



HAL
open science

Dynamic modelling of transport and adsorption processes in mesoporous solids: Application to heterogeneous catalysis and water decontamination

Rita Fayad, Aurélie Galfré, Françoise Couenne, Elsa Jolimaitre, Charles-Philippe Lienemann, Loïc Sorbier, Mélaz Tayakout-Fayolle

► To cite this version:

Rita Fayad, Aurélie Galfré, Françoise Couenne, Elsa Jolimaitre, Charles-Philippe Lienemann, et al.. Dynamic modelling of transport and adsorption processes in mesoporous solids: Application to heterogeneous catalysis and water decontamination. 9th Tokyo Conference on Advanced Catalytic Science and Technology (TOCAT), Catalysis Society of Japan, Jul 2022, Fukuoka, Japan. hal-04928783

HAL Id: hal-04928783

<https://hal.science/hal-04928783v1>

Submitted on 4 Feb 2025

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Dynamic modelling of transport and adsorption processes in mesoporous solids: Application to heterogeneous catalysis and water decontamination

Rita Fayad,^{a,*} Aurélie Galfré,^a Françoise Couenne,^a Elsa Jolimaitre,^b Loïc Sorbier,^b Charles-Philippe Lienemann^b, Mélaz Tayakout-Fayolle^a

^aUniversity Claude Bernard Lyon 1, Villeurbanne, 69100, France

^bIFP Energies Nouvelles, Solaize, 69360, France

* Corresponding author: rita.fayad@univ-lyon1.fr

Abstract:

Keywords: Ion exchange, Molecular diffusion, Dynamic modelling.

1. Introduction

Adsorption is a commonly used process in the chemical industry nowadays, since it is considered one of the most effective and economic methods for analytical purposes (i.e. chromatography) and for the treatment of waters contaminated with heavy metals¹. Another noticeable application for adsorption is the impregnation of mesoporous solids with metallic ions for the preparation of heterogeneous catalysts². In such applications, adsorption occurs through ion exchange between metal ions in the liquid solution and groups on the solid surface and is governed by diffusion processes. However, ion exchange is not easily controllable due to the complexity of the porous medium and the ionic solution³. Over the years, several researchers evaluated the aforementioned applications by modelling their physico-chemical phenomena using mathematical models for molecular diffusion (i.e. Fick's law) and adsorption (i.e. adsorption isotherms)⁴; yet omitting the non-homogeneity of the solid surface, the non-ideality of the liquid solution, and the ion exchange between the liquid phase and the solid surface.

2. Experimental (or Theoretical)

In this study, we use two impregnation techniques of alumina pellets with nickel nitrate solutions: 1) batch experiments conducted in a previous study by Catita L. et al.² (Figure 1-A), and 2) breakthrough experiments in a Continuous Stirred-Tank Reactor (CSTR) conducted in this study (Figure 1-B). In Figure 1-A), one alumina pellet is submerged in water and, then, in nickel nitrate solutions (with concentrations ranging from 100 to 300 mol/m³) for 30 seconds. Impregnation inside the pellet is after that monitored by MRI analysis. In Figure 1-B), a basket inside a CSTR is filled with alumina pellets and nickel nitrate solutions flow through the reactor. The pH, conductivity, and UV absorbance of the liquid solution exiting the reactor are measured for analysis of the impregnation process.

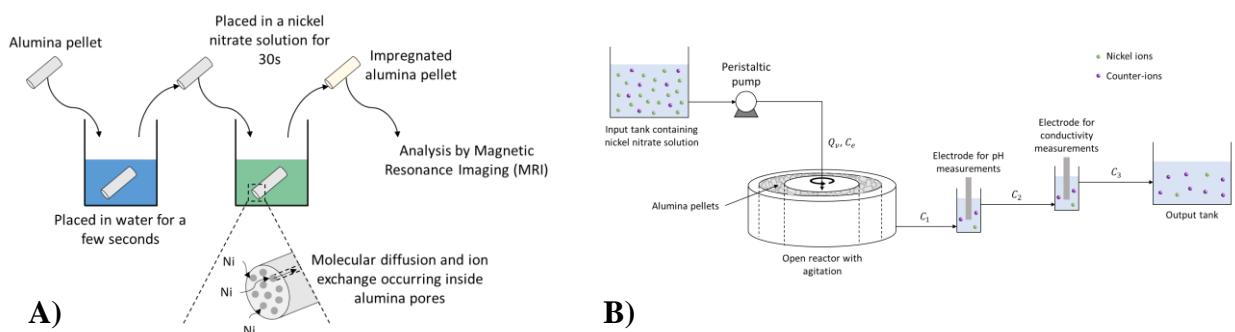


Figure 1. Description of the impregnation techniques studied: A) batch experiments employed by Catita L. et al. and B) continuous experiments applied in a CSTR in this work.

A dynamic model is developed for the abovementioned impregnation processes, in order to simulate the transport of nickel ions in the liquid solution inside the pores and the ion exchange between nickel ions from the solution and hydrogen ions on different adsorption sites on the alumina surface (each site with different

adsorbing properties). The model simulates the evolution of the nickel concentration in the liquid and adsorbed phases and the average distance travelled by nickel ions inside the alumina pellet; and compares the simulation results with the experimental results. The liquid solution is assumed to be ideal (Fick's law is used to model molecular diffusion) and the ion exchange is assumed to occur between one nickel ion and two hydrogen ions on the alumina surface. A parameter estimation technique based on the *lsqnonlin* method on MATLAB® is used to estimate the model parameters (i.e. equilibrium constants of the ion exchange) by fitting the experimental results to the simulation results.

3. Results and discussion

The model predicts the time and space evolution of the concentrations of both nickel and hydrogen ions in the liquid and adsorbed phases, inside alumina pellets. Due to the parameter estimation technique employed, the simulations agree well with the results of Catita's impregnation experiments² (Figure 2).

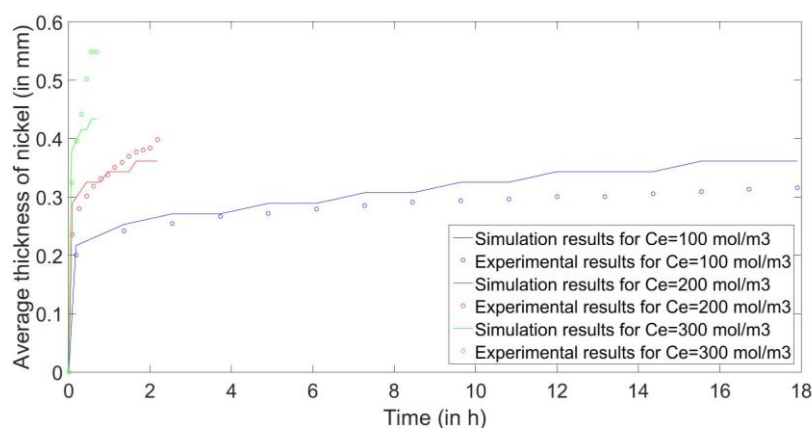


Figure 2. Comparison between simulations (solid lines) and experimental results (dots) for the average distance travelled by nickel ions inside alumina pellets impregnated with 3 impregnation solutions with different initial nickel concentrations.

Results shown in Figure 2 show that, the greater the initial nickel concentration is, the greater the distance travelled by nickel ions inside the alumina pellet but the faster the solid surface saturates; showing that diffusion is the limiting process. The model also predicts a decrease in the pH of the liquid solution inside the alumina pores (surely owing to the ion exchange between the nickel and hydrogen ions), which is later validated by the results of the adsorption experiments conducted in the CSTR (Figure 1-B).

4. Conclusions

The study is to be improved by accounting for the non-ideality of the liquid solution. Moreover, the simulation results are to be further validated at different initial conditions of pH and nickel concentration.

Acknowledgements

This conference is organized by the Catalysis Society of Japan and will be supported by many sponsors.

References

1. E. Da'na, Microporous Mesoporous Mater. 247 (2017) 145-157.
2. L. Catita, E. Jolimaitre, A.-A. Quoineaud, O. Delpoux, C. Pichon, J.-M. Schweitzer, Microporous Mesoporous Mater. 312 (2021) 110756.
3. P. Munnik, P. E. de Jongh, K. P. de Jong, Chem. Rev. 115 (2015) 6687-6718.
4. X. Liu, J. G. Khinastb, B. J. Glassera, Chem. Eng. Sci. 63 (2008) 4517-4530.