Direct numerical simulation of bubble train flow in a square mini-channel and evaluation of liquid phase residence time distribution

Martin Wörner, Bradut Ghidersa, A. Onea

Forschungszentrum Karlsruhe, Institut für Reaktorsicherheit

Multiphase Flows: Simulation, Experiment and Application
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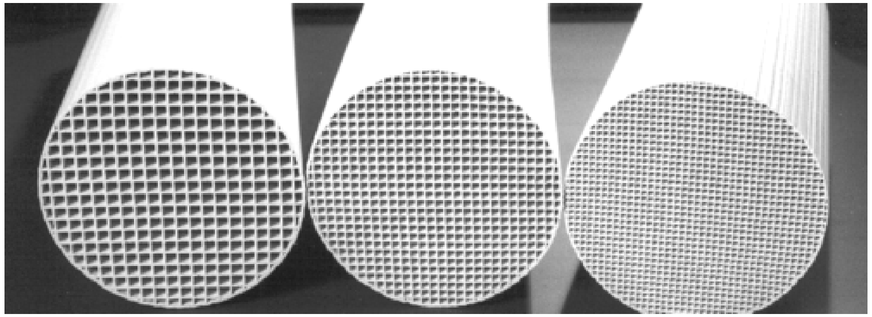
Content

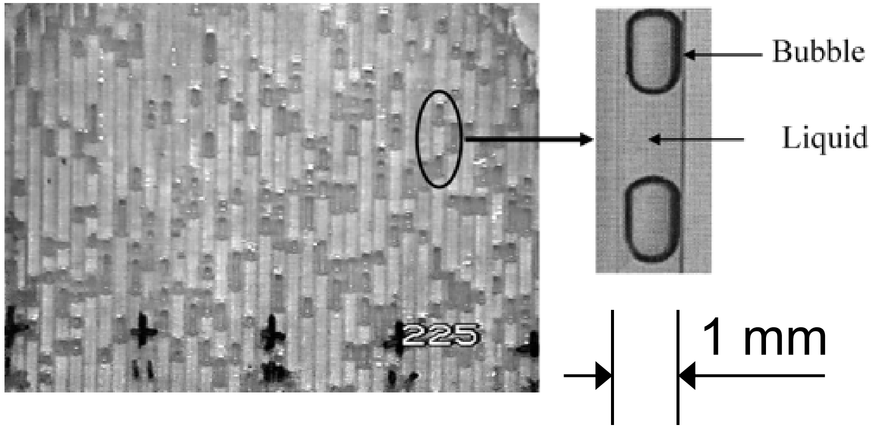
- Introduction and motivation
- Bubble train flow
  - Computational setup in DNS
  - Validation and simulation results
- Evaluation of residence time distribution
  - Procedure
  - Results of RTD for bubble train flow
  - Fitting by compartment model
- Conclusions and outlook

Introduction

Multi-fluid flow in narrow channels

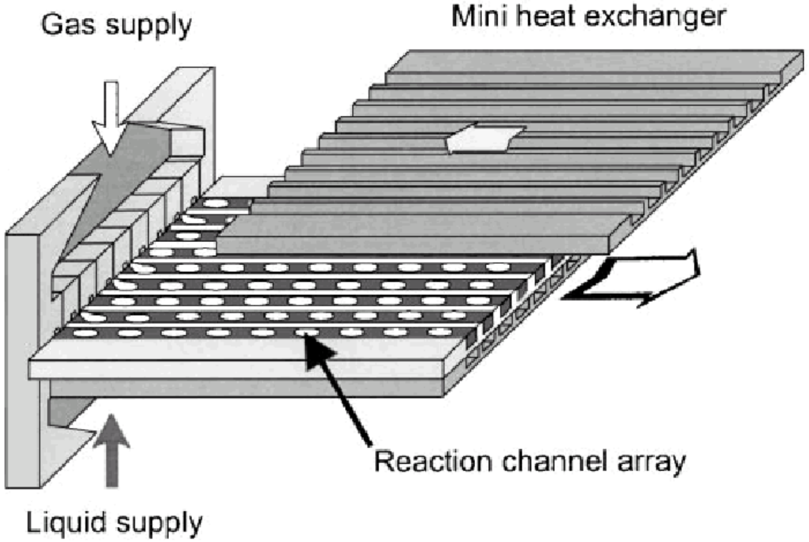
- Monolithic reactors with catalytic walls
  - Chemical inert gas bubbles segment the liquid phase and enhance its mixing





Introduction

- Micro bubble column of IMM*
  - High values of interfacial area per unit volume
    - Efficient mass transfer across interface
      (e.g. absorption, liquid-liquid extraction)
  - Defined interface geometry
    - Concept of
      „numbering up“
      instead of „scaling up“



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* Institut für Mikro-Technologie Mainz

Motivation

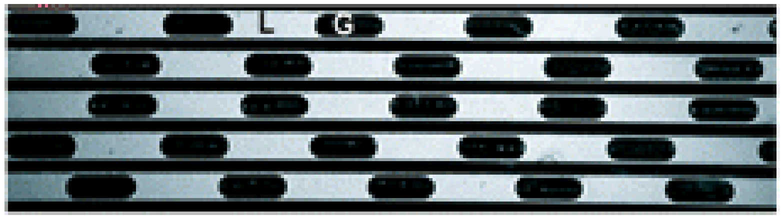
- Experimental investigation of these two-phase flows is difficult because of small dimensions and often yields integral data only
- Goal:
  - Perform direct numerical simulation of bubble train flow in a single channel to resolve local flow phenomena
  - Use DNS results to evaluate residence time distribution for liquid phase

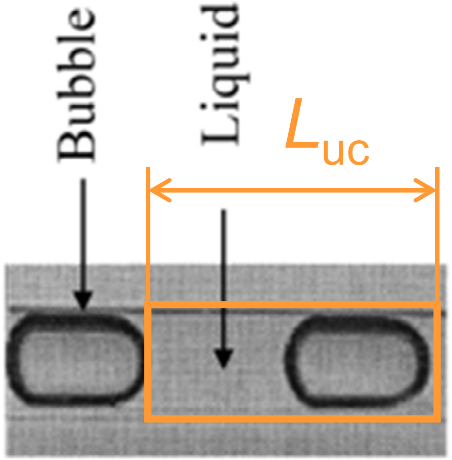
In-house code TURBIT-VOF

- Volume-of fluid method for interface tracking
  - Interface is locally approximated by plane (PLIC method)
- Governing equations for two incompressible fluids
  - Single field momentum equation with surface tension term
  - Zero divergence condition for center-of-mass velocity
  - Advection equation for liquid volumetric fraction *f*
- Solution strategy
  - Projection method resulting in pressure Poisson equation
  - Explicit third order Runge-Kutta time integration scheme
- Discretization in space
  - Finite volume formulation for regular staggered grid
  - Second order central difference approximations

Flow characterization

- Elongated bubble which fill almost the entire channel cross section (Taylor bubbles)
- Bubbles have identical shape and move with same axial velocity
- The flow is fully described by a **unit cell of length L_{uc}** consisting of a bubble and a liquid slug





uc = "unit cell"

Experiment of Thulasidas et al.*

- Square vertical channel
  - Channel cross section : 2 mm × 2 mm ($W^* = 2$ mm)
- Air bubbles in silicon oil
  - Silicon oil of different viscosity
  - Wide range of capillary numbers $Ca_B \equiv \mu_1^* U_B^* / \sigma^*$
- Specification of flow rates of air and oil
- Length of unit cell, gas content in unit cell and axial pressure drop adjust accordingly

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* Thulasidas, Abraham, Cerro, Chem. Eng. Science 50 (1995) 183-199

Numerical set up with TURBIT-VOF

- Consider one flow unit cell only (one bubble, one slug)
- Account for influence of trailing/leading unit cells by periodic boundary conditions in axial direction
- Flow is driven in vertical direction by specified axial pressure gradient and buoyancy
  - Gas and liquid flow rates adjust accordingly
- Length of flow unit cell, L_{uc}, is input parameter
  - Investigation of influence of L_{uc}

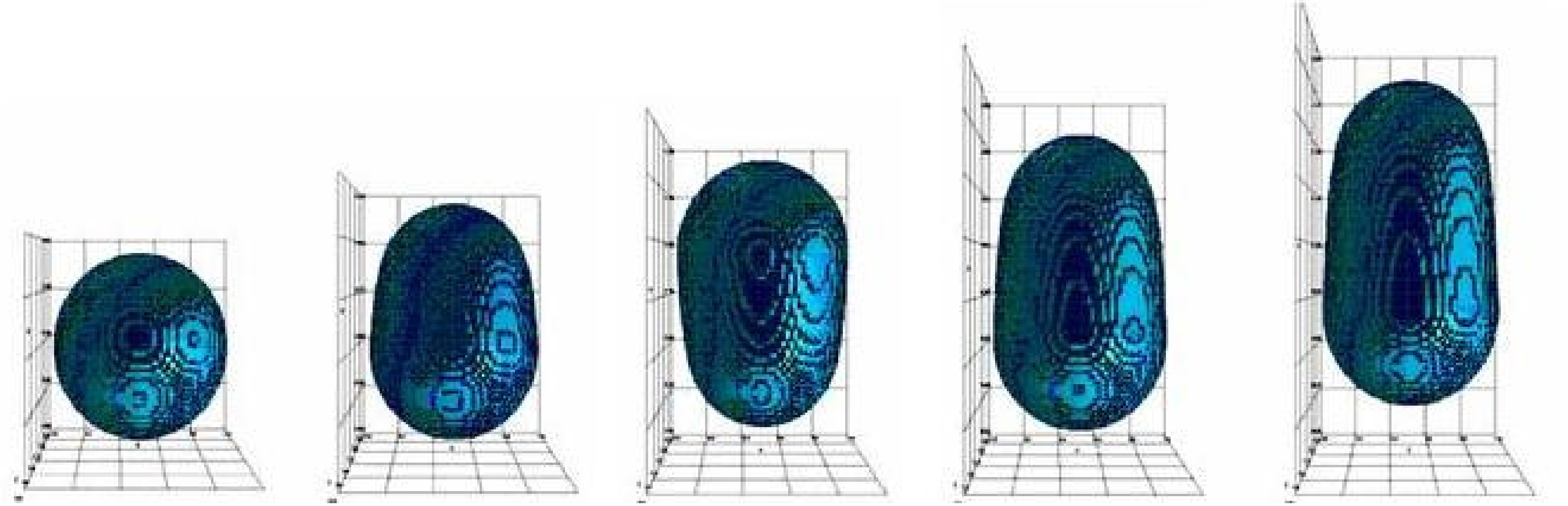
Physical parameters

- Fluid properties

Factor 10 higher than ρ and μ of air

ρ_l	ρ_g	μ_l	μ_g	σ
957 kg/m^3	11.7 kg/m^3	0.048 Pa s	1.84×10^{-4} Pa s	0.022 N/m

- Initial bubble shapes (void fraction $\varepsilon = 33\%$)

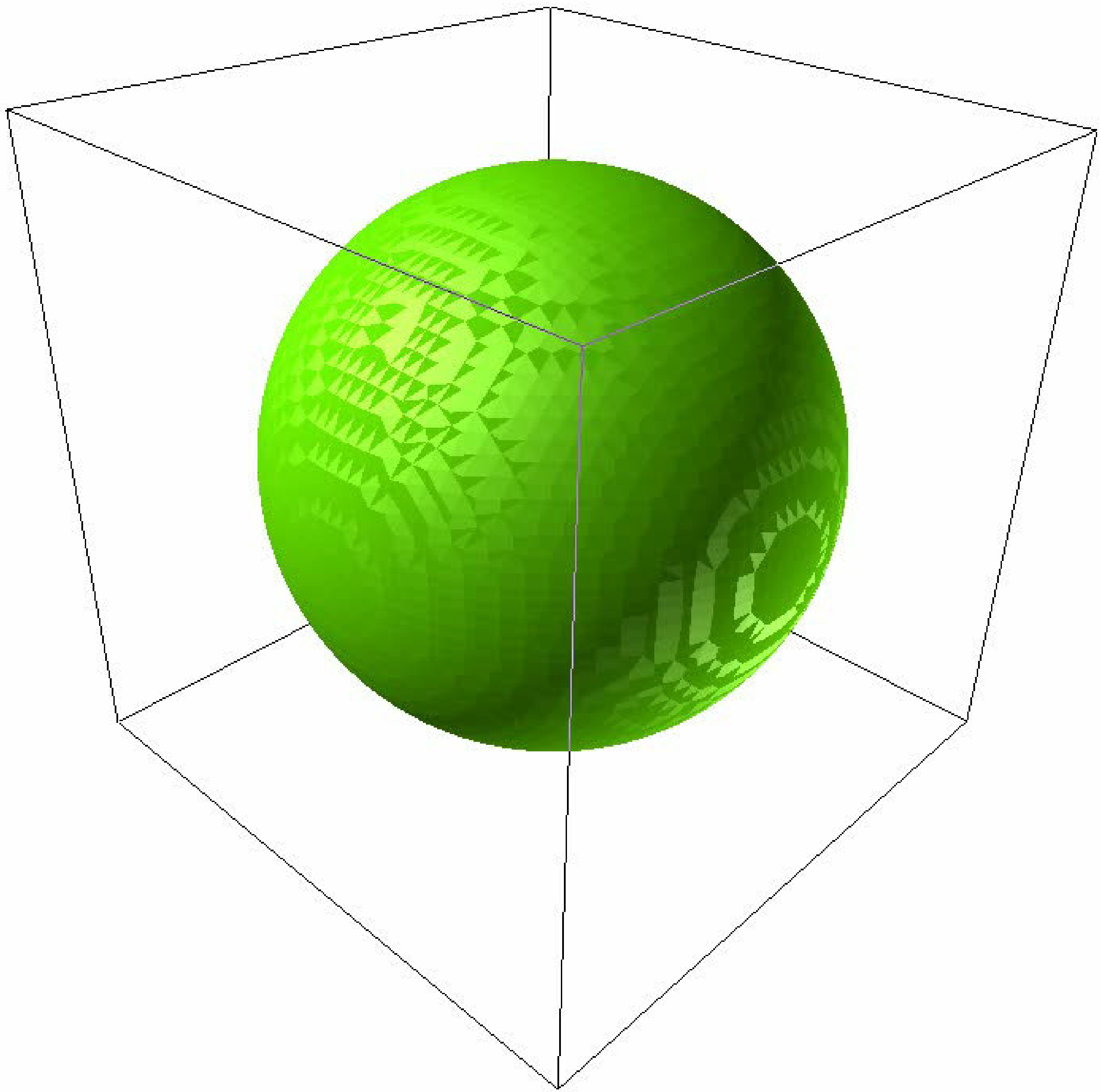


- Simulations are started from gas and liquid at rest

Computational parameters

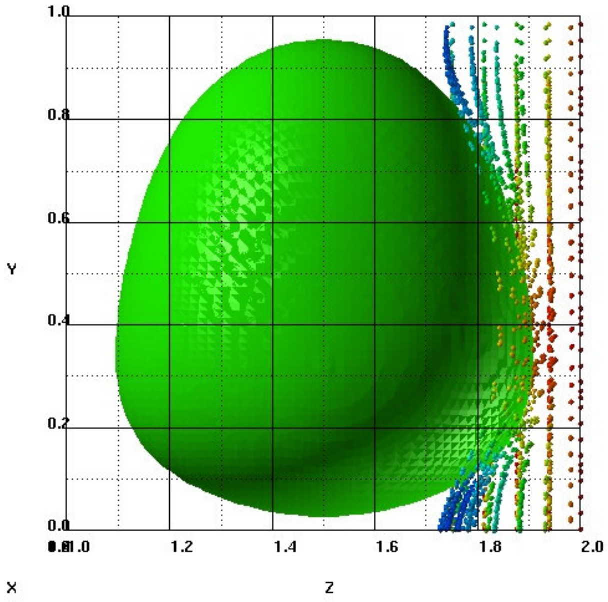
Case	L_{uc} / W	Domain	Grid	Time steps
A1	1	1 × 1 × 1	48 × 48 × 48	24,000
A2	1	1 × 1 × 1	64 × 64 × 64	60,000
B	1.25	1 × 1.25 × 1	48 × 60 × 48	24,000
C	1.5	1 × 1.5 × 1	48 × 72 × 48	26,000
D	1.75	1 × 1.75 × 1	48 × 84 × 48	26,000
E	2	1 × 2 × 1	48 × 96 × 48	28,000

Results on both grids show only slight differences

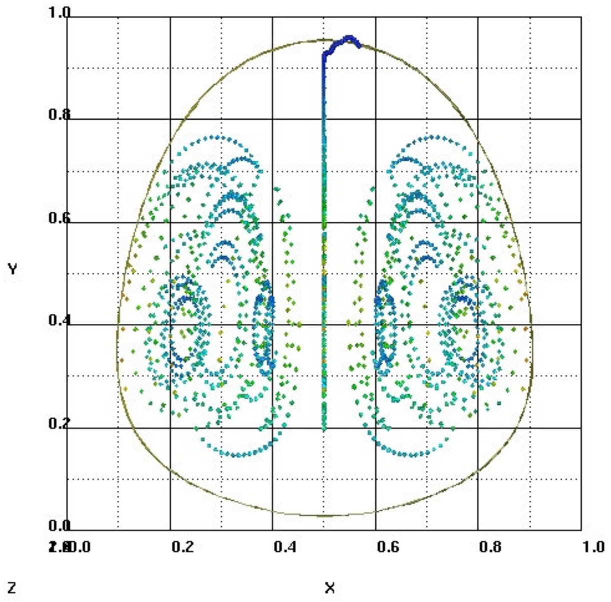


Case A2

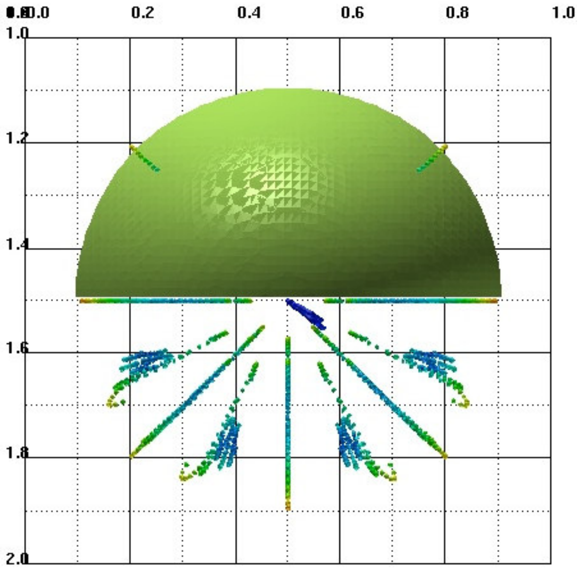
Bubble shape and trajectories of mass less particles for case A



View from side



View from side



View from top

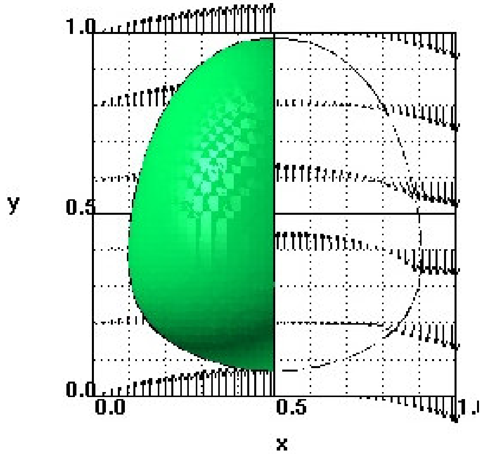
- Bubble has axisymmetric shape
- One large vortex inside the bubble
- Small azimuthal flow inside bubble

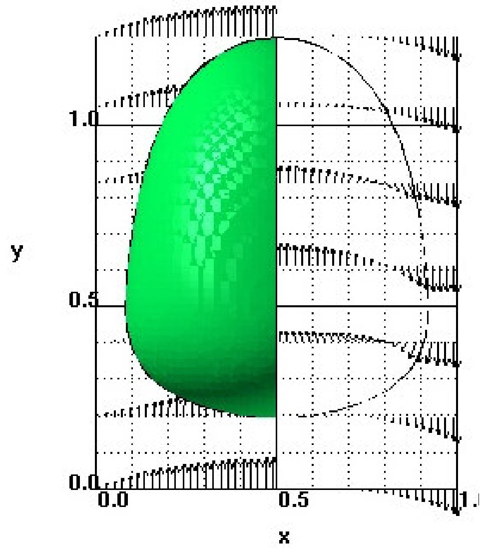
Computed bubble shape and velocity field for different values of L_{uc}

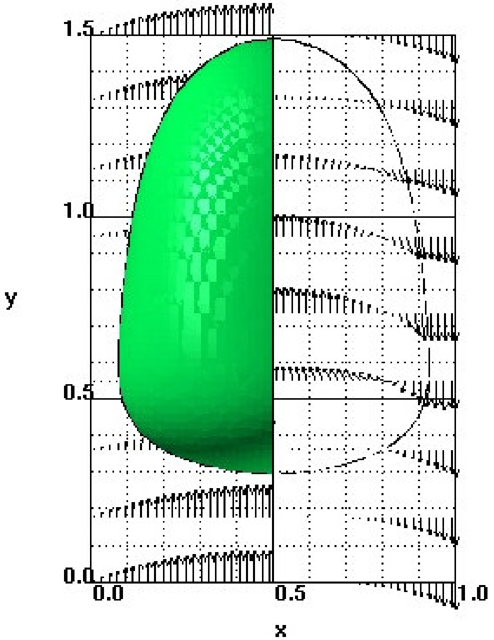
<u>Velocity field in vertical mid-plane</u>

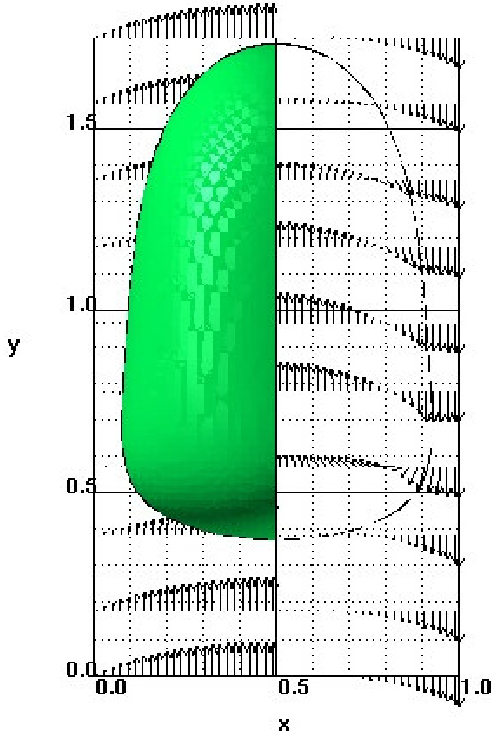
Right half: frame of reference moving with bubble

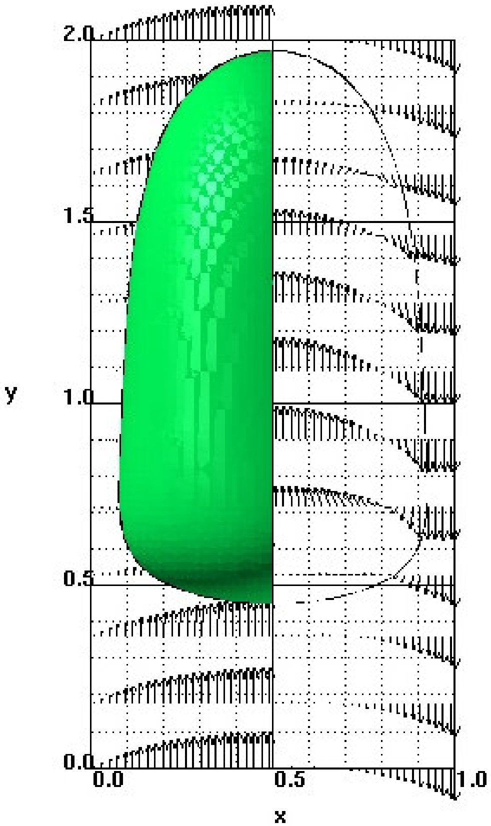
Left half: fixed frame of reference











Comparison with experiment

Non-dimensional bubble diameter

Relative velocity

Non-dimensional U_B

Case	L_{uc} / W	Ca_B	D_B / W	$(U_B – J_{total})/U_B$	U_B/J_{total}
A	1	0.204	0.81	1.80	0.445
B	1.25	0.207	0.84	1.75	0.430
C	1.5	0.215	0.85	1.75	0.430
D	1.75	0.238	0.85	1.78	0.438
E	2	0.253	0.85	1.8	0.445
Experimental data* correlated in terms of capillary number $Ca_B \equiv \mu_l U_B / \sigma$					
		0.2 – 0.25	0.82 – 0.86	1.68 – 1.84	0.435 – 0.475
			✓	✓	✓

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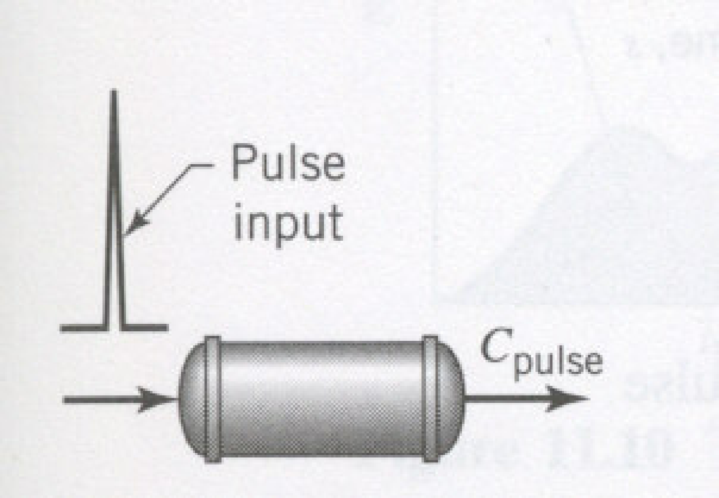
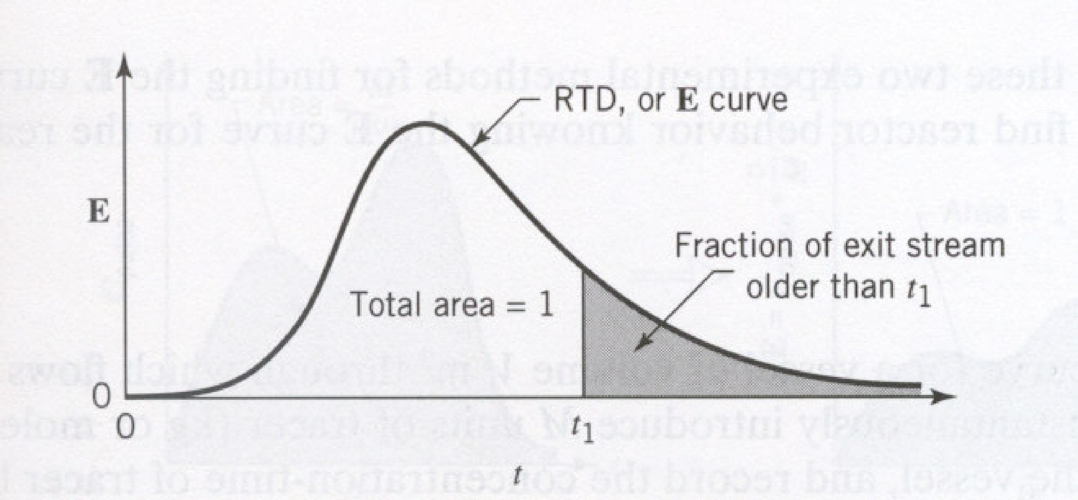
* Thulasidas, Abraham, Cerro, Chem. Eng. Science 50 (1995) 183-199

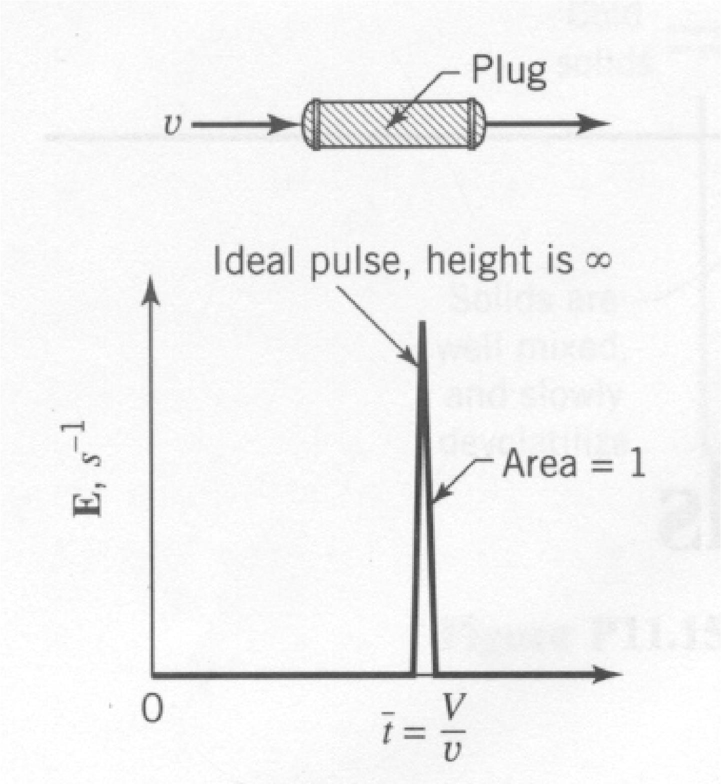
Residence time distribution

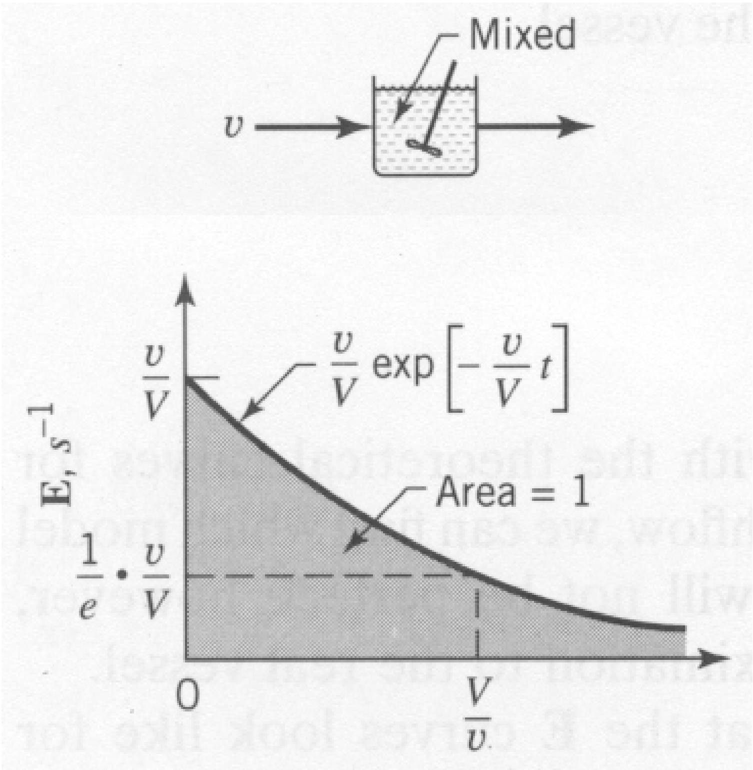
- The residence time distribution (RTD) is an important measure for characterization of any chemical reactor
  - The RTD influences yield and selectivity
- Common experimental method to determine RTD
  - Add tracer at reactor inlet as a pulse and measure the tracer concentration at the outlet





Examples for RTD





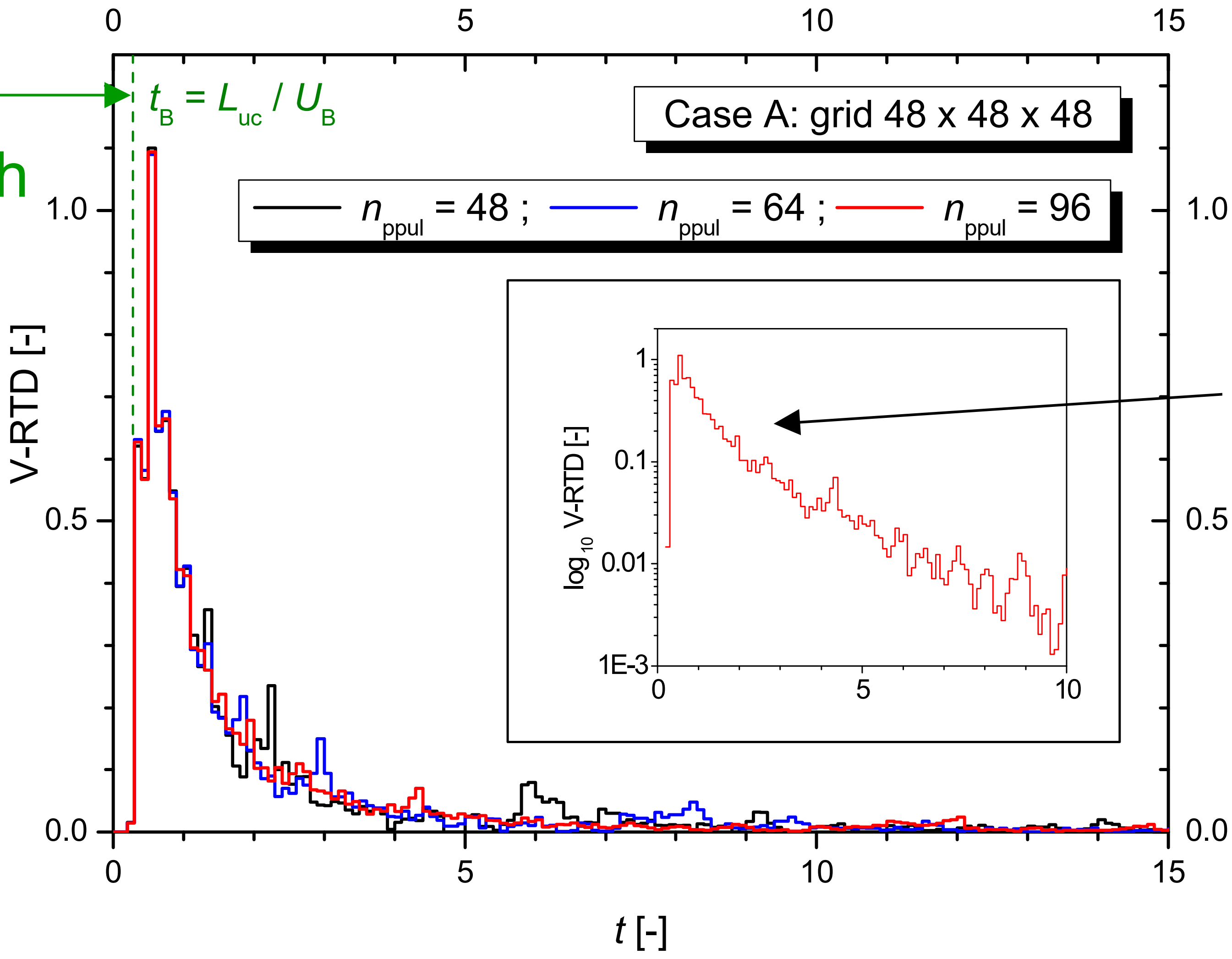
- Problems for micro reactors
  - Reaction volume is usually much smaller than the volume of inlet and the volume necessary to measure tracer at outlet
- <u>Alternative:</u> Determine RTD from DNS data

Procedure to evaluate RTD from DNS data

- Use previously computed DNS results for fully developed flow at a certain instant in time
- Introduce virtual particles in mesh cells entirely filled with liquid
  - particle distance = 1 / n_{ppul}
  - n_{ppul} = number of particles per unit length
- Track particles in fixed frame of reference
  - Problem: Velocity field in fixed frame of reference is unsteady
  - But: steady velocity field in frame of reference moving with bubble
  - Determine fluid velocity at the instantaneous particle position from its relative position to the virtually with velocity U_{B} moving bubble
- Store time the particle needs to travel an axial distance of L_{uc}
- Normalize histogram for all particles to obtain RTD

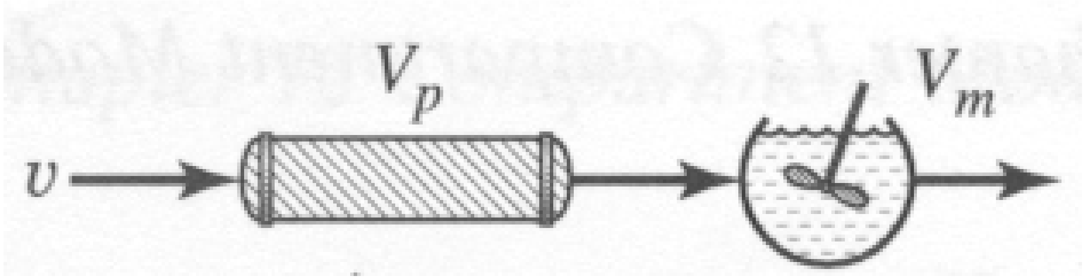
Influence of n_{ppul} for BTF Case A

Bubble breakthrough time t_B

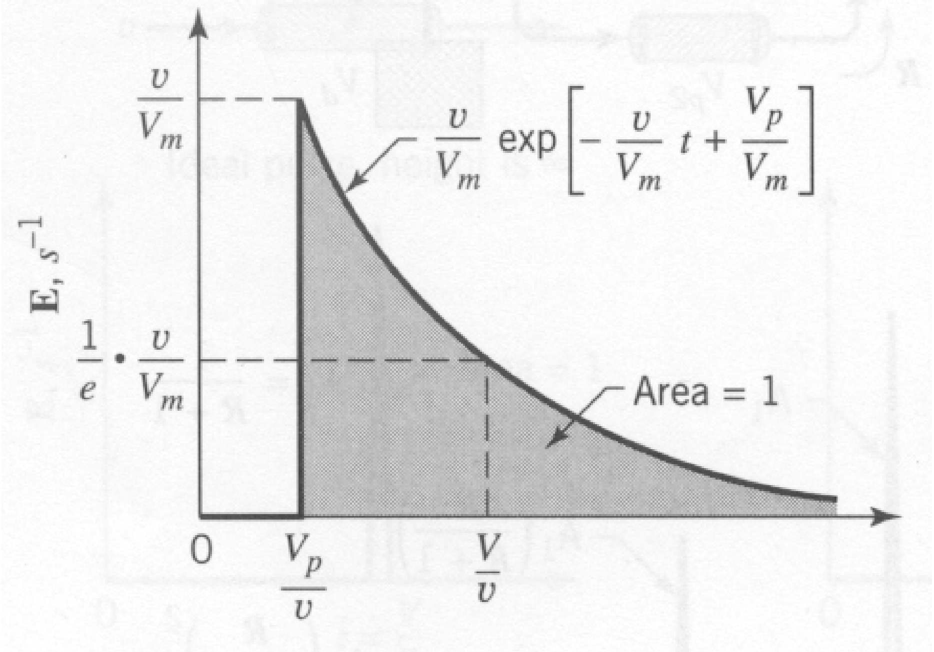


Exponential decay

Compartment model



Plug flow reactor and stirred vessel in series



$$E_{\mathrm{VRTD}} = \begin{cases} 0 & \text{for } t < L_{\mathrm{uc}}/U_{\mathrm{B}} \\ \dfrac{U_{\mathrm{L}}}{L_{\mathrm{uc}}}\exp\left(-\dfrac{U_{\mathrm{L}}}{L_{\mathrm{uc}}}\cdot t+\dfrac{U_{\mathrm{L}}}{U_{\mathrm{B}}}\right) & \text{for } t \geq L_{\mathrm{uc}}/U_{\mathrm{B}} \end{cases}$$

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Compartment model for case A

$$E_{\mathrm{VRTD}} = \begin{cases} 0 & \text{for } t < L_{\mathrm{uc}}/U_{\mathrm{B}} \\ \dfrac{U_{\mathrm{L}}}{L_{\mathrm{uc}}} \exp\left(-\dfrac{U_{\mathrm{L}}}{L_{\mathrm{uc}}} \cdot t + \dfrac{U_{\mathrm{L}}}{U_{\mathrm{B}}}\right) & \text{for } t \geq L_{\mathrm{uc}}/U_{\mathrm{B}} \end{cases}$$

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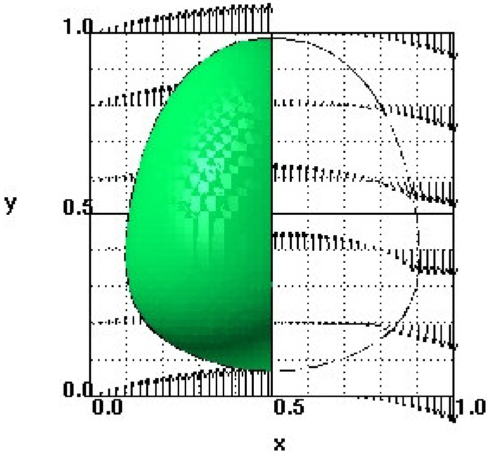
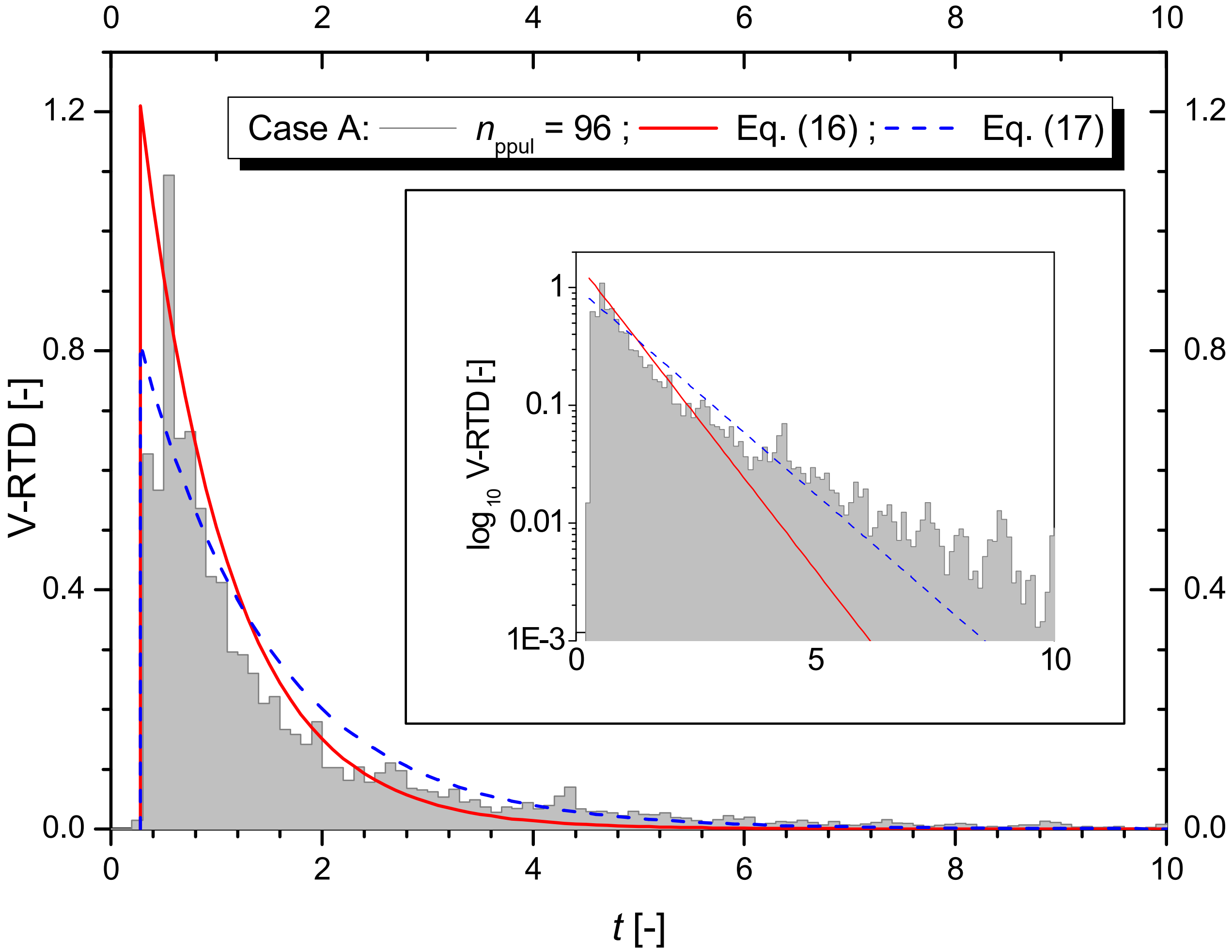
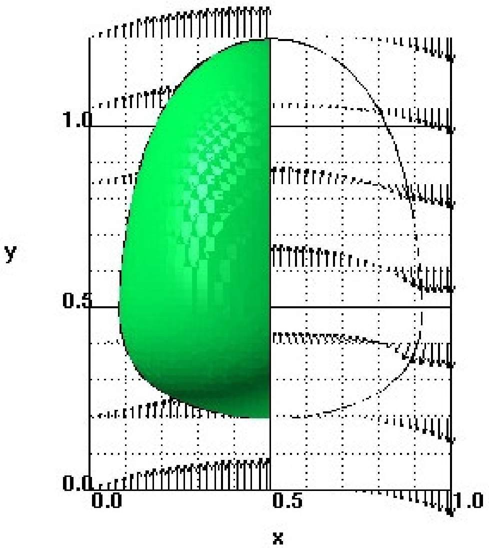
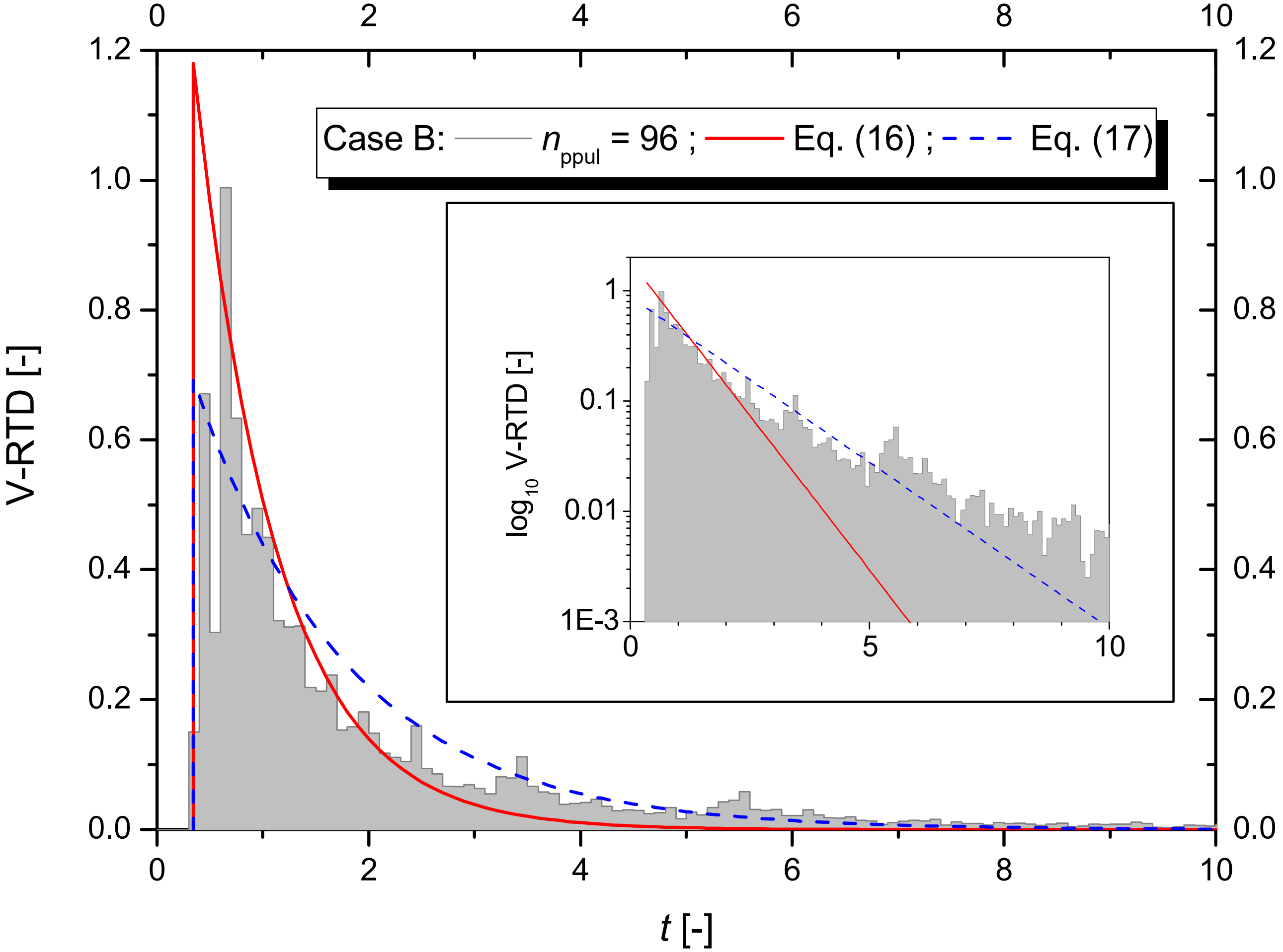


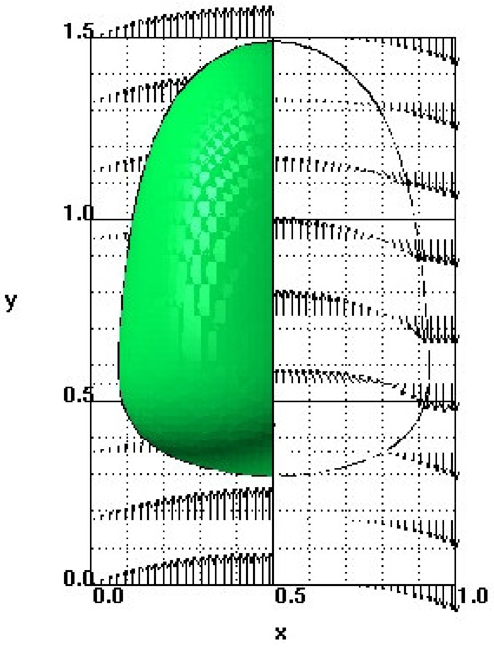


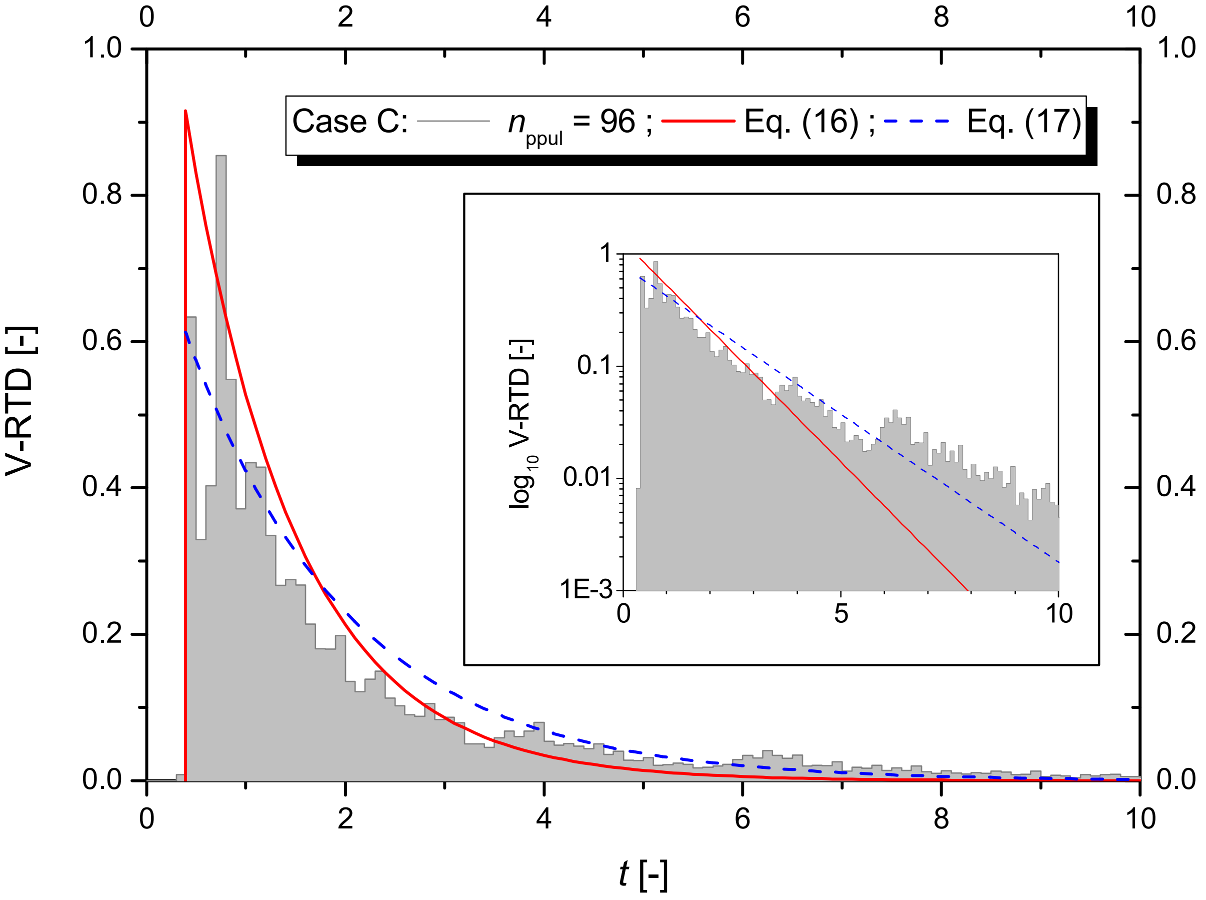
Compartment model for case B



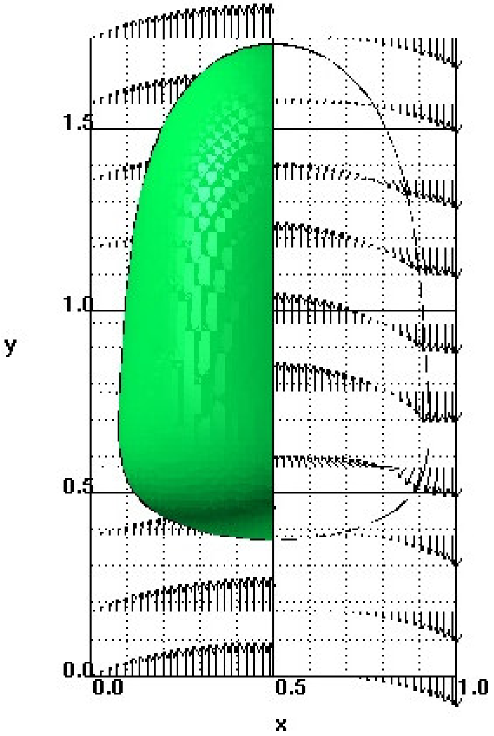


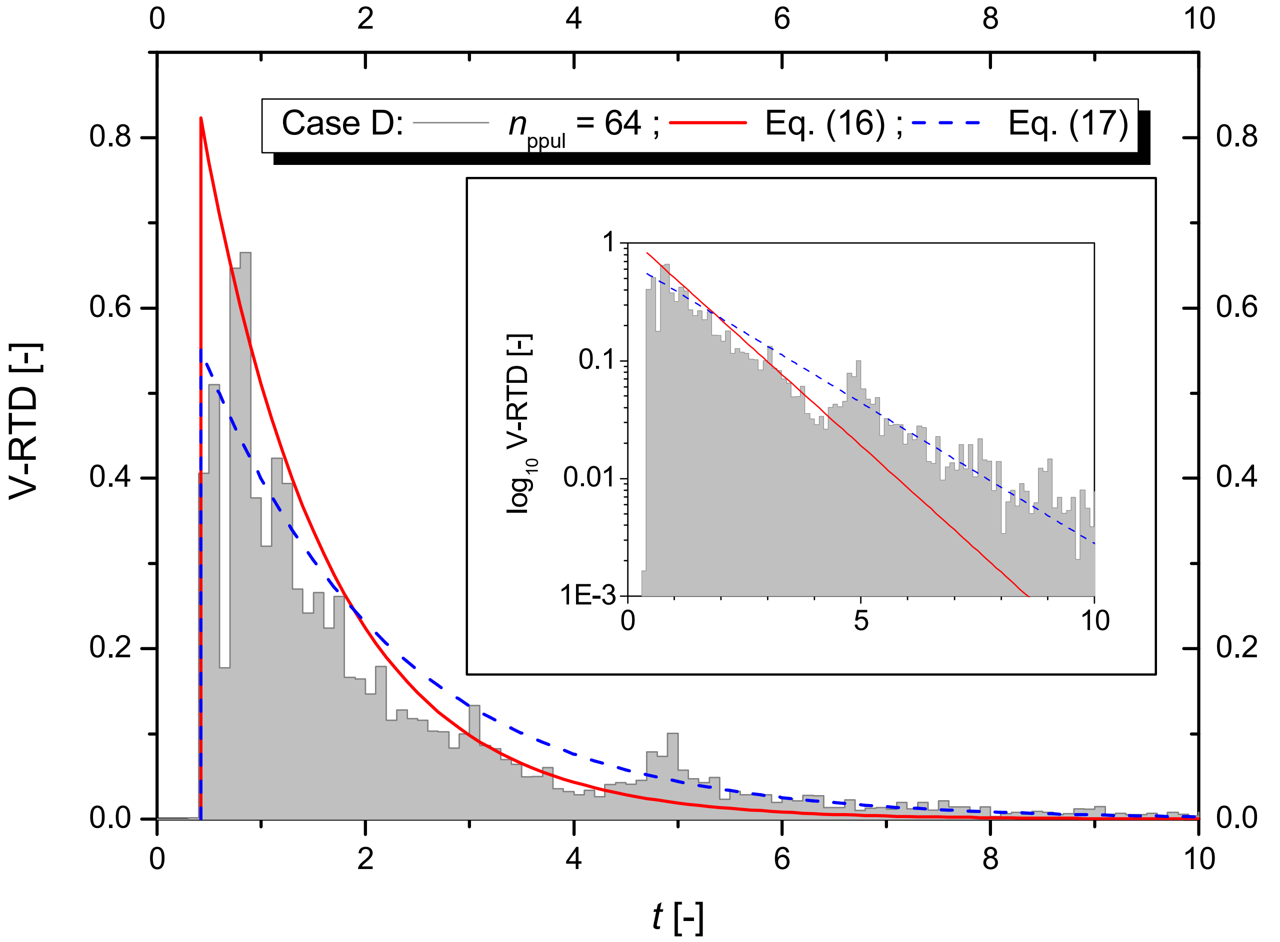
Compartment model for case C



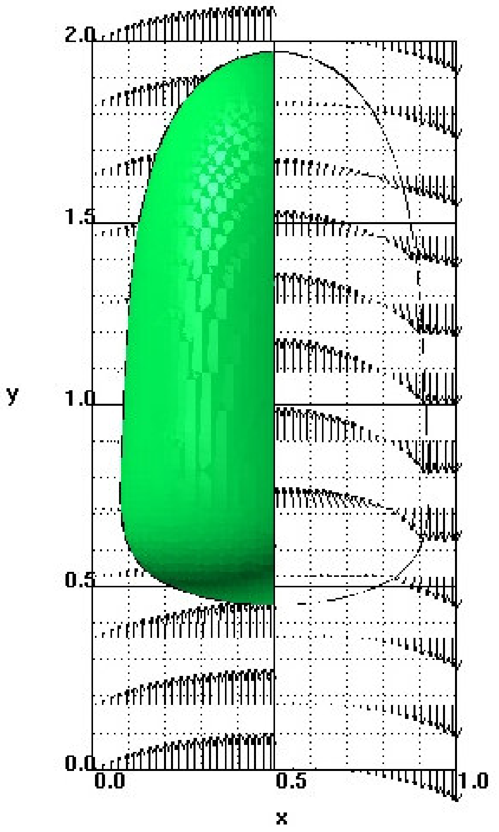


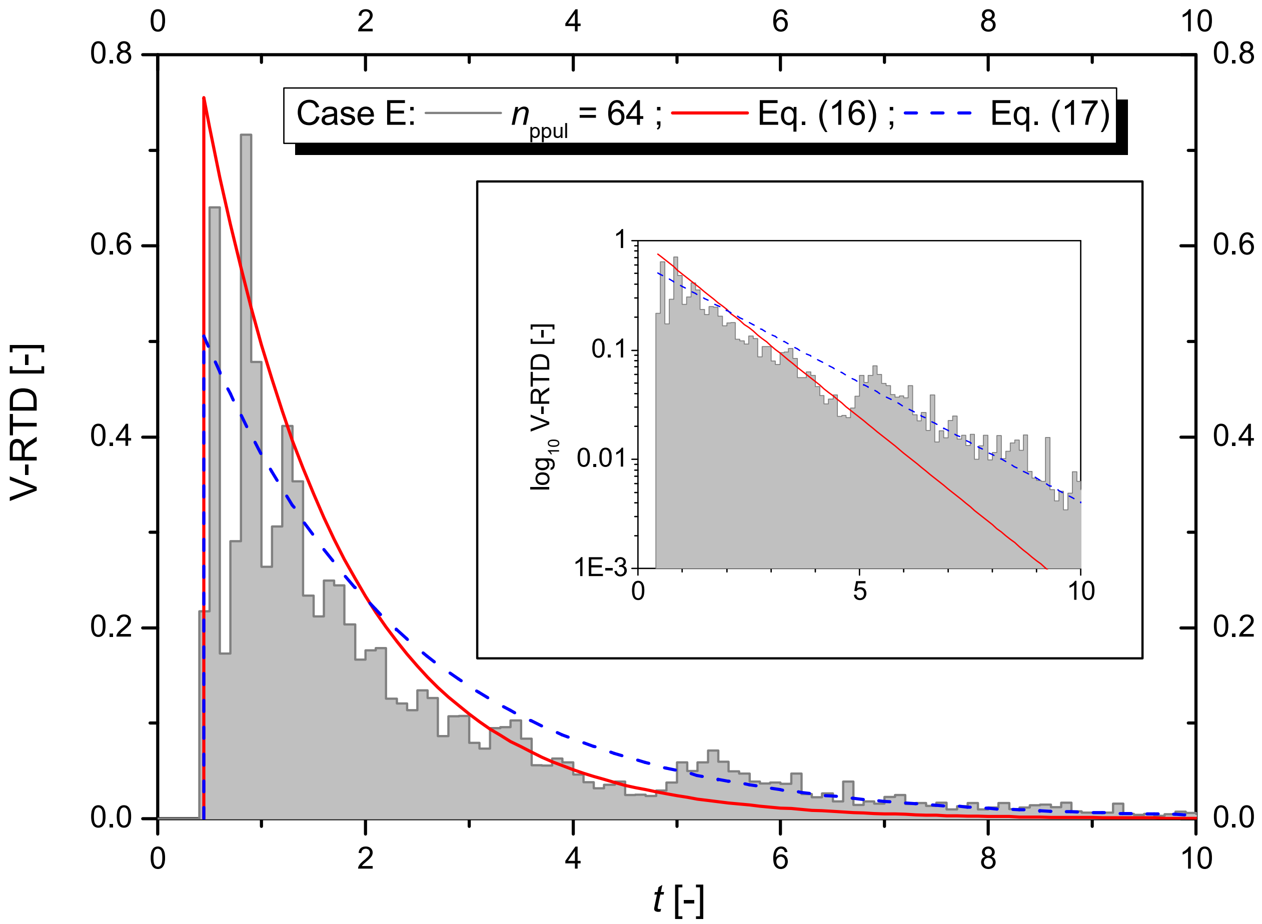
Compartment model for case D





Compartment model for case E





Conclusions

- Direct numerical simulation of bubble train flow (BTF)
  - Square vertical mini-channel of width $W = 2$ mm
  - Co-current vertical flow of air bubbles in silicon oil
  - Good agreement with experimental data from literature
- Original procedure to evaluate the liquid phase RTD
  - Introduction of mass-less particles into volume of liquid phase
  - Tracking of particles and detecting time to travel distance L_{uc}
  - Evaluated RTD is well described by compartment model with plug flow reactor and stirred vessel in series
- Outlook
  - Determine RTD for traveling distance $n_{\mathrm{uc}} \cdot L_{\mathrm{uc}}$ ($n_{\mathrm{uc}} = 2, 3, \ldots$)
  - Obtain RTD for arbitrary n_{uc} by convolution of RTD for $n_{\mathrm{uc}} = 1$ (?)