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Tailored Euler-Lagrange Model to Predict the Microfluidic Capture of Target Species

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Extended Abstract

Nano- and micro- sized functionalized particles display remarkable features that motivate and endorse their implementation in various processes as catalysts, photocatalysts, adsorbents or sensors. Although they are being integrated in multiple fields, such as water treatment or energy generation, their spotlight is in the field of biomedicine, where they are involved in the capture or release of biomolecules. These systems can be incorporated into microdevices, which constitute a profitable platform that can hugely benefit these processes [1]. Therefore, building predictive models that describe the functioning of these systems becomes a matter of interest to face their design and analysis. Two alternatives arise when considering multiphasic solid-liquid systems, the Euler-Euler approach and the Euler-Lagrange approach. The first one describes the two phases as interpenetrating continua and neglect the position in space and time of the particles. Meanwhile, the second alternative considers the discrete nature of the solid particles and tracks every one of them along the domain in every moment. In this work, two Computational Fluid Dynamics (CFD) models based on the aforementioned approaches are constructed to describe the performance of solid-liquid particulate microfluidic systems with interfacial mass transfer involved. To test and compare both models, the microfluidic capture of chromium from aqueous samples employing functionalized magnetic nanoparticles (MNPs) is selected as case study [2].

The performance of the two models is analysed in terms of the chromium capture they provide. To carry out the corresponding simulations, the system is tested introducing an aqueous solution containing 0.44 mM chromium and a suspension of amino-functionalized nanoparticles with 0.17 $mmol_{amino} \cdot g_{MNP}^{-1}$. To study the effect of the concentration of the particles and the response of both models to it, particles charges in the range 2.5-8 $g_{MNP} \cdot L^{-1}$ are considered. For that purpose, and to study the results in absence of promoted mixing, a Y-Y straight shaped microdevice is selected. Under these conditions both models are experimentally validated with a successful result. It is proved that the models can accurately predict the chromium capture in the equilibrium with deviations inferior to 2.5%. The simulations reveal that the Euler-Euler based option overestimates the chromium removal in the kinetic region up to 28%. This difference shows to turn more significant when higher particle concentrations are employed. Thus, in this work two highly valuable predictive models are reported. The Euler-Lagrange constitutes a precise and robust option to predict the functioning of microfluidic multiphasic systems. Meanwhile, the Euler-Euler alternative proves to be an attractive tool to quickly obtain capture results in equilibrium conditions.

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