Residence Time Distribution for Tubular Reactors

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Introduction: In the core of Chemical Engineering is the reactor design that include most of all scientific disciplines. The reactor, in general, are treated ideally: mixed and plug-flow patterns. Unfortunately, it is observed in the real world a very different behavior from that expected. Thus, to characterize nonideal reactors is used, among others, residence time distribution function E(t), mean residence time t_m and cumulative distribution function F(t). The aim of this present work is to determine in the COMSOL Multiphysics® a distribution of residence time of a tubular reactor that is used, didactically, in the Chemical Engineering Laboratory in Federal University of Parana.

Computational Methods: The equation that models the flow of fluid throughout the reactor is the Navier-Stokes equations.

$$\rho(u.\nabla)u = \nabla.[-pI + \mu(\nabla u + (\nabla u)^T] + F$$

Where, u is the velocity vector, ρ is the density of the fluid, μ is the viscosity, p is the pressure and F is a body force term, such as gravity.

As the flow is incompressible,

$$\rho\nabla.u = 0$$

The mesh size element was calibrated for fluid dynamics, and left to "normal" size - the highest possible for that particular calibration.

The phenomena of tracer's diffusion and convection, Figure 2, are modeled by the continuity equation together with the equation of the overall flow:

$$\frac{\partial c_i}{\partial t} + \nabla.(-D_i\nabla c_i) + u.\nabla c_i = R_i$$

$$N_i = -D_i\nabla c_i + uc_i$$

Where, c_i is the tracer's concentration, D_i is diffusivity and N_i is the diffusion flux.

Results:

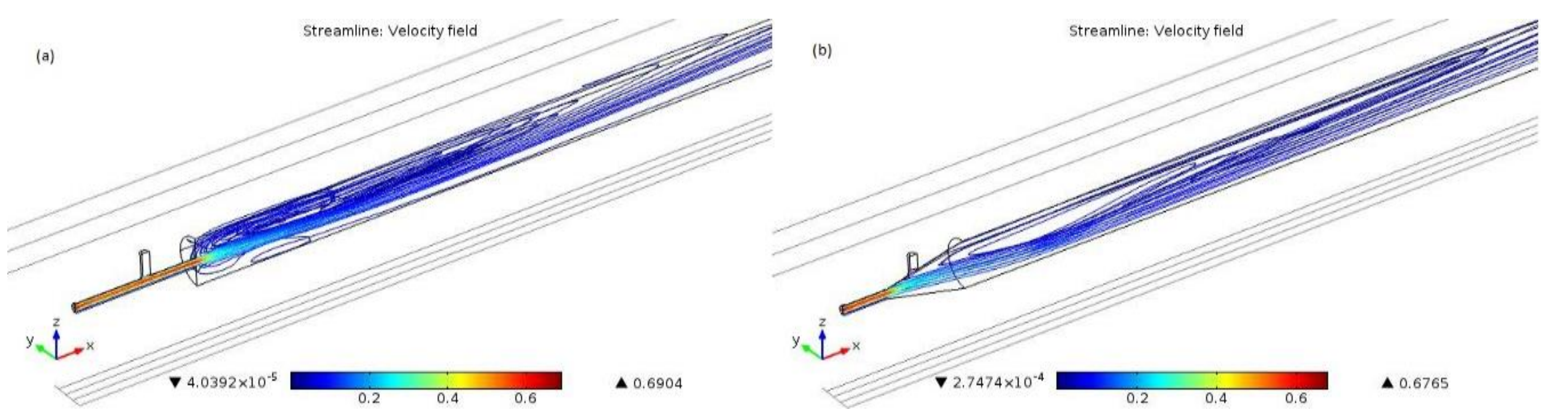

Figure 1 – (a) Original Reactor; (b) Modified Reactor

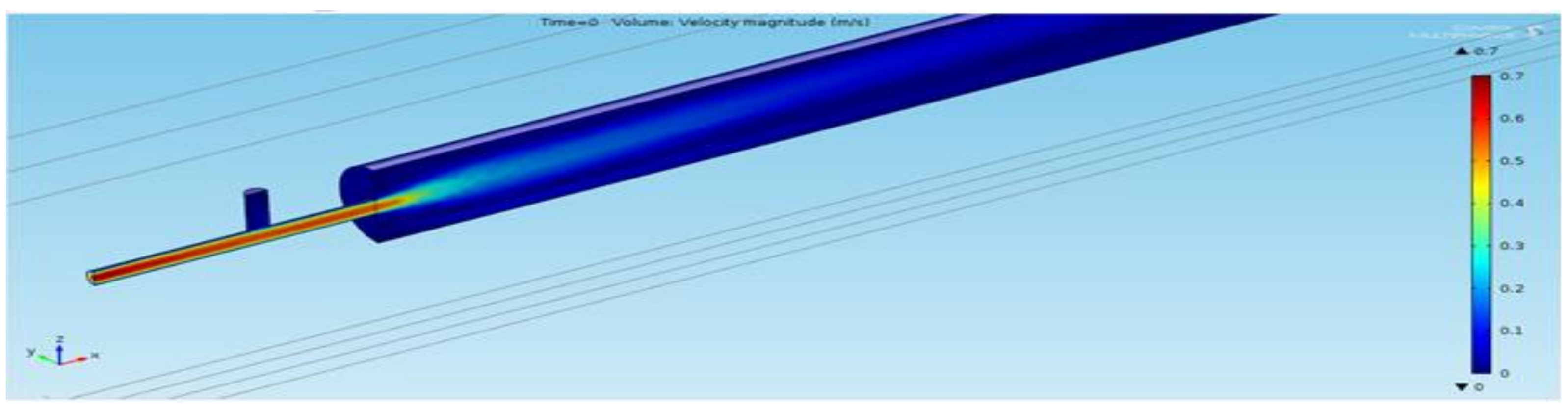

Figure 2 – Tracer injection

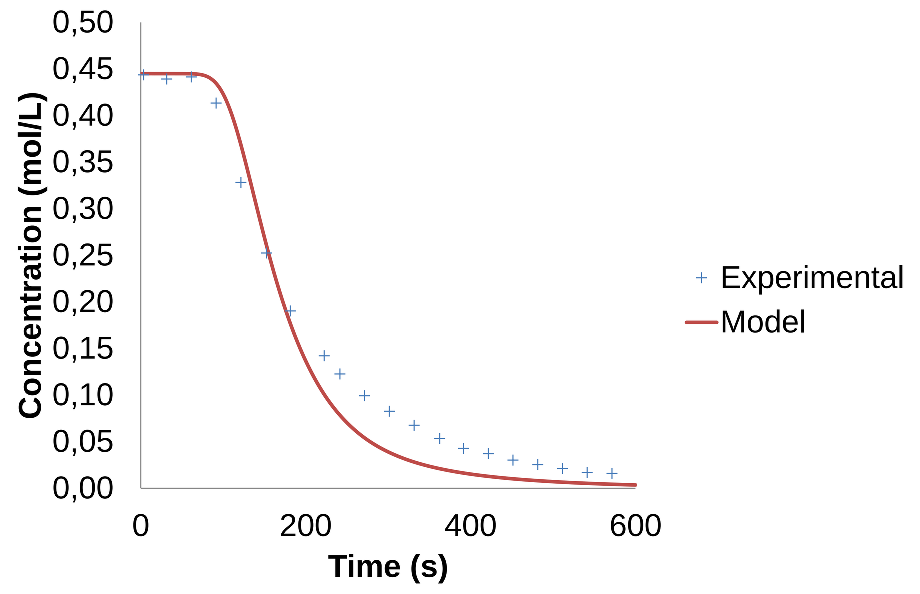

Figure 3 - Reactor outlet concentration

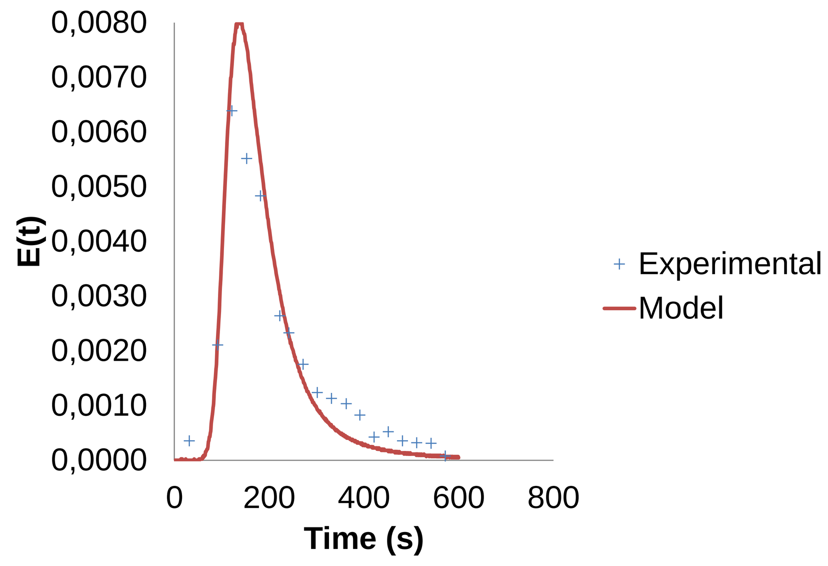

Figure 4 – RTD curve

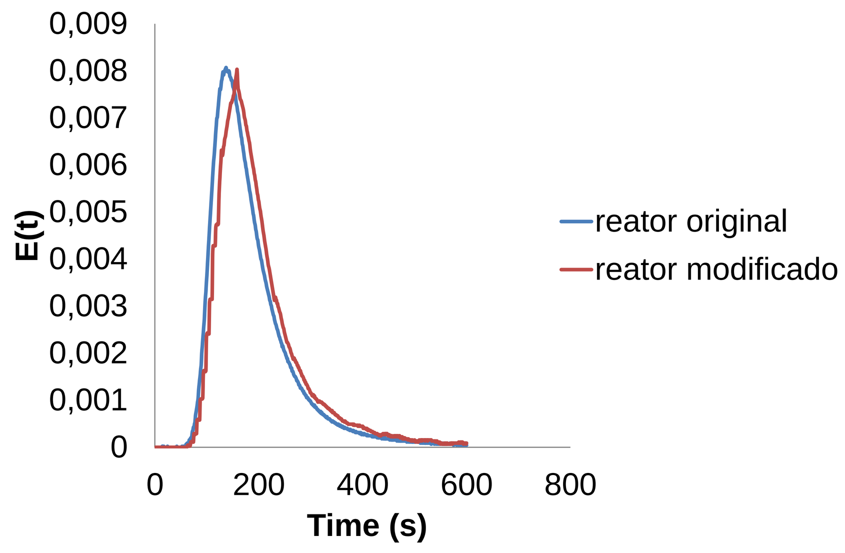

Figure 3 – RTD curve of original and modified reactor

Conclusions: it is observed that the modeling of the reactor showed good agreement with the experimental results, the correlation coefficient of 0.97, Figure 3. Furthermore, with simulation it was possible to verify the hydrodynamic behavior of the flow - preferred paths, areas of recirculation and stagnant zones - allowing to establish the non-ideality of the reactor, Figure 1. The studies showed a space-time of 6.10 min. and an average residence time of 3.05 min (original reactor) and 3.38 min (modified reactor). Importantly that closer are values of space-time and residence time average, there is an indication that the reactor will operate more adequately. However, the hydrodynamic problems are not obvious, that is why the importance of computational fluid dynamics in the analysis, design and operation of reactors.

References

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