Modeling of a Three Inputs Two-dimensional Geometry Microreactor

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Introduction: This work presents the modeling results of a microreactor with three inputs geometry (Figure 1), in relation to distributions of velocities and concentrations. The design contemplates a main channel of 30 mm and three entries (two lateral and one central channels as indicated in Figure 1(b). In order to study this geometry concerns to its fluids dynamics, ethanol and water are injected through the central channel and lateral channels, respectively. The mixture takes place whithin the main channel. The computational system used was an Intel Zeon Quad Core, 16 GB RAM, and COMSOL Multiphysics® with Chemical Reaction Engineering and CFD modules. The calculus domain is showed in Figure 1(a) and a partial mesh (total: 27,956 triangular bidimensional elements) in Figure 1(b).

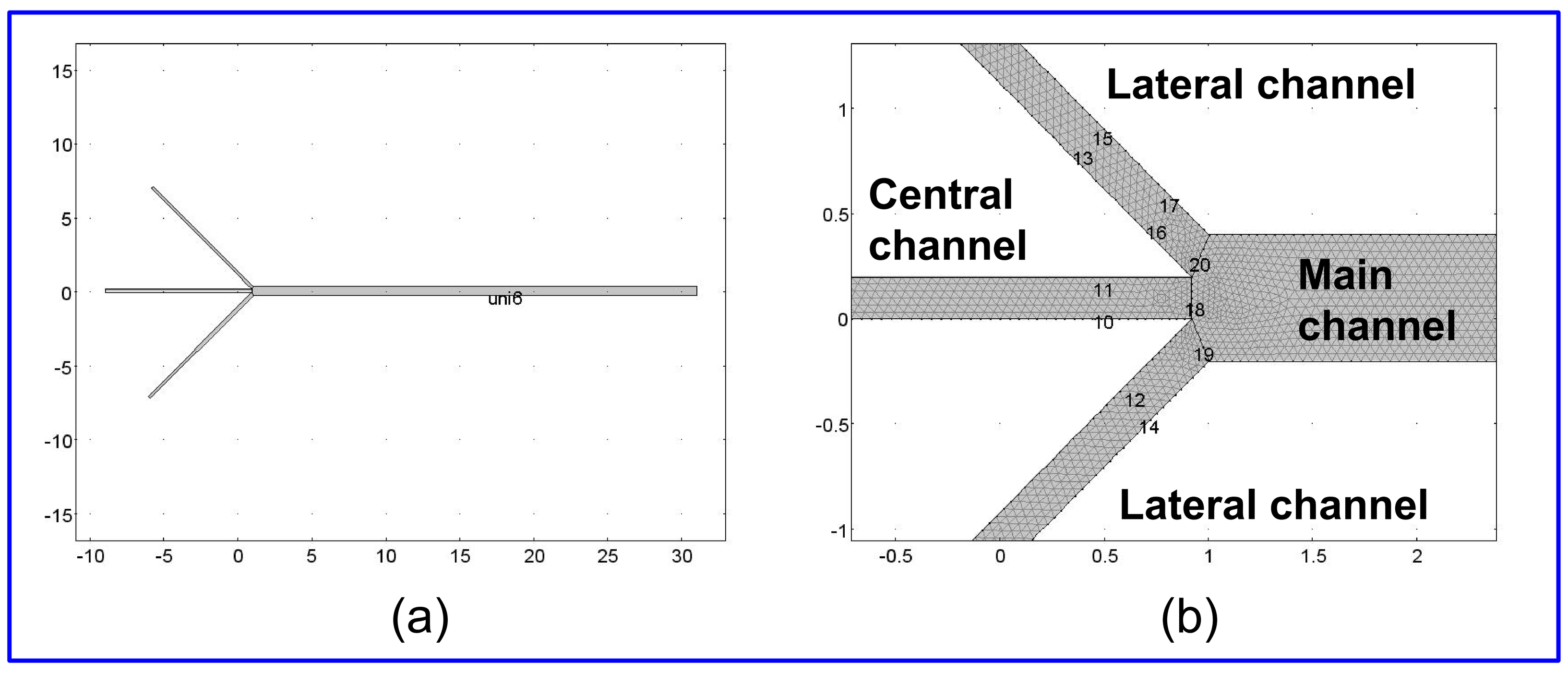


Figure 1. Three entries geometry of microreactor (a); partial mesh (b).

Computational Methods: The adopted flow values of ethanol and water (Ve and Va) were discussed and determined *a priori* with the staff responsible for the construction of the microreactor. As reading lines, we chose one line along the main channel (Figure 2(a)) and seven transversal lines (Figure 2(b)).

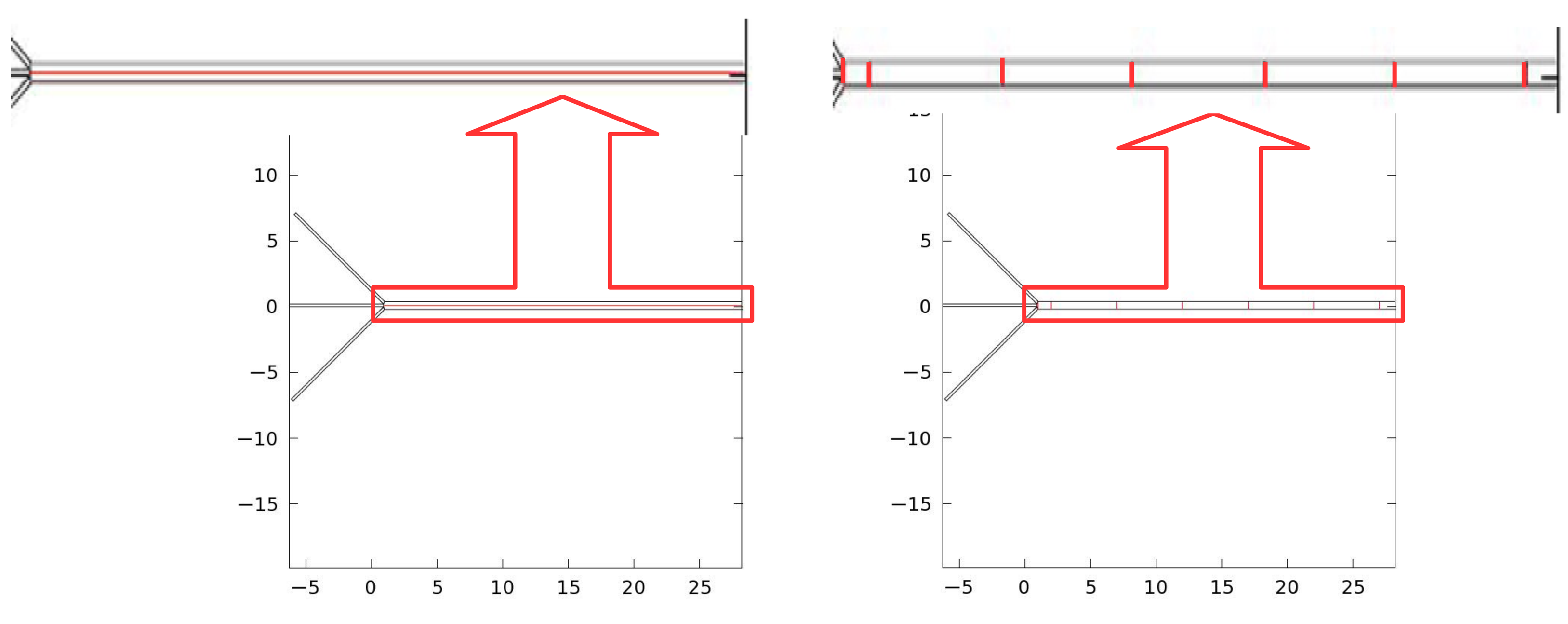


Figure 2. Reading lines along the main channel (a) and transversal lines (b).

Results: The global distributions for velocity and ethanol concentration at the beginning of the main channel are showed in Figure 3. The important point here is that the mixture is confined within the middle plane of the main channel. The quantitative numerical results for ethanol concentration taking many combinations of flow values are showed in Figure 4.

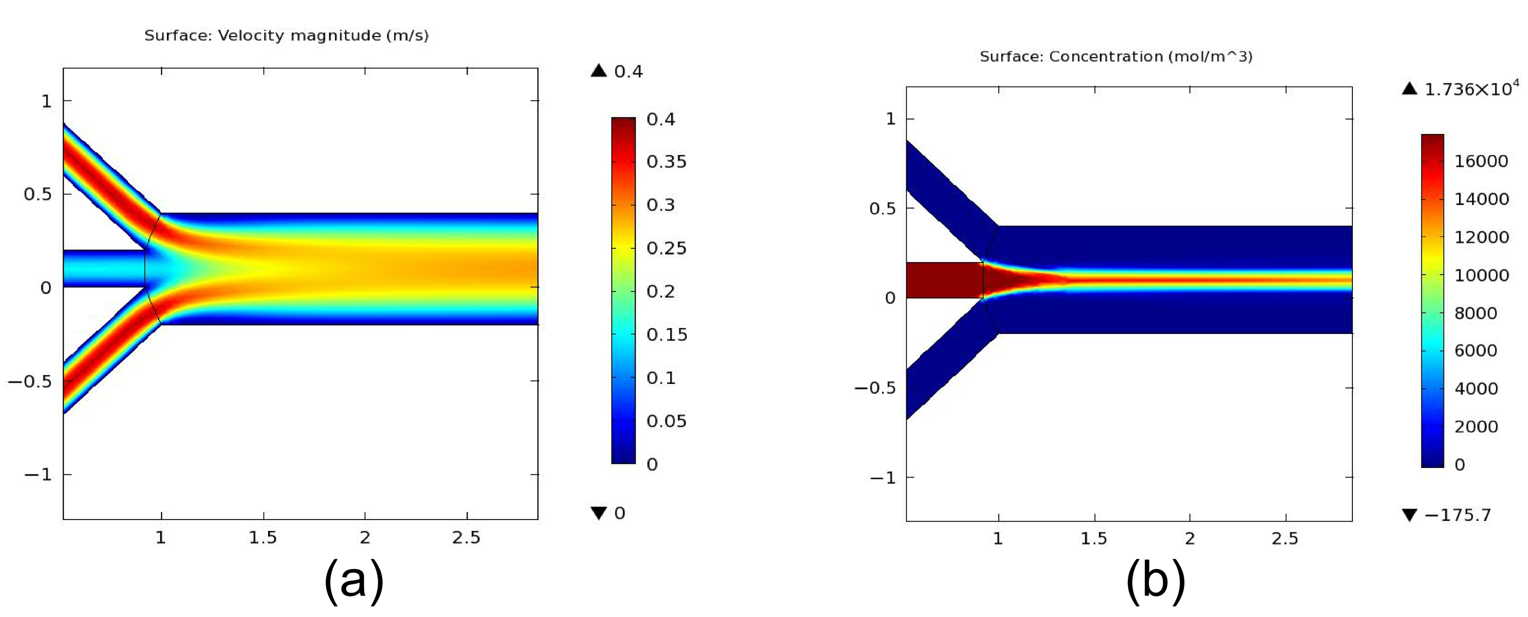


Figure 3. Velocity (a) and concentration (b) distributions.

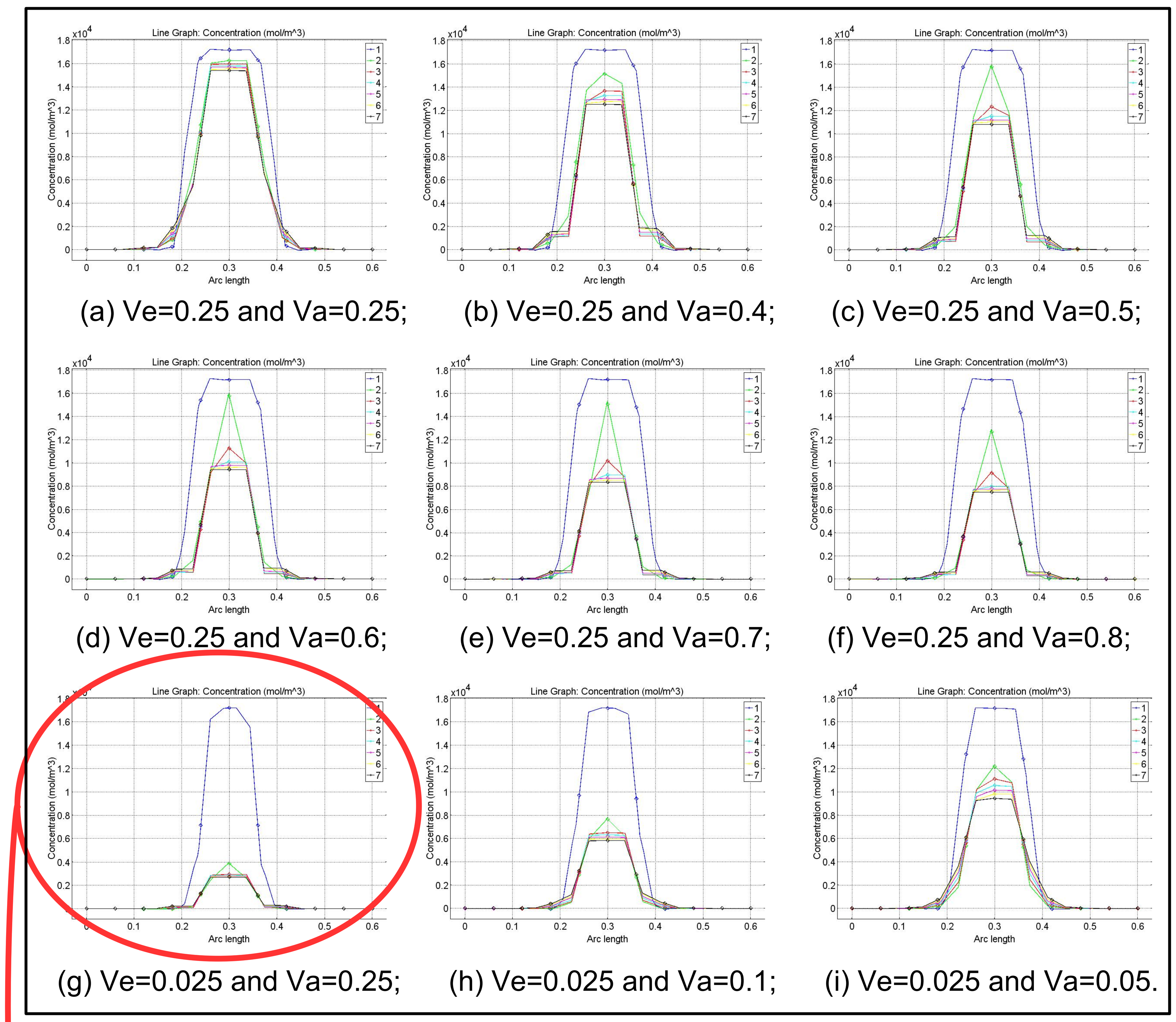
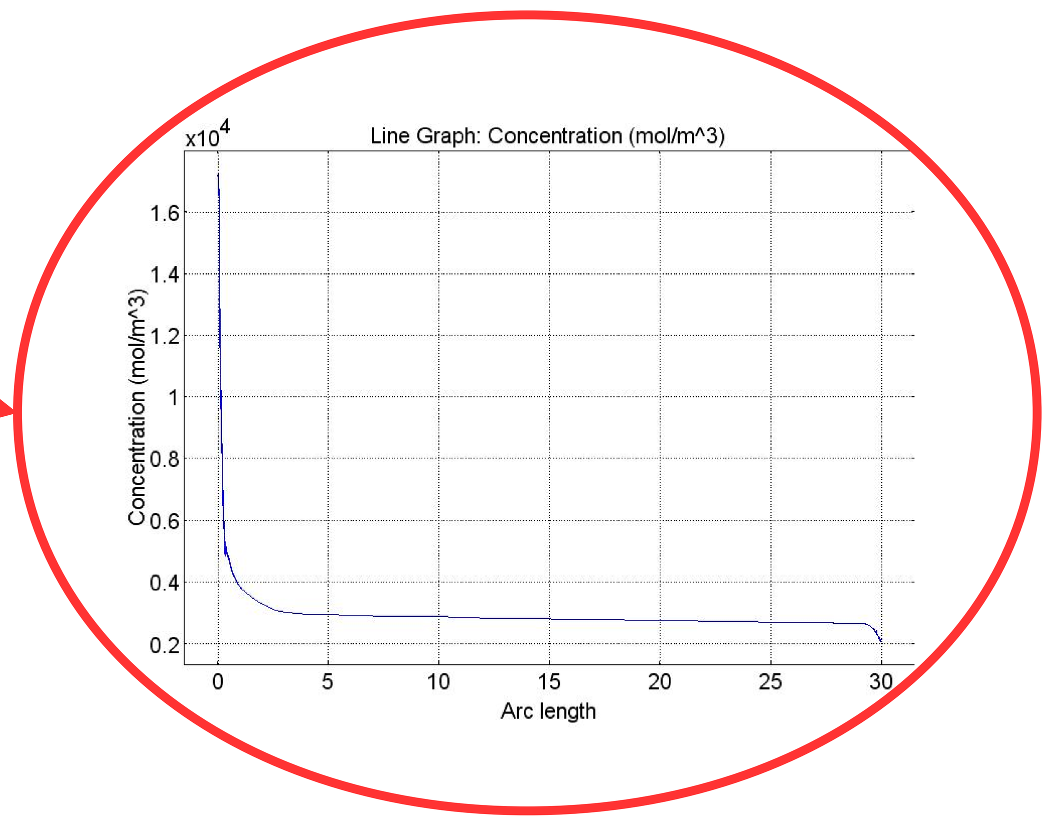


Figure 4. Ethanol concentration at transversal lines.



The result presented in Figure 4(g) was the best one, that is because in this condition the mixture takes place close to the entrance of the main channel. Therefore, the mixture is completed at 3 mm of the main channel approximately.

Figure 5. Ethanol concentration along the main channel.

These numerical responses allow insights on how fast the mixture becomes homogeneous. Then, taking into account the response of how small the required length of the main channel might be, the project makes use of such data to construct the microreactor. Figure 5 summarizes this idea, in which is presented the ethanol concentration along the main channel, for the simulation (g).

Conclusions: The factor of how fast the mixture becomes homogeneous is important for the construction of the device on ceramic, since the optimization of the geometry means lower production costs of the microreactor.

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