Reaktive Blasenströmungen
DFG SPP 1740

Numerical simulation techniques for the efficient and accurate treatment of local fluidic transport processes together with chemical reactions

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Scientific goals

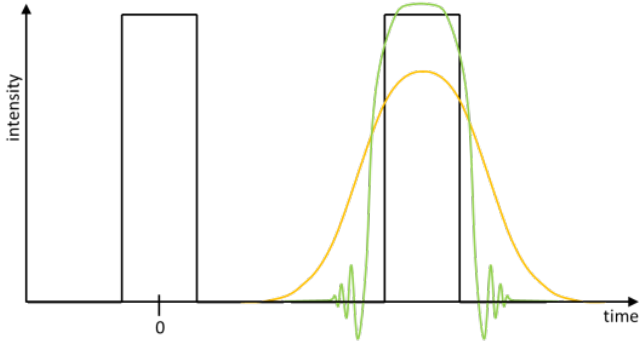
Extend the up-to-now developed and validated methodology and realize the corresponding software implementation in the CFD package FEATFLOW.

The main numerical ingredients to be combined/extended are the following:

- high-resolution Algebraic Flux Correction (AFC) stabilization schemes to suppress numerical diffusion and to prevent nonphysical oscillations
- locally adaptive Grid Deformation (GD) techniques applied on (general) unstructured meshes with the aim to obtain high-resolution computational meshes satisfying additional requirements on the relative orientation with respect to local velocity fields in order to further decrease the extent of numerical diffusion
- time-scale independent reaction modules for the treatment of mutually coupled fast chemical reactions supplemented with appropriate models to reflect the extent of segregation of the individual species

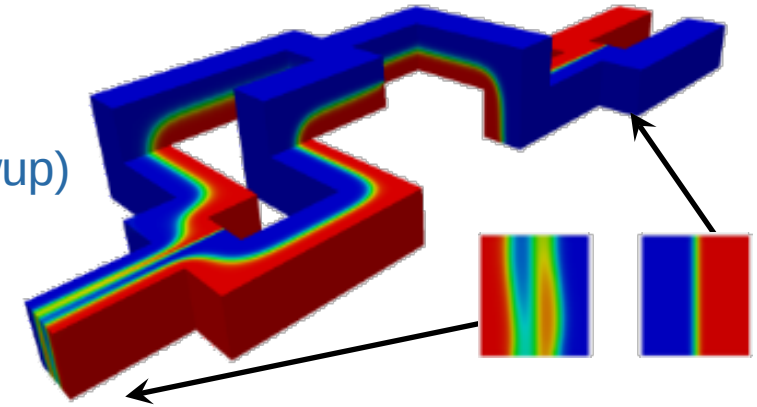
High-resolution AFC stabilization

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{v}c) - \alpha \Delta c = f(c) \qquad \text{with} \quad \alpha \longrightarrow 0$$



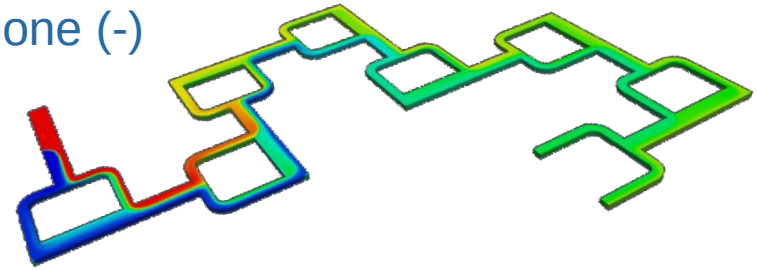
Standard discretizations face shortcomings for non-smooth solutions

- Low order methods lead to smearing
- High order methods introduce unphysical oscillations (potentially leading to simulation blowup)



Remedy: Algebraic Flux Correction method

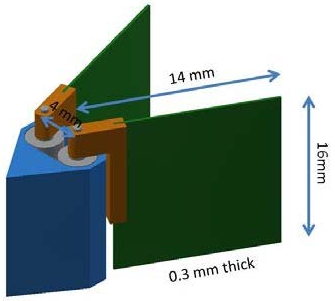
- Local extremum diminishing (+)
- Positivity preserving (+)
- Transforms the linear problem to a non-linear one (-)
- Robust and highly accurate (+)

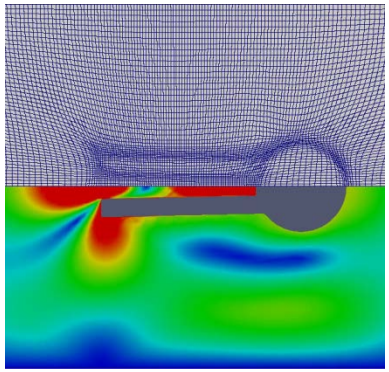


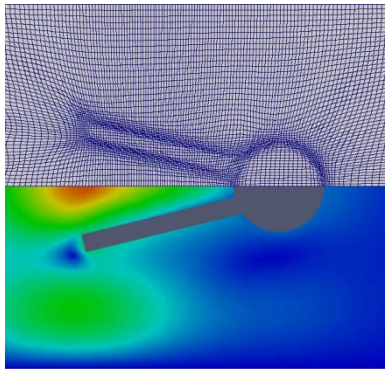
PDE-free mesh deformation method

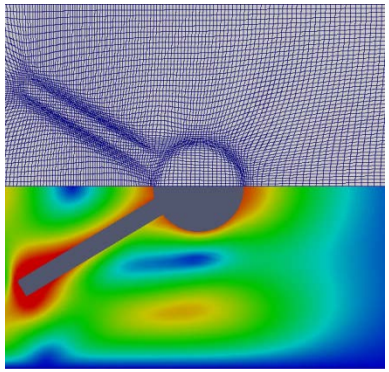
- Construction of (dynamic) monitor function (distance to interface, curvature, concentration gradients, vorticity
- Anisotropic Laplace smoothening (fast)
- Arbitrary Lagrangian-Eulerian Method (ALE) for non-stationary problems
- Handling geometrically complex/dynamic problems in the framework of FBM

Microfishes

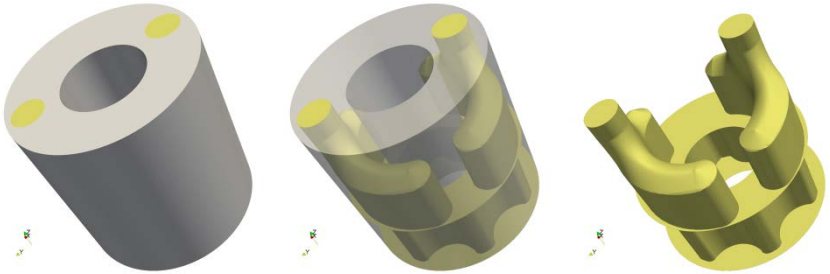


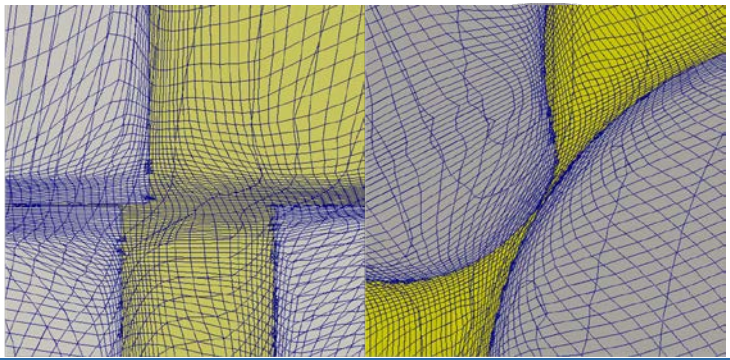






Micro gear pumps





Efficient CFD methods for coupled transport processes

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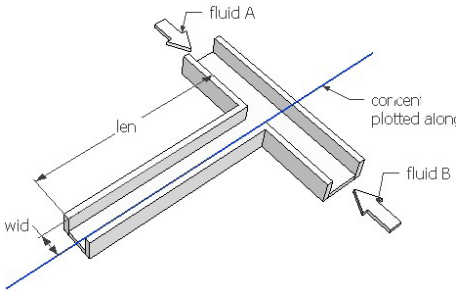
Simulation of chemical reactions (preliminary work within the SPP 1740)

$A + B \xrightarrow{k\to\infty} P$ $\partial_t\phi + u\cdot\nabla\phi = \nabla\cdot(d\nabla\phi)$ with $\phi = c_A\text{-}c_B$ Toor and Chiang



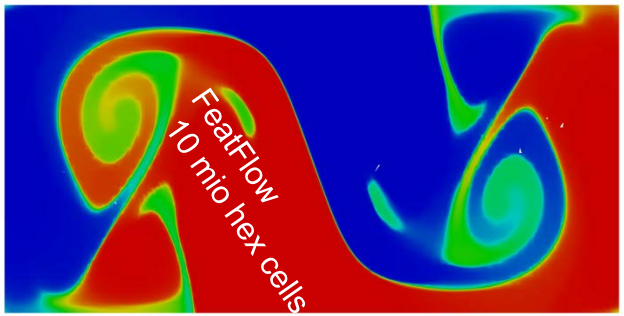
Adopted simulation technique:

Simultaneous use of two meshes /discretizations:

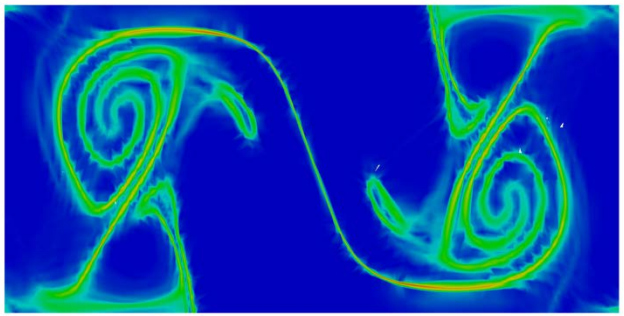
- equidistant , structured, low resolution for velocity
- deformed, structured, high resolution for passive/active scalar

Efficient and robust interpolation from mesh to mesh in parallel framework

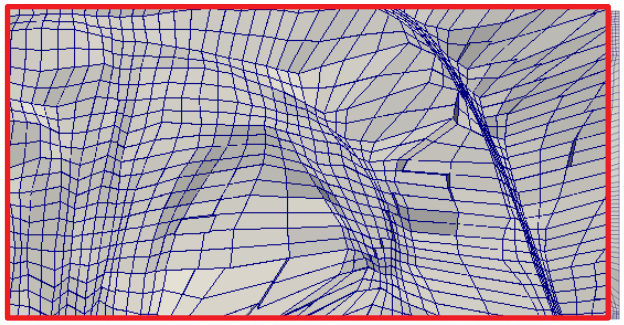
Transported scalar field ϕ



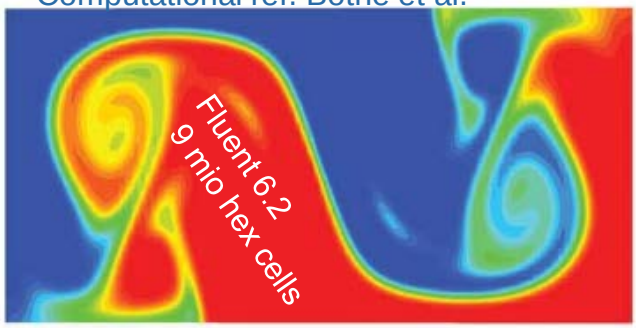
Monitor function

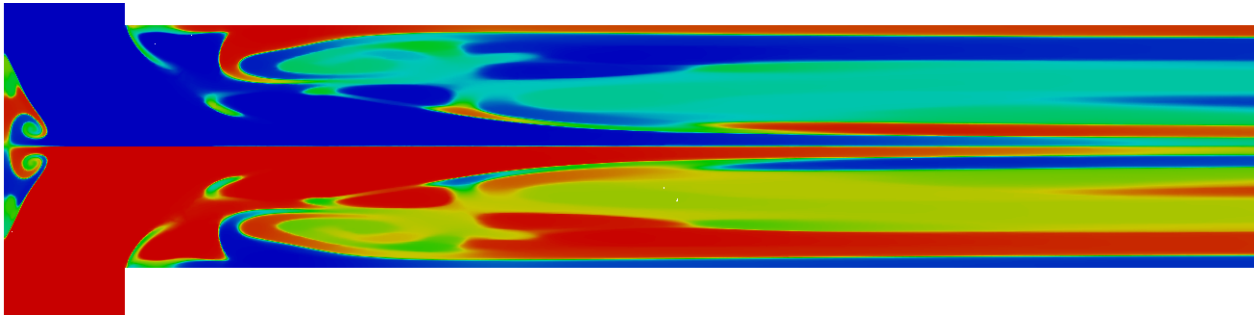


Computational mesh

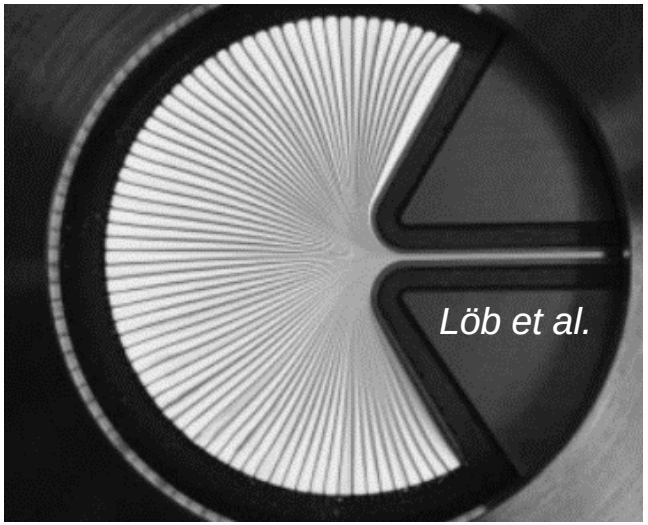


Computational ref. Bothe et al.





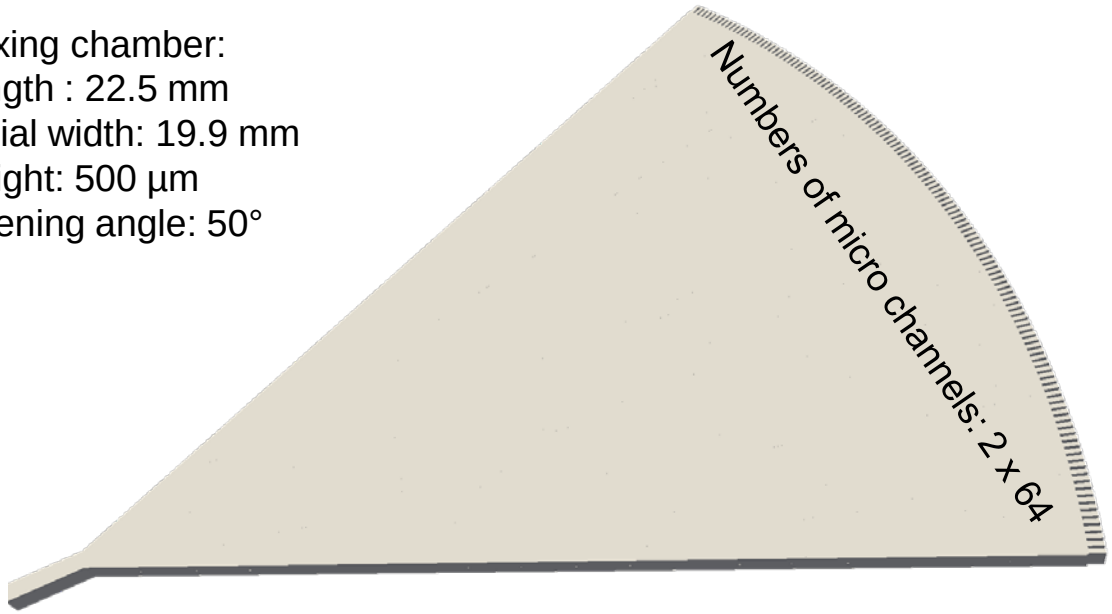
Simulation of the super-focus mixer (SFM)



Geometry of the final SFM with visualization of the reactants

Intermediate SFM geometry and operation conditions

Mixing chamber:
length : 22.5 mm
initial width: 19.9 mm
height: 500 µm
opening angle: 50°



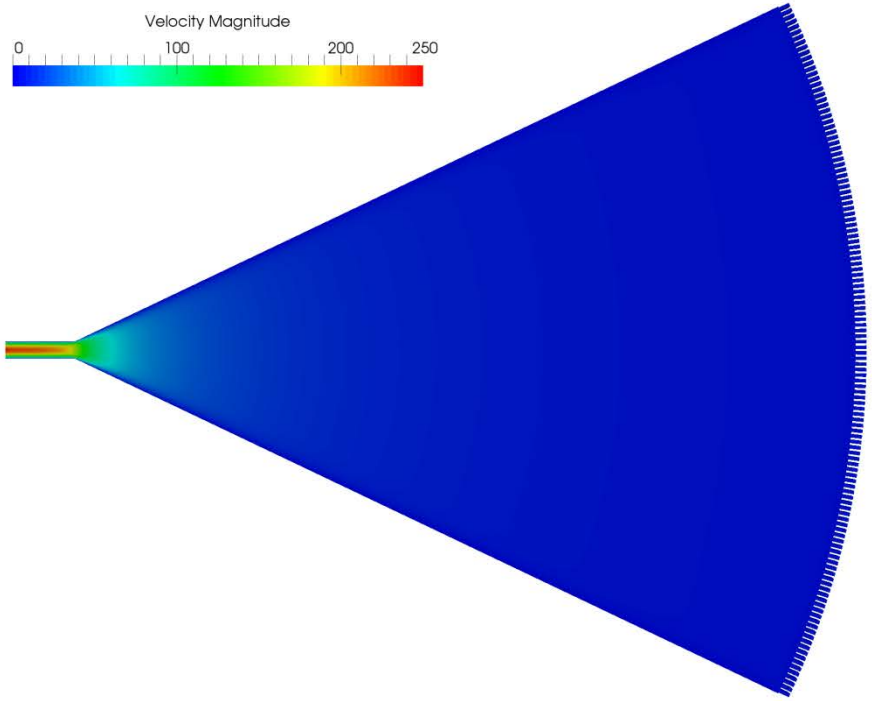
Intantaneous reaction scheme:

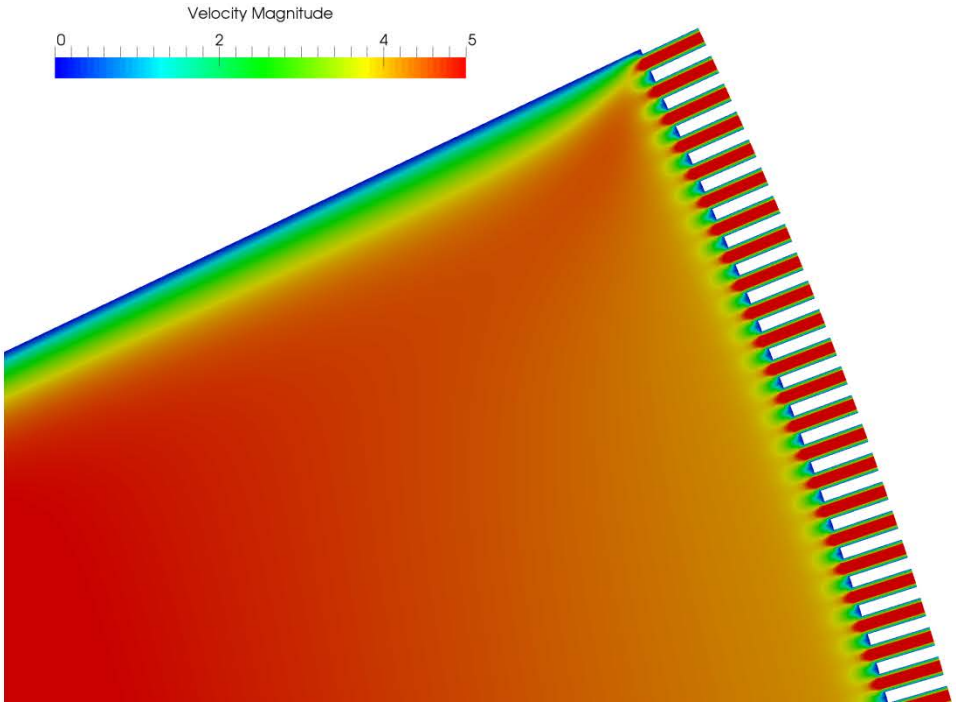
$$A + B \xrightarrow{k\to\infty} P$$

Investigated flowrates:
100 mL/h
250 mL/h
500 mL/h

$$D_{A,B} = 3.0 \cdot 10^{-10}\ m/s^2$$

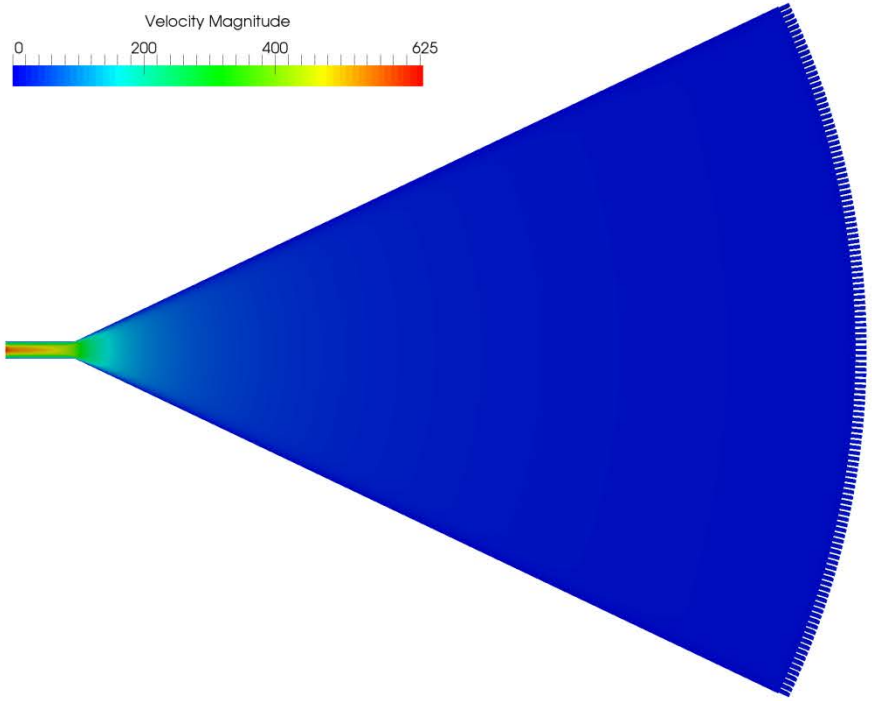
Computationally obtained flowfield in the Superfocus mixer

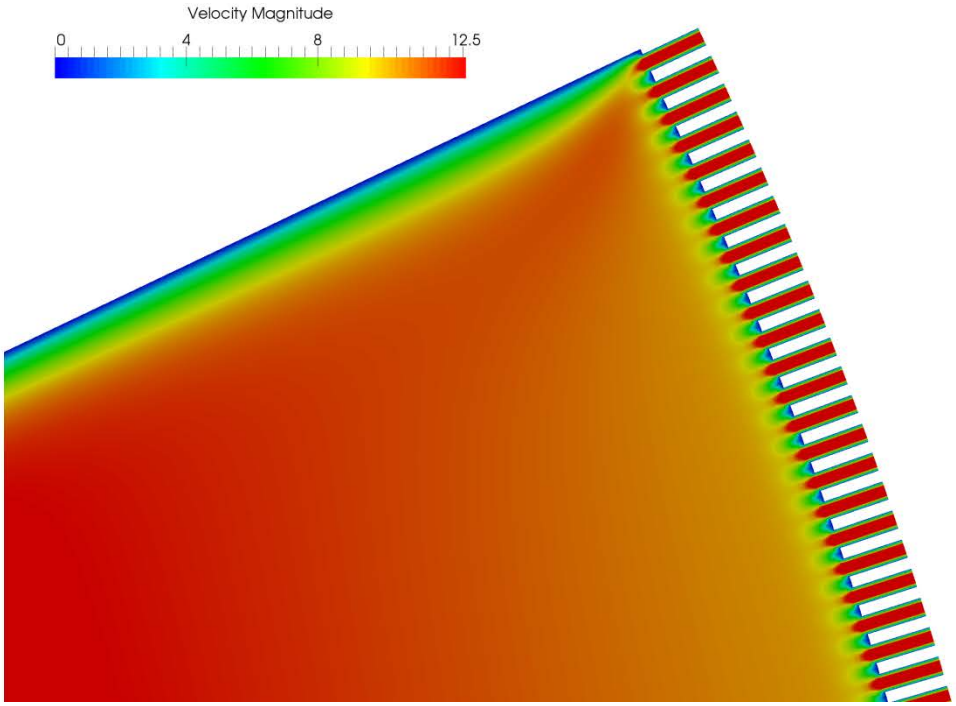




Flowrate: $\dot{V} = 100\, mL/h$

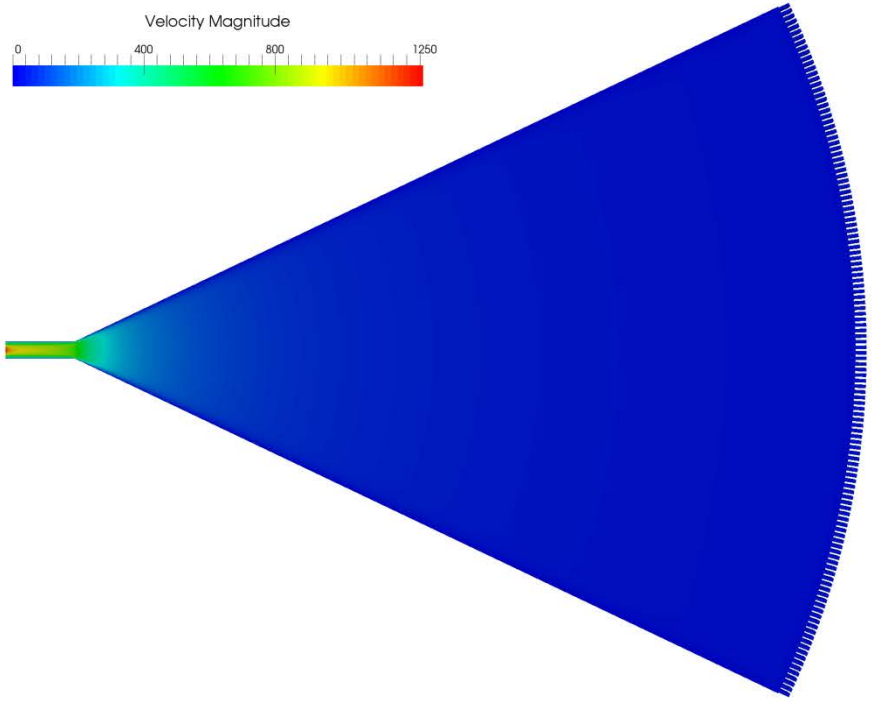
Computationally obtained flowfield in the Superfocus mixer

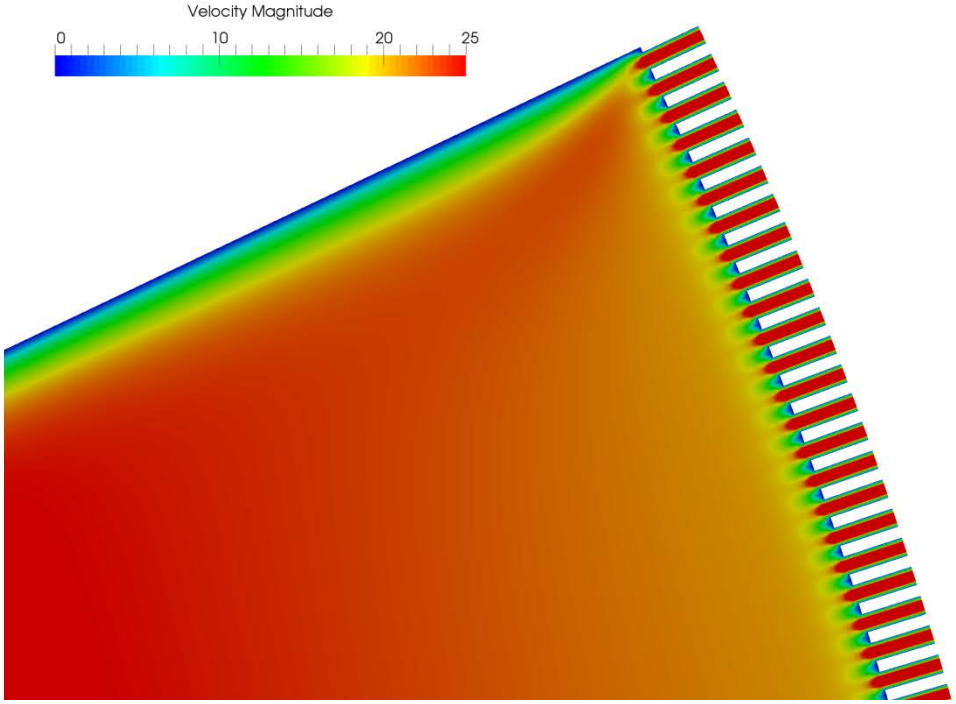




Flowrate: $\dot{V} = 250\, mL/h$

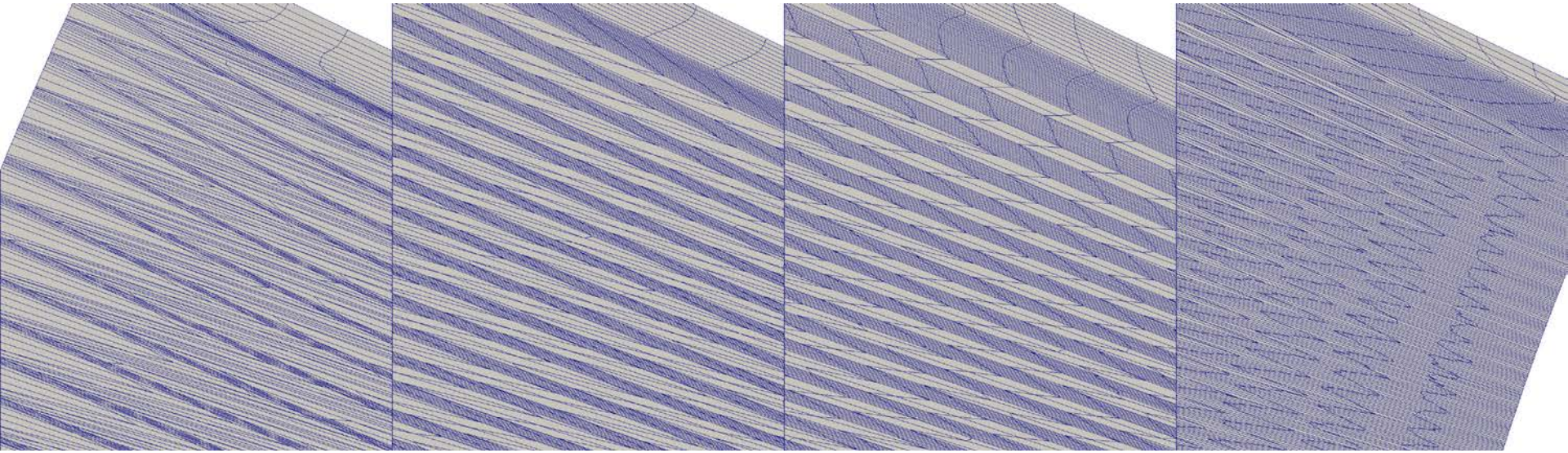
Computationally obtained flowfield in the Superfocus mixer

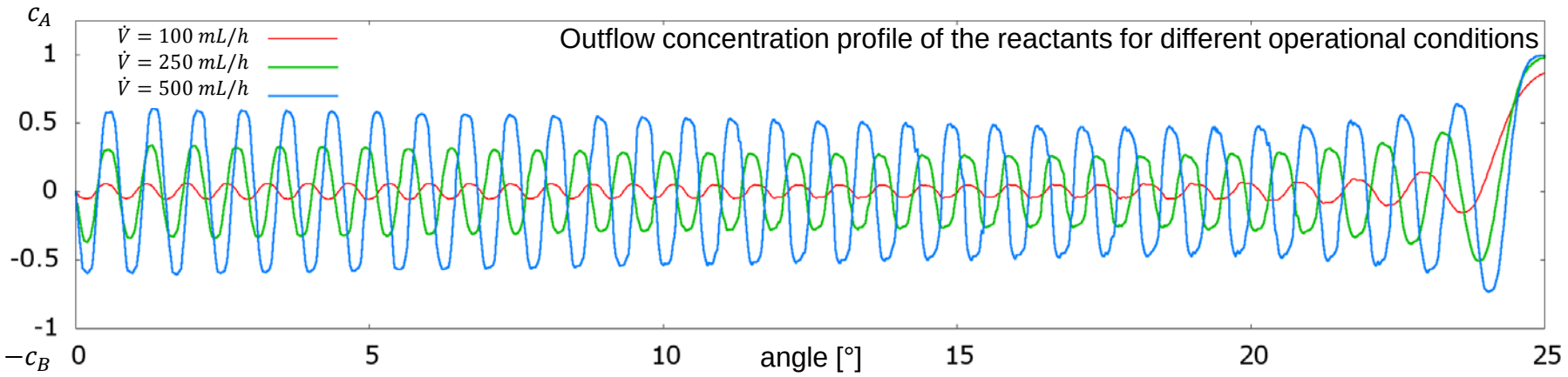




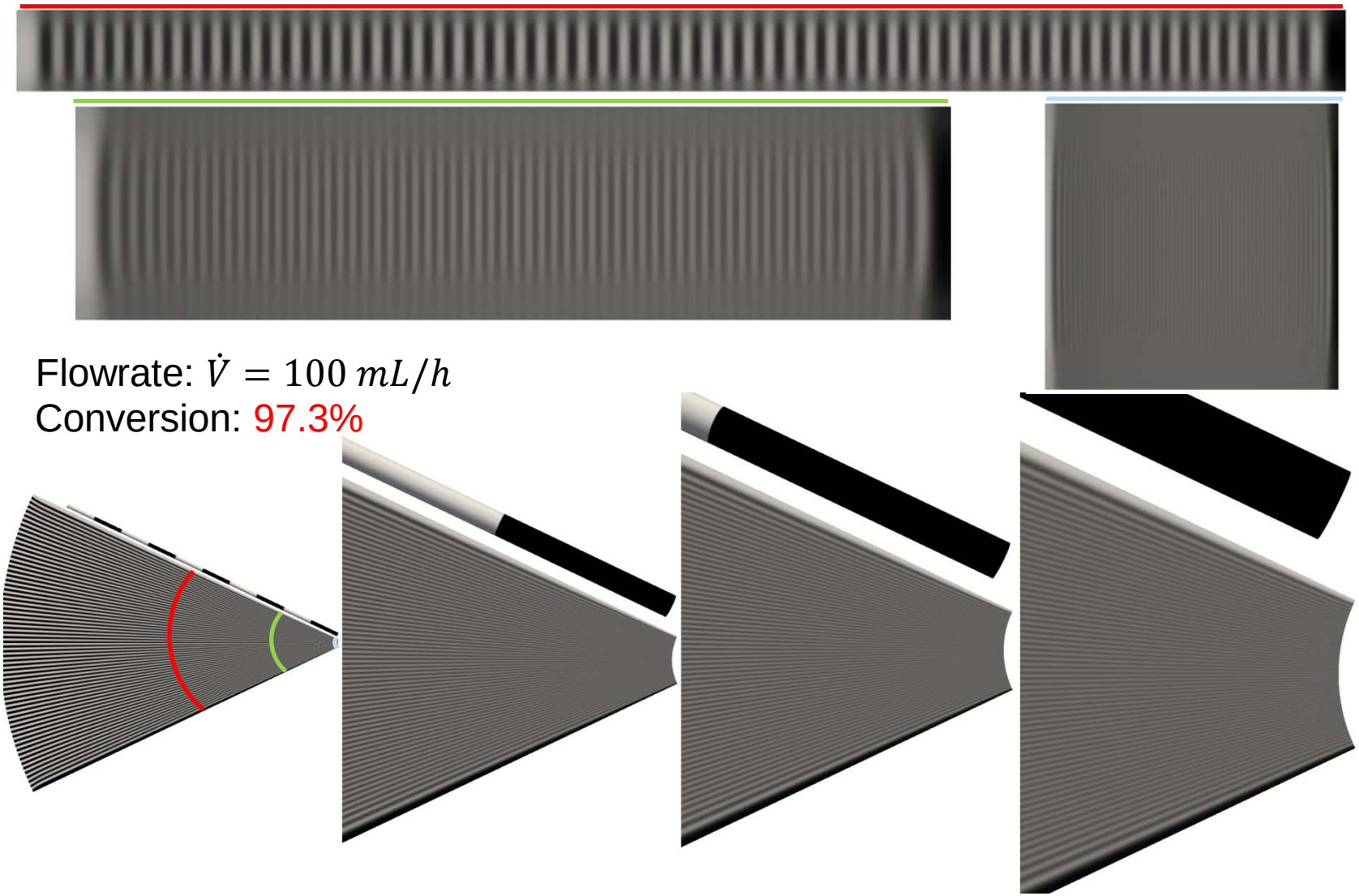
Flowrate: $\dot{V} = 500\, mL/h$

Exploiting the two-fold symmetry only the ¼ of the domain needs to be meshed. NEL(¼) = $1.2 \cdot 10^6$ elements. Velocity is interpolated in an L_2 sense to the deformed mesh.





Outflow concentration profile of the reactants for different operational conditions


Flowrate: $\dot{V} = 100\, mL/h$
Conversion: 97.3%

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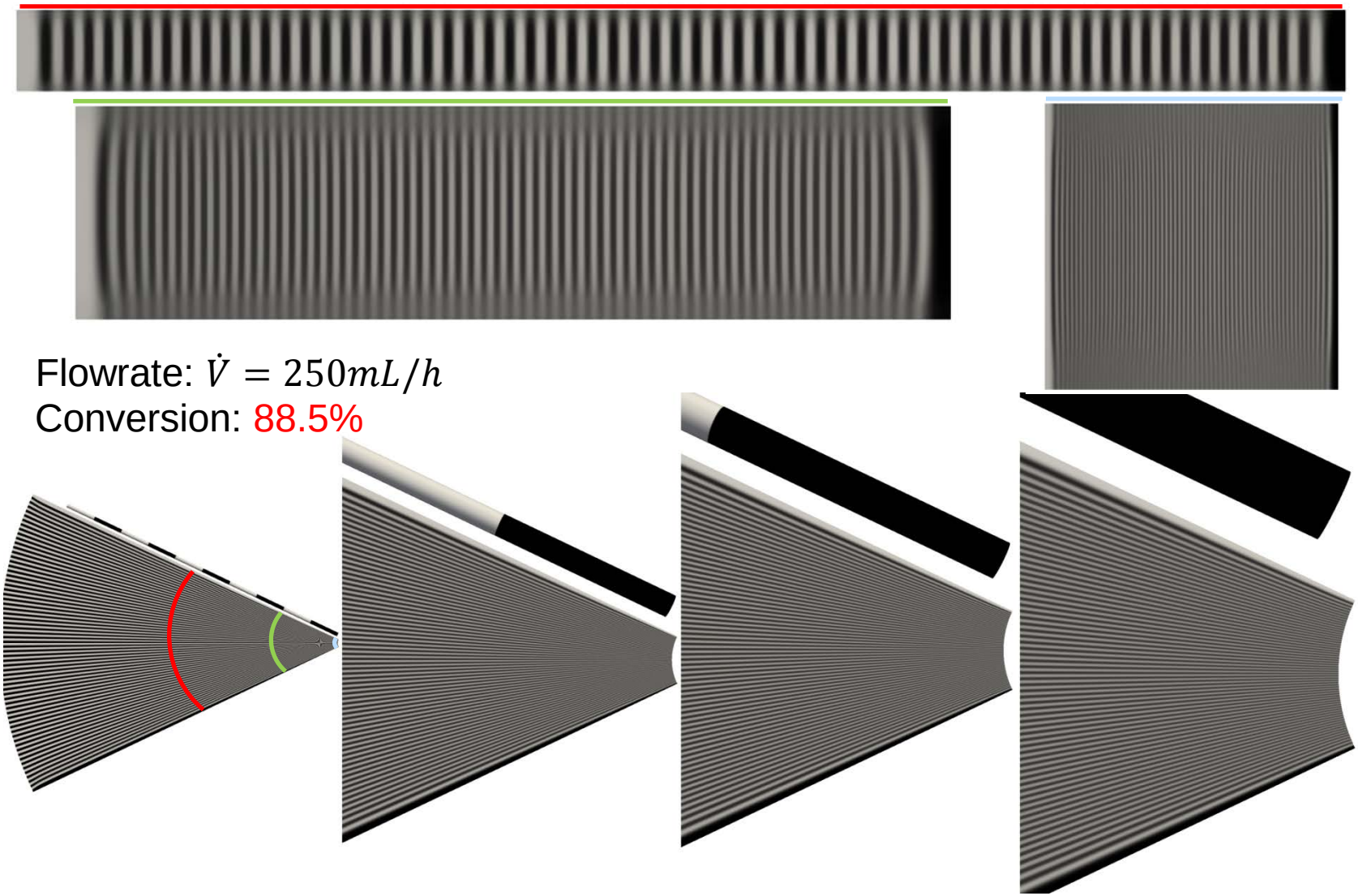

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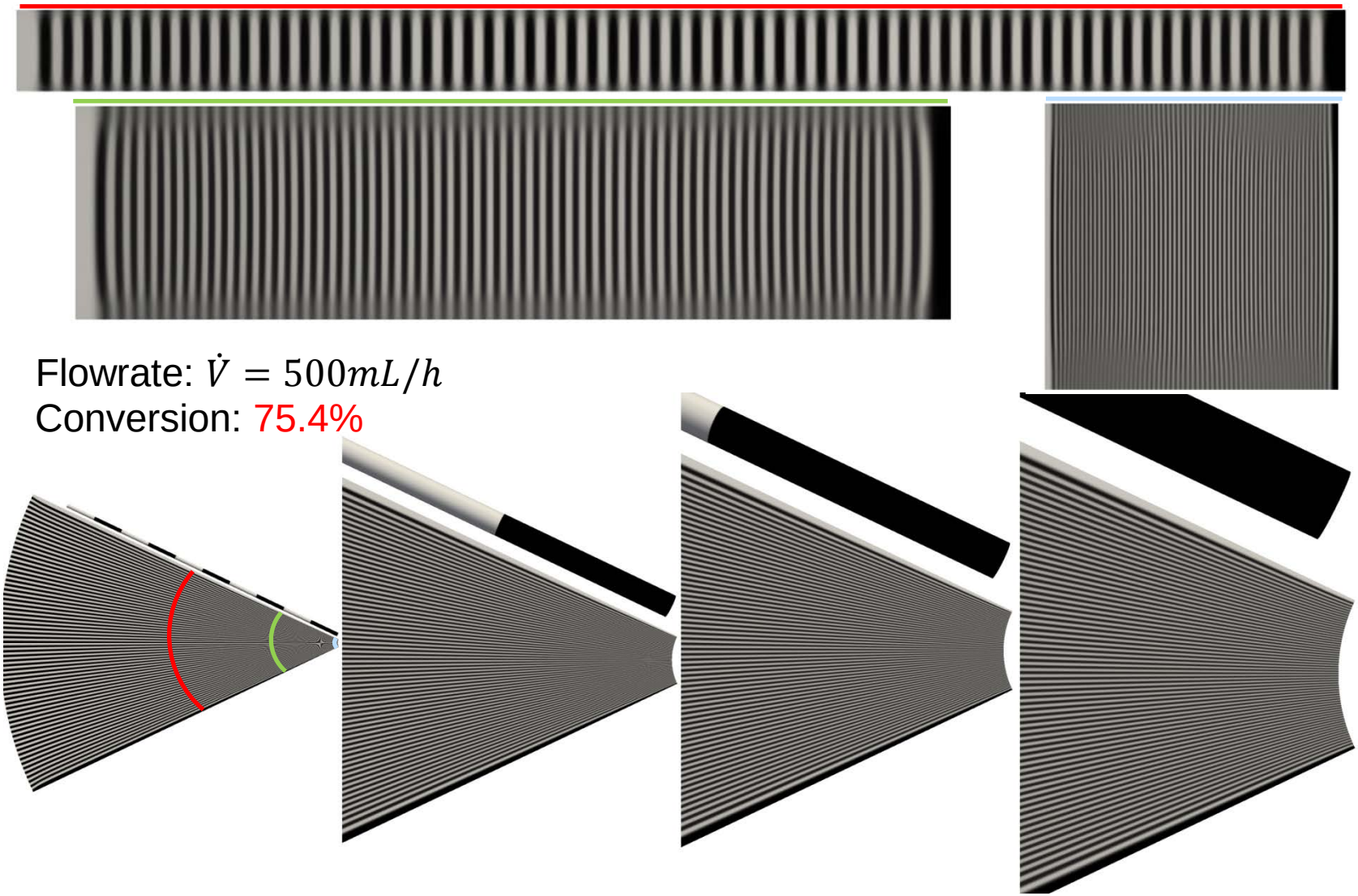

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