**Investigation of interfacial mechanisms during organic acid reactive extraction through dynamic interfacial tension measurements**

Ana-Karen Sánchez-Castañeda1, Florian Chemarin1,2, Marwen Moussa1, Violaine Athes1, Ioan-Cristian Trelea1\*.

*1 UMR 782 GMPA, AgroParisTech, INRA, Université Paris Saclay, 78850 Thiverval-Grignon, France; 2 URD Agro-Biotechnologies Industrielles, AgroParisTech 51110 Pomacle, France.*

*\*Corresponding author:* *cristian.trelea@agroparistech.fr*

**Highlights**

* Interfacial phenomena during liquid-liquid reactive extraction are analyzed
* Dynamic interfacial tension is proposed as an easy method to monitor interfacial reactions
* A mathematical model gives insights in interfacial reaction mechanisms

**1. Introduction**

3-Hydroxypropionic acid (3-HP) is an attractive platform molecule that can be converted to several materials, such as acrylic acid and biodegradable polymers. Its production by bioconversion has made remarkable advances, but its industrial commercialization is still limited by low productivities caused by product inhibition. *In situ* liquid-liquid reactive extraction assisted by a hollow fiber membrane contactor (HFMC) is a promising strategy to intensify 3-HP bioconversion [1,2]. Several points remain to be better understood, however, to develop a continuous extraction system coupled to bioconversion and maintain a low acid concentration in the medium. 3-HP extraction performed on a hollow fiber membrane contactor occurs at the interface formed inside the pores of the membrane, between two immiscible liquids. Proper interface stabilization is an important factor to avoid emulsions and direct contact of the organic phase with cells. It is also known that extraction rates can be markedly affected by interfacial mass transfer. All this highlights the need to better understand the interfacial phenomena involved during 3-HP extraction. In this study dynamic Interfacial Tension (IFT) was used to monitor concentration of the chemical species at the interface. This allows investigating the mechanisms of mass transfer during 3-HP reactive extraction, by developing a mathematical model that relates IFT with interfacial concentration of species, in addition to usual bulk concentration measurements.

**2. Methods**

The studied system consisted of 3-HP at 7 different initial concentrations (0 to 50 g/L) in the aqueous phase, and Trioctylamine (TOA) diluted in n-decanol at 20% v/v as the organic phase. For IFT measurement, both phases were put in contact in a Pendant Drop Tensiometer, putting the 3-HP solution in a syringe that creates a pendant drop inside the organic phase. In membrane contactors, mass transfer is mainly controlled by diffusion in the membrane pores. Such a configuration mimics mass transfer conditions at the interface situated in membrane pores. A previously developed mathematical model that successfully describes interfacial equilibrium of the chemical species in the considered extraction system [3] was combined with a mass transfer model adapted to the geometry and physical conditions of the pendant drop method. Then, the Gibbs equation that relates IFT with interfacial species concentration combined with the Langmuir-Freundlich adsorption isotherm were used to compare model predictions with dynamic IFT measurements.

**3. Results and discussion**

Dynamic IFT values were chiefly related to interfacial 3-HP/TOA complex concentration formed in reactive extraction, calculated by the model. IFT value of the organic phase with water was 10.24 mN/m, and this value decreased when 3-HP initial concentration increased. The lowest measured value was 6.36 mN/m with an initial concentration 3-HP of 50 g/L. These values are low enough to make potentially difficult the interface stabilization in the pores. Results showed that observed mass transfer in the pendant drop tensiometer could not be explained by molecular diffusion only and involved local convection in the organic phase [4]. The model allows one to estimate adsorption and desorption rates of chemical species at the liquid-liquid interface and the interfacial concentration of the acid-amine complex, the main surface-active species. Insights in the interfacial reaction mechanisms obtained in this study will be useful to determine the rate-limiting mechanisms (adsorption, desorption, reaction, diffusion, convection) in HFMC.

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| Initial [3-HP] (g/L) |

Figure 1. Dynamic Interfacial Tension at different initial 3-HP concentrations. Filled circles: experimental values. Lines: model results.

**4. Conclusions**

Information obtained from this study validates assumed mass transfer and reaction mechanisms and sets the stage for model-based process optimization in the HFMC configuration.

**References**

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