

Modelling of solute and solvent transport through nanofiltration membranes

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1. Introduction

This work proposes a methodology for modelling the transport of defined solutes and solvents through nanofiltration membranes, by using mathematical models based on a mechanistic or a chemometric approach, or on their combination, which will be referred to as hybrid modelling.

The situations under study are the transport/rejection of non-spherical solutes from aqueous media by nanofiltration, and the transport of defined solvents using solvent resistant nanofiltration membranes. For the first case, the rejection of a number of solutes (*n*-alcohols and di-alcohols) with different chain length, polarity, symmetry and functional group position (butanol, hexanol, octanol, 1,4-butanediol, 1,6-hexanediol, 1,8-octanediol and 3-hexanol) was studied experimentally using a Desal 5-DK (GE Osmonics, USA) nanofiltration membrane. For the second case, the permeation of water, *n*-butanol, *iso*-butanol and *tert*-butanol as single solvents as well as their binary mixtures

was studied, using a STARMEM 240 (Grace Davison, USA) solvent resistant nanofiltration membrane.

2. Approach

The global approach followed in this work is schematically described in Fig. 1. The input matrix of values composed by the solvent/solute/membrane characteristic parameters and by defined process operational conditions is fed either to mechanistic models or to chemometric models. Depending on the system under study, a hybrid modelling approach might be followed by combining mechanistic with chemometric models. The output matrix encloses information about solvent flux and solute rejection for a given nanofiltration membrane.

The mechanistic model for aqueous nanofiltration is based on the widely used hydrodynamic model, for which a mathematical description of the solute size was developed using its “Geometric radius”, where the molecular geometry is represented by a prolate revolution ellipsoid [1]. Additionally, the preferential orientation of

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Tadashi Uragami



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Solute and Solvent Transport Through Nanoporous Ceramic Membranes Thomas Hilfer, 2011 **Science and Technology of Separation Membranes** Tadashi Uragami, 2017-02-10 Offers a comprehensive overview of membrane science and technology from a single source Written by a renowned author with more than 40 years experience in membrane science and technology and polymer science Covers all major current applications of membrane technology in two definitive volumes Includes academic analyses applications and practical problems for each existing membrane technology Includes novel applications such as membrane reactors hybrid systems and optical resolution as well as membrane fuel cells

Advanced Materials for Membrane Preparation Maria Giovanna Buonomenna, G. Golemme, 2012 The need to reduce pollution and the waste of energy and resources imposes a wider diffusion of environmentally friendly membrane systems The expanding domain of membrane operations demands tailored materials with unprecedented performances and resistance

Ceramic Materials Research Trends Paul B. Lin, 2007 Ceramics are refractory inorganic and non metallic materials They can be divided into two classes traditional and advanced Traditional ceramics include clay products silicate glass and cement while advanced ceramics consist of carbides SiC pure oxides Al₂O₃ nitrides Si₃N₄ non silicate glasses and many others Ceramics offer many advantages compared to other materials They are harder and stiffer than steel more heat and corrosion resistant than metals or polymers less dense than most metals and their alloys and their raw materials are both plentiful and inexpensive Ceramic materials display a wide range of properties which facilitate their use in many different product areas This book presents new and important international research in this dynamic field **Comprehensive**

Membrane Science and Engineering Enrico Drioli, Lidietta Giorno, Enrica Fontananova, 2017-07-20 Comprehensive Membrane Science and Engineering Second Edition Four Volume Set is an interdisciplinary and innovative reference work on membrane science and technology Written by leading researchers and industry professionals from a range of backgrounds chapters elaborate on recent and future developments in the field of membrane science and explore how the field has advanced since the previous edition published in 2010 Chapters are written by academics and practitioners across a variety of fields including chemistry chemical engineering material science physics biology and food science Each volume covers a wide spectrum of applications and advanced technologies such as new membrane materials e g thermally rearranged polymers polymers of intrinsic microporosity and new hydrophobic fluoropolymer and processes e g reverse electrodialysis membrane contractors membrane crystallization membrane condenser membrane dryers and membrane emulsifiers that have only recently proved their full potential for industrial application This work covers the latest advances in membrane science linking fundamental research with real life practical applications using specially selected case studies of medium and large scale membrane operations to demonstrate successes and failures with a look to future developments in the field Contains comprehensive cutting edge coverage helping readers understand the latest theory Offers readers a variety of

perspectives on how membrane science and engineering research can be best applied in practice across a range of industries Provides the theory behind the limits advantages future developments and failure expectations of local membrane operations in emerging countries

Porous Membranes Annarosa Gugliuzza,Wanqin Jin,2025-08-04 The book is essential for anyone seeking a deep understanding of porous membranes as it offers valuable insights into manufacturing methods innovative applications and strategies for optimizing membrane design to meet critical project demands across various fields Porous Membranes Breakthroughs in Manufacturing and Applications is a comprehensive guide to discovering the world of porous membranes and their applications This volume gives a global perspective of basic concepts featuring manufacturing approaches and potential applications where control of pore size and shape and distribution can be decisive for the success of a membrane process In depth explanations elaborate on the key role assigned to a membrane s pores in directing events that are crucial for the mandatory targets imposed by a project s requirements Further discussions on how to manage and characterize materials from a molecular to macro scale to achieve highly defined architecture to enable high performing separations are explored Advances and innovation are central themes providing useful solutions to current critical aspects and existing bottlenecks in the control of structural and chemical features of targeted membranes This cross disciplinary discussion opens new routes for membrane science in expanding fields including water management environmental remediation recovery of targeted compounds food and health Readers will find this book Introduces the strict relationship between extensively ordered porous membranes and enhanced productivity Explores new approaches based on new membrane pore concepts Emphasizes the feasibility and reliability of the proposed techniques within the context of a potential scale up analyzing critical issues and traits Focuses on the role of porous membranes in some strategic membrane operations providing clear evidence about the fundamental role of structure separation properties for the success of membrane processes dedicated to natural resource management Audience Researchers in chemistry biology biomedicine materials science textiles and electronics who are involved with membranes and materials technologists and product managers from industry including those responsible for research and development building prototypes and commercial devices will find this book to be especially valuable Applied Science & Technology Index ,2000 *Chemical Abstracts* ,2002 *Organically-modified Ceramic Membranes for Solvent Nanofiltration* Cheryl Raditya Tanardi,2015 **Ceramic Membranes Applied in Separation Processes** Dionisio da Silva Biron,Venina dos Santos,Mara Zeni,2017-05-18 This book covers diverse types of ceramic membranes applied in separation processes The authors present the preparation methods and well as the main application of ceramic membranes Modules microfiltration and ultrafiltration are topics described within the text The final chapter focuses on water and wastewater treatment by membranes separation processes

Organic Solvent Nanofiltration in the Peptide Industry Patrizia Marchetti,2013 In recent years the application of membrane technology to molecular separation processes has stimulated interest and showed great potential in a number of

industrial fields Ultrafiltration membranes have been successfully applied to downstream separation of therapeutically active peptides to overcome some of the limitations of the conventional techniques in terms of costs scale up selectivity and solvent recovery In this research project Organic Solvent Nanofiltration of peptide solutions is studied and this understanding is applied to the development of innovative membrane based purification strategies for industrial case studies Basic understanding of transport mechanisms was approached by investigating solvent transport through ceramic nano and ultrafiltration membranes and developing a predictive phenomenological model for the transport of solvents and solvent mixtures Effects of solvent membrane interactions strongly affected the solvent permeation through nanofiltration membranes while they were found to be negligible in the ultrafiltration range The effect of the organic solvent on the permeation of neutral and charged solutes monovalent salts a small molecule and peptides in organic water mixtures was studied with particular attention to the role of preferential solvation in the solvent mixture It was found that the solvent composition and the complex association of counter ions and buffers highly affect membrane permeation and rejection of organic molecules It is proposed that all these components change the relative solute membrane affinity Since permeation of peptides in organic water mixtures is affected by complicated matrices of input parameters a Design of Experiment approach was proposed to efficiently investigate the nanofiltration of model peptides in acetonitrile water solutions Statistical models for solvent flux peptide and ion rejection were obtained by Analysis of Variance and interpreted from a phenomenological point of view The statistical models were used to assist process development for two industrial case studies 1 concentration and salt solvent exchange of a first therapeutic peptide were optimised based on the integration of the statistical DoE models with the process simulation for concentration and diafiltration 2 the nanofiltration assisted synthesis of a second therapeutic peptide based on the coupling between nanofiltration and reaction in one unique process was developed and compared to the established process by techno economical analysis The so called Reactive Peptide Nanofiltration was found to be advantageous in terms of economics efficacy impact on the market and on the environment In conclusion nanofiltration was found to be a solid and competitive technique for application to peptide processes On the basis of the results of this research Lonza decided to invest in a new nanofiltration plant for the downstream of peptides with ceramic membranes The advantages of nanofiltration technology in terms of development of more efficient materials stable in critical solvents and harsh acid basic conditions improvement of membrane performances selectivity lifetime and integration of nanofiltration with other techniques in hybrid processes seem therefore promising in overcoming the hesitancy of industries to modify the established processes and invest in new nanofiltration plants by making the payback period for the return of investment more attractive It is plausible to think that this technology will shortly become a primary choice for new separation and purification processes

Ceramic Membranes for Liquid Phase Separations Reid Alan Peterson, 1994 **Ionic and Molecular Transport Through Active Nanoporous Membranes** Fabien Wildhaber, Philippe Renaud (Physiker, Schweiz), 2014

Recent Advances in Gas Separation by Microporous Ceramic Membranes N.K. Kanellopoulos, 2000-09-26 This book is dedicated to the rapidly growing field of microporous ceramic membranes with separating layers of pore diameter less than 2nm. The chapters of this book bring forward a wide range of issues namely fundamentals of complex sorption and transport processes in micropore structures, highly innovative methods of preparation of microporous membranes and examples of their possible commercial applications. This book presents insights by distinguished investigators who have contributed significantly to the advance of research efforts in the diverse topics described herein. Recently significant progress has been made with respect to the development of novel microporous asymmetric membranes mainly involving modification by means of deposition of additional material within the pores of the substrates. Most state of the art technologies aiming in the development of microporous ceramic membrane are presented in the third section of the book. These include several material deposition methods and techniques on macroporous or mesoporous supports and substrates from the liquid or vapour phase namely those involving sol gel, zeolite and chemical vapour deposition techniques. In addition to the above mentioned methods, the classical technique of carbonizing polymeric deposits along with one of the novel techniques of plasma treating organically deposited Langmuir-Blodgett films are also presented. Nanophase mixed ionic-electron membranes for enhanced oxygen transport are described which pose a strong candidacy for a number of significant commercial applications.

Study of the Separation by Organic Solvent Nanofiltration of Diluted Solutes Using Commercial, Dense and Porous Membranes and Their Derivatives by Deposition of Polyelectrolyte Nanolayers Mahbub Morshed, 2019 The objective of this study was to improve the OSN separation performance of commercial membranes for metathesis applications in which highly diluted catalysts are used. In this work, commercial polymeric membranes were first studied to characterize their performance in organic media using very dilute solute-solvent binary mixtures. Based on a literature review, it was shown that the PERVAP4060 membrane, of which PDMS is the dense active layer, was a promising candidate for organic solvent nanofiltration (OSN). As a porous membrane, the AMS and PAN commercial supports have also been taken into account. In this study, we considered the modification on the surface to improve the separation properties of polymeric OSN membranes. Ar/O₂ plasma and/or polyelectrolyte multilayers were used for the preparation of new prototype membranes. Unmodified and modified membranes were tested under OSN conditions using binary feed mixtures. Several highly dilute solutes, organophosphorus ligand R-BINAP, phase transfer catalyst ToABR and linear alkanes have been studied. Both R-BINAP and ToABR were used in the range of 0.0001 to 0.5% by weight and most experiments were subsequently performed with 0.05% solute concentrations in toluene. It has been shown that PDMS can retain 80% R-BINAP and about 93% ToABr in toluene. After modification by the LBL deposition, the rejection is improved with the modified PERVAP4060 membranes, leading to an 88% rejection of R-BINAP with a deposit of 10 PAH-PSS polyelectrolyte bilayers at the surface and this rejection being able to reach 95% when the number of bilayers is 20. ToABr rejection

increases to 97% with the ten bilayered membranes. The performance of the membrane was studied under different pressures of between 1 and 40 bar; the high rejection still observed in these OSN conditions strongly supports a solution diffusion transfer mechanism through the PDMS. The treatment of ternary mixtures mimicking the catalyst/solute/solvent mixture corresponding to the hydroformylation has also been studied; no evidence of coupling was detected and the highest retention remained unchanged. On the other hand, the improvement of the rejection also observed from the porous membranes after modification. The rejection of C44 in the AMS was reached 75% after modification by ten bilayers of PDDA/PSS, whereas it was only 25% before modification. In the modified PAN, the rejection of the solutes obtained is in the range of 37 to 50%, whereas it was only 3 to 7% by weight before modification. The disadvantage of the porous membrane, however, is the sharp decrease in flux after the deposition of the multiple layers.

Size-selective Transport of Uncharged Solutes Through Multilayer Polyelectrolyte Membranes Xiaoyun Liu, 2003

Solvent Transport Through Nanofiltration Membranes Dario R. Machado, Tekhniyon, Makhon tekhnologi le-Yisra'el. Fakultah le-handasah khimit, 1998

The Analysis of Solute Transport Through Size Selective Membranes Using Polydisperse Dextrans Seiichi Mochizuki, 1992

A Study of Solvent and Macrosolute Transport Mechanisms in Asymmetric Ultrafiltration Membranes Alan S.

Michaels, 1981

Ceramic Membranes Vitaly Gitis, Gadi Rothenberg, 2016-08-22

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