Turbulence and residence time distribution in micromixers

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Summary

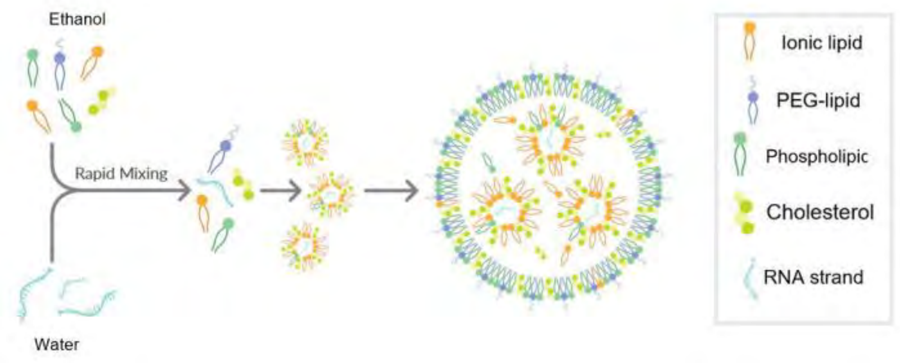
1. Introduction
2. Meshing
3. Model
4. Results
5. Conclusion and Future Works

Introduction

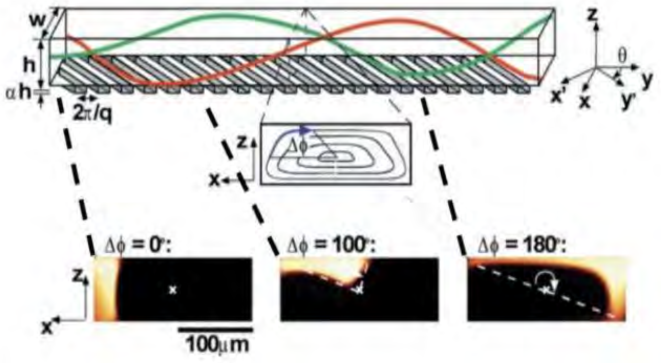
Micromixers devices rely on the geometry to promote mixture within the channel

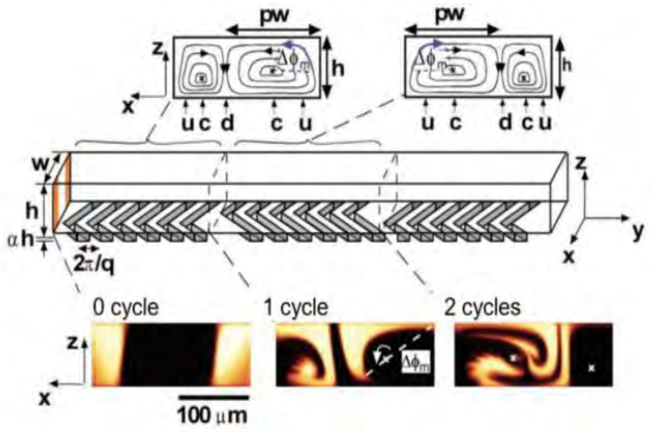
LNPs are formed through rapid mixing of 2 solutions

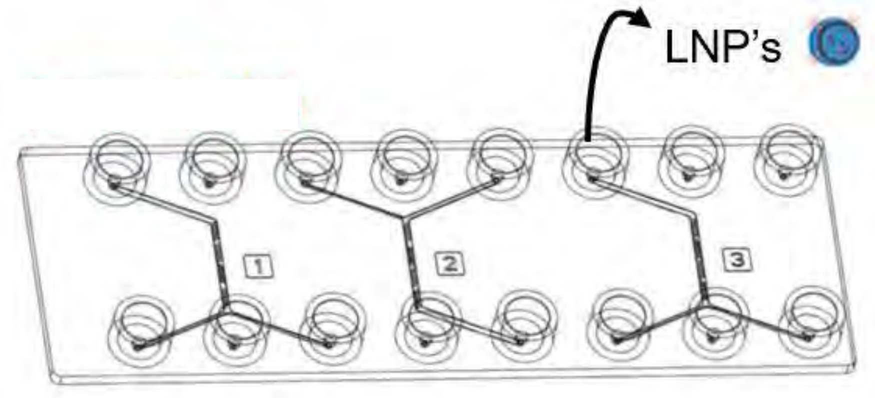
- ✓ Reproducible flow
- ✓ Low dispersivity



Herringbone mixers have ridges and grooves on the walls to generate secondary flows in the channel

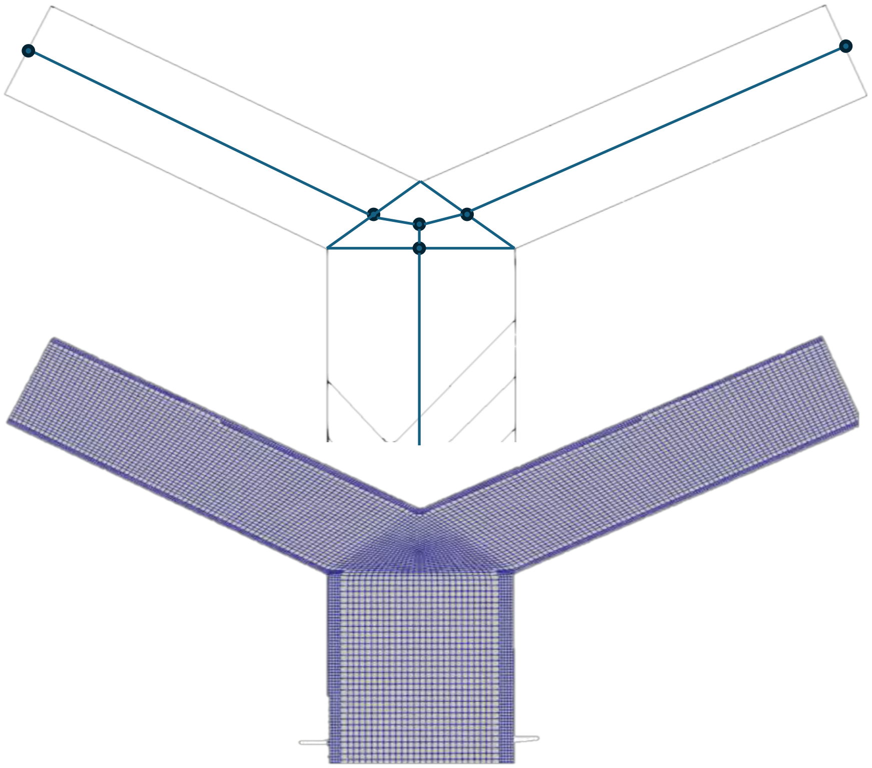






Geometry designed with Blender

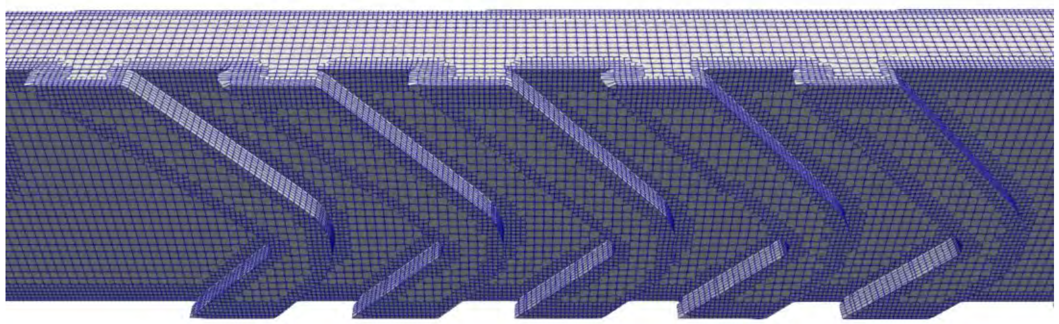
blockMesh > surfaceFeatureExtract > snappyHexMesh



One background block does not suffice for proper meshing

Total of 15 blocks to accomodate the geometry

Better refinement of ridges

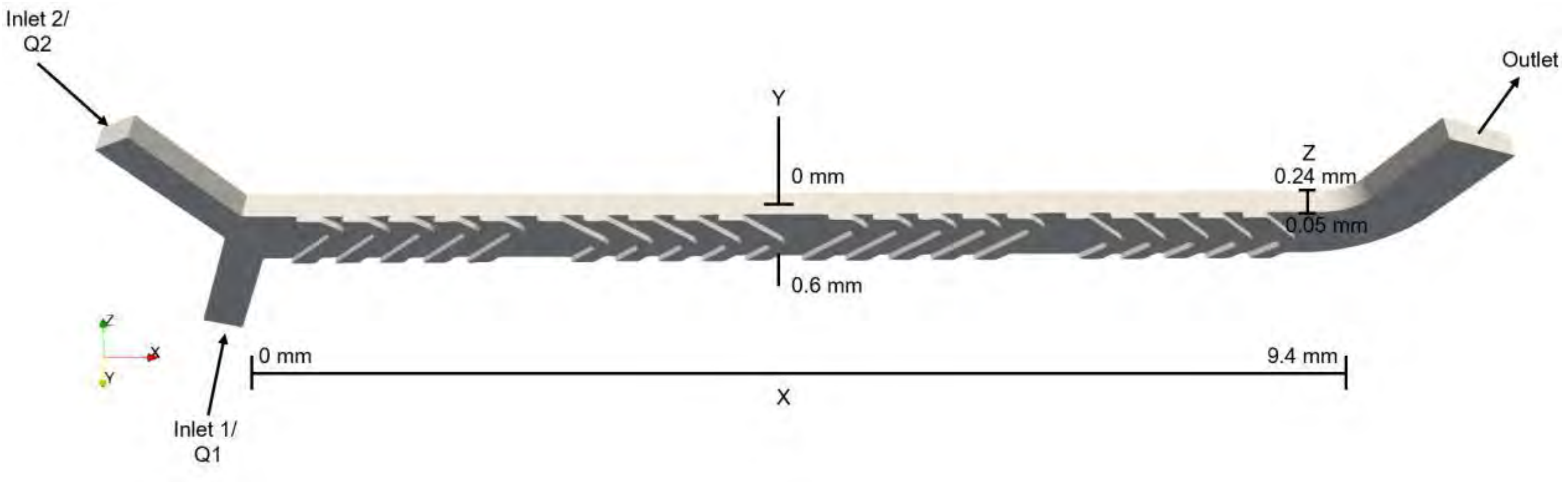


Boundaries: Inlet 1 & 2; Walls; Outlet

Number of cells = 303k => Result of grid convergence test

GCI = 0.3%

V = 1.373 mm^3

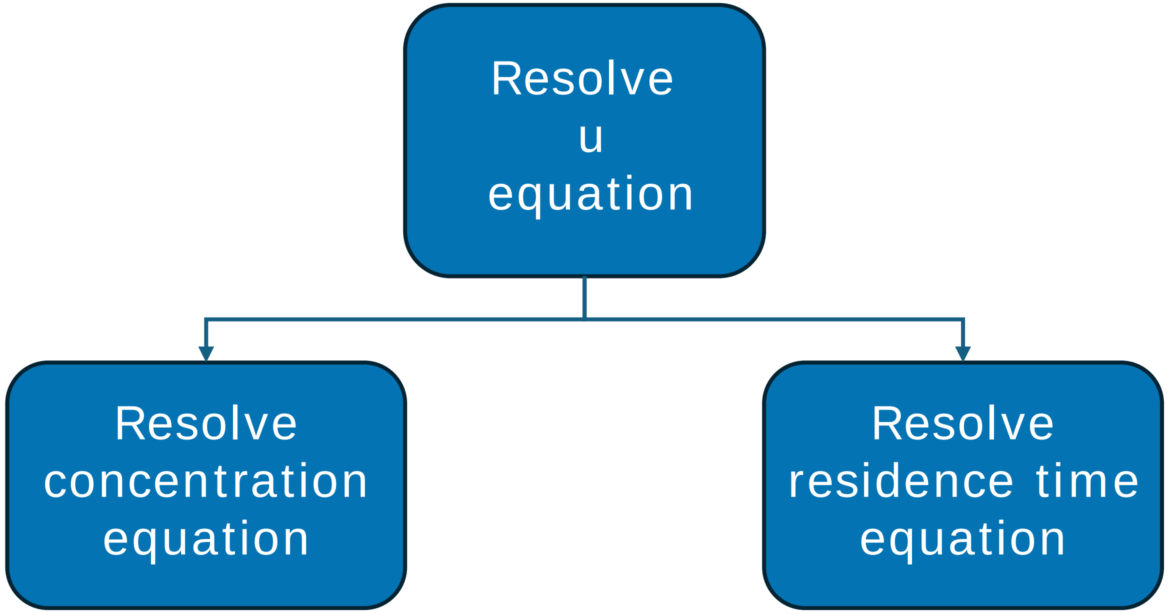


Model

Microfluidic device with 2 inlets to mix water – containg mRNA - and ethanol – containing lipids.

System: single phase; incompressible; steady state

SIMPLE solver used for simulations.



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Navier-Stokes equations:

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho(\vec{u} \cdot \nabla)\vec{u} = -\nabla P + \mu \nabla^2 \vec{u} + \rho \vec{g}$$

$$\nabla \cdot \vec{u} = 0$$

Turbulent modeling considered RANS k-ω SST

Resolve concentration equation

Resolve residence time equation

Model

Microfluidic device with 2 inlets to mix water – containg mRNA - and ethanol – containing lipids.

System: single phase; incompressible; steady state

SIMPLE solver used for simulations.

Resolve u equation

Transport equation for concentration of component A – ethanol

$$\frac{\partial C_A}{\partial t} + \nabla \cdot \vec{u} C_A - \nabla \cdot D_T \nabla C_A = 0$$

Due to turbulent modeling, turbulent diffusion is included:

$$D_T = D_A + \frac{v_{tur}}{Sc_{tur}}$$

Resolve residence time equation

Microfluidic device with 2 inlets to mix water – containg mRNA - and ethanol – containing lipids.

System: single phase; incompressible; steady state

SIMPLE solver used for simulations.

Resolve u equation

Resolve concentration equation

Transport equations for residence time of system:

$$\frac{\partial \tau}{\partial t} + \nabla \cdot \vec{u}\tau = 1$$

Boundaries conditions:

- Inlet 1 & 2:

  Uniform velocity

  Ethanol concentration set to 1 $\frac{\text{mol}}{\text{m}^3}$ at Inlet 1

  Inlet residence time equals 0

  k values calculate - assuming a eddy viscosity ratio of 1

- Outlet:

  Pressure fixedValue set to 0

- Walls:

  noSlip condition − velocity at the wall equals zero

  omegaWallFunction

- 2 inlets velocities simulated

Simulation	FRR	TFR/ mL/min	Q1/ mL/min	Q2/ mL/min
A	4	4	0.80	3.20
B	4	20	4.00	16.00

- Transport conditions

$v/ \frac{mm^2}{s}$	$D_A/ \frac{mm^2}{s}$	Sc_{tur}
1	0.001	0.9

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Post-processing

Mixing Index:

$$MI = 1 - \frac{\sigma_m}{\bar{C}} = 1 - \frac{\left[\frac{\sum Q_i (C_i - \bar{C})}{\sum Q_i}\right]^{1/2}}{\bar{C}}$$

Turbulence Intensity:

$$Int \equiv \frac{\sqrt{\frac{1}{3}\left(u_x'^2 + u_y'^2 + u_z'^2\right)}}{\sqrt{\bar{u}_x^2 + \bar{u}_y^2 + \bar{u}_z^2}} = \frac{\sqrt{\frac{2}{3}k}}{\sqrt{\bar{u}_x^2 + \bar{u}_y^2 + \bar{u}_z^2}}$$

- **Low Turbulence:** Int ≤ 1%
- **Medium Turbulence:** 1% ≤ Int ≤ 5%
- **High Turbulence:** 5% ≤ Int ≤ 20%

$$fV(\%) = \frac{V(Intensity \geq 1\%)}{V_{total}}$$

Residence Time:

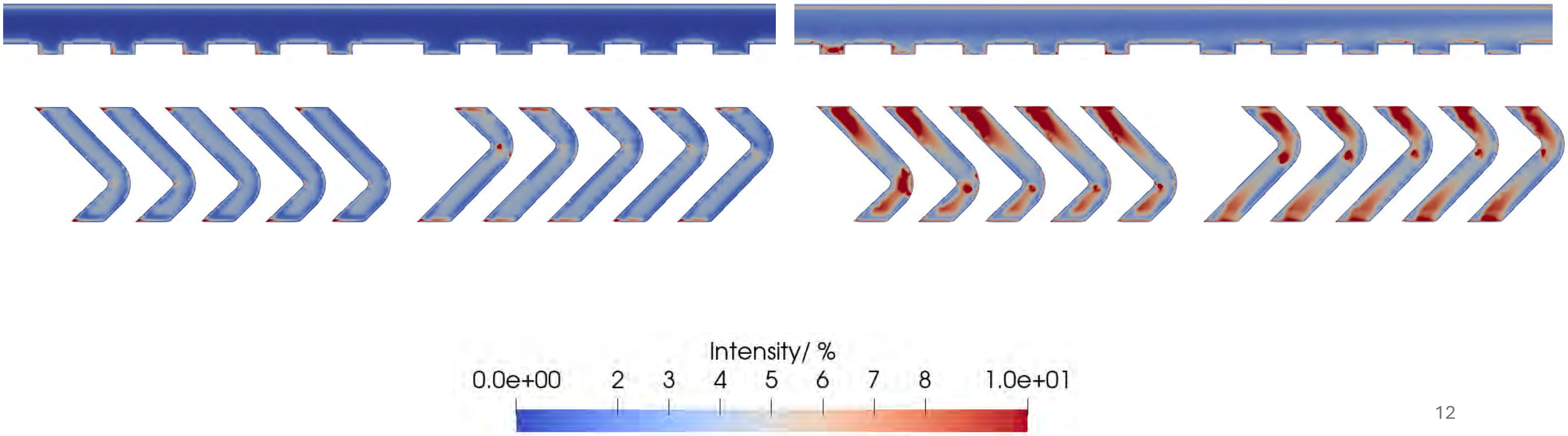
$$\mu = \frac{\sum Q_i \tau}{\sum Q_i}$$

$$\frac{\sigma}{\mu} = \frac{\left[\frac{\sum Q_i (\tau_i - \mu)}{\sum Q_i}\right]^{1/2}}{\left[\frac{\sum Q_i \tau}{\sum Q_i}\right]}$$

Localized turbulence:

TFR = 4 mL/min

TFR = 20 mL/min

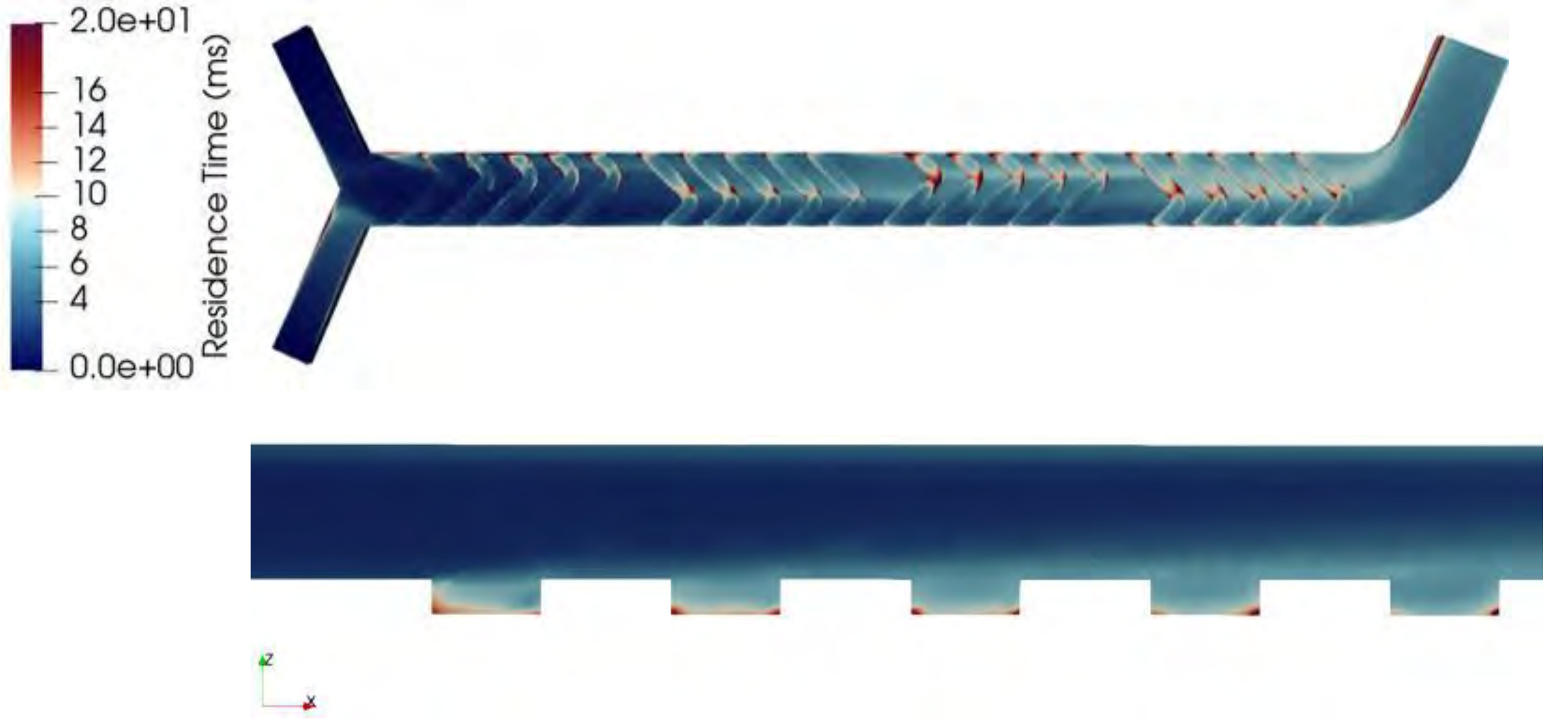


Localized residence time:

Localized time residence higher at the edges of the grooves

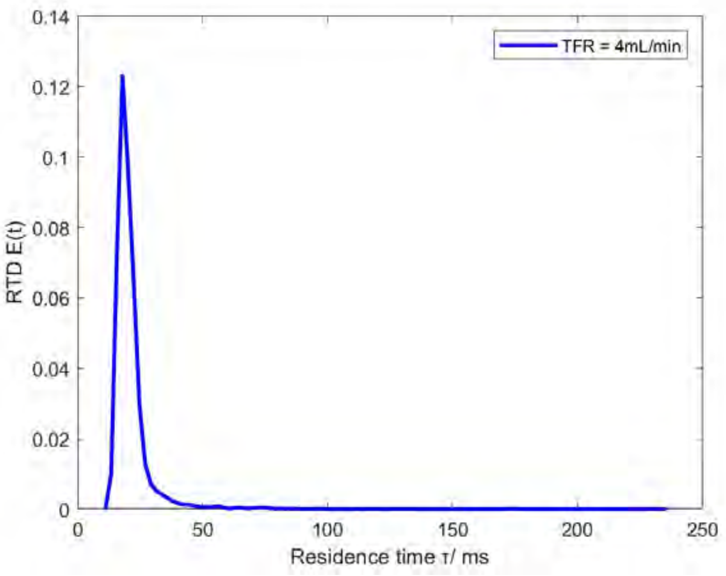
Free stream at main channel

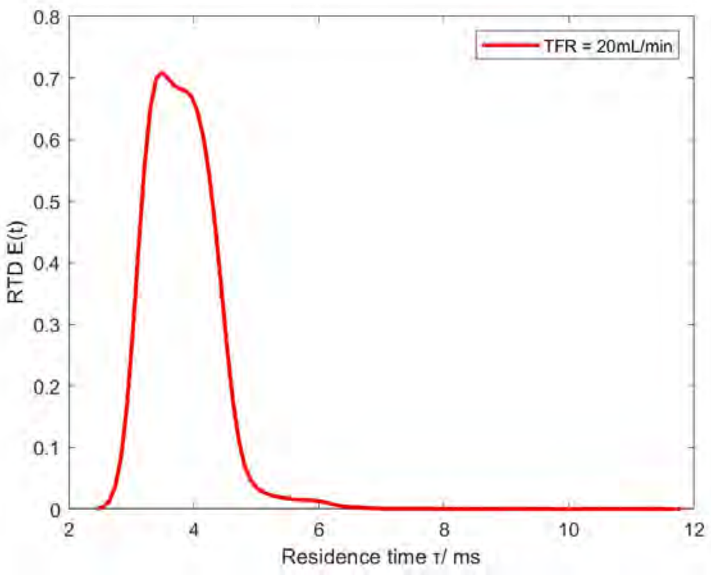
TFR = 4 mL/min

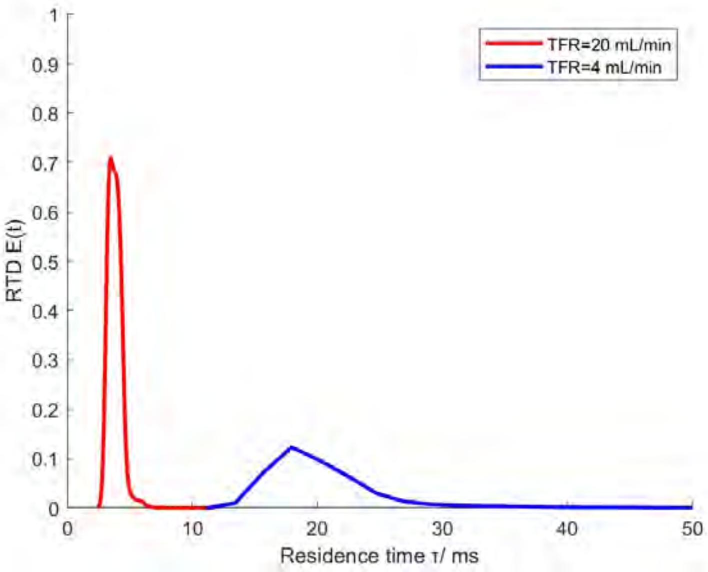


Localized residence time:

Age of the fluid at the outlet is the post processed in MatLab:







TFR / mL/min	MI / %	$fV{:}I \geq 1\%$	$fV{:}I \geq 5\%$	V/TFR / ms	μ / ms	σ/μ
4	95.91	4.55	0.01	20.59	21.31	0.44
20	99.56	75.37	13.77	4.12	3.82	0.15

Conclusion and Future Works

Conclusion

- Mixing indexes above 90% - higher flow rate resulting in better mixing
- Turbulence is observed close to the channel walls
- Higher localized residence time at the edges of the grooves
- RTD is wider at lower flow rates

Future Works

- Pressure drop analysis to evaluate viable operating conditions
- Correlation of simulation results with experimental particle size distribution

Thanks for the attention!

Acknowledgments

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