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MATHEMATICAL MODELING AND SIMULATION OF FLOW IN
DOMAINS SEPARATED BY LEAKY SEMIPERMEABLE
MEMBRANE INCLUDING OSMOTIC EFFECT*

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Dedicated to Professor K. R. Rajagopal on the occasion of his 60th birthday

Abstract. In this paper, we propose a mathematical model for flow and transport processes of diluted solutions in domains separated by a leaky semipermeable membrane. We formulate transmission conditions for the flow and the solute concentration across the membrane which take into account the property of the membrane to partly reject the solute, the accumulation of rejected solute at the membrane, and the influence of the solute concentration on the volume flow, known as osmotic effect.

The model is solved numerically for the situation of a domain in two dimensions, consisting of two subdomains separated by a rigid fixed membrane. The numerical results for different values of the material parameters and different computational settings are compared.

Keywords: leaky semipermeable membrane, osmotic pressure, transmission conditions, finite element method

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1. INTRODUCTION

Membranes play an important role in many applications. For example, biological membranes act as selective barriers between or around living cells, artificial mem-

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branes are used for separation purposes in laboratory or in industry, like in dialysis, water purification, seawater desalinization or removing of microorganisms from dairy products. In this paper, we consider the flow of a volume (solvent) and a solute in domains separated by a leaky semipermeable membrane which is modeled as an interface allowing the solvent to go through, but reflects a high amount of the solute. We consider the solution to be diluted, i.e. the mass concentration of the solute is low, and thus, we assume that the solute concentration does not influence the solvent density.

The most commonly used driving forces of the flow through a semipermeable membrane are pressure and concentration gradients. This process is known as filtration, and in literature, see e.g. Kedem and Katchalsky [4], Patlak et al. [7], Cheng [1], Kocherginsky [5], is described by two equations, one for the solute flux and one for the volume flux. They involve three parameters which model the membrane properties: the filtration coefficient or hydraulic conductivity of the membrane, the solute reflection coefficient (describing the property of the membrane to partly reject the solute), and the solute permeability of the membrane. Although general, this approach describing the total volume fluxes through the membrane is limited due to the fact that the effects of the processes considered are taken in average. This might be sufficient, e.g. for experimental needs, however, if we want to model the flow of the solvent and the transport of concentration in domains separated by a membrane, we need suitable transmission conditions at the membrane which lead to well posed models. In the case of reaction-diffusion processes in domains separated by a membrane, effective transmission conditions were derived in Neuss-Radu and Jäger [6] by means of multi-scale techniques, starting from a microscopic model of the processes in the membrane, and letting the scale parameter (ratio between the thickness of the membrane and the dimension of the domain) tending to zero. The flow of miscible mixtures through a membrane could be also studied in the context of the theory of mixtures, see e.g. Rajagopal and Wineman [8], and Tao et al. [10]. In this context, the processes inside the membrane are resolved starting from the balance of mass, momentum and energy. However, this approach has its own difficulties, namely the specification of boundary conditions.

In this paper, we propose a mathematical model for flow and transport processes in domains separated by a leaky semipermeable membrane. The model is formulated on the macroscopic scale: the membrane is a fixed and rigid interface, separating the flow domains. Thus, the processes inside the membrane are not resolved, however, their effective contributions are included phenomenologically in the transmission conditions. We consider the membrane to be symmetric, i.e. the transmission properties of the membrane from both sides are the same.

The model presented here takes into account the free flow of the solvent through the membrane, the accumulation of the rejected solute in the neighborhood of the

membrane, and the formation of the concentration polarization layer, as well as the influences of the solute concentration on the volume flow, via the osmotic effect.

The transmission conditions at the membrane for the solvent consist in continuity of the normal component of the solvent velocity, while the tangent component is set to zero, and continuity of normal stresses. The vanishing of the tangential component corresponds to no-slip in the tangential direction on the membrane. Other conditions, like the partial slip condition in the tangential direction, see Hron et al. [5], could also be imposed. In our model, the osmotic pressure is considered to be a component of the fluid stress at the membrane. The transmission conditions for the solvent velocity do not include the effects of the curvature of the membrane on the flow of the solvent. However, a quantitative description of the curvature effects is up to now an open question.

For the solute concentration, the transmission conditions consist in the continuity of the normal fluxes, and the requirement that just a fraction of the convective flux permeates through the membrane. The accumulation of the reflected solute at the membrane leads to jumps in the solute concentration across the membrane.

The model is introduced gradually starting with the formulation of the equations for the fluid flow and the transport of the solute in the bulk, together with the transmission conditions for the situation when the osmotic effect is neglected. Thus, the process of concentration buffering is modeled first, see Section 2 and Section 3. In Section 4, the general model including the osmotic effect is formulated. Via the osmotic pressure, which is a function of solute concentration, the flow equations for the solvent are also coupled with the transport equation for the solute, yielding a fully coupled model. In Section 5, the method used for the computation of the numerical solution is described, while in Section 6 the numerical simulations are presented. The simulations are done for several values of the system's parameters: different values for the membrane reflection coefficient, different functions for the inlet pressure, as well as different dependencies of the osmotic pressure on the solute concentration are considered. A comparison of the full model and the model without osmotic effect yields the following important conclusion: in the case when the osmotic pressure is included, the pressure difference across the bulk domain is reduced as the osmotic pressure of the reflected solvent concentration increases, leading to a decline in the permeate solvent flux through the membrane. This is in agreement with literature, e.g. Cheng [1].

2. FORMULATION OF THE EQUATIONS IN THE BULK DOMAINS

The mathematical model for the processes in the bulk domains consists of the Navier-Stokes equations describing the flow of the diluted solution, together with the convection-diffusion equation modeling the solute transport. This system of governing equations takes the form

$$(2.1) \quad \operatorname{div} \mathbf{v} = 0,$$

$$(2.2) \quad \varrho \frac{\partial \mathbf{v}}{\partial t} + \varrho [\operatorname{grad} \mathbf{v}] \mathbf{v} = -\operatorname{grad} p + 2 \operatorname{div}(\mu \mathbf{D}),$$

$$(2.3) \quad \frac{\partial c}{\partial t} + (\operatorname{grad} c) \cdot \mathbf{v} = \operatorname{div}(D_c \operatorname{grad} c),$$

where \mathbf{v} is the velocity vector of the solvent, p the hydrodynamical pressure, c the concentration of the solute and \mathbf{D} the symmetric part of the velocity gradient, $\mathbf{D} = \frac{1}{2}(\operatorname{grad} \mathbf{v} + (\operatorname{grad} \mathbf{v})^T)$. The solution parameters: ϱ the density, μ the kinematic viscosity and D_c the diffusivity are considered to be constant as we want to primarily model the effects of the transport through the membrane.

We recast the equations (2.1)–(2.3) to non-dimensional variables, defined by

$$(2.4) \quad \mathbf{X} = \frac{\mathbf{x}}{L^*}, \quad \mathbf{V} = \frac{\mathbf{v}}{V^*}, \quad C = \frac{c}{C^*}, \quad P = \frac{p}{P^*},$$

where L^* and V^* are the characteristic length and velocity, respectively. The non-dimensionalized concentration C takes values between $(0, 1)$. Since diluted solutions are considered, the values of C should be small, below 0.05. For consistency, we choose

$$(2.5) \quad P^* = \varrho(V^*)^2.$$

From now on, for simplicity of notation, we use instead of capitals the small letters for the non-dimensional variables. Thus, the system of the governing equations is transformed to

$$(2.6) \quad \operatorname{div} \mathbf{v} = 0,$$

$$(2.7) \quad \frac{\partial \mathbf{v}}{\partial t} + [\operatorname{grad} \mathbf{v}] \mathbf{v} = -\operatorname{grad} p + \frac{2}{\operatorname{Re}} \operatorname{div}(\mathbf{D}),$$

$$(2.8) \quad \frac{\partial c}{\partial t} + (\operatorname{grad} c) \cdot \mathbf{v} = \frac{1}{\operatorname{Pe}} \operatorname{div}(\operatorname{grad} c),$$

with standard notation for the Reynolds number $\operatorname{Re} = \varrho L^* V^* / \mu$, and the Péclet number $\operatorname{Pe} = L^* V^* / D_c$.

The system of governing equations (2.6)–(2.8) has to be complemented with initial conditions, boundary conditions at the outer boundaries, and transmission conditions at the separating membrane. As already pointed out in the introduction, the complex processes inside the membrane will not be resolved. The membrane is modeled as a fixed and rigid interface separating the bulk regions.

In the formulation of the transmission conditions across the membrane, the following aspects have been taken into account: first, the separating properties of the membrane with respect to the solvent, which lead to the buffering of solute concentration at the membrane, and second, connected with the first aspect, the influence of the concentration accumulation on the volume flow, known as the osmotic effect. Our model has features similar to other models existing in literature, see e.g. Kedem and Katchalsky [4]. However, the important difference is that we do not formulate equations only for the total volume fluxes across the membrane, as is done in the existing literature, but we give transmission conditions, which can be used to describe the influence of the membrane on the processes in the bulk regions.

The transmission conditions across the membrane will be formulated in the next two sections. However, let us remark already at this stage that due to the osmotic effect induced by the presence of the membrane, the final model will be a fully nonlinear coupled system.

3. MODELING OF CONCENTRATION BUFFERING

In this section we discuss and model the effect of the concentration buffering at the leaky semipermeable membrane which is characteristic e.g. for diluted polymeric solutions with relatively small diffusivity (high Péclet number).

The effect of concentration buffering (sometimes called the concentration polarization) is caused by the free transport of the solvent through the membrane while the solute carried by the solvent to the membrane is partially reflected by the membrane and consequently accumulated in front of it.

First, we consider the 1D stationary case, where we can find the analytic solution of the system. Next, we generalize the model to 2D.

3.1. 1D model

For the stationary case in 1D, due to the incompressibility of the fluid, the system of the N-S equations provides a unique constant solution of the velocity, which we denote by u . The governing equation for the concentration reduces to an ordinary differential equation where the known constant velocity u enters. Our domain of interest is the interval $\langle -1, 1 \rangle$ and we place the membrane at position $x = 0$. The

solvent can go through the membrane freely, thus the velocity remains constant in the whole domain. We set the solvent velocity in the direction of the positive axis.

We denote by c^- the concentration on the interval $\langle -1, 0 \rangle$, and by c^+ the concentration on the interval $\langle 0, 1 \rangle$, see Fig. 3.1. The governing model for concentrations c^- and c^+ is given by

$$(3.1) \quad \begin{aligned} -1 \leq x \leq 0 & & 0 \leq x \leq 1 \\ -D_c \frac{d^2 c^-}{dx^2} + u \frac{dc^-}{dx} = 0, & & -D_c \frac{d^2 c^+}{dx^2} + u \frac{dc^+}{dx} = 0, \end{aligned}$$

$$(3.2) \quad \begin{aligned} c^-(-1) = c_{\text{in}}, & & -D_c \frac{dc^+}{dx}(1) = 0, \end{aligned}$$

$$(3.3) \quad -D_c \frac{dc^-}{dx}(0) + \sigma u c^-(0) = 0, \quad -D_c \frac{dc^-}{dx}(0) + u c^+(0) = u(1 - \sigma) c^-(0),$$

where σ is called the membrane reflection coefficient and describes the property of the membrane to be leaky semipermeable. More precisely, the parameter σ takes the values between 0 and 1, and it specifies the fraction of the convective flux of the solute molecules which is reflected back by the membrane. Accordingly, $(1 - \sigma)$ specifies the fraction being allowed to pass through the membrane. The ideal semipermeable membrane (i.e. a membrane that perfectly separates solute from solvent) would be then described by the reflection coefficient $\sigma = 1$.

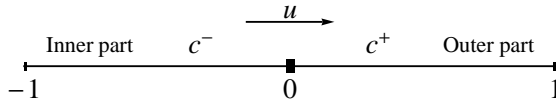


Figure 3.1. 1D description of membrane surroundings. Membrane is placed at point $x = 0$.

The conditions for concentrations on the membrane imply the natural assumption on the continuity of the solute fluxes $D_c(dc^-/dx)(0) - u c^-(0) = D_c(dc^+/dx) - u c^+(0)$ across the membrane. The membrane condition for c^- means that the σ fraction of the convective flux is reflected back, and that there is no fraction of diffusive flux through the membrane.

The analytic solution of system (3.1)–(3.3) is

$$(3.4) \quad c^-(x) = -\frac{c_{\text{in}}(1 - \sigma + \sigma e^{x u/D_c})}{-1 + \sigma - \sigma e^{-u/D_c}}, \quad c^+(x) = -\frac{c_{\text{in}}(1 - \sigma)}{-1 + \sigma - \sigma e^{-u/D_c}}.$$

The plotted solutions for different parameter values are given in Fig. 3.2. We mention the formation of the concentration polarization layer, and the discontinuity in the solute concentration at the membrane. As one can see, the influence of velocity and diffusivity on the concentration polarization layer are of a similar effect: with

higher velocity and lower diffusivity the boundary layer is more distinguishable and steeper. This behavior qualitatively agrees with the experimental results found for example in Scott et al. [9]. In the next subsection, the transmission conditions for the concentration at the membrane are generalized to higher dimensional setting.

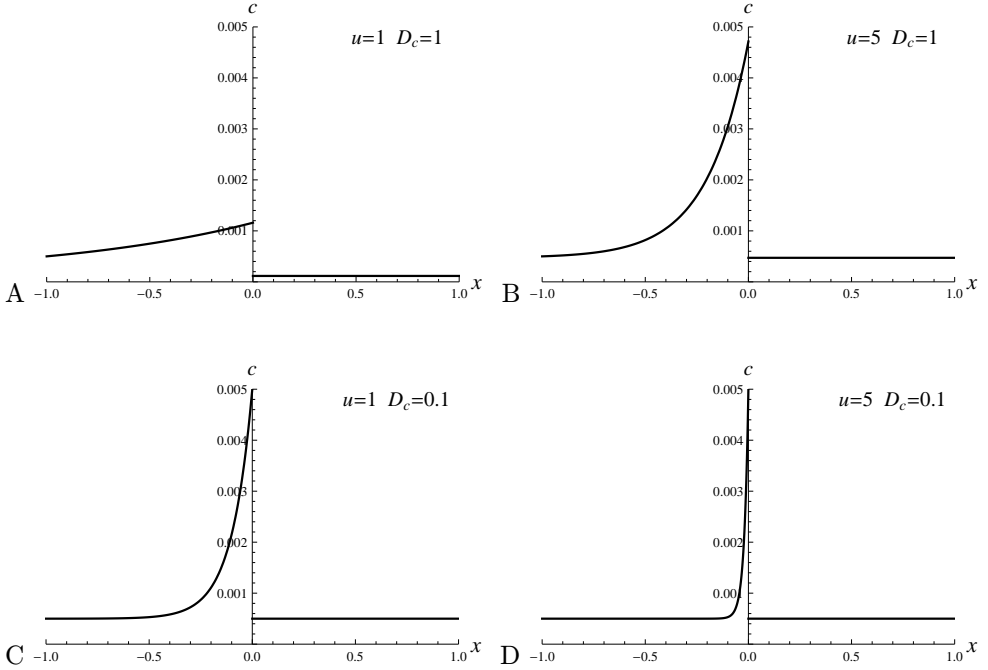


Figure 3.2. Concentration profiles for $c_{\text{in}} = 5 \times 10^{-4}$ and $\sigma = 0.9$. Four plots for different velocity and diffusivity setting: A) $u = 1$, $D_c = 1$, B) $u = 5$, $D_c = 1$, C) $u = 1$, $D_c = 0.1$, D) $u = 5$, $D_c = 0.1$.

3.2. Generalization of the transmission conditions to higher dimensions

We consider a domain Ω consisting of two subdomains Ω^+ and Ω^- in \mathbb{R}^n separated by an interface Γ_m representing the membrane, see the 2-dimensional situation in Fig. 3.3. Thus we have

$$\Omega = \Omega^+ \cup \Gamma_m \cup \Omega^-.$$

The restrictions of functions defined on Ω to the subdomains Ω^+ and Ω^- are denoted by the superscripts $+$ and $-$, respectively.

The transmission conditions for the solvent flow at the membrane now consist of the continuity of the normal component of the velocity, the no-slip condition in the tangential direction with the respect to the membrane interface, and of the continuity

of normal stresses

$$(3.5) \quad \mathbf{v}^+ \cdot \boldsymbol{\tau} = -\mathbf{v}^- \cdot \boldsymbol{\tau} = 0, \quad \mathbf{v}^+ \cdot \mathbf{n}^+ = -\mathbf{v}^- \cdot \mathbf{n}^- = \mathbf{v} \cdot \mathbf{n}^+,$$

$$(3.6) \quad [-(p^- - p^+)I + \frac{2}{\text{Re}}(\mathbf{D}^- - \mathbf{D}^+)]\mathbf{n}^- = 0\mathbf{n}^-,$$

where \mathbf{n}^+ , \mathbf{n}^- are the outer unit normal vectors on Γ_m with respect to the domains Ω^+ , Ω^- , and $\boldsymbol{\tau}$ is the tangential unit vector satisfying $\mathbf{n}^+ \cdot \boldsymbol{\tau} = \mathbf{n}^- \cdot \boldsymbol{\tau} = 0$.



Figure 3.3. 2D computational domain with dimensions $\langle -5, 5 \rangle \times \langle 0, 1 \rangle$; boundaries Γ_1 and Γ_3 are impermeable walls, Γ_4 is the inlet and Γ_2 is the outlet. Γ_m is the inner boundary representing the zero-thickness membrane.

Concerning the transmission conditions for the solute concentration, we require continuity of the normal fluxes across the membrane, and the condition modeling the partial reflection of the solute at the membrane. If we assume that the velocity \mathbf{v} satisfies $\mathbf{v} \cdot \mathbf{n}^- \geq 0$, then these conditions have the form

$$(3.7) \quad -\frac{1}{\text{Pe}} \text{grad } c^- \cdot \mathbf{n}^- + \sigma c^- \mathbf{v} \cdot \mathbf{n}^- = 0,$$

$$-\frac{1}{\text{Pe}} \text{grad } c^+ \cdot \mathbf{n}^+ + c^+ \mathbf{v} \cdot \mathbf{n}^+ = -(1 - \sigma) c^- \mathbf{v} \cdot \mathbf{n}^-.$$

The main disadvantage of this formulation is the directional dependence of the conditions for the concentration. Since the buffering occurs in the case of outflow while in the case of inflow the washout of concentration from the membrane is observed, we have to know explicitly the direction of the flow. One of the possible generalizations of the transmission conditions for concentration (3.7), assuming symmetric properties of the membrane from both sides, is

$$(3.8) \quad \frac{1}{\text{Pe}} \text{grad } c^- \cdot \mathbf{n}^- = (\sigma c^-) \mathbf{v} \cdot \mathbf{n}^- + (1 - \sigma)(c^- - c^+) \min(0, \mathbf{v} \cdot \mathbf{n}^-),$$

$$\frac{1}{\text{Pe}} \text{grad } c^+ \cdot \mathbf{n}^+ = (\sigma c^+) \mathbf{v} \cdot \mathbf{n}^+ + (1 - \sigma)(c^+ - c^-) \min(0, \mathbf{v} \cdot \mathbf{n}^+).$$

It is easy to see that (3.8) reduces to (3.7) if $\mathbf{v} \cdot \mathbf{n}^- \geq 0$, and on the other hand, for the case $\mathbf{v} \cdot \mathbf{n}^- \leq 0$ we obtain an analogous condition for the outflow in the opposite direction.

The complete model for higher dimensions thus consists of the equations (2.1)–(2.3), together with the boundary conditions at the outer boundary, and the transmission conditions (3.5), (3.6), and (3.8).

For the numerical simulation of the concentration buffering in two dimensions, we use the following computational setting. We consider the domain from Fig. 3.3, with the fixed and rigid membrane Γ_m . The domain Ω^- on the left side of the membrane is prolonged, since there the most interesting accumulation of concentration occurs. We assume the pressure driven flow, where the fluid of a given concentration enters the channel on the boundary Γ_4 , and the filtrate leaves the channel on the boundary Γ_2 . The walls of the channels Γ_1 and Γ_3 are impermeable for both the concentration and the velocity. The form of the boundary conditions at the outer boundaries is

$$(3.9) \quad \Gamma_4: \left[-p\mathbf{I} + 2\frac{1}{\text{Re}}\mathbf{D} \right] \mathbf{n} = -p_{\text{in}}\mathbf{n}, \quad c = c_{\text{in}},$$

$$(3.10) \quad \Gamma_1, \Gamma_3: \mathbf{v} = \mathbf{0}, \quad \left(\frac{1}{\text{Pe}} \text{grad } c + c\mathbf{v} \right) \cdot \mathbf{n} = 0,$$

$$(3.11) \quad \Gamma_2: \left[-p\mathbf{I} + 2\frac{1}{\text{Re}}\mathbf{D} \right] \mathbf{n} = 0\mathbf{n}, \quad \frac{1}{\text{Pe}} \text{grad } c \cdot \mathbf{n} = 0,$$

where c_{in} is a constant inlet concentration and p_{in} is a constant or a periodical function of time. The transmission conditions on the membrane are (3.5), (3.6), and (3.8). Since we solve the time-dependent problem, we specify the initial conditions as a rest state ($\mathbf{v} = 0$ and $c = 0$).

The computational results are shown in Section 6.

4. EXTENSION OF THE MODEL BY OSMOTIC EFFECT

In this section, we take into account the effect of the solute concentration on the volume flow, via the osmotic pressure. In literature on filtration problems, this effect is included in the transmembrane volume flux, see e.g. Kedem and Katchalsky [4] where the following formula is derived from thermodynamical considerations:

$$(4.1) \quad J_v = L_p(\Delta p - \sigma\Delta\pi).$$

Here, L_p is the filtration coefficient or hydraulic conductivity, Δp is the pressure difference across the membrane and $\Delta\pi$ is the difference in osmotic pressures across the membrane $\Delta\pi = \pi(c^+) - \pi(c^-)$.

In our approach, the osmotic pressure $\pi(c)$ is included in the normal stresses of the fluid at the membrane. Thus, the transmission conditions for the flow have the

form

$$(4.2) \quad \mathbf{v}^+ \cdot \boldsymbol{\tau} = -\mathbf{v}^- \cdot \boldsymbol{\tau} = 0, \quad \mathbf{v}^+ \cdot \mathbf{n}^+ = -\mathbf{v}^- \cdot \mathbf{n}^- = \mathbf{v} \cdot \mathbf{n}^+,$$

$$(4.3) \quad \left[-(p^- - p^+) \mathbf{I} + 2 \frac{1}{\text{Re}} (\mathbf{D}^- - \mathbf{D}^+) \right] \mathbf{n}^- = -(\pi(c^-) - \pi(c^+)) \mathbf{n}^-.$$

For the osmotic pressure of the solution, we use the representation

$$(4.4) \quad \pi(c) = P_1 c + P_2 c^2,$$

where P_1 and P_2 are constants, see e.g. Cheng [1] and Coleman et al. [2].

The complete model describing the filtration problem in the domain Ω containing the membrane Γ_m thus consists of the equations (2.1)–(2.3) on the subdomains Ω^+ , and Ω^- , together with the boundary conditions (3.9)–(3.11) at the outer boundary, the transmission conditions (3.8) for the solute concentration, and the transmission conditions (4.2), (4.3) for the flow. As one can see, the equations for the flow and the transport equation for the solvent are now fully coupled via the transmission condition (4.3).

For numerical simulations of the model including the osmotic effect, we consider the setting from Subsection 3.2. The results are compared for the transmission model without and with the osmotic pressure effect in Section 6.

5. NUMERICAL METHOD

We use the standard Galerkin finite element method to solve the PDE system consisting of equations (2.6)–(2.8) on the domain introduced in Fig. 3.3 and of boundary conditions (3.9)–(3.11). The standard weak formulation of the system is derived separately on the two subdomains Ω^+ and Ω^- , where the coupling between them is provided through the requirement of continuous velocity on the membrane and the transmission conditions (4.3) and (3.8).

The time discretization is done by the Crank-Nicholson scheme. The discretization in space is done by the finite element method. By \mathcal{T}_h we denote a set of quadrilaterals covering our domain Ω . We assume that \mathcal{T}_h is regular in the usual sense and the membrane Γ_m coincides with the edges of the mesh. Since the fluid is incompressible, we have to choose a pair of finite element spaces known to be stable for problems with the incompressibility constraint. One possible choice is the conforming biquadratic/discontinuous linear approximation pair Q_2/P_1^{disc} .

While the velocity is required to be continuous on the membrane and can be approximated by globally continuous functions, the concentration is allowed to be discontinuous on the membrane and thus has to be splitted into two continuous

variables c^+ and c^- defined on Ω^+ and Ω^- , respectively. The global concentration variable is defined as

$$(5.1) \quad c(\mathbf{x}) = \begin{cases} c^+(\mathbf{x}) & \text{if } \mathbf{x} \in \Omega^+, \\ c^-(\mathbf{x}) & \text{if } \mathbf{x} \in \Omega^-. \end{cases}$$

The concentrations c^+ , c^- can be approximated by either Q_2 or Q_1 finite element spaces.

The spaces for the unknowns $(\mathbf{v}, p, c) \in (V, P, C)$ are approximated in the case of the $Q_2, P_1^{\text{disc}}, Q_2$ finite elements as

$$(5.2) \quad V_h = \{\mathbf{v}_h \in [C(\Omega)]^2, \mathbf{v}_h|_T \in [Q_2(T)]^2 \forall T \in \mathcal{T}_h, \mathbf{v}_h = \mathbf{0} \text{ on } \Gamma_1\},$$

$$(5.3) \quad P_h = \{p_h \in L^2(\Omega), p_h|_T \in P_1(T) \forall T \in \mathcal{T}_h\},$$

$$(5.4) \quad C_h = \{c_h \in C(\Omega^+) \cup C(\Omega^-), c_h|_T \in Q_2(T) \forall T \in \mathcal{T}_h\}.$$

Let us denote by \mathbf{v}_h^n the approximation of $\mathbf{v}(t^n)$, by c_h^n the approximation of $c(t^n)$, and by p_h^n the approximation of $p(t^n)$.

The nonlinear discrete system can be written in the form

$$(5.5) \quad \begin{aligned} \left(\mathbf{M}_v + \frac{\tau}{2}\mathbf{A}_v(\mathbf{v}_h^{n+1})\right)\mathbf{v}_h^{n+1} + \tau\mathbf{B}^T p_h^{n+1} &= F(\mathbf{v}_h^n, c_h^n, c_h^{n+1}), \\ \mathbf{B}\mathbf{v}_h^{n+1} &= 0, \\ \left(\mathbf{M}_c + \frac{\tau}{2}\mathbf{A}_c(\mathbf{v}_h^{n+1})\right)c_h^{n+1} &= G(\mathbf{v}_h^n, c_h^n, \mathbf{v}_h^{n+1}, c_h^{n+1}) \end{aligned}$$

where \mathbf{M}_v and \mathbf{M}_c represent the corresponding mass matrices, \mathbf{B} is the discrete divergence operator, $\mathbf{A}_v(\mathbf{v}_h)$ and $\mathbf{A}_c(\mathbf{v}_h)$ are the operators representing the convection and diffusion parts of the corresponding equations and F, G are the remaining terms coming from the previous time level and from the boundary conditions. This can be written still in a more compact way as

$$(5.6) \quad \mathcal{F}(\mathbf{X}) = 0,$$

where $\mathbf{X} = (\mathbf{v}_h^{n+1}, p_h^{n+1}, c_h^{n+1})$ is the unknown vector in the time step n . The system (5.6) is solved using the quasi-Newton iteration method of the form

$$(5.7) \quad \mathbf{X}^{k+1} = \mathbf{X}^k - \omega^k \left[\frac{\partial \mathcal{F}}{\partial \mathbf{X}}(\mathbf{X}^k) \right]^{-1} \mathcal{F}(\mathbf{X}^k),$$

where the parameter $\omega^k \in [0, 1]$ is the damping factor improving the convergence of the quasi-Newton method.

The block structure of the Jacobian matrix $\partial\mathcal{F}/\partial\mathbf{X}$ is

$$(5.8) \quad \frac{\partial\mathcal{F}}{\partial\mathbf{X}}(\mathbf{X}) = \begin{pmatrix} \square & \square & \square \\ \square & 0 & 0 \\ \square & 0 & \square \end{pmatrix},$$

and the matrix is approximated by finite differences from the residual vector $\mathcal{F}(\mathbf{X})$

$$(5.9) \quad \left[\frac{\partial\mathcal{F}}{\partial\mathbf{X}}\right]_{ij}(\mathbf{X}) \approx \frac{[\mathcal{F}]_i(\mathbf{X} + \varepsilon\mathbf{e}_j) - [\mathcal{F}]_i(\mathbf{X} - \varepsilon\mathbf{e}_j)}{2\varepsilon},$$

where \mathbf{e}_j are the unit basis vectors in \mathbb{R}^d .

One iteration of the used method can be summarized in the following steps:

1. Let \mathbf{X}^n be a starting guess.
2. Set the residuum vector $\mathbf{R}^n = \mathcal{F}(\mathbf{X}^n)$ and the Jacobian matrix

$$\mathbf{A} = \frac{\partial\mathcal{F}}{\partial\mathbf{X}}(\mathbf{X}^n).$$

3. Solve for the correction δ :

$$\mathbf{A}\delta = \mathbf{R}^n.$$

4. Find the optimal step length ω .
5. Update the solution $\mathbf{X}^{n+1} = \mathbf{X}^n - \omega\delta$.

This numerical approach works well for moderate values of Reynolds and Péclet numbers, which is our case. For high values of Reynolds or Péclet number, i.e. the convection dominated problem, one would have to modify the discretization by including some suitable stabilization terms.

6. NUMERICAL SIMULATIONS

Numerical solutions of the model are computed for the computational setting described in Subsection 3.2 for Reynold's number $\text{Re} = 1$ and Péclet number $\text{Pe} = 100$. In each set of plots, we compare the model without the osmotic effect with the full transmission model. Hereby, we consider linear or quadratic osmotic pressure dependence on concentration, and two different values of the reflection coefficient σ . The following physical quantities are plotted:

- the distribution of solute concentration in the domain Ω , see Fig. 6.1,
- the values of the hydrodynamical pressure on the central cut-line $\langle -5, 5 \rangle \times [0, 0.5]$, see Fig. 6.2,

- the time evolution of the concentration, pressure, and the total flux, at the middle point of the membrane $[0, 0.5]$, see Figs. 6.3–6.6.

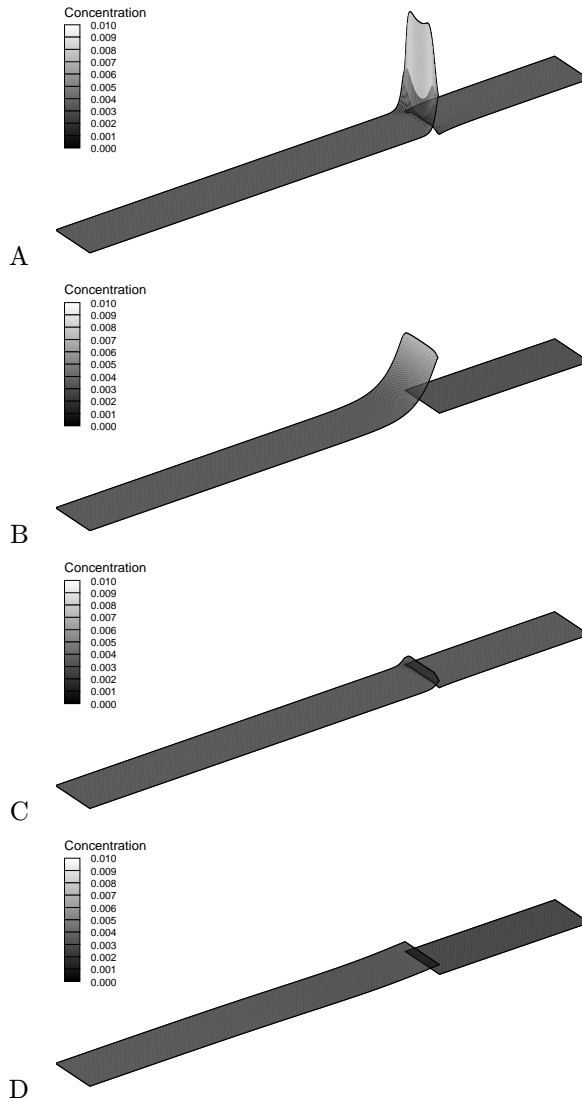


Figure 6.1. Concentration distribution at steady state. Four plots for different parameter settings; without osmotic pressure: A) $\sigma = 0.9$, $P_1 = P_2 = 0$; with osmotic pressure: B) $\sigma = 0.9$, $P_2 = 0$, C) $\sigma = 0.5$, $P_2 = 0$, D) $\sigma = 0.9$, $P_2 = 5 \cdot P_1$.

Fig. 6.1 presents the steady state of the concentration distribution in the whole domain. As one can see, the shape of the concentration layer strongly differs. In the case of simulation without inclusion of osmotic pressure (case A), the concentration

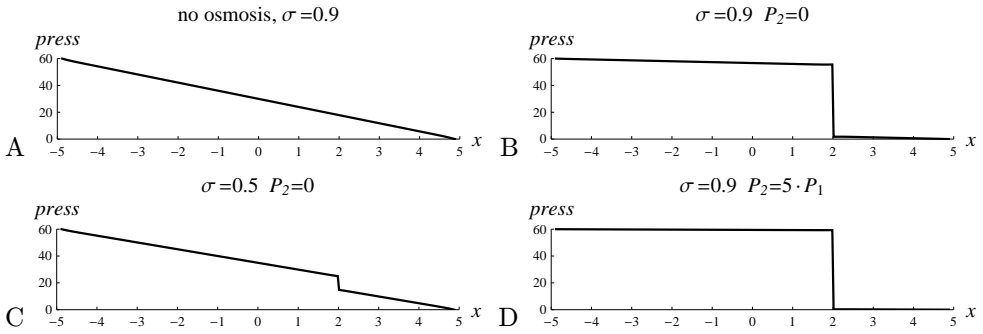


Figure 6.2. Hydrodynamic pressure on centerline at steady state. Four plots for different parameter settings; without osmotic pressure: A) $\sigma = 0.9$, $P_1 = P_2 = 0$; with osmotic pressure: B) $\sigma = 0.9$, $P_2 = 0$, C) $\sigma = 0.5$, $P_2 = 0$, D) $\sigma = 0.9$, $P_2 = 5 \cdot P_1$.

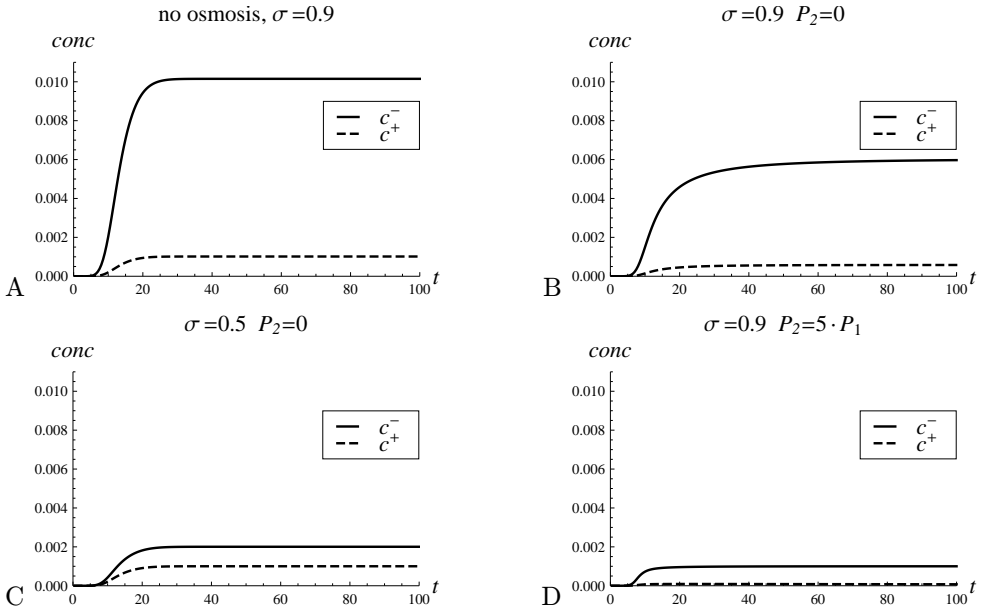


Figure 6.3. Time evolution of concentration at midpoint of the membrane (MP) for different parameter combinations; without osmotic pressure: A) $\sigma = 0.9$, $P_1 = P_2 = 0$; with osmotic pressure: B) $\sigma = 0.9$, $P_2 = 0$, C) $\sigma = 0.5$, $P_2 = 0$, D) $\sigma = 0.9$, $P_2 = 5 \cdot P_1$.

at the membrane is higher towards the walls, than in the middle part. This is caused by the non-decelerated parabolic velocity profile. In the middle part, the velocity is higher than close to the walls, thus it carries away more of the concentration. This phenomenon is not observed for the cases where the velocity at the membrane rapidly

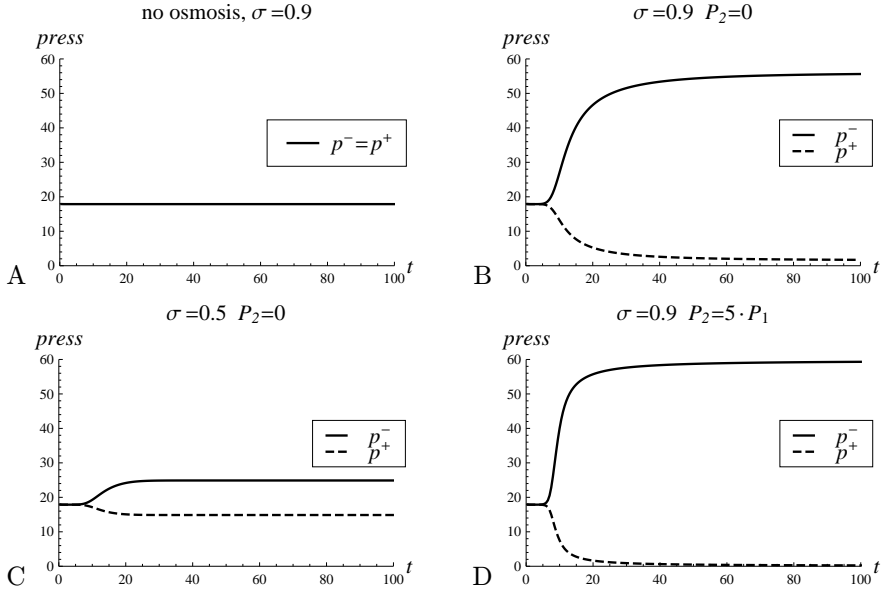


Figure 6.4. Time evolution of hydrodynamical pressure at midpoint of the membrane (MP) for different parameter combinations; without osmotic pressure: A) $\sigma = 0.9$, $P_1 = P_2 = 0$; with osmotic pressure: B) $\sigma = 0.9$, $P_2 = 0$, C) $\sigma = 0.5$, $P_2 = 0$, D) $\sigma = 0.9$, $P_2 = 5 \cdot P_1$.

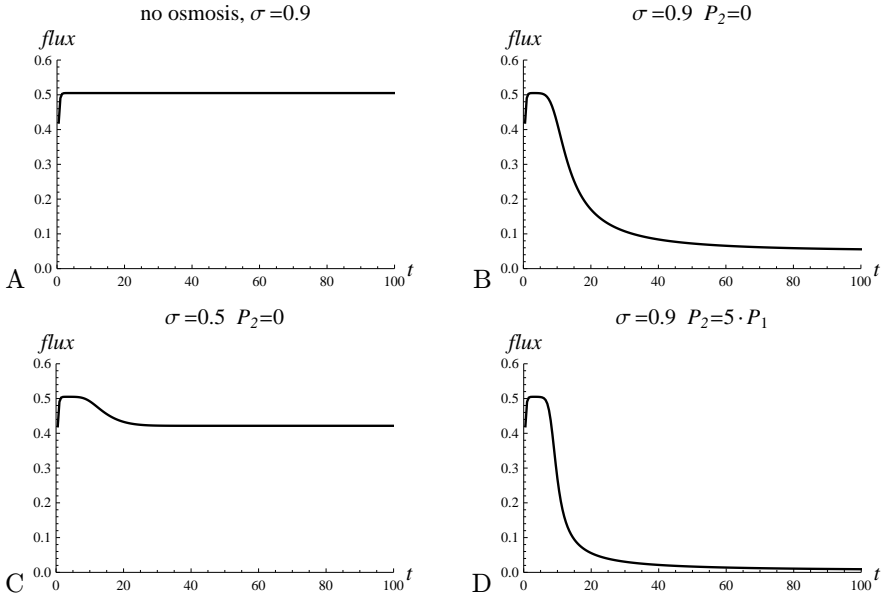


Figure 6.5. Time evolution of total solvent flux through Γ_m for different parameter combinations; without osmotic pressure: A) $\sigma = 0.9$, $P_1 = P_2 = 0$; with osmotic pressure: B) $\sigma = 0.9$, $P_2 = 0$, C) $\sigma = 0.5$, $P_2 = 0$, D) $\sigma = 0.9$, $P_2 = 5 \cdot P_1$.

drops like in the settings of B) and D), as can be seen in Fig. 6.5 and Fig. 6.6. For the settings C) and D) with low reflection coefficient and quadratic osmotic pressure dependence, a small concentration layer is created compared to the setting with higher σ and linear dependence of osmotic pressure, settings A) and B).

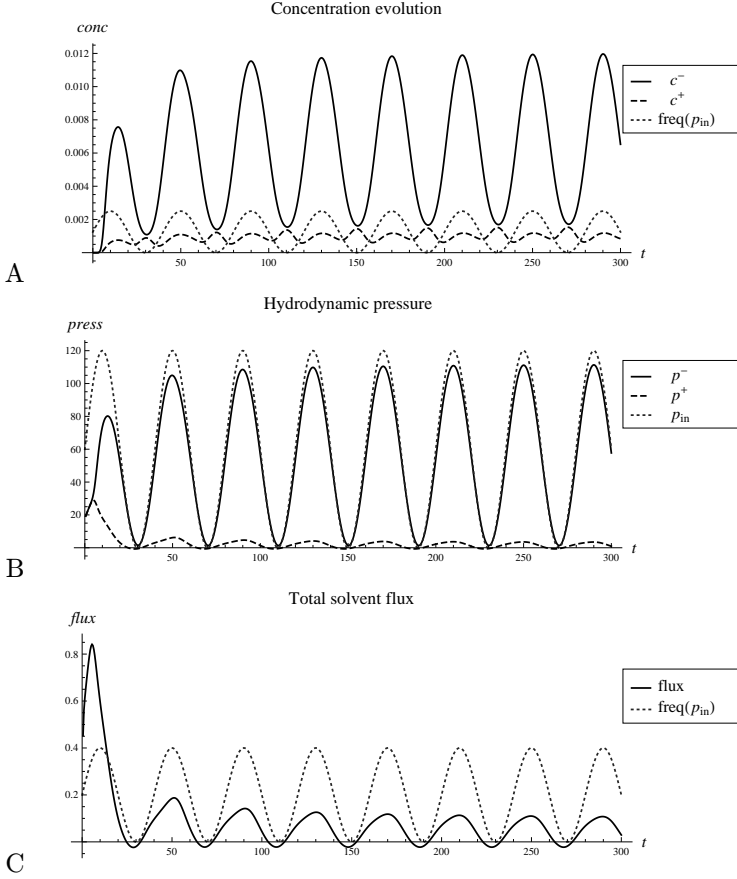


Figure 6.6. Time evolution of various quantities for periodic pressure inlet $p_{\text{in}} = p_0(1 + \sin(\pi t/20))$, $\sigma = 0.9$, $P_2 = 0$; A) concentration on MP, B) pressure on MP, C) total solvent flux through Γ_m . Dotted profile represent the frequency of the pressure inlet oscillations.

Profiles of hydrodynamical pressure are presented in Fig. 6.2. In the case of computational setting without osmosis, the equations for velocity and concentration are not fully coupled and thus the hydrodynamical pressure is a solution of the classical Navier-Stokes equations, and has a linear profile. For the settings including osmosis jumps in pressure occur. As one can see in the case of small σ , the concentration layer at the membrane is not so significant, see Fig. 6.3, and thus it does not evoke

high difference in the osmotic pressures which could act against the fluid pressure, see Fig. 6.4. In the case of the quadratic osmotic pressure dependence on the concentration, the compensation of the pressures occurs even though the drop in concentration is not so high as for the case in Fig. 6.3B.

Figs. 6.3–6.5 present the time evolution of individual physical quantities at the middle point of the membrane. Since the values of the concentration and of the pressure are discontinuous at the membrane, we plot the traces of these functions from both sides of the membrane; the solvent flux is continuous across the membrane. At the beginning of the computation, there are no jumps since at that time no concentration layer at membrane has been created. During this time the solvent flux is constant and highest. After the creation of the concentration layer, the flux decreases corresponding to the induced hydrodynamical pressure drop.

The last set of graphs in Fig. 6.6 shows the solution for computation with time periodic inlet pressure $p_{\text{in}} = p_0(1 + \sin(\pi t/20))$. As one can see, after a short initial phase, the solution becomes periodic with the same frequency as the enforcing pressure condition. In this setting we can observe that the solvent flux changes its direction at the time when the forcing pressure is lowest. This is the manifestation of the osmotic effect, since the concentration on the left-hand side of the membrane is higher than the concentration on the right-hand side, which creates the pressure force acting against the inflow pressure.

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