Mathematical modelling of membrane separation

This thesis concerns mathematical modelling of membrane separation. The thesis consists of introductory theory on membrane separation, equations of motion, and properties of dextran, which will be the solute species throughout the thesis. Furthermore, the thesis consist of three separate mathematical models, each with a different approach to membrane separation.

The first model is a statistical model investigating the interplay between solute shape and the probability of entering the membrane. More specific the transition of solute particles from being spherical to becoming more elongated as prolate ellipsoids with the same volume. The porous membrane is assumed isotropic such that the model reduces to a two dimensional model. With this assumption ellipsoids with the same volume reduces to ellipses with the same area. The model finds the probability of entering the pore of the membrane. It is found that the probability of entering the pore is highest when the largest of the radii in the ellipse is equal to half the radius of the pore, in case of molecules with circular radius less than the pore radius. The results are directly related to the macroscopic distribution coefficient and the rejection coefficient.

The second model is a stationary model for the flux of solvent and solute in a hollow fibre membrane. In the model we solve the time independent equations for transport of solvent and solute within the hollow fibre. Furthermore, the flux of solute and solvent through the membrane is coupled through the boundary conditions. The model investigates how the true and observed rejection coefficient depends on the transmembrane pressure, the average inlet velocity, and the molecular weight. Furthermore, the effect of concentration dependent viscosity on the rejection coefficients is investigated. The results show that the true rejection coefficient is increasing as a function of increasing transmembrane pressure, increasing inlet velocity, and decreasing molecular weight. Furthermore, it is found that a concentration dependent viscosity decreases the true rejection. The observed rejection is increasing for decreasing molecular weight and increasing inlet velocities. The observed rejection can be either increasing or decreasing as a function of increasing transmembrane pressure. Moreover, the observed rejection is reduced when the viscosity depends on the concentration. The study is a time dependent model of back-shocking. During back-shocking the pressure difference across the membrane is reversed for a given time. This implies that the concentration polarization at the membrane surface is flushed away. When the pressure is reversed back to normal the membrane performs better resulting in an increased average flux. Two models models of the problem was made.

In a two dimensional model, limited to capture the dynamics close to the membrane, a positive effect was observed on both the observed rejection and the average solvent flux. Furthermore, an analytical upper estimate for the optimal back-shock time is given. In a three dimensional model, where the flow within the entire hollow fibre is modelled, the mentioned upper estimate is used to obtain a positive effect on both the observed rejection and the average solvent flux. Moreover, the effect of a concentration dependent viscosity was investigated. It was found that the average flux compared to the steady-state solution increased when the viscosity depends on the concentration.
This paper concerns mathematical modeling and computational fluid dynamics of back-shocking during hollow fibre ultrafiltration of dextran T500. In this paper we present a mathematical model based on first Principles, i.e., solving the Navier-Stokes equation along with the continuity equation for both the solute and the solvent. We investigate the validity of the estimate on the optimal back-shock time, i.e., the back-shock time needed to achieve the highest permeate flux, published in a previous paper by the authors (Vinther et al., Predicting optimal back-shock times in ultrafiltration hollow fibre membranes, J. Membr. Sci. 470 (2014) 275-293 [33]). Furthermore, the simulations have been performed with two different inlet velocities, i.e., crossflow velocities and are clone with and without a concentration dependent viscosity. This enables us, for the first time, to investigate the effect of different inlet velocities and the effect of a concentration polarization on the observed rejection and the permeate flux, as a function of different back-shock times. In all cases the average permeate flux and the observed rejection during one period of back-shocking were found to be higher than the steady-state values - representing the long time behavior of a similar separation process performed without back-shocking - when using the optimal back-shock time. It is concluded that the estimate of the optimal back-shock time is in good agreement with the optimal time found in the simulations performed in this paper. Furthermore, it is found that the optimal back-shock time increases when the viscosity is allowed to depend on the concentration. It is found that this can be explained by a decrease in the velocity tangential to the membrane due to the increase in viscosity where the concentration is high - resulting in a longer time for the concentration polarization to be convected tangentially along the membrane surface. The ratio between the average flux over a back-shock cycle and the steady-state flux is found to increase with increasing inlet velocity. Furthermore, this ratio increases when the viscosity depends on the concentration. This is due to the relatively lower steady-state value when the viscosity depends on the concentration. Moreover, an increase in observed rejection is found when using back-shocking. The increase in observed rejection is found to be largest when the inlet velocity is high and the viscosity depends on the concentration. (C) 2015 Elsevier B.V. All rights reserved.
Mathematical modelling of dextran filtration through hollow fibre membranes

In this paper we present a mathematical model of an ultrafiltration process. The results of the model are produced using standard numerical techniques with Comsol Multiphysics. The model describes the fluid flow and separation in hollow fibre membranes. The flow of solute and solvent within the hollow fibre is modelled by solving the Navier-Stokes equation along with the continuity equation for both the solute and the solvent. The flux of solute and solvent through the membrane are given by the solution diffusion model, since ultrafiltration occurs at high rejections. For a given set of parameters describing the characteristics of the membrane, effect on the observed and the intrinsic rejection of the membrane are investigated for the different working parameters: inlet velocity, molecular weight, and transmembrane pressure.
Furthermore, the model investigates the effect of a concentration dependent viscosity. The model shows that both the observed and intrinsic rejection increase when the inlet velocity increases. Moreover, the intrinsic rejection increases as a function of transmembrane pressure, but the observed rejection has a characteristic maximum. Therefore, the observed rejection can either increase or decrease as a function of pressure. The influence of a concentration dependent viscosity is to increase the concentration on the membrane surface. This leads to a decrease in both the observed and the intrinsic rejection, when compared to a constant viscosity. For small values of the solute permeability the concentration dependent viscosity decreases the volumetric flux through the membrane at high pressures. This effect is due to a very high concentration at the membrane surface. The model is related to experimental data. There is a good qualitative and a reasonable quantitative agreement between simulations and experimental data.
Predicting optimal back-shock times in ultrafiltration hollow fibre modules through path-lines

This paper presents a two dimensional mathematical model of back-shocking in ultrafiltration. The model investigates the effect of back-shocking on concentration polarization. The model shows a positive effect on both the volumetric flux and the observed rejection when back-shocking is applied as compared to the steady-state solution. Furthermore, the effect of changing different parameters such as inlet velocity, forward and backwards pressure on the back-shock time, the increase in volumetric flux and observed rejection, is presented. Moreover, two analytical estimates for the optimal back-shock time derived from calculating the path-lines during a back-shock cycle are presented. Both of these expressions are in good agreement with the results obtained from the mathematical model and data collected from the literature. Based on this, a simple expression for an optimal back-shock time in a multi-parameter problem is provided.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Mathematics
Pages: 275-293
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Membrane Science
Volume: 470
ISSN (Print): 0376-7388
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.13 SJR 2.062 SNIP 1.72
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2 SNIP 1.771 CiteScore 5.89
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.433 SNIP 1.935 CiteScore 5.42
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.452 SNIP 2.001 CiteScore 5.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Mathematical modeling of the hypothalamic-pituitary-adrenal gland (HPA) axis, including hippocampal mechanisms

This paper presents a mathematical model of the HPA axis. The HPA axis consists of the hypothalamus, the pituitary and the adrenal glands in which the three hormones CRH, ACTH and cortisol interact through receptor dynamics. Furthermore, it has been suggested that receptors in the hippocampus have an influence on the axis. A model is presented with three coupled, non-linear differential equations, with the hormones CRH, ACTH and cortisol as variables. The model includes the known features of the HPA axis, and includes the effects from the hippocampus through its impact on CRH in the hypothalamus. The model is investigated both analytically and numerically for oscillating solutions, related to the ultradian rhythm seen in data, and for multiple fixed points related to hypercortisolemic and hypocortisolemic depression. The existence of an attracting trapping region guarantees that solution curves stay non-negative and bounded, which can be interpreted as a mathematical formulation of homeostasis. No oscillating solutions are present when using physiologically reasonable parameter values. This indicates that the ultradian rhythm originate from different mechanisms. Using physiologically reasonable parameters, the system has a unique fixed point, and the system is globally stable. Therefore, solutions converge to the fixed point for all initial conditions. This is in agreement with cortisol levels returning to normal, after periods of mild stress, in healthy individuals. Perturbing parameters lead to a bifurcation, where two additional fixed points emerge. Thus, the system changes from having a unique stable fixed point into having three fixed points. Of the three fixed points, two are stable and one is unstable. Further investigations show that solutions converge to one of the two stable fixed points depending on the initial conditions. This could explain why healthy people becoming depressed usually fall into one of two groups: a hypercortisolemic depressive group or a hypocortisolemic depressive group.
Statistical modelling of the interplay between solute shape and rejection in porous membranes

The structural conformation of complex molecules, e.g., polymers and proteins, is determined by several factors like composition of the basic structural units, charge, and properties of the surrounding solvent. In absence of any chemical or physical interaction solute–solute and/or solute–membrane, it can be expected that the possibility for a solute particle to enter the membrane pore will only depend upon the relation between such molecular conformation and pore size. The objective of the present study is to use geometric and statistical modelling to determine the effect of particle elongation – from spherical to being increasingly prolate ellipsoidal – on the possibility of entering the pore, and, in turn, on the macroscopic distribution coefficient, $K$, and overall retention during filtration. The model showed that the value of $K$ was maximal when the longer of the radii in the prolate ellipsoid was approximately equal to the radius of the pores, in case the spherical size of the particle was smaller than the membrane pore. Furthermore, for spherical particles larger than the pore, such a maximum was found to occur after the smaller of the radii was smaller than the pore radius. Either for spherical particles bigger or smaller than the pore radius, $K$ was monotonically decreasing towards zero as the particles became more elongated. When relating the values of $K$ to the friction model, the maximal rejection coefficient was found to reach a characteristic minimum when changing shape. The results suggested that the retention during porous membrane filtration can be manipulated when working with solute particles prone to alter conformation via, e.g., adding proper functional groups to the molecule, or modifying charge density/distribution by varying pH.

General information
State: Published
Organisations: Department of Mathematics, Applied functional analysis, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Dynamical systems, Computer Aided Process Engineering Center, Membrane Technology group
Authors: Vinther, F. (Intern), Pinelo, M. (Intern), Brøns, M. (Intern), Jonsson, G. (Intern), Meyer, A. S. (Intern)
Pages: 261-269
Publication date: 2012
Main Research Area: Technical/natural sciences

Publication information
Journal: Separation and Purification Technology
Volume: 89
ISSN (Print): 1383-5866
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.78 SJR 1.023 SNIP 1.394
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.078 SNIP 1.504 CiteScore 3.75
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.257 SNIP 1.54 CiteScore 3.5
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.325 SNIP 1.678 CiteScore 3.62
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.409 SNIP 1.732 CiteScore 3.2
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.35 SNIP 1.64 CiteScore 3.48
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
The minimal model of the hypothalamic–pituitary–adrenal axis

This paper concerns ODE modeling of the hypothalamic–pituitary–adrenal axis (HPA axis) using an analytical and numerical approach, combined with biological knowledge regarding physiological mechanisms and parameters. The three hormones, CRH, ACTH, and cortisol, which interact in the HPA axis are modeled as a system of three coupled, nonlinear differential equations. Experimental data shows the circadian as well as the ultradian rhythm. This paper focuses on the ultradian rhythm. The ultradian rhythm can mathematically be explained by oscillating solutions. Oscillating solutions to an ODE emerges from an unstable fixed point with complex eigenvalues with a positive real parts and a non-zero imaginary parts. The first part of the paper describes the general considerations to be obeyed for a mathematical model of the HPA axis. In this paper we only include the most widely accepted mechanisms that influence the dynamics of the HPA axis, i.e. a negative feedback from cortisol on CRH and ACTH. Therefore we term our model the minimal model. The minimal model, encompasses a wide class of different realizations, obeying only a few physiologically reasonable demands. The results include the existence of a trapping region guaranteeing that concentrations do not become negative or tend to infinity. Furthermore, this treatment guarantees the existence of a unique fixed point. A change in local stability of the fixed point, from stable to unstable, implies a Hopf bifurcation; thereby, oscillating solutions may emerge from the model. Sufficient criteria for local stability of the fixed point, and an easily applicable sufficient criteria guaranteeing global stability of the fixed point, is formulated. If the latter is fulfilled, ultradian rhythm is an impossible outcome of the minimal model and all realizations thereof. The second part of the paper concerns a specific realization of the minimal model in which feedback functions are built explicitly using receptor dynamics. Using physiologically reasonable parameter values, along with the results of the general case, it is demonstrated that un-physiological values of the parameters are needed in order to achieve local instability of the fixed point. Small changes in physiologically relevant parameters cause the system to be globally stable using the analytical criteria. All simulations show a globally stable fixed point, ruling out periodic solutions even when an investigation of the ‘worst case parameters’ is performed.

General information
State: Published
Organisations: Roskilde Universitet
Authors: Vinther, F. (Intern), Andersen, M. (Ekstern), Ottesen, J. T. (Forskerdatabase)
Pages: 663-690
Publication date: 2011
Main Research Area: Technical/natural sciences
Matematisk modellering af membranseparation

Department of Informatics and Mathematical Modeling
Period: 01/04/2010 → 20/03/2014
Number of participants: 7
Phd Student:
Vinther, Frank (Intern)
Supervisor:
Meyer, Anne S. (Intern)
Sørensen, Mads Peter (Intern)
Main Supervisor:
Brøns, Morten (Intern)
Examiner:
Hassager, Ole (Intern)
Davis, Robert H. (Ekstern)
Jönsson, Ann-Sofi (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD