

Design optimization of a bioreactor for ethanol production using CFD simulation and genetic algorithms

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The search for new ways to provide fuel for the society has been constantly increasing. One of the great challenges for scientists and academic researchers is to provide fuels without jeopardizing the environment. An interesting alternative is the bioethanol production from sugar cane or other kinds of biomass, like corn, beet, *etc.* The production of sugar cane ethanol is economically feasible only at large scales, such as 45 thousand liters per hour, for instance. At these scales, any efficiency improvement can result in a very significant overall optimization in terms of production rates and environmental impacts as well. Due to the difficulty to do experimental analyses, the expensive materials that are used and time limitations, Computational Fluid Dynamics tools (CFD) constitute an alternative of great potential to study the flow inside the bioreactors, and to better cope with their intrinsic design difficulties. Most of the studies, however, were developed for small-scale reactors. Large-scale bioreactors, usually applied at industrial bioethanol production, must be studied more carefully because fluid velocity profiles, shear stresses, and other physical conditions may be considerably different compared with small-scale bioreactor. The bioreactor should be able to provide optimum conditions to the bio-chemical or mechanical process. The bioreactor design has a great influence in the flow conditions, with respect to mass transfer, shear stress, mixing, control of pH, temperature and substrate conditions. Some flow conditions can be a bad influence on the bio-chemical reactions inside the bioreactor. Stagnant zones keep the sugar cane juice inside the reactor for longer or shorter than necessary for an optimum glucose to ethanol conversion. In both cases, stagnant zones are prejudicial to bioethanol production. An alternative to control the flow inside the reactor and get yields improvements is to modify structural parameters. The definition of the geometry has a great influence in the flow and consequently in the bio-chemical reaction. The aim of this study is to provide an optimized structure design for a continuous reactor applied to bioethanol production from sugar cane juice. A simple test case was analyzed in which different outlet tube heights were simulated, intending to optimize the velocities inside the bioreactor. The flow inside the bioreactor was determined by the ANSYS CFX 13 commercial software. To find the ideal structural parameters, the flow simulations are coupled with an optimization

process based on a specialized genetic algorithm. The genetic algorithm chosen here was the Modified Genetic Algorithm II, the MOGA II, an improved version of MOGA that uses five different operators for reproduction: selection, classical cross-over, directional cross-over, mutation and elitism. At each step of the reproduction process, one of the five operators is chosen and applied to the current individual. The directional cross-over assumes that a direction of improvement can be detected comparing the fitness values of two individual references, and this comparison is made in the same generation. This kind of cross-over improves the algorithm convergence. The MOGA II is implemented in the ModeFRONTIER 4.3 commercial software. This software allows the coupling between the ANSYS CFX 13 solver and MOGA II, automating the process. Schematically, the coupling between the CFD solver and the optimization platform works in this order: structure generation, mesh generation, fluid solver, optimization and new parameters definition, new structure generation, and so successively, until the stop criterion is reached.

Results and Conclusions

Were tested 46 different values of outlet tube height, and the best value was determined. To select the best parameters a Genetic Algorithm, MOGA II, was applied by ModeFRONTIER 4.3 commercial software coupled with ANSYS CFX 13. Despite the initial tests were limited to limited computational efforts a good performance was obtained. The knowledge about the optimized structure provides a bioreactor yield improvement, material economy and environmental impact reduction. Future works are concerned in tests validation and verification through an experimental prototype fabrication and improvements on CFD modeling.

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