Evaluation of residence time distribution for bubble train flow in a square mini-channel by direct numerical simulation

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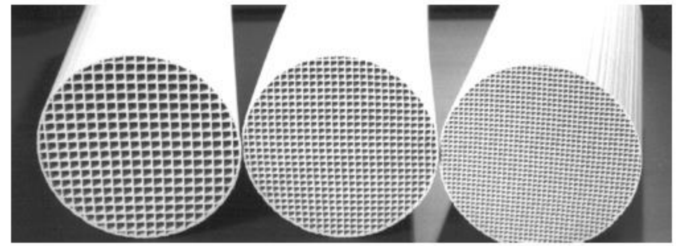
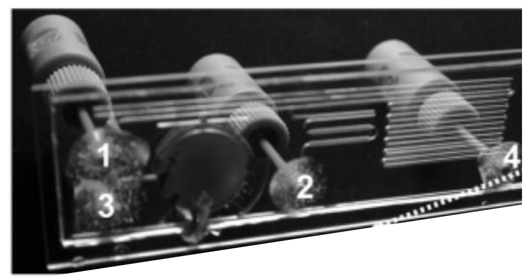
Outline

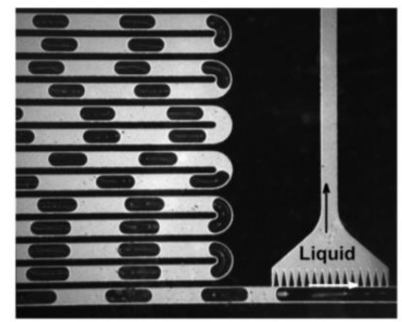
- Introduction and motivation
- Bubble train flow (BTF)
  - Computational setup
  - Simulation results and validation
- Residence time distribution (RTD)
  - Procedure to evaluate RTD
  - Results for RTD of bubble train flow
  - Model for the RTD
- Conclusions and outlook

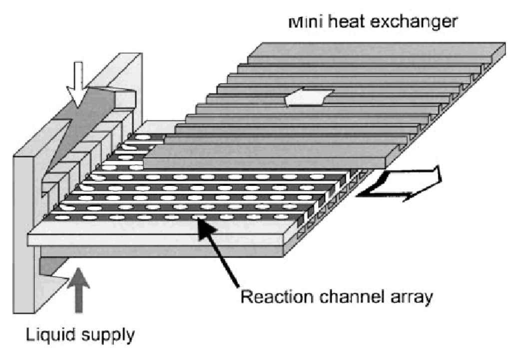
Gas-liquid flow in narrow channels with rectangular cross section

- Examples for devices
  - Monolithic reactors with catalytic walls
  - Micro-channel network (MIT)
  - Micro bubble column (IMM)
- Advantages
  - Enhanced mixing in liquid slug
  - Reduced axial dispersion
  - Efficient mass transfer across interface







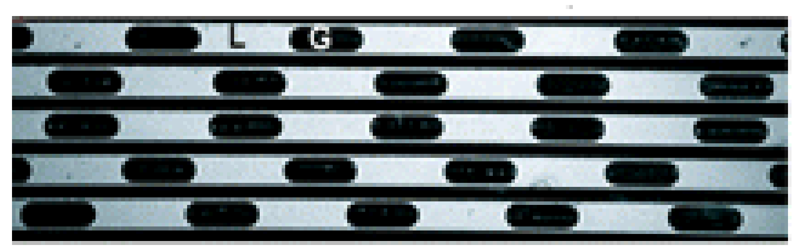


Motivation

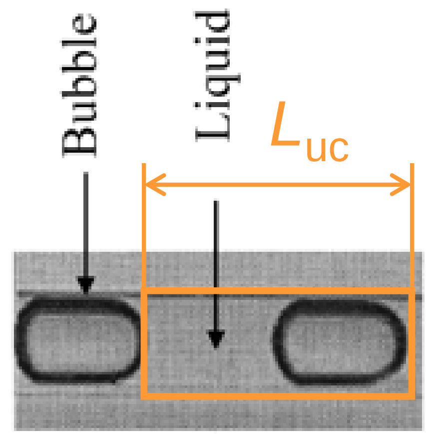
- Experimental investigation of these two-phase flows is difficult because of small dimensions and often yield integral data only
- <u>Goal:</u>
  - Perform direct numerical simulation (DNS) of bubble train flow in a single channel to resolve local flow phenomena
  - Use DNS results to evaluate residence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

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 one bubble and one liquid slug



uc = "unit cell"

Numerical set up

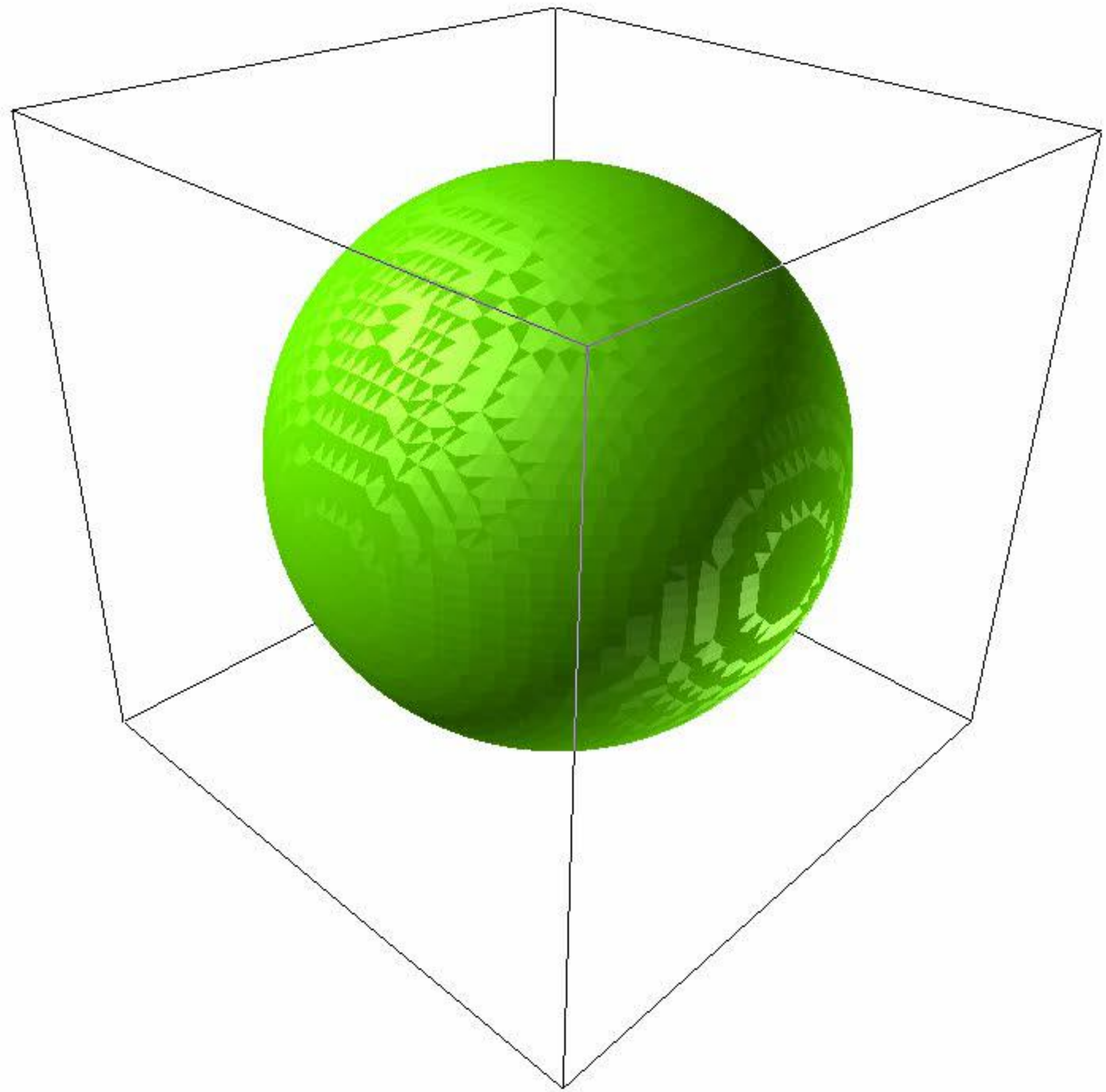
- In-house code TURBIT-VOF
  - Navier-Stokes eq. with surface tension term for two incompressible fluids
  - Volume-of-fluid method (interface is locally approximated as plane)
- Consider one flow unit cell only (one bubble, one slug)
- Account for influence of trailing/leading unit cells by periodic boundary conditions in axial direction
- Co-current upward vertical flow driven by specified pressure gradient
- Length of flow unit cell, L_{uc}, is input parameter
  - simulations for different values of L_{uc} and fixed void fraction $\varepsilon = 33\%$
- Comparison with experiments of Thulasidas et al.*
  - Air bubbles in silicon oil
  - Square channel with 2mm $\times$ 2mm cross section ($W = 2$mm)

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

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



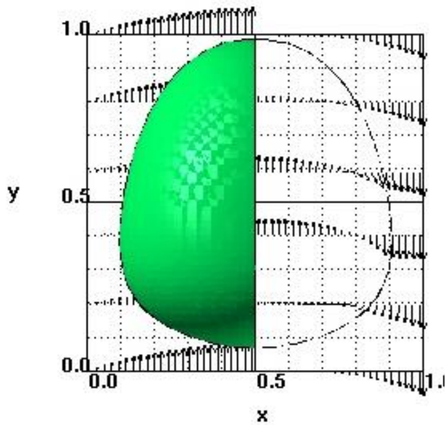
Case A2

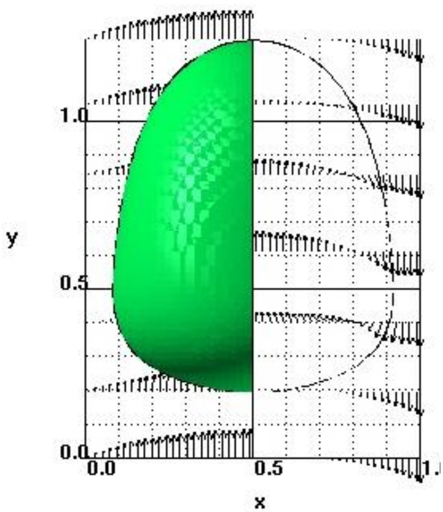
Computed bubble shape and velocity field for different values of L_{uc}

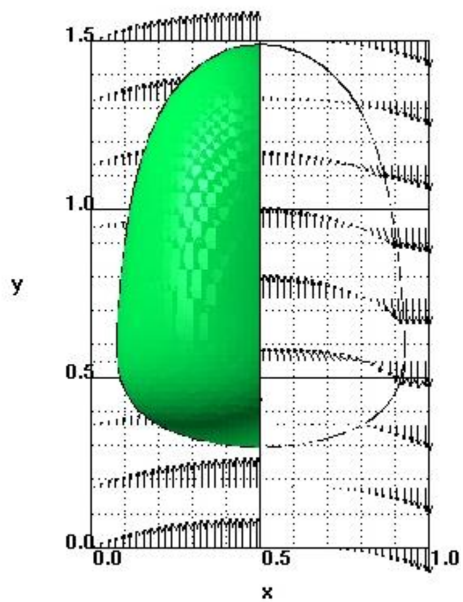
<u>Velocity field in vertical mid-plane</u>

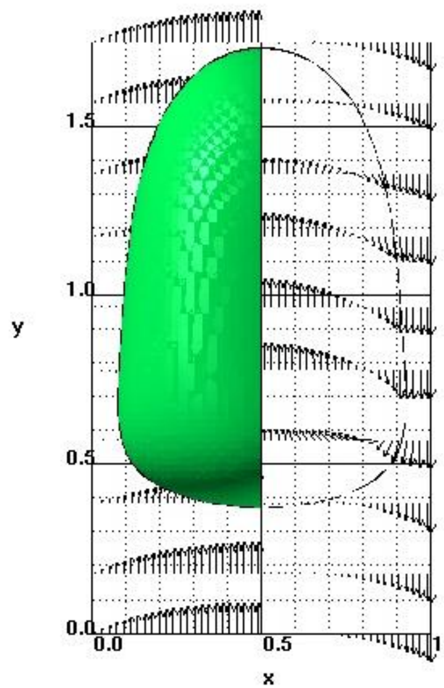
Right half: frame of reference moving with bubble

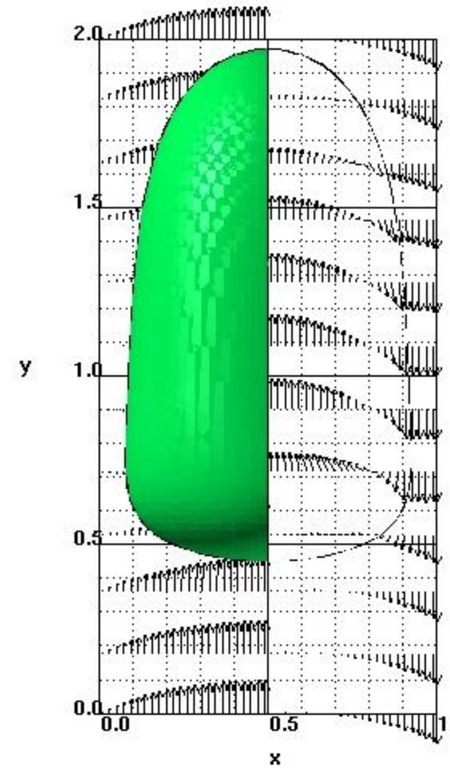
Left half: fixed frame of reference











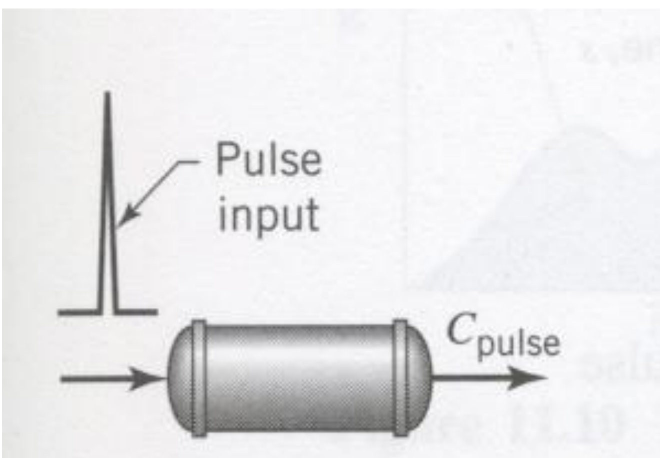
Comparison with experiment

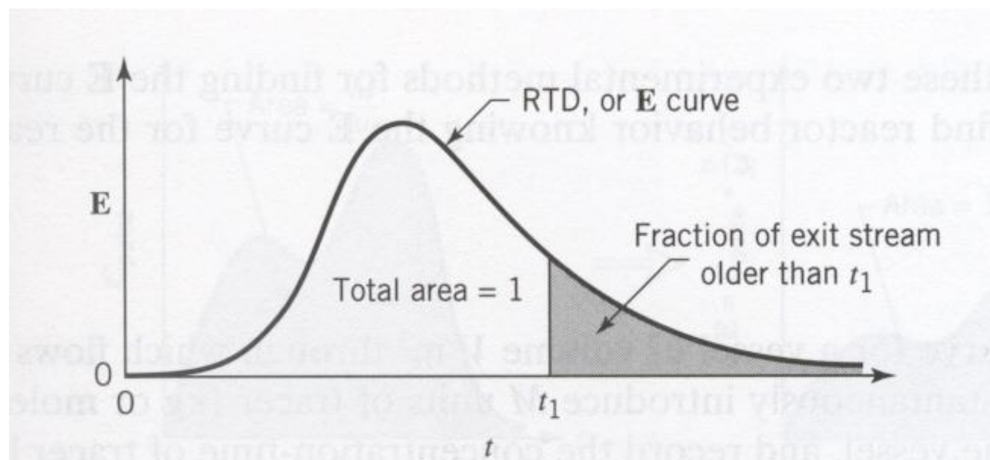
Case	L_{uc} / W	Ca_B	D_B / W (Non-dimensional bubble diameter)	$(U_B - J_{total})/U_B$ (Relative velocity)	U_B/J_{total} (Non-dimensional U_B)
A	1	0.204	0.81	1.80	0.445
B	1.25	0.207	0.84	1.75	0.430
C	1.5	0.215	0.85	1.75	0.430
D	1.75	0.238	0.85	1.78	0.438
E	2	0.253	0.85	1.8	0.445
Experimental data* correlated 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 ✓

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

Residence time distribution

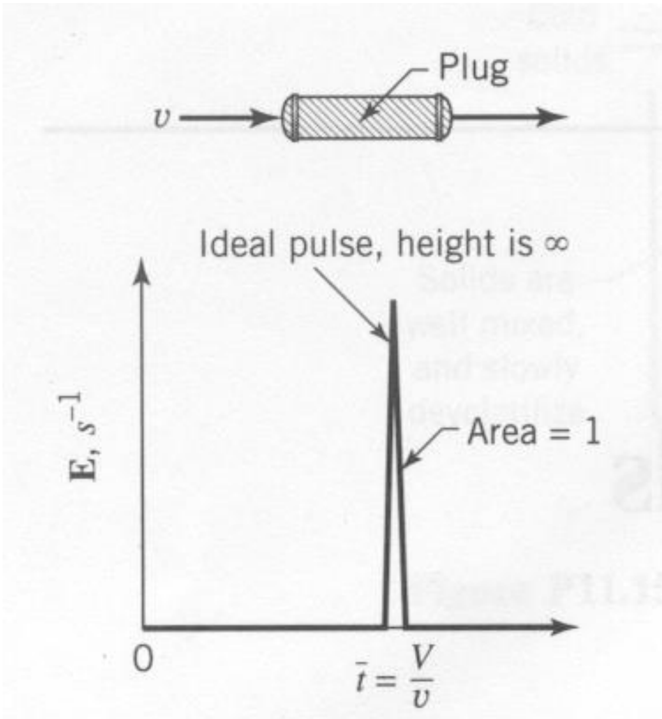
- The residence time distribution (RTD) is an important measure for characterization of any chemical reactor
  - The RTD influences yield and selectivity
- Common experimental method to determine RTD*
  - Add tracer at reactor inlet as a pulse and measure the tracer concentration at the outlet

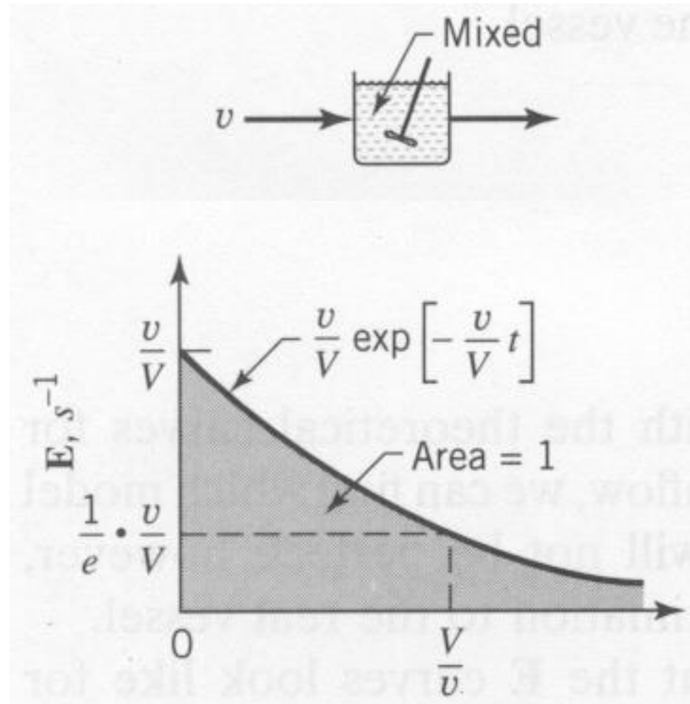




* Figures are taken from book "Chemical Reaction Engineering" by O. Levenspiel

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 fully developed DNS results for a certain instant in time
- Introduce virtual particles in mesh cells entirely filled with liquid
  - particle distance = 1 / 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 instant particle position from its relative position to the bubble, which is virtually moved with velocity U_B
- Store time the particle needs to travel an axial distance of L_{uc}
- Normalize histogram for all particles to obtain two RTD curves
  - *E**: no special weighting of particle residence times
  - *E*: weighting of particle residence time by axial velocity at release

RTD for single phase planar Poiseuille flow

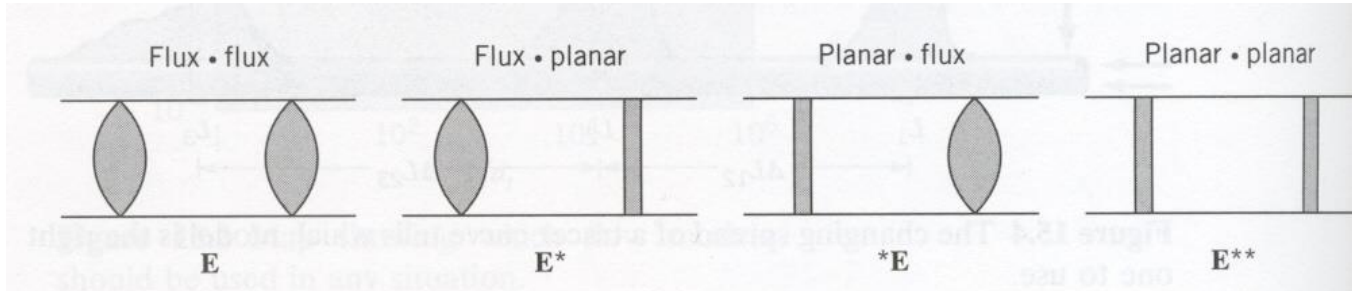
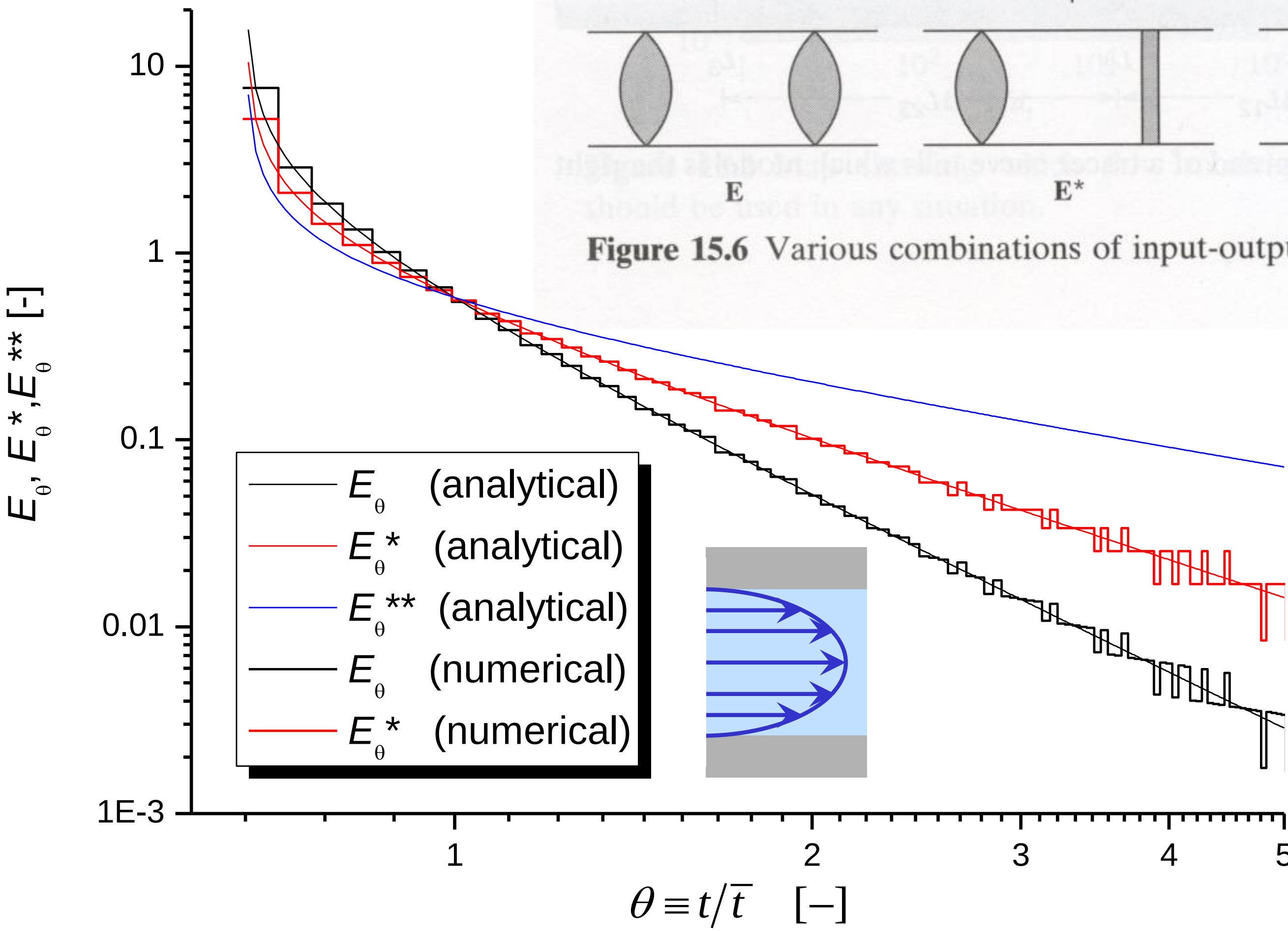


Figure 15.6 Various combinations of input-output methods.



For $\theta \equiv t/\bar{t} \geq 2/3$:

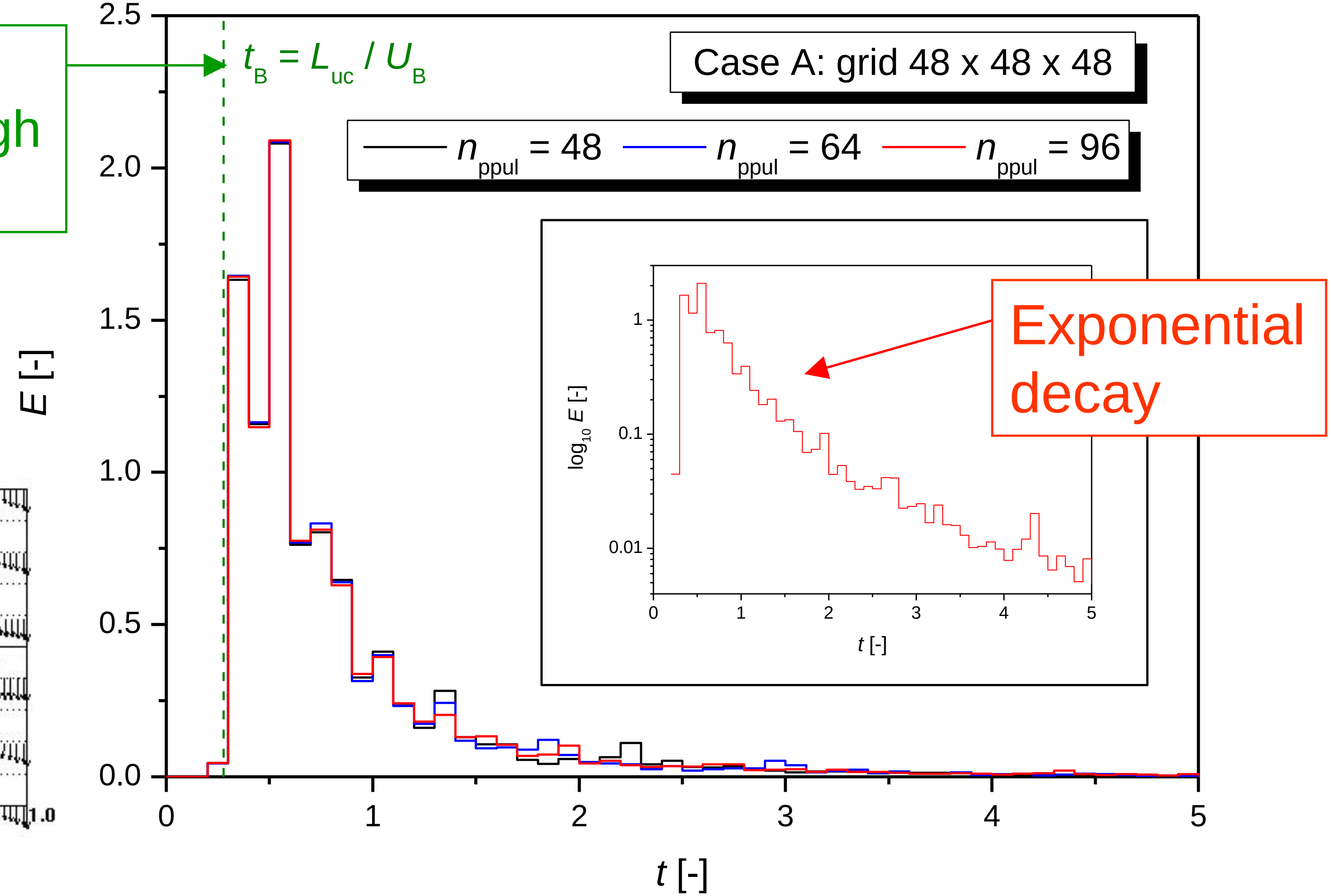
$$E_\theta(\theta) = \bar{t} \cdot E = \frac{1}{3\theta^3}\left(1 - \frac{2}{3\theta}\right)^{-\frac{1}{2}}$$

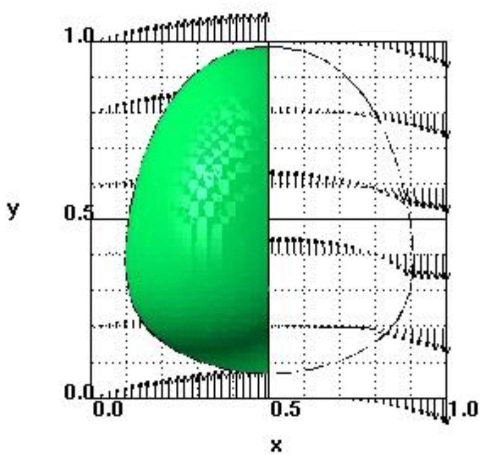
$$E_\theta^*(\theta) = \bar{t} \cdot E^* = \frac{1}{2\theta^2}\left(1 - \frac{2}{3\theta}\right)^{-\frac{1}{2}}$$

$$E_\theta^{**}(\theta) = \bar{t} \cdot E^{**} = \frac{1}{2\theta}\left(1 - \frac{2}{3\theta}\right)^{-\frac{1}{2}}$$

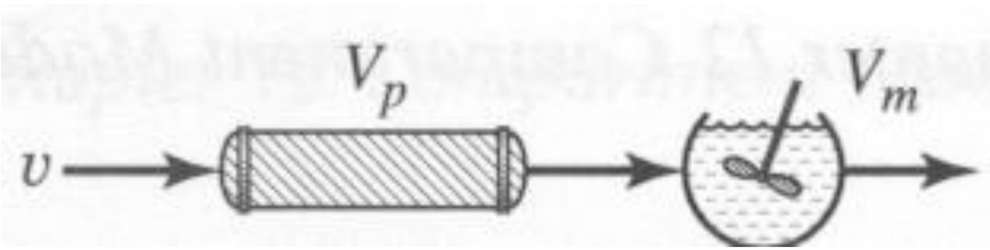
Influence of n_{ppul} for BTF case A

Bubble breakthrough time t_B

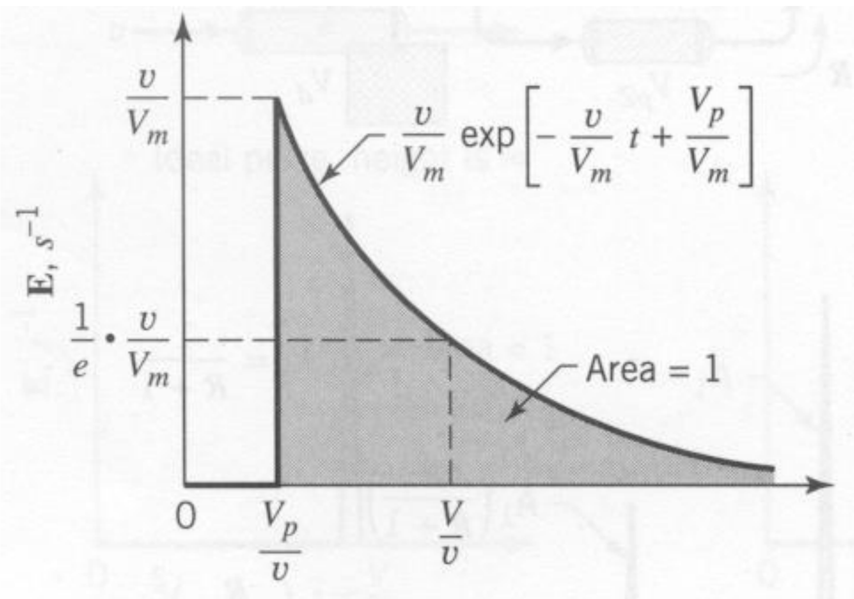




Compartment model



Plug flow reactor and stirred vessel in series (single phase flow)



$$E = \begin{cases} 0 & \text{for } t < L_{uc}/U_B \\ \frac{U_L}{L_{uc}} \exp\left(-\frac{U_L}{L_{uc}} \cdot t + \frac{U_L}{U_B}\right) & \text{for } t \geq L_{uc}/U_B \end{cases}$$

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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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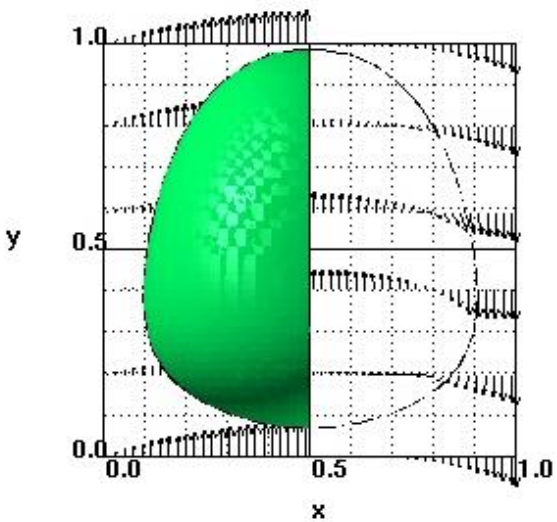
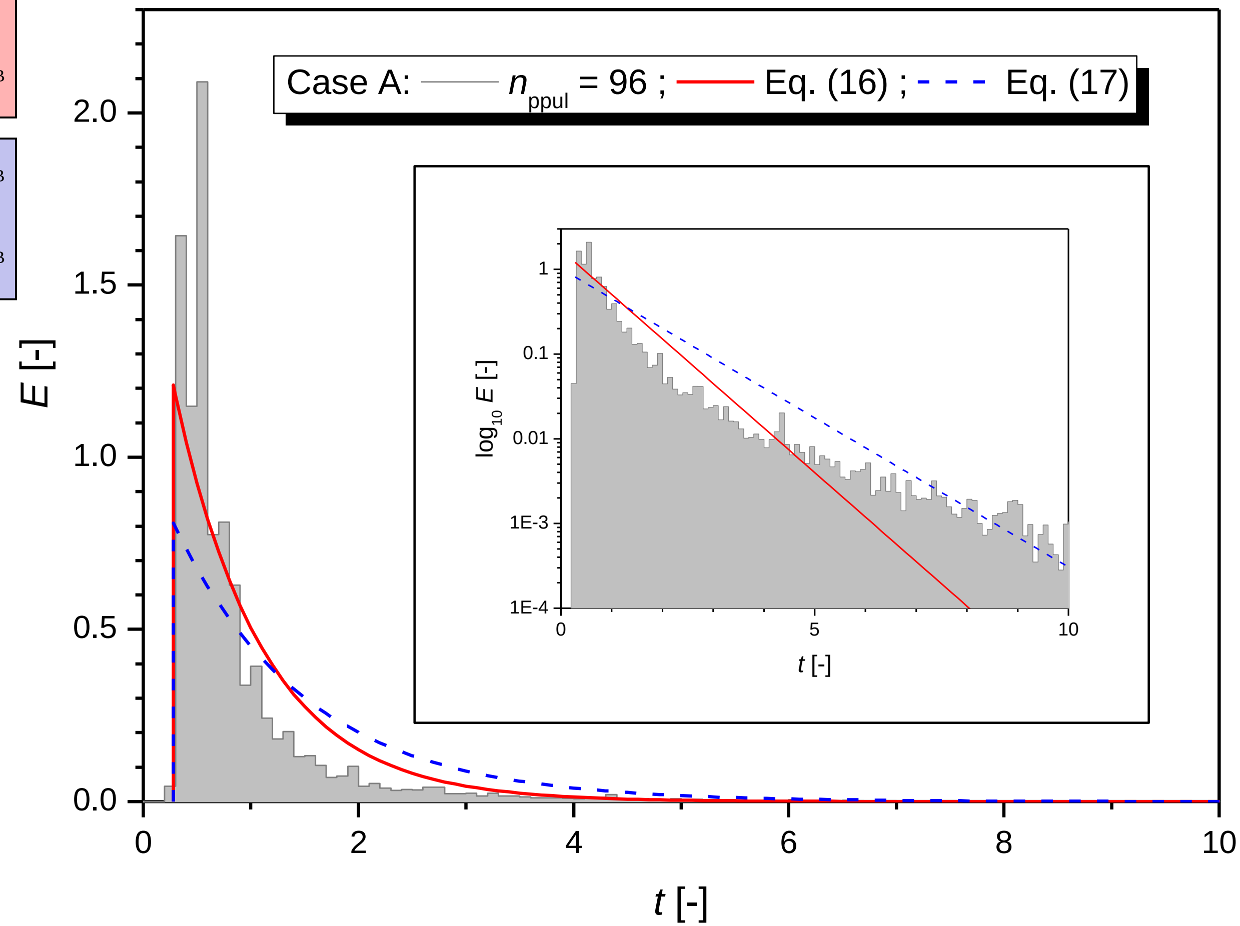
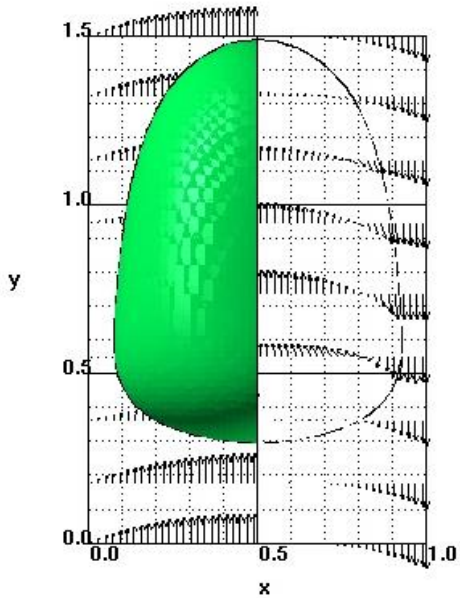
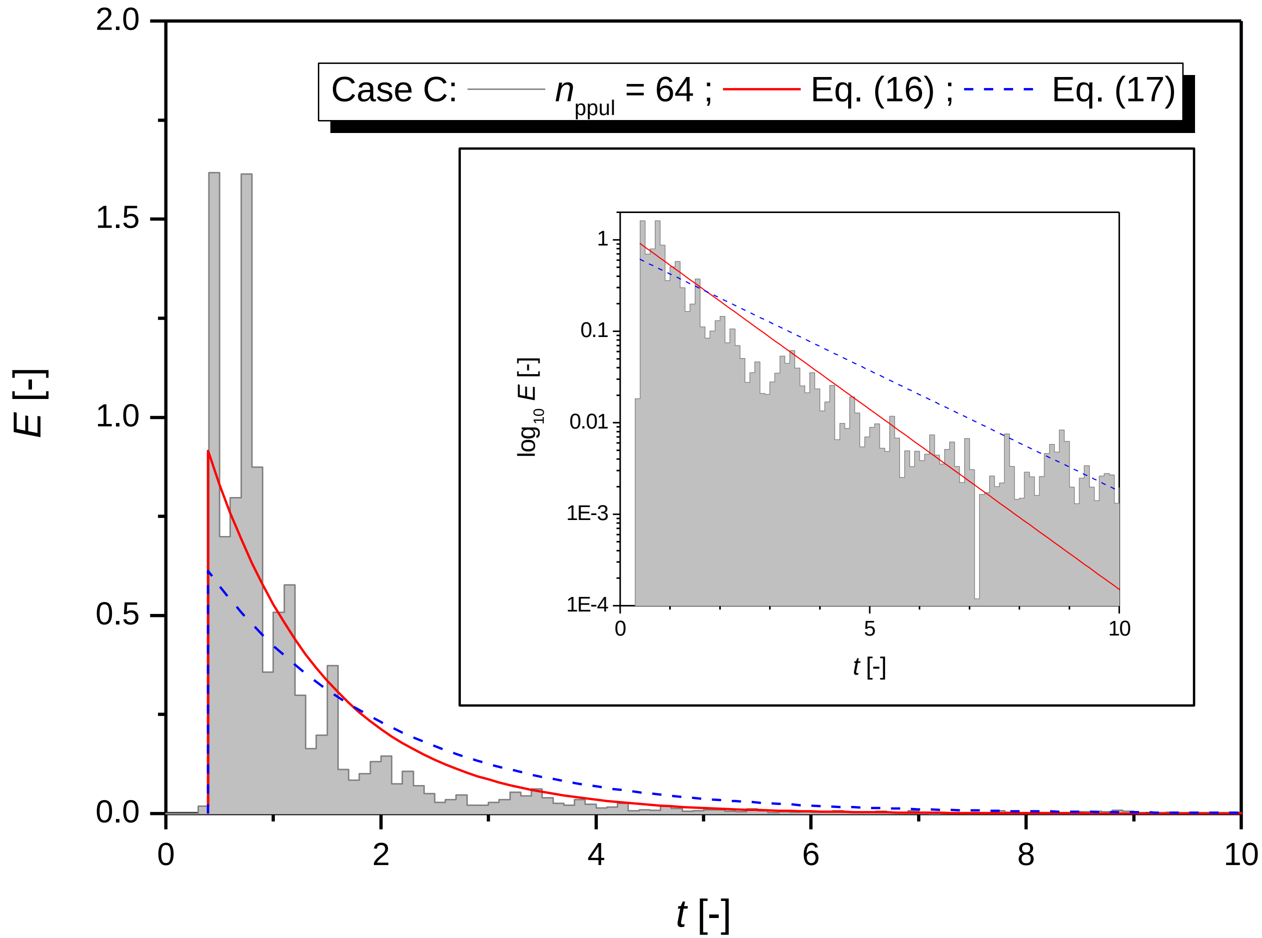


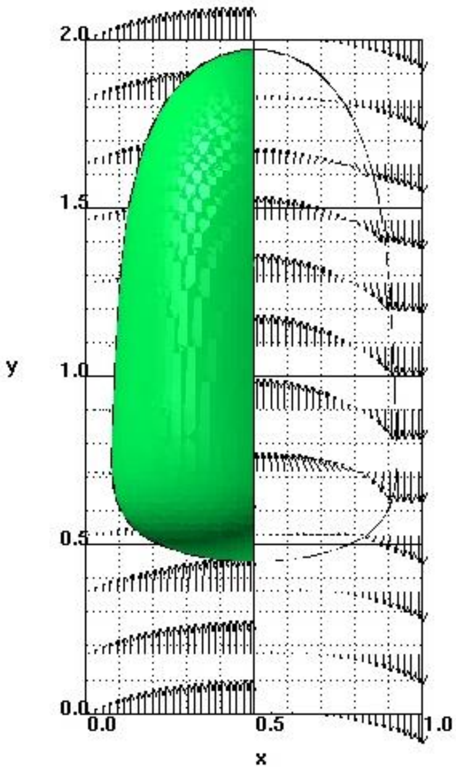


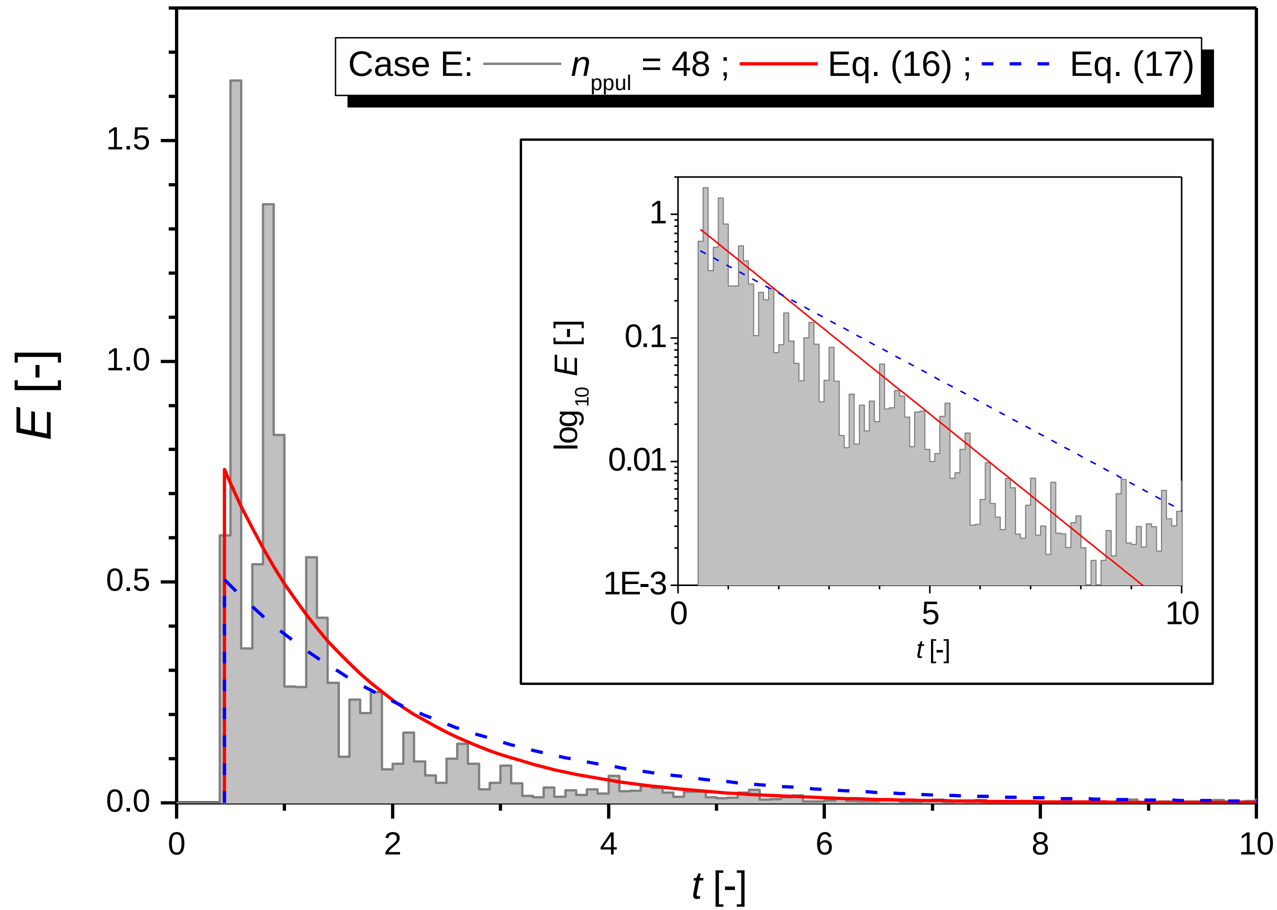
Compartment model for case C



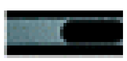
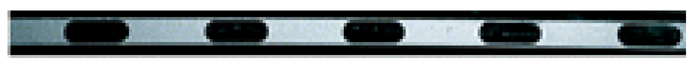


Compartment model for case E





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 can be approximated by compartment model with plug flow reactor and stirred vessel in series
- Outlook  
  - Identifying better model for liquid RTD of unit cell (?)
  - Determine RTD for traveling distance $n_{uc} \cdot L_{uc}$ ($n_{uc} = 2, 3, \ldots$)
  - Obtain RTD for arbitrary n_{uc} by convolution of RTD for $n_{uc} = 1$ (?)