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In partnership with Clermont-Auvergne University, IFPEN has developed a tool for predicting and scaling-up the performance of aerated bioreactors used in bio-based fuel production. This tool, based on numerical fluid mechanics, combines hydrodynamics, rheology, matter transfer and simplified microorganism metabolism.

## Biofuel production: a major challenge for the energy transition

As an alternative to fossil fuels, ethanol derived from lignocellulosic biomass is associated with a **reduction in greenhouse gas emissions** while not competing with food-related agriculture. In order to reduce the production costs of this biofuel using enzymatic processes, one important lever is **the optimization of enzyme production through filamentous fungi fermentation**.

One of the main challenges associated with this step is **the extrapolation of cultures from the laboratory scale**, where tests are conducted, to industrial-scale production. That is because the supply of oxygen and substrates to microorganisms must remain optimal **to maximize enzymatic productivity**, a task made complex due to the non-Newtonian rheology of the fermentation medium (which reduces the transfer and mixing functions) and the sensitivity of the fungi to the shear stress generated by mechanical stirring.

## Development of experimental methods to construct a reliable database

Since the exchange surface between the gas and liquid plays an essential role in oxygen supply to microorganisms, it is important to be able **to predict the bubble sizes and volume fractions in the fermenters.**

Bubble sizes in various media (fermentation filtrate, model media) were characterized using **an optical sensor technique** developed at IFPEN during previous research [1], but never before applied to non-Newtonian media [2]. These original measurements were reinforced by the determination of the gas/liquid transfer coefficient ( $k_L a$ ) in each of the systems studied, and the combination of the different results led to **the development of a robust transfer coefficient ( $k_L$ ) model incorporating the impact of rheology and shear stress.**

In addition, hydrodynamic characterizations - Mixing Time (via colorimetry and image processing) and Velocimetry (by Pavlov tube\* ) - were conducted in the same aerated viscous media in order to build a **numerical model validation database.**

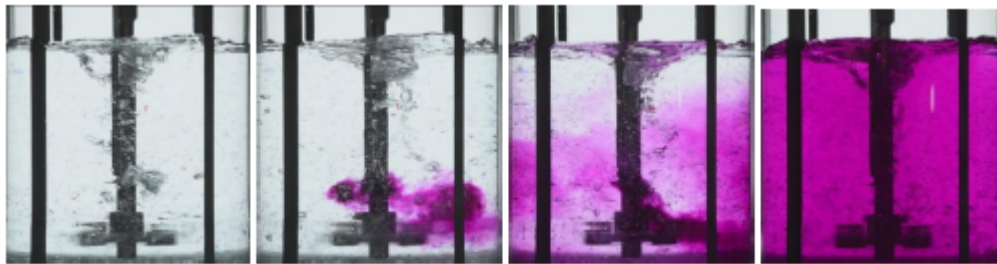


Figure 1: Illustration of the mixing in water mechanism, at several points in time (photographs), from injection (a) through to complete mixing (d)

\* Instrument used to determine the speed of a fluid, including for the two-phase scenario, from a pressure difference measurement

## Use of predictive numerical methods

For the purposes of numerical simulation, a model was developed on the basis of a Eulerian two-phase approach [3] and an averaged description of velocity fields\*\*. This model also integrates the oxygen transfer phenomena and the consumption metabolism for different substrates.

It allows **the prediction, at all scales (laboratory, pilot unit, industrial), of sugar and dissolved oxygen concentration ranges**, as well as the associated global protein (enzyme) productivity. It also provides a distribution of local enzyme productivity, as illustrated in [figure 2](#) below, for two different-sized fermenters.

These calculations also highlighted an increase in metabolism heterogeneities with dimensional extrapolation, caused by substrate heterogeneities between zones. Consequently, there are **potential differences in the behavior of microorganisms** between the top and bottom of the fermenters.

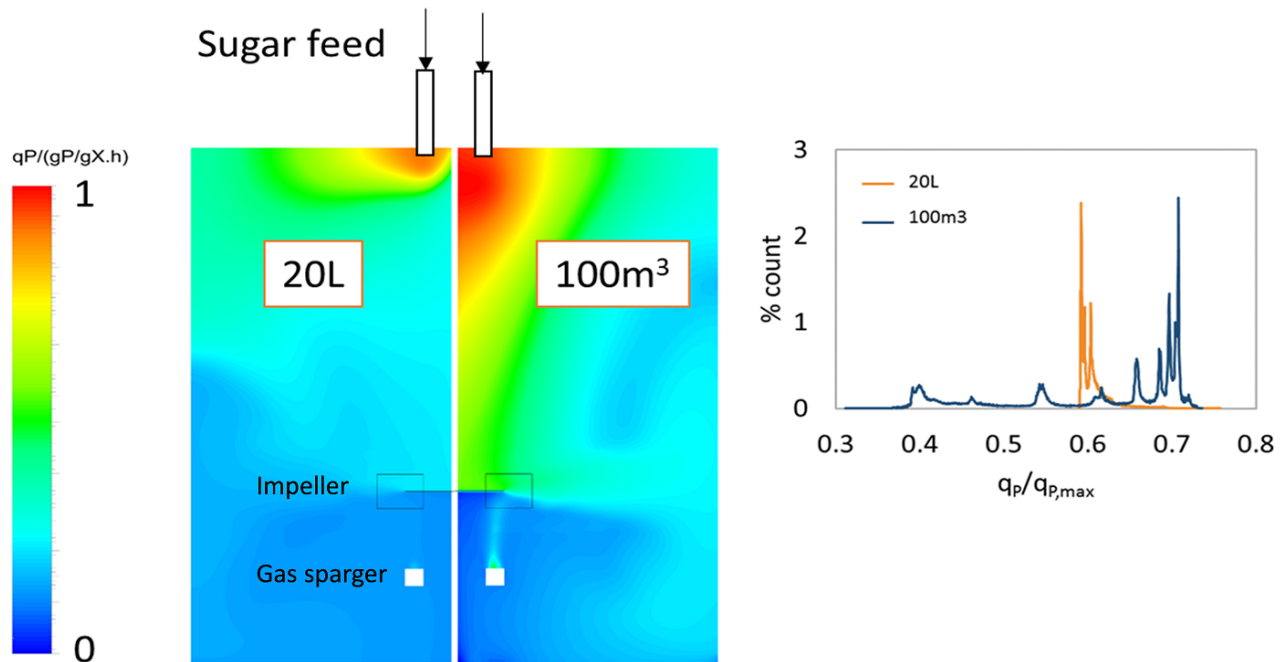


Figure 2: Standardized protein (enzyme) productivity ranges in two fermenters of 20 L and 100 m<sup>3</sup>, and associated productivity distributions

\*\* RANS approach : [Reynolds Averaged Navier-Stokes equations](#)

## Towards increased incorporation of substrate variability

However, the metabolic model employed does not take into account the sensitivity of the microorganism to time-related and geometric variations in substrate composition. To fine-tune productivity predictions in large-sized fermenters, it is therefore necessary **to evaluate the model's ability to adapt to such fluctuations.**

Tests **to better characterize this aspect of the microorganism's behavior** are currently also underway in dual-zone fermenters, using a "scale-down" approach\*\*\*.

Finally, the model will soon be used to validate stirring technologies and substrate injection methods aimed at ensuring the required level of homogeneity of substrates **in order to maintain the optimal productivity of industrial fermenters.**

\*\*\* Thesis underway by T. Goncalves Roque (IFPEN/AgroParisTech)

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## References:

- [1] Maximiano Raimundo P., Analyse et modélisation de l'hydrodynamique locale dans les colonnes à bulles (Local hydrodynamic analysis and modeling in bubble columns), Thèse de doctorat, Université de Grenoble, 2015.
- [2] Cappello, V., Plais C., Vial, C., Augier, F. (2020). Bubble size and liquid-side mass transfer

coefficient measurements in aerated stirred tank reactors with non-newtonian liquids. Chemical Engineering Science, 211, 115280. DOI:10.1016/j.ces.2019.115280.

[3] Cappello V., Plais C., Vial C., Augier F., Scale-up of aerated bioreactors: CFD validation and application to the enzyme production by *Trichoderma reesei*. Chemical Engineering Science, 229 (2021), 116033. DOI:10.1016/j.ces.2020.116033.

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