Analysis and modelling of the reaction-mixture interaction on the extrapolation of the aerobic and anaerobic fermenters

UNIVERSITÉ Clermont Auvergne

Ecole doctorale Sciences Pour l'Ingénieur

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Introduction

Context

The massive use of **fossil fuels** for industrial development and human activities leads to a **pollution of soils, air and water**. This source of energy is also **limited in quantity unlike "renewable" energies**, which are now **real sources** to be exploited.

Within this framework, we are interested in the **"dark fermentation"** process, which consists in the **decomposition of organic substrates** thanks to **microorganisms** in agitated bioreactors (*figure 1*). They are also called **fermenters**, and are used to **produce biohydrogen and other molecules** of commercial interest. It is a well-known process but still needs to be optimized.

An **optimum process** needs a **good homogeneity** of the reactional environment while **limiting the energy consumption** by the impellers. Hence, it is necessary to better understand the **hydrodynamics** and the concomitant **heat and mass transfer** within the fermenter in order to select the **best operating conditions** of the bioreactor and their impact on the mixture.

Objectives

- To develop and validate a numerical tool based on **CFD (*Computational Fluid Dynamics*)** (***figure 6***), based on **Navier-Stokes** equations, leading to assist in the **design of gas-liquid reactors** by including all of the involved physical phenomena.
- The simulations will have to take into account the **multiphase flows** as well as the of **heat and mass transfer**.
- To develop a method of **optical trajectography** to measure the Lagrangian velocity field (***figure 9***), and a method of **PIV (*Particle Image Velocimetry*)** to measure the Eulerian velocity field (***figure 5***).
- Estimate the **quality of the mixing and the mass transfer** in fermenters of **variable size and design** to understand the scale effects in Newtonian and non-Newtonian fluids.

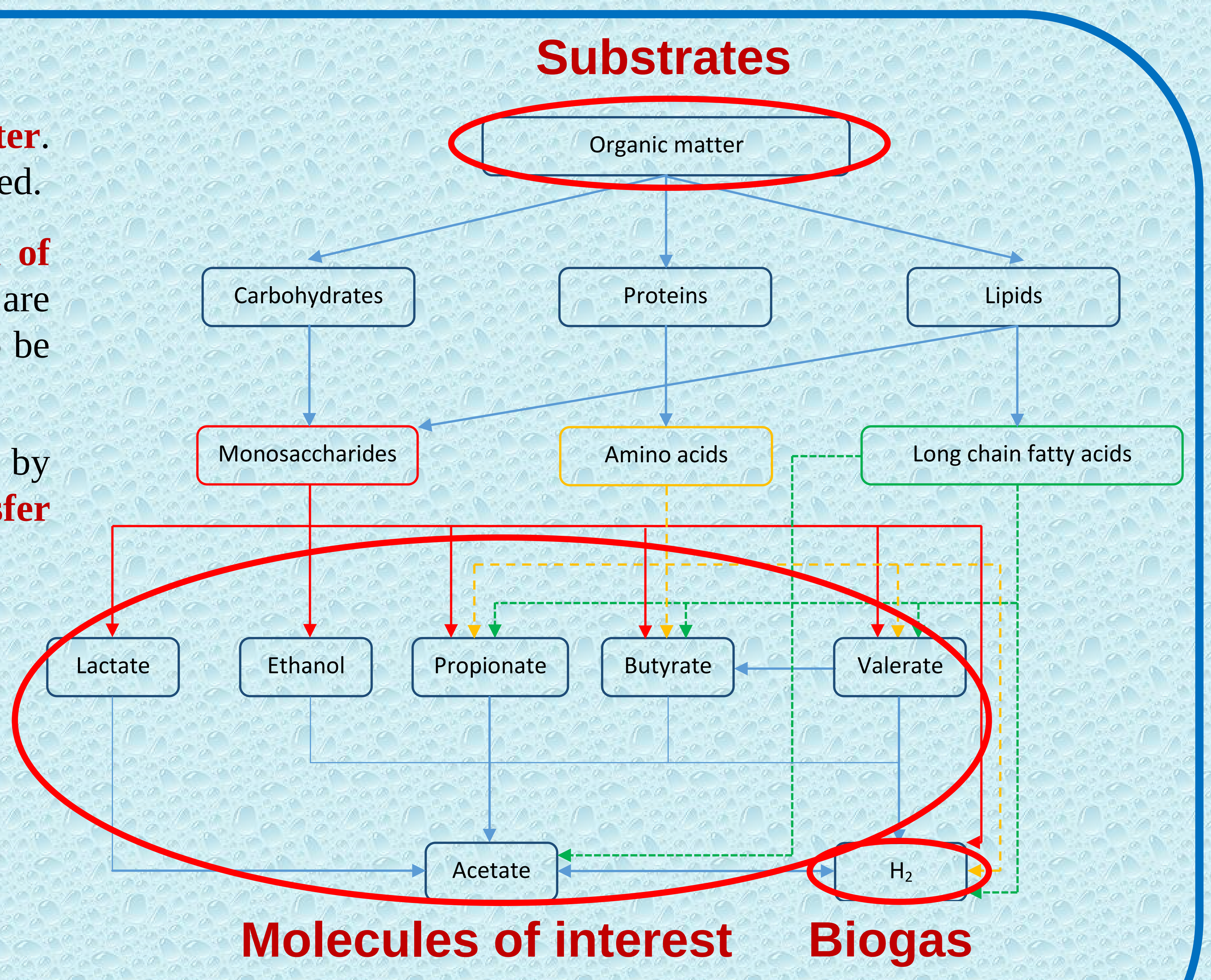

***Figure 1**. Simplified chemical mechanisms which govern dark fermentation process*

Implementation of the CFD model

- ***Definition of the physical domain***
  Implementation of the **domain limits** and the **objects** within it (***figure 2***).
- ***Mesh Grid***
  Definition of the **mesh size and structure** around the objects and the physical domain limits (***figure 3***).
- ***Turbulence model***
  Choosing the most suitable turbulent model for this simulation. A variant of the ***k-ε* model** was chosen in our case.
- ***Boundary conditions***
  Selection of the **boundary conditions** of the flow configuration and the **fluid properties** (ex : ***Newtonian***). **No-slip** on the solid boundaries and **stress free** at the upper liquid-air interface.
- ***Numerical parameters***
  Choosing the **parameters of calculation** (ex: number of iterations, relaxation control, output,…).

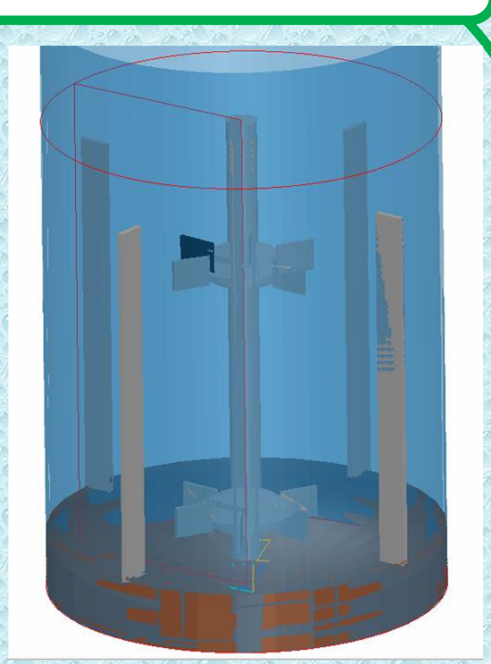

***Figure 2**. Modelling of the bioreactor*

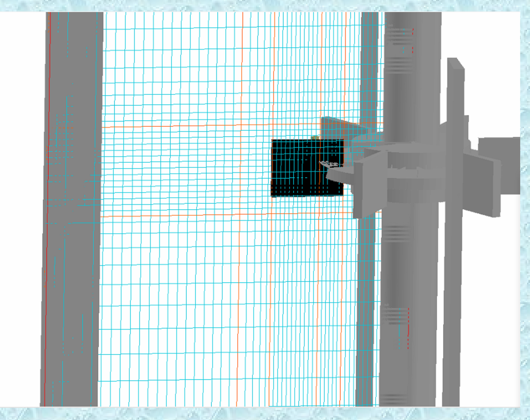

***Figure 3**. Mesh grid of the bioreactor*

Results of the model reliability

- ***Grid independent***
  Choosing the **mesh grid** that allows computing solutions that do **not depend** significantly on the **mesh resolution**.

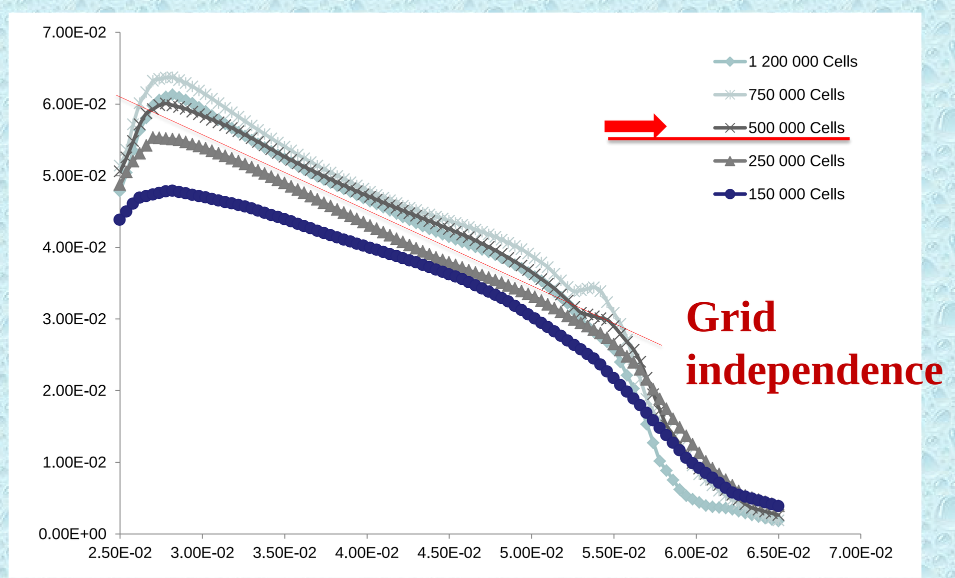

***Figure 4**. Flow speed profile out of the high impeller for each mesh size*

- ***Comparison to experiments :***
  Comparison with the **PIV data**

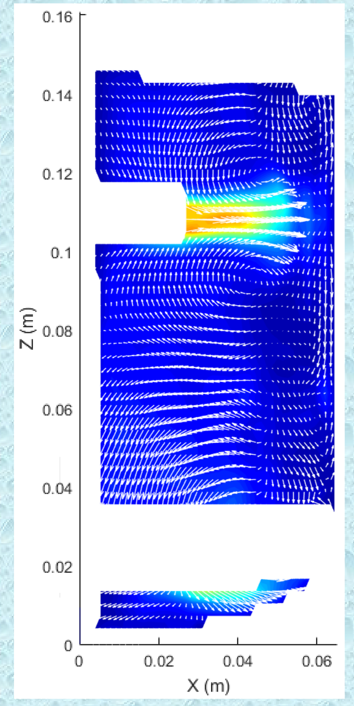

***Figure 5**. Velocity field from PIV at 40 rpm (experimental)*

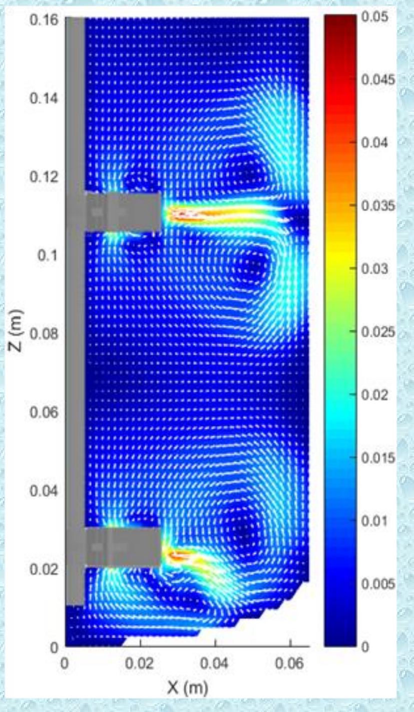

***Figure 6**. Velocity field from CFD at 40 rpm (simulation)*

- ***Convergence***
  Stabilization of the values.
- ***Negligible Residuals :***
  The **smallest possible** values of the residuals, which measure **numerical error**.

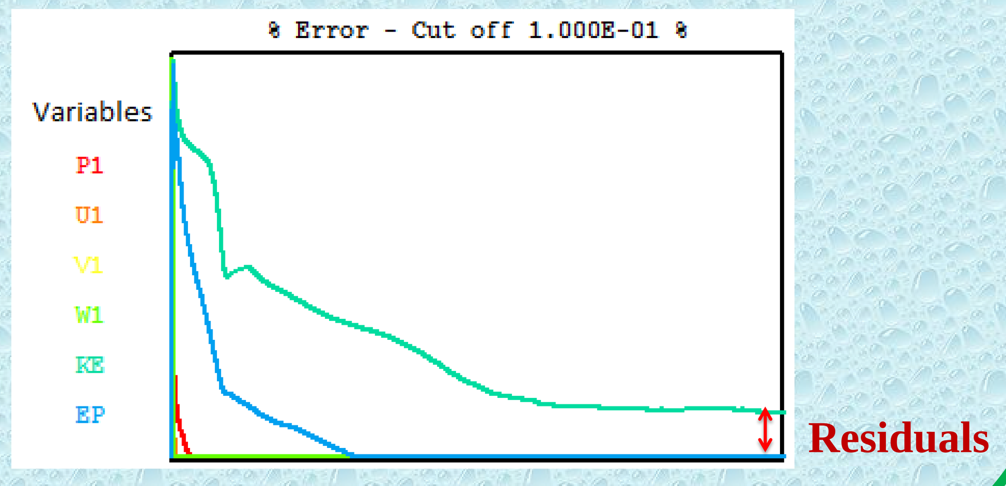

***Figure 7**. Residuals plotted against the number of iterations at 40 rpm*

Conclusions and perspectives

Conclusions

- As it can be seen in the ***figures 4 ,5, 6 and 7***, the **model** has been **correctly set up**, with a good agreement between experimental and numerical data.
- Hence, the first **test on complex fluids** (ex: ***non-Newtonian***) can be performed with a strong basis, which needs to be **reinforced by new PIV measurement** for these types of fluids.
- The new experimental tool of **optical trajectography**, coupled with the study of **heat and mass transfer** should allow us to **better characterize real media** which are complex fluids in order to **enhance biohydrogen production** in this bioreactor.

Complexification of the model

- ***Material and heat transfer***
  Study of **distributive mixing** within the liquid phase (*ex: **mixing time***) and the **dispersive mixing** at the interface, as well as **heat transfer**.
- ***Power consumption***
  Study of the **torque on impellers**, comparing it to the experimental data in order to estimate **power consumption** due to mechanical mixing in the reactor.
- ***Multiphase simulation***
  Study of a **solid suspension** (simulating microorganisms) in the liquid phase.
- ***Non-Newtonian fluids***
  New simulations where the **viscosity** is a function of the **shear rate**.

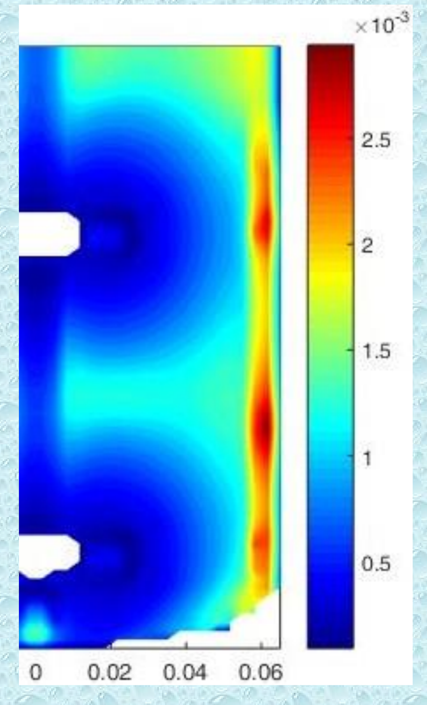

***Figure 8**. Viscosity field in CFD (simulation)*

- ***GENTRA (CFD particle tracking)***
  Simulation of **particle tracking** in the reactor and comparison with **optical trajectography**.

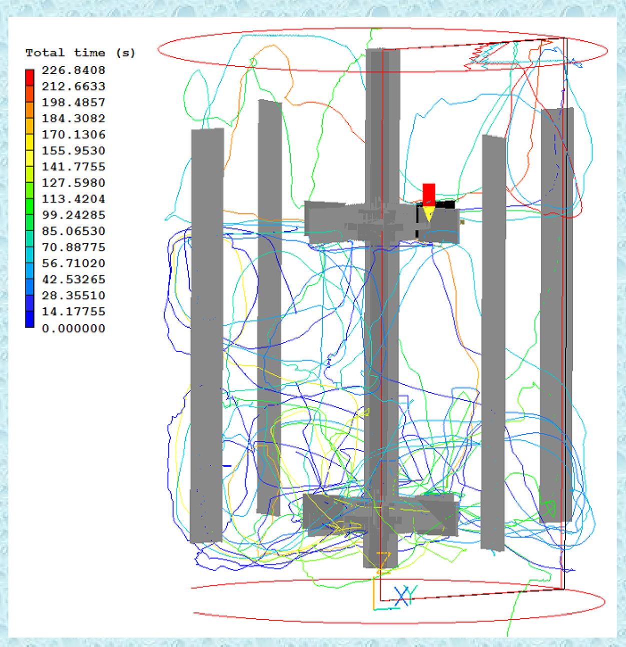

***Figure 9**. Particle tracking in CFD (simulation)*