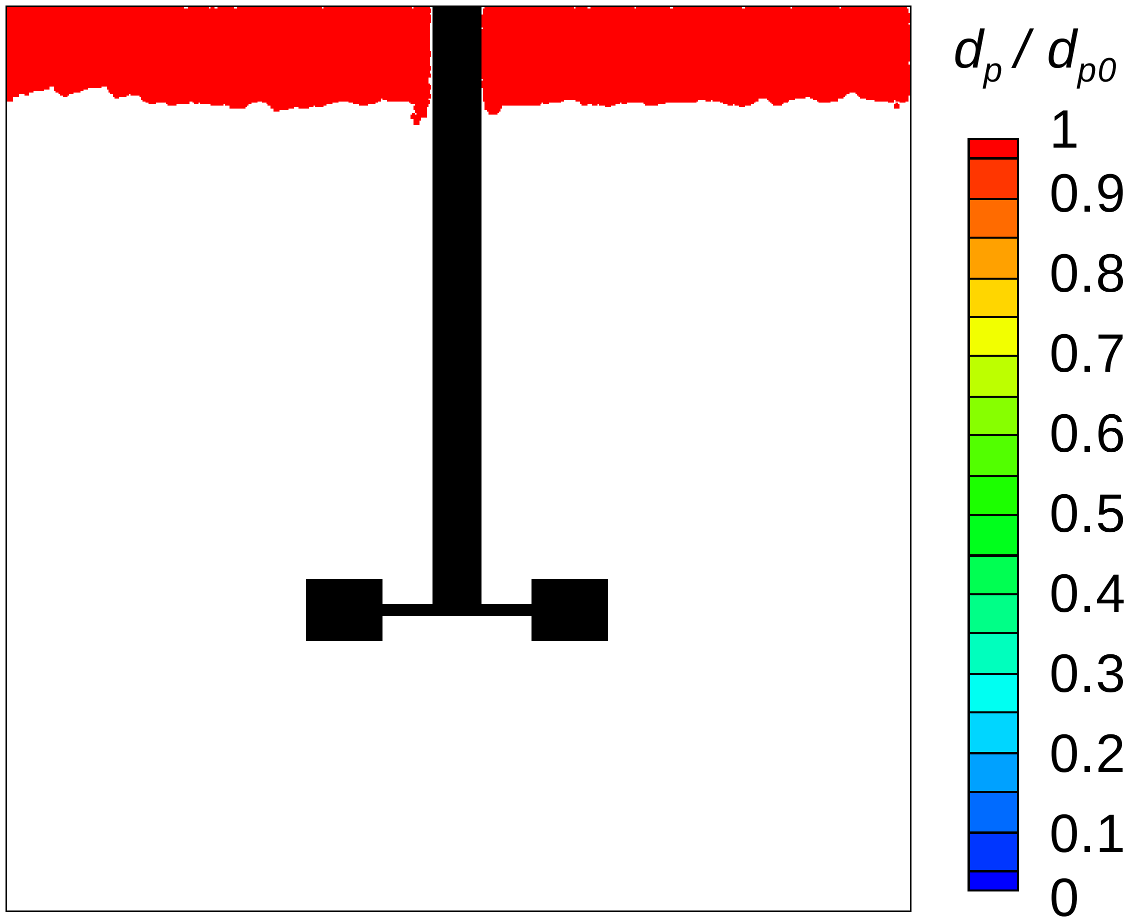
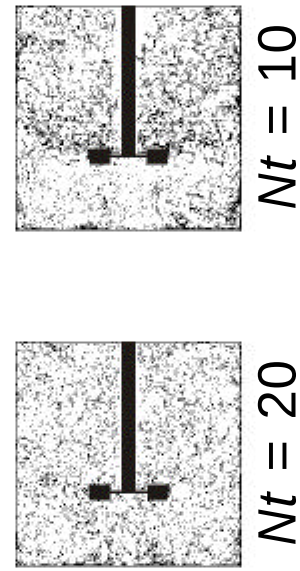
Results

Animation spatial particle distribution: $0 < Nt \leq 60$





The particles are 5 times enlarged

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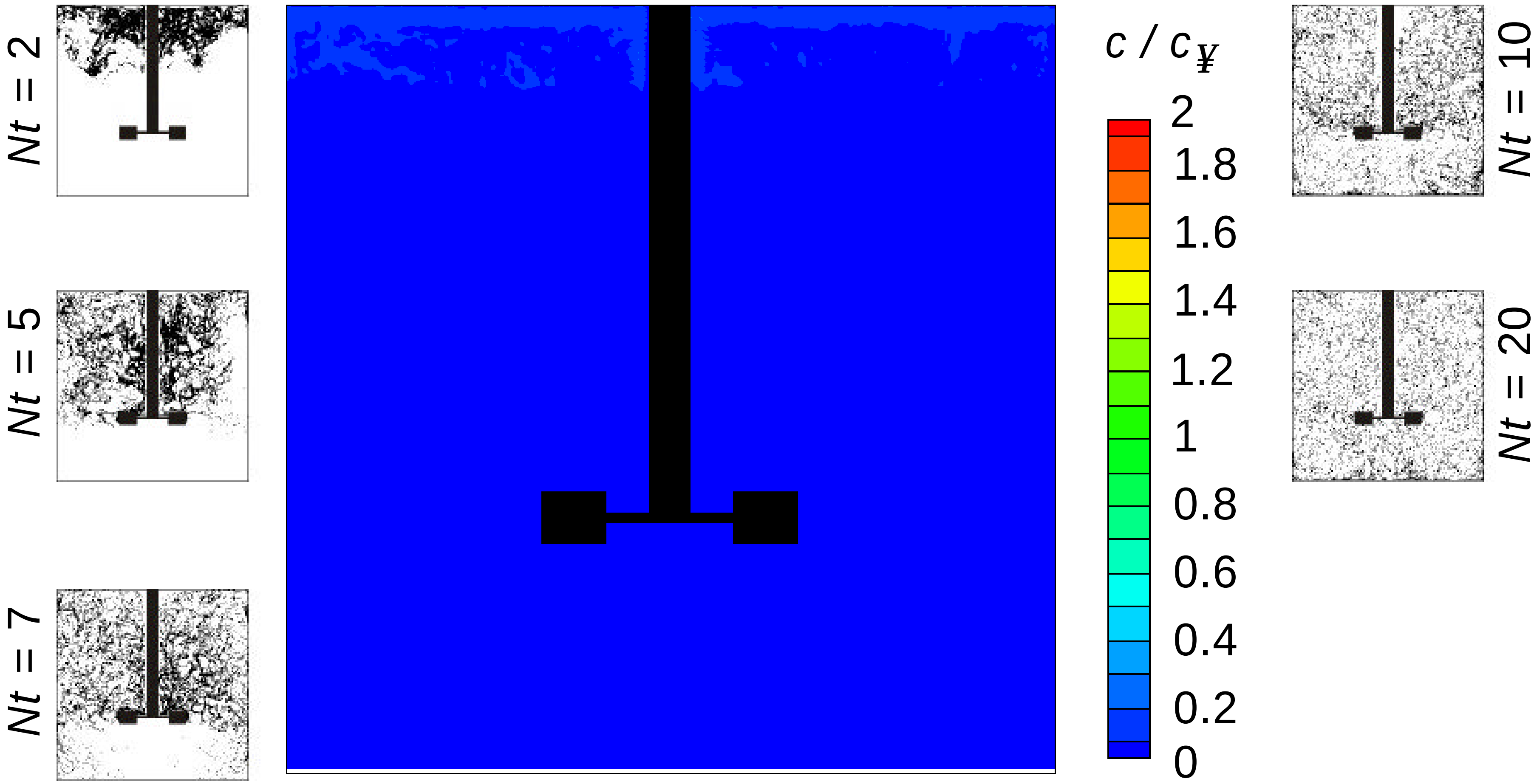
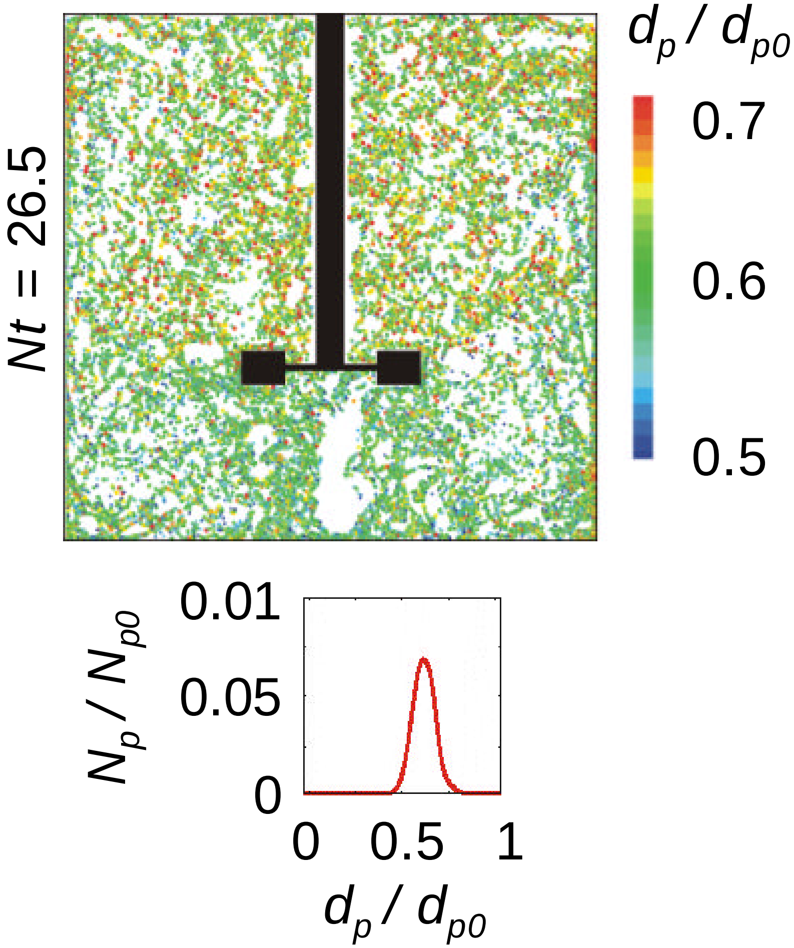
Results, cont'd

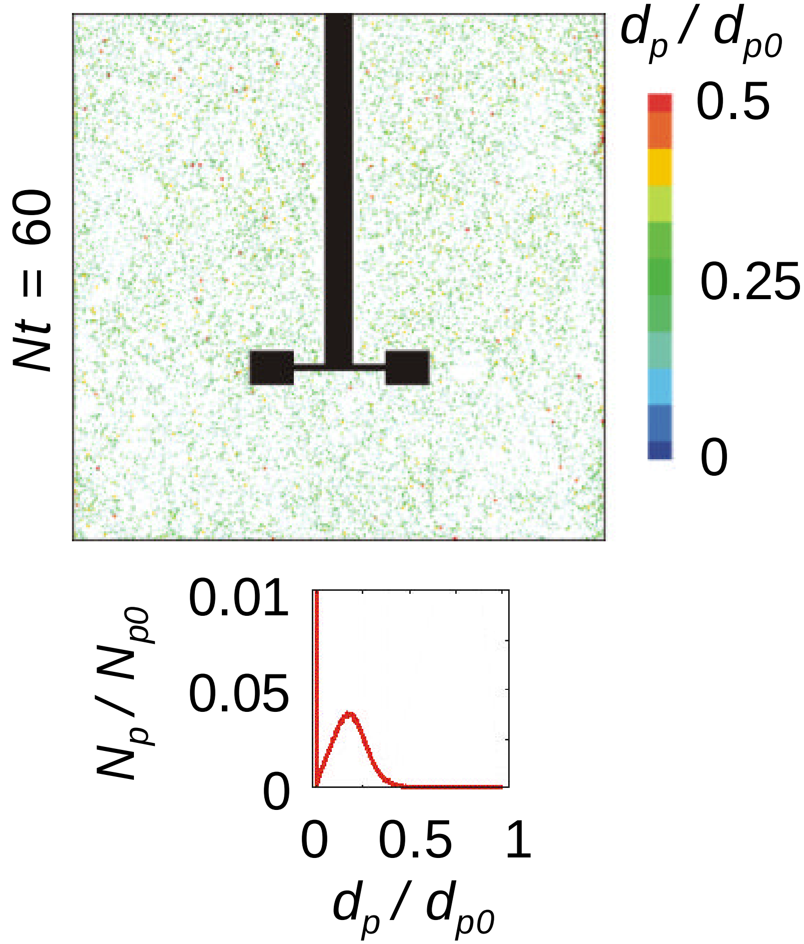
Animation concentration distribution: $0 < Nt \leq 20$



Results, cont'd

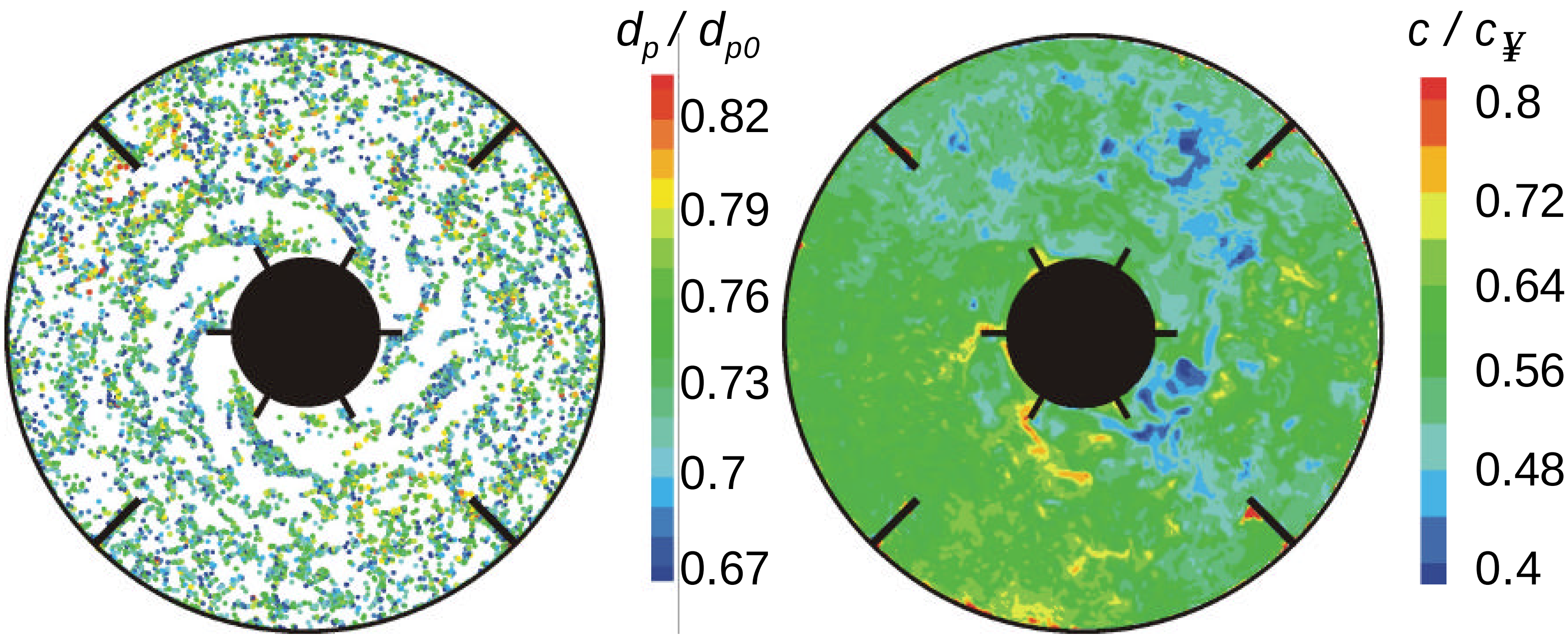
Snapshots spatial particle distributions (particles 10 times enlarged)





Results, cont'd

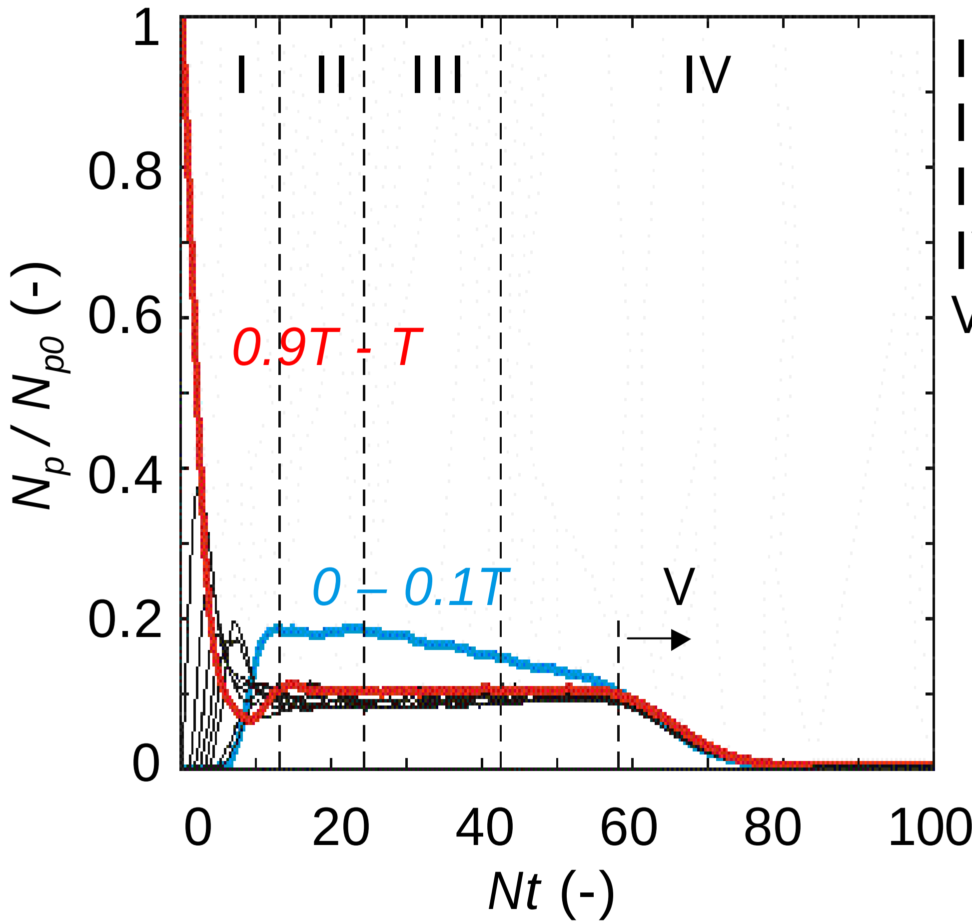
Snapshot of spatial particle and concentration distribution at $Nt = 15$



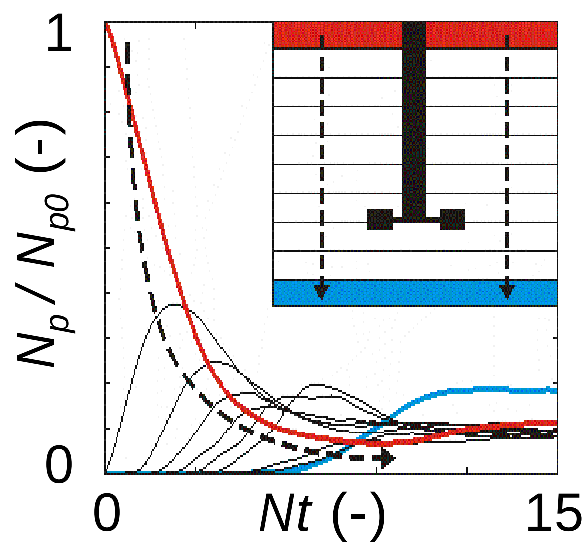
The particles are 10 times enlarged

Results, cont'd

Solubility stages



I: Mixing & Dispersing (0 ≤ *Nt* < 12)
II: Quasi steady-state (12 ≤ *Nt* < 24)
III: Resuspension (24 ≤ *Nt* < 42)
IV: Dissolution (*Nt* ≥ 42)
V: Homogeneous suspension (*Nt* ≥ 58)



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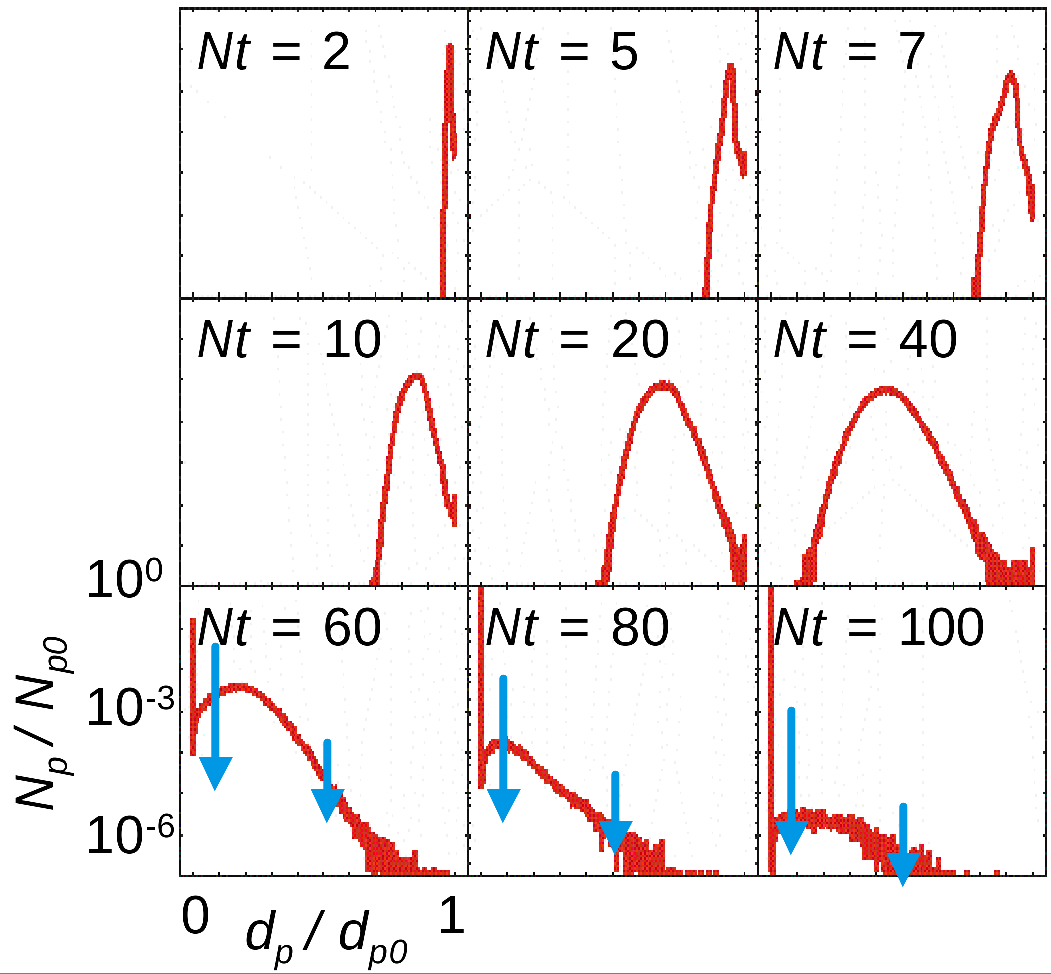
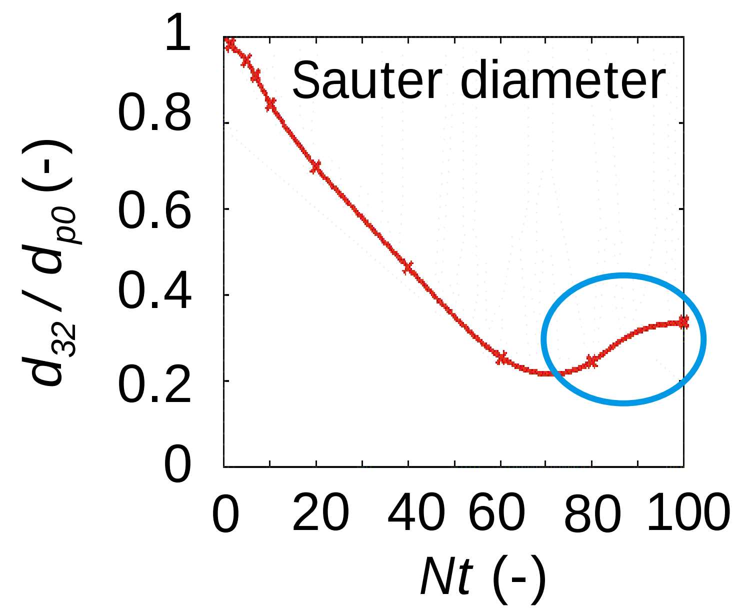
Results, cont’d

Evolution particle size distribution in time





$Sh = 2 + 0.6Re_p^{0.5}Sc^{0.33}$ [1]

d_p ® 0 → Sh ® 2 → f_m μ d_p → $d(d_p)/dt$ μ d_p^{-1}

[1] Ranz and Marshall (1952)

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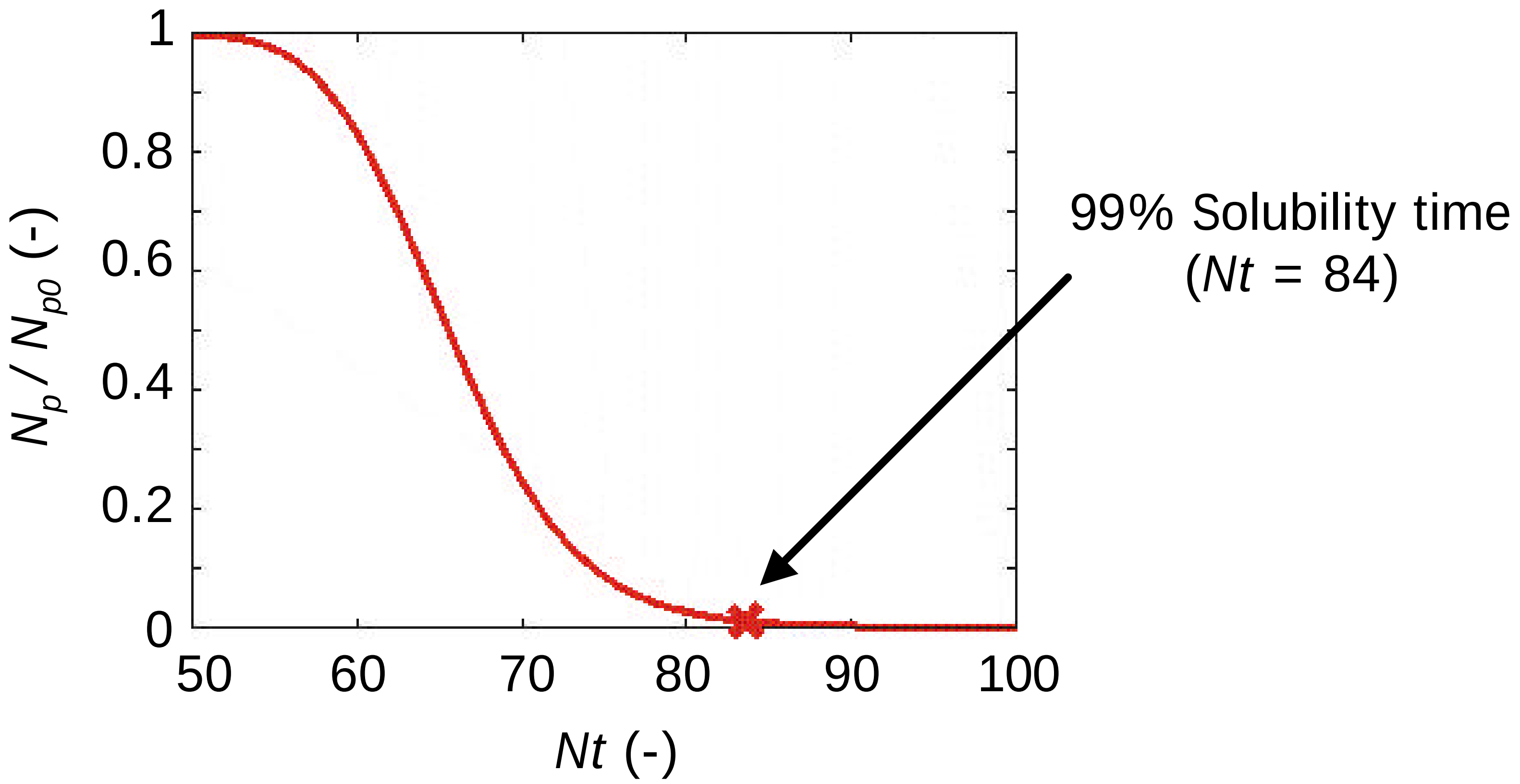
Results, cont'd

Solubility time



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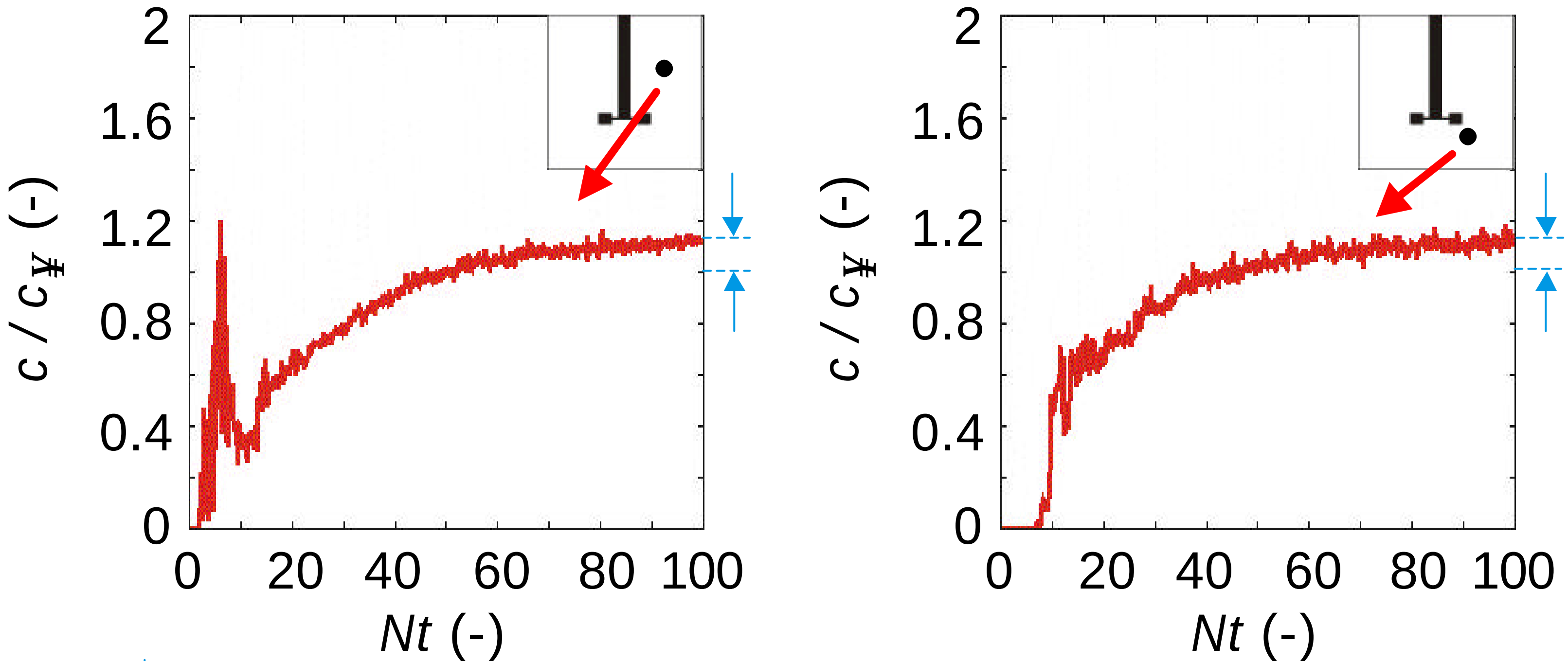
Results, cont'd

Concentration profiles



Unphysical mass increase: 0.12% each impeller revolution

→ Due to newly developed immersed boundary technique

Conclusions…

- Solubility time at most one order of magnitude larger than mixing time scale
- Four stages identified: mixing and dispersing, quasi steady-state, resuspension, dissolution
- Decreasing particle inertia: streaky patterns disappear
- Non-homogeneous mixing effects: development PSD
- Scalar transport matches particle transport
- Unphysical scalar mass increase is due to newly developed immersed boundary technique

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… and perspectives

- LES including scalar mixing in conjunction with particle transport has become a promising possibility to study multi-phase processes in lab-scale reactors

- Improvements:
  - Collision algorithm
  - Inclusion hydrodynamic interactions between particles
  - Immersed boundary technique for scalars

- Future direction: crystallization process
  - Nucleation
  - Attrition
  - Agglomeration

Acknowledgement

This work was sponsored by the Netherlands National Computing Facilities for the use of supercomputer facilities, with financial support from the Netherlands Organization for Scientific Research (NWO).

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