Flow Modeling in Long Surface Patterned Micromixers Using Division in Multiple Geometrical Subunits

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INTRODUCTION: Optimization of mixing in microfluidic devices is a popular application of computational fluid dynamics software packages, such as COMSOL Multiphysics. However, it has to be noted that even very performant mixing topologies, such as the use of ridge-groove surface features, require multiple mixing units. This in turn requires very high resolution meshing, in particular when looking for solutions for the convection-diffusion equation governing the reactant or chemical species distribution. For the typical length of microfluidic mixing channels, analyzed using finite element analysis, this becomes computationally challenging due to the large number of elements that need to be handled. In this work we describe a methodology using the COMSOL 5.3a CFD and Chemical Reaction Engineering modules, in which large geometries are split into subunits, allowing the governing equations to be evaluated on higher resolution meshing.

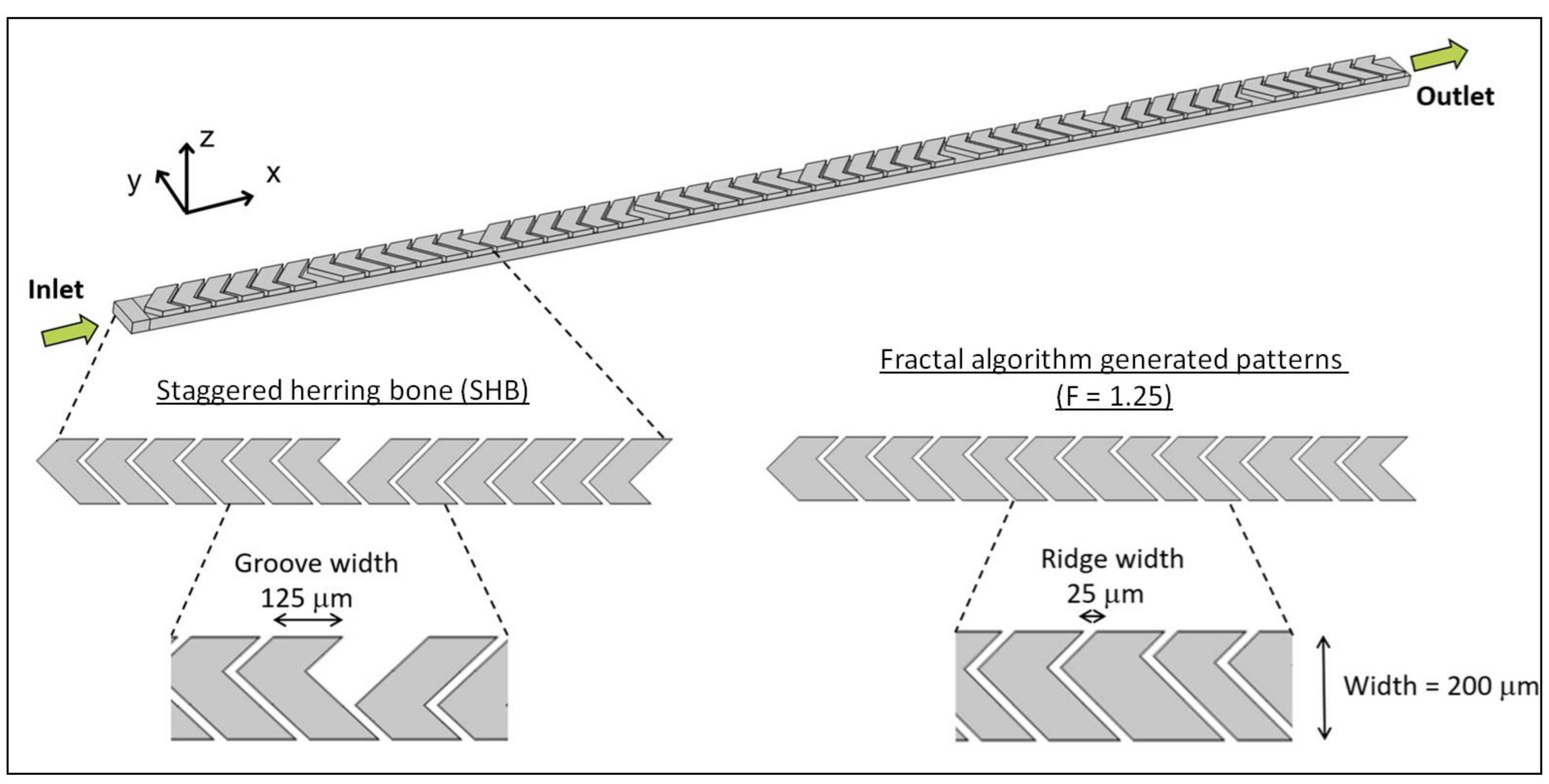


Figure 1. General topology of the micromixers investigated; Snapshot of the ridge/groove profile: (left) of a full mixing unit for an SHB design; and (right) of a mixing section generated based on the fractal algorithm.

MICROCHANNEL GEOMETRIES: The micromixer geometry used in this work involves the patterning of slanted ridge/grooves on the channel walls to control the transversal flows. The ridge/grooves follow either a periodic pattern (SHB [1]) or one generated by a fractal algorithm [2]:

$$W(x) = \sum_{n=0}^{\infty} \frac{\sin(2^n x)}{2^{n(2-F)}}$$

GOVERNING EQUATIONS:

Navier-Stokes equations:

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u}\right) = -\nabla P + \eta \nabla^2 \boldsymbol{u}$$

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

Concentration-diffusion equation:

$$\frac{\partial c}{\partial t} = D\nabla^2 c - \boldsymbol{u} \cdot \nabla c$$

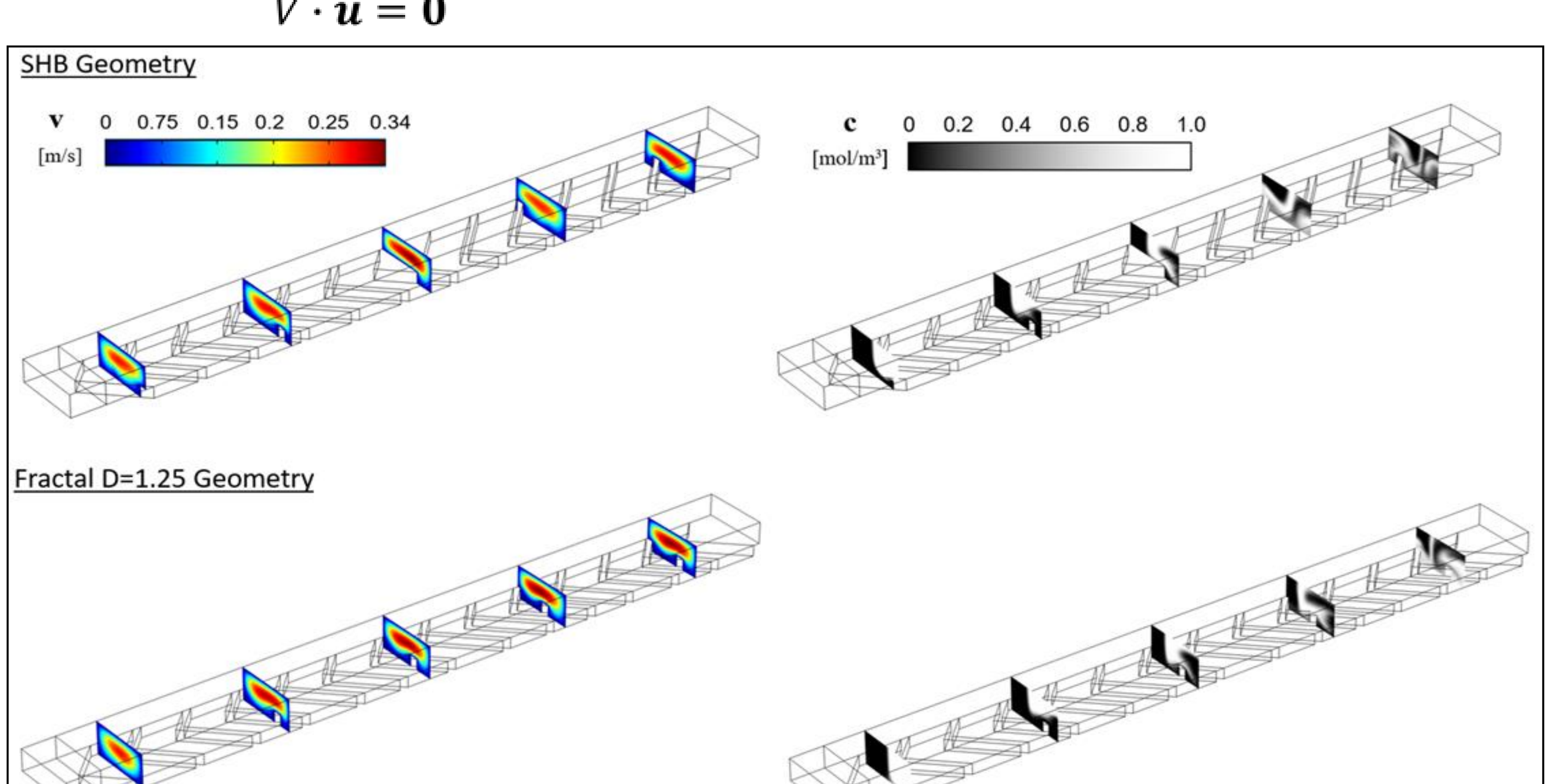
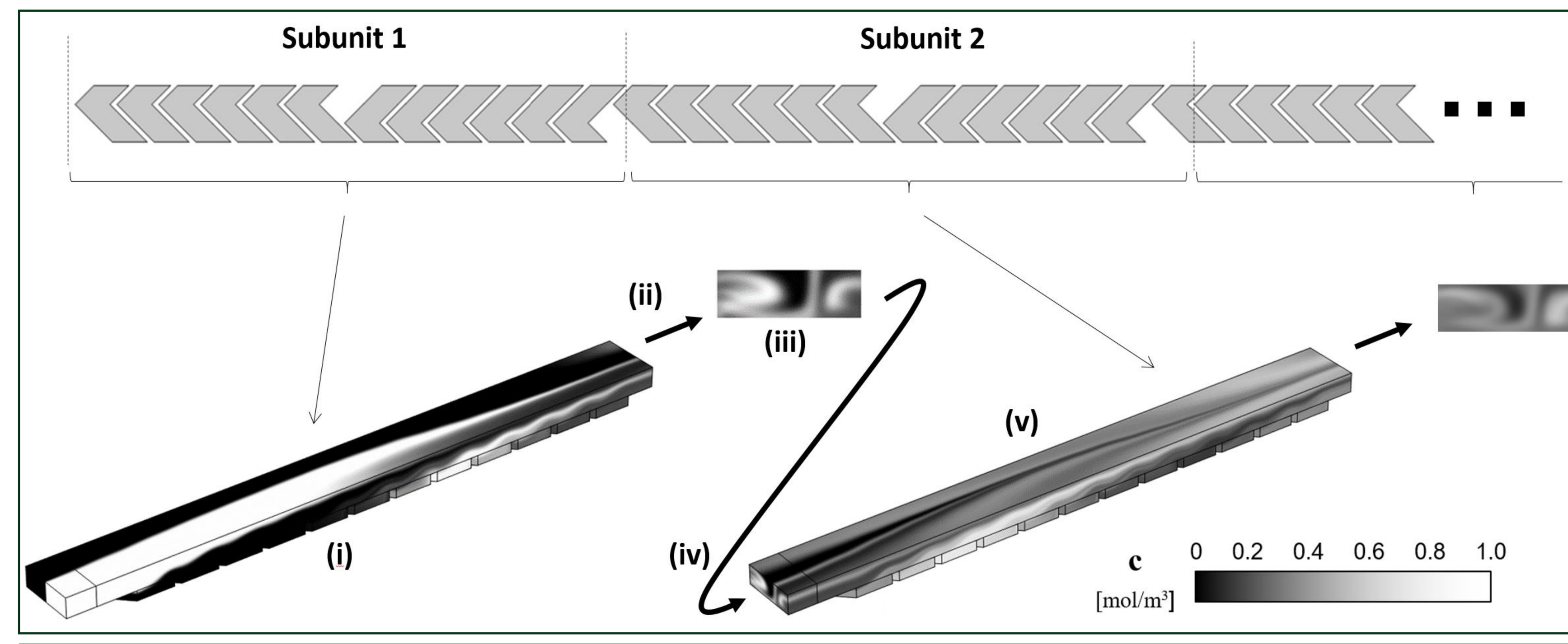


Figure 2. (left) Velocity magnitude and (right) concentration distribution for the SHB and fractal F=1.25 micromixer geometries.

PROBLEM SEGMENTATION:



(i) The Navier-Stokes and concentration-diffusion equations are solved for the first geometrical unit of the channel, with the desired inlet boundary conditions.

(ii) Once the solution is obtained, a "Cut Plane" section is generated in the "Results" tab, near the outlet of the section.

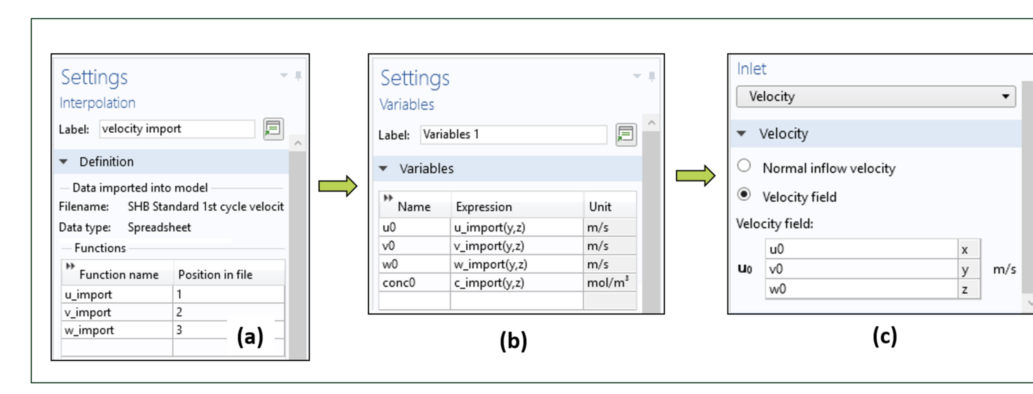
(iii) The "Export" feature is used to save the data across the plane generated in step (ii), for the velocity components and the concentration, respectively. Each resulting exported text-based file contains aside from the variables of interest the two spatial coordinates across the cut-plane.

(iv) The data obtained at the outlet of one cycle is used as the inlet condition for the next cycle. To achieve this, in the model corresponding to the next cycle, under the "Definitions" tab two interpolation functions are generated that use the data generated in step (iii) (Fig 4a). These interpolation functions are then used to define a new set of variables (4b) that allow the mapping of the solutions onto the inlet of the new cycle (4c).

(v) The inlet conditions for the new cycle are set, and the model can be solved to obtain the flow field and concentration distribution. Steps (ii) though (v) can be repeated to obtain the velocity and concentration along extensive mixing systems.

Figure 3. Steps of the used partitioning method in geometrical sub-units.

Figure 4. Steps for transferring boundary conditions from one sub-section model to the subsequent one.



MESHING COMPARISON: By partitioning the channel's geometry into multiple subunits of roughly equivalent size, we can significantly increase the meshing resolution of the numerical simulation.

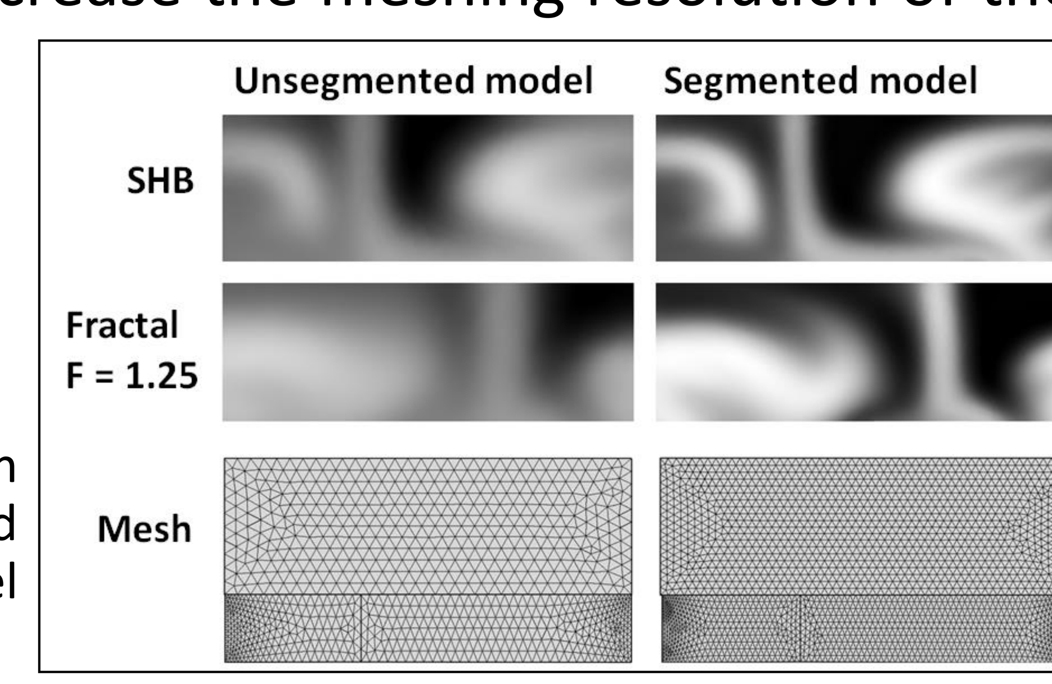


Figure 5. Mesh comparison between the segmented and unsegmented channel geometries (Re≈20).

RESULTS: the computational results have been compared with fluorescence confocal microscopy images of dye distribution in this type of mixers, with good qualitative results.

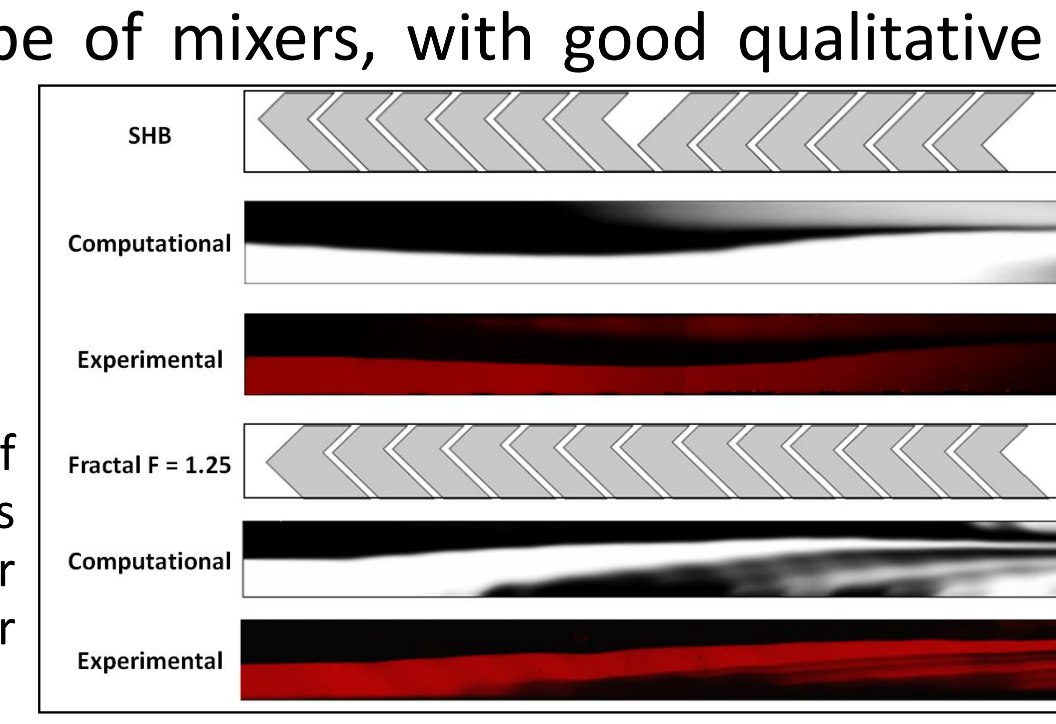


Figure 6. Comparison of concentration distributions along the *xy* plane for different microchannel mixer configurations

CONCLUSIONS: high-quality numerical simulations can be acquired in CFD modules in COMSOL Multiphysics 5.3a by partitioning channel geometries into smaller subunits and solving iteratively. The methods proposed in this study have general applicability, to other transport problems.

ACKNOWLEDGEMENTS:

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