12

Mathematical model

We recall the model for transport of surfactants, derived in Sect. 1.1.4. In Sect. 1.1.4 the concentration of the surfactant is denoted by $S(x,t)$, the velocity field by $\mathbf{u}$ and the diffusion coefficient by D_Γ. For simplicity we assume D_Γ to be constant. By a rescaling we can take $D_\Gamma = 1$. In this and the next chapter we use a different notation for the unknown concentration and for the velocity field, namely $u = u(x,t)$ and $\mathbf{w} = \mathbf{w}(x,t)$, respectively. With this notation the convection-diffusion equation for the unknown concentration takes the following form, cf. (1.25):

$$\dot{u} + u \,\mathrm{div}_\Gamma \mathbf{w} = \mathrm{div}_\Gamma \nabla_\Gamma u, \tag{12.1}$$

where $\dot{u}$ denotes the material derivative of $u(x,t)$. Using the definitions of the material derivative and of the Laplace-Beltrami operator this equation can be written as

$$\frac{\partial u}{\partial t} + \mathbf{w} \cdot \nabla u + u \,\mathrm{div}_\Gamma \mathbf{w} - \Delta_\Gamma u = 0. \tag{12.2}$$

Remark 12.0.5 In (12.2) we do not model ad- or desorption effects. These would lead to a source term f of the form $f = f(u_\Omega)$, where u_Ω denotes the concentration of u in Ω_i ($i = 1$ or $i = 2$) evaluated at the interface Γ. Suitable models for f are hard to derive. In the remainder we restrict ourselves to (12.2), i.e., we do not treat models that include ad- or desorption effects.

In this chapter we consider weak formulations of the convection-diffusion problem (12.2). These weak formulations form the basis for the finite element methods treated in Chap. 13. We distinguish two cases, namely surfactant transport on a *stationary* or on a *non-stationary* interface.

12.1 Surfactant transport on a stationary interface

In this section we assume that the interface Γ is stationary, sufficiently smooth, bounded and $\partial\Gamma = \emptyset$, i.e. Γ does not have a boundary. Before we turn to the weak formulation of the convection-diffusion problem (12.2) we first consider the so-called *Laplace-Beltrami equation*, which is an important model problem that is often used in the literature. This equation models a pure diffusion process on a given sufficiently smooth surface (in our case, interface) Γ. It reads as follows: For a given f determine u such that

$$-\Delta_\Gamma u = f \quad \text{on} \quad \Gamma.$$

Since $-\int_\Gamma \Delta_\Gamma u \, ds = \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma 1 \, ds = 0$ we introduce the assumption $\int_\Gamma f \, ds = 0$. A well-posed weak formulation is as follows: For given $f \in L_0^2(\Gamma) := \{ v \in L^2(\Gamma) : \int_\Gamma v \; ds = 0 \}$, determine $u \in H_*^1(\Gamma)$, with $H_*^1(\Gamma) := \{ v \in H^1(\Gamma) : \int_\Gamma v \; ds = 0 \}$, such that

$$\int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v \; ds = \int_\Gamma f v \; ds \qquad \text{for all} \;\; v \in H_*^1(\Gamma). \tag{12.3}$$

The bilinear form $(u, v) \to \int_\Gamma \nabla_\Gamma u \nabla_\Gamma v \; ds$ is continuous and elliptic on $H_*^1(\Gamma)$ and thus, using the Lax-Milgram lemma, it follows that this weak formulation has a unique solution u. Furthermore, it can be shown that this solution has the regularity property $u \in H^2(\Gamma)$ and $\|u\|_{H^2(\Gamma)} \leq c\|f\|_{L^2(\Gamma)}$, with a constant c independent of f, cf. [92].

We now consider a weak formulation of the convection-diffusion problem in (12.2). We use the results presented in the abstract Hilbert space setting in Sect. 2.2.3, in particular Theorem 2.2.7. We apply the abstract results with the Hilbert spaces $V = H_*^1(\Gamma)$, $H = L_0^2(\Gamma)$. In case of a stationary interface we have $\mathbf{w} \cdot \mathbf{n} = 0$ and thus $\mathbf{w} \cdot \nabla u = \mathbf{w} \cdot \nabla_\Gamma u$. Using this we can rewrite (12.2) as

$$\frac{\partial u}{\partial t} + \mathrm{div}_\Gamma(\mathbf{w} u) - \Delta_\Gamma u = 0. \tag{12.4}$$

We introduce the bilinear form

$$\hat{a}(u, v) = \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v + \mathrm{div}_\Gamma(\mathbf{w} u)\, v \, ds, \quad u, v \in H_*^1(\Gamma).$$

A sufficiently smooth solution u of (12.4), if it exists, satisfies $\int_\Gamma \frac{\partial u}{\partial t} v \, ds + \hat{a}(u, v) = 0$ for all $v \in H_*^1(\Gamma)$. We introduce the following weak formulation of (12.4), cf. (2.29) in Sect. 2.2.3:

Find $u \in W^1(0, T; H_*^1(\Gamma))$ such that

$$\begin{aligned} \frac{d}{dt}(u(t), v)_{L^2(\Gamma)} + \hat{a}(u(t), v) = 0 \quad \text{for all} \;\; v \in H_*^1(\Gamma), \; t \in (0, T), \\ u(0) = u_0. \end{aligned} \tag{12.5}$$

The space $W^1(0,T;H^1_*(\Gamma))$ is as defined in Sect. 2.2.3, i.e. $W^1(0,T;H^1_*(\Gamma)) = \{ v \in L^2(0,T;H^1_*(\Gamma)) : v' \in L^2(0,T;H^1_*(\Gamma)') \text{ exists} \}$, where v' denotes the weak time derivative of v. This space has the following continuous embedding property, cf. (2.28),

$$W^1(0,T;H^1_*(\Gamma)) \hookrightarrow C([0,T];L^2_0(\Gamma)). \tag{12.6}$$

Based on Theorem 2.2.7 and Remark 2.2.7 we derive the following well-posedness result:

Theorem 12.1.1 *Assume* $\mathbf{w} \in H^1(\Gamma)^3$ *and* $\|\operatorname{div}\mathbf{w}\|_{L^\infty(\Gamma)} \le c$. *For each* $u_0 \in L^2_0(\Gamma)$ *there exists a unique solution* u *of* (12.5) *and the linear mapping* $u_0 \to u$ *is continuous from* $L^2_0(\Gamma)$ *into* $W^1(0,T;H^1_*(\Gamma))$.

Proof. We apply Theorem 2.2.7 with the ellipticity condition replaced by the Garding inequality, cf. Remark 2.2.8. Using the smoothness assumption on the velocity field $\mathbf{w}$ it follows that $\hat{a}(\cdot,\cdot)$ is continuous on $H^1_*(\Gamma) \times H^1_*(\Gamma)$. Using the Green formula (14.15) and $\mathbf{w}\cdot\mathbf{n} = 0$ we get

$$\int_\Gamma \operatorname{div}_\Gamma(\mathbf{w}u)\, u\, ds = -\int_\Gamma u\mathbf{w}\cdot\nabla_\Gamma u\, ds = -\int_\Gamma \operatorname{div}_\Gamma(\mathbf{w}u)\, u\, ds + \int_\Gamma \operatorname{div}_\Gamma\mathbf{w}\, u^2\, ds,$$

and thus $\int_\Gamma \operatorname{div}_\Gamma(\mathbf{w}u)\, u\, ds = \frac{1}{2}\int_\Gamma \operatorname{div}_\Gamma \mathbf{w}\, u^2\, ds$. Using this we obtain with suitable constants $\gamma_V > 0$ and γ_H:

$$\begin{aligned}\hat{a}(u,u) &= \|\nabla_\Gamma u\|^2_{L^2(\Gamma)} + \frac{1}{2}\int_\Gamma \operatorname{div}_\Gamma\mathbf{w}\, u^2\, ds \\ &\ge \gamma_V \|u\|^2_{H^1_*(\Gamma)} - \gamma_H \|u\|^2_{L^2(\Gamma)} \quad \text{for all } \ u \in H^1_*(\Gamma).\end{aligned}$$

Hence $\hat{a}(\cdot,\cdot)$ satisfies the Garding condition. □

In Chap. 13 we treat finite element discretizations of the variational problems in (12.3) and (12.5).

12.2 Surfactant transport on a non-stationary interface

We now consider the case in which the interface may vary in time. We assume that for all $t \in [0,T]$ the interface $\Gamma(t)$ is *sufficiently smooth*. Precise sufficient smoothness conditions on $\Gamma(t)$ are formulated in Sect. 2 in [94]. Below we consider two weak formulations of the convection-diffusion equation (12.2). The first one, which is introduced in [94], is a variational problem *in space only*, in which the test space depends on time. The second one is a *space-time* variational problem. We introduce both, because as we will see in Chap. 13, these two formulations induce different finite element discretization approaches with their own merits.

The first weak formulation is taken from [94]. The smoothness assumptions on $\Gamma(t)$ are such that the space-time interface

$$\Gamma_* := \cup_{t\in[0,T]}\Gamma(t) \times \{t\}$$

is a three-dimensional hypersurface in $\mathbb{R}^4$. On this hypersurface one can define the corresponding Sobolev space of all functions for which all weak first derivatives exist. As usual, this space is denoted by $H^1(\Gamma_*)$. On $H^1(\Gamma_*)$ the norm equivalence

$$\|u\|^2_{H^1(\Gamma_*)} \sim \|u\|^2_{L^2(\Gamma_*)} + \|\nabla_\Gamma u\|^2_{L^2(\Gamma_*)} + \|\dot{u}\|^2_{L^2(\Gamma_*)}, \quad u \in H^1(\Gamma_*),$$

holds, with $\dot{u} = \frac{\partial u}{\partial t} + \mathbf{w}\cdot\nabla u$ the material derivative. In the analysis below we need a smoothness property of the velocity field $\mathbf{w}$. In the remainder of this section we assume

$$\mathbf{w} \in H^1(\Gamma_*)^3, \quad \|\mathrm{div}_\Gamma \mathbf{w}\|_{L^\infty(\Gamma_*)} < \infty.$$

We introduce the following weak formulation of (12.2):

Find $u \in H^1(\Gamma_*)$ such that for almost all $t \in (0,T)$:

$$\int_{\Gamma(t)} \dot{u}v + uv\,\mathrm{div}_\Gamma\mathbf{w} + \nabla_\Gamma u \cdot \nabla_\Gamma v\, ds = 0 \;\; \forall\, v(\cdot,t) \in H^1\big(\Gamma(t)\big), \qquad (12.7)$$
$$u(\cdot,0) = u_0.$$

Clearly, a strong solution of (12.2) is a solution of (12.7). The following result is proved in [94].

Theorem 12.2.1 *Assume $u_0 \in H^1(\Gamma(0))$. Then there exists a unique solution of the variational problem* (12.7).

Proof. For a proof we refer to [94]. □

In the variational formulation (12.7) we use different trial and test spaces, namely $H^1(\Gamma_*)$ and $H^1\big(\Gamma(t)\big)$, respectively. Note, however, that for any $v \in H^1(\Gamma_*)$ we have $v(\cdot,t) \in H^1\big(\Gamma(t)\big)$ for almost all $t \in [0,T]$. This is due to the fact that from $\int_0^T \int_{\Gamma(t)} \nabla_\Gamma v\cdot\nabla_\Gamma v + v^2\, ds\, dt < \infty$ it follows (Fubini's theorem) that $\int_{\Gamma(t)} \nabla_\Gamma v \cdot \nabla_\Gamma v + v^2\, ds < \infty$ for almost all $t \in [0,T]$.

For a space-time variational formulation we introduce a test space consisting of functions in $L^2(\Gamma_*)$ for which the weak *spatial* first derivatives exist, i.e.

$$H^{1,0}(\Gamma_*) := \left\{\, v \in L^2(\Gamma_*) : \; \|\nabla_\Gamma v\|_{L^2(\Gamma_*)} < \infty \,\right\},$$

which is a Hilbert space w.r.t. the norm

$$\|v\|^2_{H^{1,0}(\Gamma_*)} = \|v\|^2_{L^2(\Gamma_*)} + \|\nabla_\Gamma v\|^2_{L^2(\Gamma_*)}.$$

The weak formulation is as follows:

Find $u \in H^1(\Gamma_*)$ such that:

$$\begin{aligned} \int_0^T \int_{\Gamma(t)} \dot{u}v + uv\,\mathrm{div}_\Gamma \mathbf{w} + \nabla_\Gamma u \cdot \nabla_\Gamma v \, ds\, dt = 0 \quad \forall\, v \in H^{1,0}(\Gamma_*), \\ u(\cdot, 0) = u_0. \end{aligned} \tag{12.8}$$

This formulation is a well-posed problem:

Theorem 12.2.2 *Assume $u_0 \in H^1(\Gamma(0))$. Then there exists a unique solution of the variational problem* (12.8)*.*

Proof. On $H^1(\Gamma_*) \times H^{1,0}(\Gamma_*)$ we introduce the bilinear form

$$a(u, v) := \int_0^T \int_{\Gamma(t)} \dot{u}v + uv\,\mathrm{div}_\Gamma \mathbf{w} + \nabla_\Gamma u \cdot \nabla_\Gamma v \, ds\, dt,$$

which is continuous. Let $u \in H^1(\Gamma_*)$ be the solution of (12.7). Integration of the identity in (12.7) over $t \in [0, T]$ results in

$$a(u, v) = 0 \quad \text{for all} \;\; v \in C^\infty(\overline{G}_T).$$

Since $C^\infty(\overline{G}_T)$ is dense in $H^{1,0}(\Gamma_*)$ is follows that u is a solution of (12.8). We now prove uniqueness, using a Gronwall argument. A corollary of the Gronwall lemma is as follows (cf. lemma 29.3 in [256]): if $f \in C([0, T])$, $f(t) \geq 0$ for all $t \in [0, T]$, and there exists a constant C such that

$$f(\tau) \leq C \int_0^\tau f(t)\, dt \quad \text{for all} \;\; \tau \in [0, T],$$

this implies that $f(t) = 0$ for all $t \in [0, T]$. Let $w \in H^1(\Gamma_*)$ be a solution of (12.8) with $w(\cdot, 0) = u_0 = 0$. Define $f(t) := \int_{\Gamma(t)} w(s, t)^2\, ds$. A variant of the embedding property (12.6) yields that f is continuous on $[0, T]$. Clearly $f(0) = 0$, $f \geq 0$ on $[0, T]$. Take a $\tau \in (0, T]$. By the differentiation rule (14.21b) we obtain

$$\begin{aligned} f(\tau) = f(\tau) - f(0) &= \int_0^\tau \frac{d}{dt} \int_{\Gamma(t)} w^2\, ds\, dt \\ &= \int_0^\tau \int_{\Gamma(t)} 2\dot{w}w + w^2 \mathrm{div}_\Gamma \mathbf{w}\, ds\, dt. \end{aligned}$$

We use (12.8) with a test function v given by $v(\cdot, t) = w(\cdot, t)$ for $t \leq \tau$, $v(\cdot, t) = 0$ otherwise. Then we obtain

$$\begin{aligned} \int_0^\tau \int_{\Gamma(t)} \dot{w}w\, ds\, dt &= -\int_0^\tau \int_{\Gamma(t)} w^2 \mathrm{div}_\Gamma \mathbf{w}\, ds\, dt - \int_0^\tau \int_{\Gamma(t)} \nabla_\Gamma w \cdot \nabla_\Gamma w\, ds\, dt \\ &\leq -\int_0^\tau \int_{\Gamma(t)} w^2 \mathrm{div}_\Gamma \mathbf{w}\, ds\, dt. \end{aligned}$$

Hence, we get

$$f(\tau) \leq \|\mathrm{div}_\Gamma \mathbf{w}\|_{L^\infty(\Gamma_*)} \int_0^\tau f(t)\, dt.$$

Application of the Gronwall corollary yields $f(t) = \int_{\Gamma(t)} w(x,t)^2\, ds = 0$ for all $t \in [0,T]$. Hence $w = 0$ a.e. on Γ_*, which implies uniqueness. $\square$

We compare the weak formulations in (12.7) and (12.8). In both formulations we use the same trial space $H^1(\Gamma_*)$. In (12.7) we have, for each $t \in (0,T)$, a variational formulation and a corresponding test space on the interface $\Gamma(t)$. In (12.8) the variational formulation and the corresponding test space are on the space-time domain Γ_*. This difference in the variational problems leads to (very) different finite element discretization methods, treated in Chap. 13.