Multicomponent diffusion coefficient determination in metallurgy by a reduced adjoint system

Benny Malengier

NfaM^2 Research Group, Department of Mathematical Analysis, Faculty of Engineering, Ghent University, Belgium

E-mail: `bm@cage.ugent.be`

Abstract. This work focuses on a ternary diffusion model, with unknown nonlinear interdiffusion coefficients. Multicomponent diffusion processes are important in metallurgy, eg for the production of high Si-steel by diffusion annealing. A least-squares approach is applied, using the adjoint equation to drive the optimization process. To speed up computations further, freeform determination of the unknown coefficients $D_{ij}(u, v)$ is used in 2 dimensions, combined with a mapping strategy to space coordinates. This results in a reduced adjoint equation of the same form as the direct equation.

1. Introduction

Diffusion processes in metallurgy are described by Fick's laws of diffusion, leading to models described by partial differential equations (PDE), see [1]. In practical applications, the material properties enter the model via the diffusion coefficient and this coefficient can depend nonlinearly on the solution of the PDE. Due to the complicated micro behaviour (phase changes, hole formation, migration), it is often more straightforward to apply a macro-diffusion coefficient hiding the underlying processes which are experimentally hard to determine.

In [2] a model and numerical discretisation suitable to the solution of the diffusion process is proposed, as well as an experimental technique usable in the determination of the unknown diffusion coefficient by an inverse method. The solution of the diffusion problem can be obtained by different techniques (e.g. finite differences [3]), however the experiment is fixed: known concentration distribution over the entire sample at discrete time steps.

The determination of unknown coefficients from such experiments is in general an *ill-posed* problem. Apart from the question of existence and uniqueness of the determined variables, the lack of stability implies that small measurement errors may lead to large deviation of the determined diffusion from its true value. However, the determination of the unknowns by inverse modeling in parabolic PDE is common practice, see eg [4, 5] and references therein. The ill-posedness is generally handled by introducing a generalized solution defined by the minimum of an appropriate error functional, as well as the application of regularization. Stabilization can furthermore be achieved by doing a discretization of the coefficient space, instead of considering the infinite dimensional problem.

Here we will apply the adjoint or costate method to determine the gradient of the penalty functional, see eg. [6]. The adjoint method has the disadvantage that the resulting adjoint equation can be of a different form than the original equation, hence requiring a different solution

method. We consider a nonlinear diffusion problem, of which the common adjoint equation is a variable coefficient linear convection-diffusion problem. Furthermore, in the adjoint equation derivatives of the unknown coefficient function can appear, making a linear interpolation scheme for the determination of the coefficient function not ideal (ie. a discontinuous derivate can increase the computation time drastically).

To avoid these complications, we apply a mapping strategy, which correlates the changes of the unknown parameters to the change of the diffusion coefficient in specific space-time points. This yields the possibility of using a reduced adjoint equation consisting solely of a variable coefficient diffusion problem, without the appearance of derivatives of the unknown diffusion coefficient.

The use of a freeform or unbiased determination of a coefficient function has been proposed in eg. [7] for a 1D-diffusion problem arising in soil sciences. The weak smoothness of a piecewise linear parametrization there leads to the use of a piecewise cubic Hermite interpolation, which is not readily extended to 2D. The problem of the amount of degrees of freedom and the optimal position of the interpolation points is also not considered in our work.

Application of the reduced adjoint equation has some correspondance to the technique of linearization of the original problem, as done in [4]. However, by only considering the linearization in the adjoint problem, we avoid the complications in determining the unknown nonlinear diffusion coefficient from the linearized diffusion coefficient. This means of course that a nonlinear forward problem must be solved, but this is not necessarily problematic. Note that having discrete time measurements that are far apart, makes neither techniques relying on knowledge of the change over time applicable, eg. [5], nor equation error methods as in [8].

In Section 2 we give our setting: diffusion of a multicomponent coating in an iron steel bar. We also describe the experiments that are possible in order to determine the unknown diffusion coefficient, and briefly sketch the numerical discretization used to solve the forward problem. In the next section we give the set-up for the inverse problem. In Section 4 we present the adjoint system and our mapping strategy, and we end this article in section 5 with a numerical example.

2. Multicomponent diffusion example

When considering heat induced diffusion of a surface coating into a steel substrate, we only need to consider a one dimensional model. When the coating consists of several components, a multicomponent diffusion model is required. This leads for two components to the *nonlinear diffusion equation* for $x \in \Xi \equiv (0, W)$ and $t \in I \equiv (0, T)$:

$$\partial_t u(x,t) - \partial_x \left(D_{11}(u,v)\partial_x u(x,t) + D_{12}(u,v)\partial_x v(x,t) \right) = 0 \tag{1}$$

$$\partial_t v(x,t) - \partial_x \left(D_{21}(u,v)\partial_x u(x,t) + D_{22}(u,v)\partial_x v(x,t) \right) = 0$$

$$u(x,0) = u_0(x), \quad v(x,0) = v_0(x) \tag{2}$$

$$\partial_x u(0,t) = 0 = \partial_x u(W,t), \quad \partial_x v(0,t) = 0 = \partial_x v(W,t), \tag{3}$$

where W is the width of the sample and T is the end time of the experiment. $u(x,t), v(x,t)$ are the two components diffusing into our substrate, and u_0, v_0 are smooth initial concentrations. The boundary condition (3) indicates no-flow boundaries.

Measurements of the practical sample are done as follows, [9]. The sample is cooled, effectively stopping the diffusion process. It is cut, so that the internal composition can be measured in a Scanning Electron Microscope (SEM) equipped with EDS (Energy Dispersive Spectroscopy). This gives the concentration expressed in atomic percentage, which can be converted to a standard concentration (mol/mm^3).

As the measurement destroys the sample, one starts with a batch of identical samples (same initial condition), and takes measurements at specific time steps. This translates in additional

conditions,

$$u(x, t_m) = u_k(x), \quad v(x, t_m) = v_m(x), \qquad m = 1, 2, \ldots, M. \tag{4}$$

Many solution methods have been proposed for problem (1)-(3). We follow a *method of lines* approach. The space discretization is done by *finite volumes*, in which the interval is split in N cells, and the value of the concentration in the midpoint of the cell follows from the inflow and outflow balance, ie. the flux $D_{ij}(u)\partial_x u$ and $D_{ij}(v)\partial_x v$ on the edges. We obtain an ODE system of $2N$ equations, which is then solved by a stiff ODE solver (we have used the Netlib lsoda implementation, [10]).

3. Least squares approach and parametrization

The experiments can in general not be obtained continuously in space. So assume the data is given as a finite dimensional vector $\mathbf{m} \in \mathbb{R}^n$. Let $\mathbf{f}$ be the vector of coefficient functions, which is to be determined. Denote by $\mathbf{m}(\mathbf{f})$ the corresponding observation computed by solving the direct problem for given $\mathbf{f}$, and by $\mathbf{m}^*$ the experimental observations, possibly disturbed by measurement errors.

The inverse problem reads: find a coefficient function $\mathbf{f}$, which solves

$$\mathbf{m}(\mathbf{f}) = \mathbf{m}^*. \tag{5}$$

The solution does not exist in general, so we define a generalized solution by a least squares approach: find $\mathbf{f}^*$ which minimizes

$$J(\mathbf{f}) = \frac{1}{2}\|\mathbf{m}(\mathbf{f}) - \mathbf{m}^*\|_2^2. \tag{6}$$

Here, $\|\cdot\|$ denotes the Euclidian norm.

The coefficient functions are given as multi-valued functions $f(u, v)$. It is sufficient to describe them on over the effective solution path in the solution space. For simplicity though, we will determine them over a rectangle $\Omega = [u_{\min}, u_{\max}] \times [v_{\min}, v_{\max}]$, keeping in mind that only in the limited subdomain which the solution of the direct problem attains, the coefficient functions can be identified, $\Omega_{\text{sol}} \subset \Omega$.

A coefficient function f, which is continuous and piecewise analytic on Ω, is replaced by a parametrization $f(u, v) = f_{\mathbf{p}}(u)$, which is defined by a finite number of parameters $\mathbf{p}$. For this we define a rectangular mesh over Ω with rs nodes, and consider the finite element space χ with piecewise bilinear polynomials as basis functions. Given a partition $u_{\min} = u_1 < u_2 < \cdots < u_{r-1} < u_r = u_{\max}$ and equally for v, with $v_{\max} = v_s$, an element is given by $\Omega_e = [u_i, u_{i+1}] \times [v_i, v_{i+1}]$ with width $a = u_{i+1} - u_i$ and height $b = v_{i+1} - v_i$. The basis functions corresponding to a node of the mesh in this element are then given by

$$\phi_{i+1,j+1} = \frac{1}{4}(1 + \xi)(1 + \eta), \quad \phi_{i,j+1} = \frac{1}{4}(1 - \xi)(1 + \eta), \tag{7}$$

$$\phi_{i,j} = \frac{1}{4}(1 - \xi)(1 - \eta), \quad \phi_{i+1,j} = \frac{1}{4}(1 + \xi)(1 + \eta), \tag{8}$$

$$\xi = 2\frac{u - u_i}{a}, \quad \eta = 2\frac{v - v_i}{b}, \quad (u, v) \in \Omega_e. \tag{9}$$

Denoting by $\psi_{i,j}$ the global node function constructed by collecting the basisfunctions corresponding to node i, j in all adjacent elements, our parametrisation of f is given by

$$f(u, v) = \sum_{i,j} p_{i,j}\psi_{i,j}(u, v), \quad (u, v) \in \Omega, \tag{10}$$

or considering only one element

$$f(u,v) = p_{i,j}\phi_{i,j}(u,v) + p_{i+1,j}\phi_{i+1,j}(u,v) + p_{i,j+1}\phi_{i,j+1}(u,v) + p_{i+1,j+1}\phi_{i+1,j+1}(u,v), \quad (11)$$

$(u,v) \in \Omega_e$.

Additionaly, in the case of positive coefficients, we restrict the parameters to

$$p_{i,j} > 0. \tag{12}$$

The interpolation method based on bilinear basis functions is only continuous, and not continuously differentiable. This restricts how it can be used in the inverse algorithm. The computational time of constructing and using the interpolation on the other hand is considerably lower than the alternative of using more elaborate 2D-interpolations. The use of linear interpolation is important for another reason. It guarantees that the change of one parameter $p_{i,j}$ has a minimal influence on the coefficient function, i.e. if $p_{i,j}$ changes, then f only changes in the elements where node i,j is a corner of. Spline based interpolation methods do not have this property and show a global dependance.

The inverse problem is now reduced to finding the parameter vector in the coefficient space, $\mathbf{p} \in \mathbb{R}_+^{\nu \cdot (rs)}$, where ν is the number of unknown coefficient functions. The problem can be summarized as: Find $\mathbf{p}^* \in \mathbb{R}_+^{\nu \cdot (rs)}$ which minimizes

$$J(\mathbf{p}) = \frac{1}{2}\|\mathbf{m}(\mathbf{p}) - \mathbf{m}^*\|_2^2. \tag{13}$$

This functional J is minimized by constructing an adjoint problem to calculate its gradient. As this depends on the direct problem formulation, we return to the formulation given in Sec. 2.

4. The adjoint problem

Use of an adjoint problem is a standard method to solve inverse problems. For problem (1)-(4) it is derived by considering the variation in the diffusion coefficients as arising from a variation in the parameters. This is used to determine the resulting variation of the functional J.

To simplify the setup, consider the L_2 least squares function

$$J(\mathbf{p}) = \frac{1}{2}\left\|\sqrt{\sum_j \delta(t - t_j)}\,(u(\mathbf{p}) - u^*)\right\|_{L_2(\Xi \times I)}^2 + \frac{1}{2}\left\|\sqrt{\sum_{j=1} \delta(t - t_j)}\,(v(\mathbf{p}) - v^*)\right\|_{L_2(\Omega \times I)}^2, \quad (14)$$

where δ is the Dirac measure, and $u^*(x,t), v^*(x,t)$ are suitable interpolations of the measurement over the entire domain. It is straightforward to determine the variation of (14), and rewrite it using the sensitivity equation of (1)-(3). The reduced ajoint equation resulting from this is the end value problem:

$$\partial_t \psi_u(x,t) + \partial_x\left(D_{11,\mathbf{p}}\partial_x\psi_u(x,t) + D_{21,\mathbf{p}}\partial_x\psi_v(x,t)\right) = (u(x,t) - u^*)\sum_{j=1,\dots,M}\delta(t - t_j) \quad (15)$$

$$\partial_t \psi_v(x,t) + \partial_x\left(D_{12,\mathbf{p}}\partial_x\psi_u(x,t) + D_{22,\mathbf{p}}\partial_x\psi_v(x,t)\right) = (v(x,t) - v^*)\sum_{j=1,\dots,M}\delta(t - t_j) \quad (16)$$

$$-\partial_x\left(D_{11,\mathbf{p}}\psi_u(0,t) + D_{21,\mathbf{p}}\psi_v(0,t)\right) = 0 = -\partial_x\left(D_{11,\mathbf{p}}\psi_u(W,t) + D_{21,\mathbf{p}}\psi_v(W,t)\right),$$

$$-\partial_x\left(D_{12,\mathbf{p}}\psi_u(0,t) + D_{22,\mathbf{p}}\psi_v(0,t)\right) = 0 = -\partial_x\left(D_{12,\mathbf{p}}\psi_u(W,t) + D_{22,\mathbf{p}}\psi_v(W,t)\right), \quad (17)$$

$$\psi_u(x,T) = 0, \quad \psi_v(x,T) = 0 \tag{18}$$

Remember that for the adjoint equation, $u(x,t)$ and $v(x,t)$ are known input functions resulting from the solution of the direct problem with a given paremeter $\mathbf{p}$, and hence the diffusion

coefficients $D_{ij,\mathbf{p}}$ can also be viewed as functions over $\Xi \times I$, $D_{ij,\mathbf{p}} \equiv D_{ij}(x,t)$, making the adjoint equation a variable coefficient linear parabolic system with a source term at discrete time steps.

If ψ_u, ψ_v are the solution of the above adjoint sythem, we can write the variation of the cost functional J as

$$\delta J(\mathbf{p}) = \int_T \int_\Xi \delta D_{11} \partial_x u \partial_x \psi_u + \delta D_{12} \partial_x v \partial_x \psi_u + \delta D_{21} \partial_x u \partial_x \psi_v + \delta D_{22} \partial_x v \partial_x \psi_v. \tag{19}$$

Eq. (19) does not yet allow to determine the gradient $\nabla_\mathbf{p} J$ as δD_{ij} is still unknown. Using the expression

$$\delta D_{ij} = \partial_u D_{ij} \delta u + \partial_v D_{ij} \delta v + \nabla_\mathbf{p} D_{ij} \cdot \delta \mathbf{p},$$

is no option as the variations $\delta u, \delta v$ are unknown. The terms arising with these variations are precily the terms we want to avoid. Handling them is only possible by adding the terms resulting from them to the reduced adjoint equation to obtain the full adjoint equation.

The solution to calculating (19) is by using a mapping strategy which maps δD_{ij} to $\delta \mathbf{p}$. First let us note that in the right-hand side of (19) we need the variation of the coefficient at a specific space-time point $(x_{k+\frac{1}{2}}, t_l)$, where we indicate with $k + \frac{1}{2}$ the midpoint of our space discretization, as that is where we calculate concentrations with the finite volume method used in the direct problem. We have that

$$
\begin{aligned}
\delta D(x_{k+\frac{1}{2}}, t_l) &= \delta D(u(x_{k+\frac{1}{2}}, t_l), v(x_{k+\frac{1}{2}}, t_l), \mathbf{p}) \\
&= \delta p_{ij} \psi_{ij}(u_{kl}, v_{kl}) + \delta p_{i+1,j} \psi_{i+1,j}(u_{kl}, v_{kl}) + \delta p_{i,j+1} \psi_{i,j+1}(u_{kl}, v_{kl}) \\
&\quad + \delta p_{i+1,j+1} \psi_{i+1,j+1}(u_{kl}, v_{kl}) \quad \text{with } (u(x_{k+\frac{1}{2}}, t_l), v(x_{k+\frac{1}{2}}, t_l)) \in \Omega_e \\
&= \sum_{ij} m_{ijk}^l \delta p_{ij} = \left(\delta \mathbf{p}^T \mathbf{M}^l \right)_k,
\end{aligned}
$$

which defines the mapping matrix $\mathbf{M}^l \in \mathbb{R}^{rs \times K}$ for every time step t_l as a sparse matrix with four non-zero elements in every column. The supscript T indicates the transpose operation. In the above, K, is the number of cells in our space grid $\{x_k\}_{k=0}^K$ over Ξ.

We have a mapping matrix at every timestep for every coefficient function, $\mathbf{M}_{11}, \mathbf{M}_{12}, \mathbf{M}_{21}, \mathbf{M}_{22},$. These matrices allow us to determine $\delta D_{11}, \delta D_{12}, \delta D_{21}, \delta D_{22}$, and can be calculated after the direct problem has been solved for a specific parameter set $\mathbf{p} = (\mathbf{p}_{11}, \mathbf{p}_{12}, \mathbf{p}_{21}, \mathbf{p}_{22})$, where we have indicated that the full parameter consists of the parameter sets of every coefficient function separately.

As noted, the choice of a finite volume solution method means the data is obtained in the midpoints of the control volumes, so at $x_{k+\frac{1}{2}}$, and not in the nodes. To approximate the derivative in space of a function in the midpoints by the values of the function in the midpoints themselves introduce the notation, $\mathbf{L} \in \mathbb{R}^{K \times K}$:

$$\mathbf{L} = \begin{pmatrix} \frac{-1}{\Delta_{\frac{1}{2}}} & \frac{1}{\Delta_{\frac{1}{2}}} & & \\ \frac{-1}{\Delta_{\frac{1}{2}} + \Delta_{\frac{3}{2}}} & 0 & \frac{1}{\Delta_{\frac{1}{2}} + \Delta_{\frac{3}{2}}} & \\ & \ddots & \ddots & \\ & \frac{-1}{\Delta_{K-\frac{5}{2}} + \Delta_{K-\frac{3}{2}}} & 0 & \frac{1}{\Delta_{K-\frac{5}{2}} + \Delta_{K-\frac{3}{2}}} \\ & & \frac{-1}{\Delta_{K-\frac{3}{2}}} & \frac{1}{\Delta_{K-\frac{3}{2}}} \end{pmatrix}, \tag{20}$$

with $\Delta_{k+\frac{1}{2}} = \frac{1}{2}(\Delta_k + \Delta_{k+1})$, $\Delta_k = x_{k+1} - x_k$.

We can now numerically determine the value of (19) as

$$
\begin{aligned}
\delta J(\mathbf{p}) \;=\; & \sum_{k=0}^{K-1}\sum_{l=0}^{L-1} (\delta D_{11}\partial_x u \partial_x \psi_u + \delta D_{12}\partial_x v \partial_x \psi_u + \delta D_{21}\partial_x u \partial_x \psi_v \\
& + \delta D_{22}\partial_x v \partial_x \psi_v)|_{x=x_{k+\frac{1}{2}},\,t=t_l}\, \Delta x \Delta t,
\end{aligned}
\tag{21}
$$

where the remaining unknowns in (21) can be calculated as follows. We have that $\partial_x u(x_{k+\frac{1}{2}}) = (\mathbf{L}\,\mathbf{u})_k$, where $\mathbf{u}$ is the vector with elements $u(x_{k+\frac{1}{2}})$, and the same for ψ_u, ψ_v and v. If we next introduce the vector $\mathbf{g}_{11}^l$ with elements $g_i = (\mathbf{L}\,\mathbf{u})_i(\mathbf{L}\,\psi_{\mathbf{u}})_i \Delta_i \Delta t$ taken at $t = t_l$, and similarly for the other terms, we obtain for the variation of the functional

$$
\begin{aligned}
\delta J(\mathbf{p}) \;=\; & \sum_{l=0}^{L-1}\sum_{k=0}^{K-1}\left[\left(\delta\mathbf{p}_{11}^T\mathbf{M}_{11}^l\right)_k \mathbf{g}_{11,k}^l + \left(\delta\mathbf{p}_{12}^T\mathbf{M}_{12}^l\right)_k \mathbf{g}_{12,k}^l + \left(\delta\mathbf{p}_{21}^T\mathbf{M}_{21}^l\right)_k \mathbf{g}_{21,k}^l \right. \\
& \left. + \left(\delta\mathbf{p}_{22}^T\mathbf{M}_{22}^l\right)_k \mathbf{g}_{22,k}^l \right] \\
\;=\; & \sum_{l=0}^{L-1}\left[\delta\mathbf{p}_{11}^T\mathbf{M}_{11}^l\mathbf{g}_{11}^l + \delta\mathbf{p}_{12}^T\mathbf{M}_{12}^l\mathbf{g}_{12}^l + \delta\mathbf{p}_{21}^T\mathbf{M}_{21}^l\mathbf{g}_{21}^l + \delta\mathbf{p}_{22}^T\mathbf{M}_{22}^l\mathbf{g}_{22}^l \right].
\end{aligned}
\tag{22}
$$

It follows that the gradient of the functional can be calculated by

$$
\partial_{p_{ij},r} J(\mathbf{p}) = \sum_{l=0}^{L-1}(\mathbf{M}_{ij}^l\mathbf{g}_{ij}^l)_r.
\tag{23}
$$

The inverse algorithm is then

(i) Choose a valid starting value $\mathbf{p}_1$, $i = 1$.

(ii) Obtain solution $u_i(x,t), v_i(x,t)$ of the direct problem (1)-(3) for $\mathbf{p}_i$

(iii) Solve adjoint problem (15)-(18) for $\mathbf{p}_i$ and u_i, v_i.

(iv) Calculate $\mathbf{M}_{11}^l, \mathbf{M}_{12}^l, \mathbf{M}_{21}^l, \mathbf{M}_{22}^l$ and $\mathbf{g}_{11}^l, \mathbf{g}_{12}^l, \mathbf{g}_{21}^l, \mathbf{g}_{22}^l$ for all l.

(v) Determine the gradient of the cost functional with (23).

(vi) Determine a new value p_{i+1} by application of a suitable gradient optimization method (eg. conjugate gradient method).

(vii) Stop if stopping criterium is satisfied, otherwise: $i = i + 1$ and go to (ii).

As the adjoint equation is of the same form of the direct problem (but now a linear variable coefficient diffusion problem), the same solution method can be used as for the direct problem. The reaction term on the right hand side must be treated carefully due to the appearance of a Dirac measure. One has to solve the problem over the interval (t_j, t_{j+1}), starting from t_{j+1} without reaction, from which one obtains the solution $\bar{\psi}_u(x,t_j), \bar{\psi}_v(x,t_j)$. Next one has to apply the reaction as

$$
\psi_u(x,t_j) = \bar{\psi}_u(x,t_j) + (u(x,t_j) - u^*),
$$

$$
\psi_v(x,t_j) = \bar{\psi}_v(x,t_j) + (v(x,t_j) - v^*).
$$

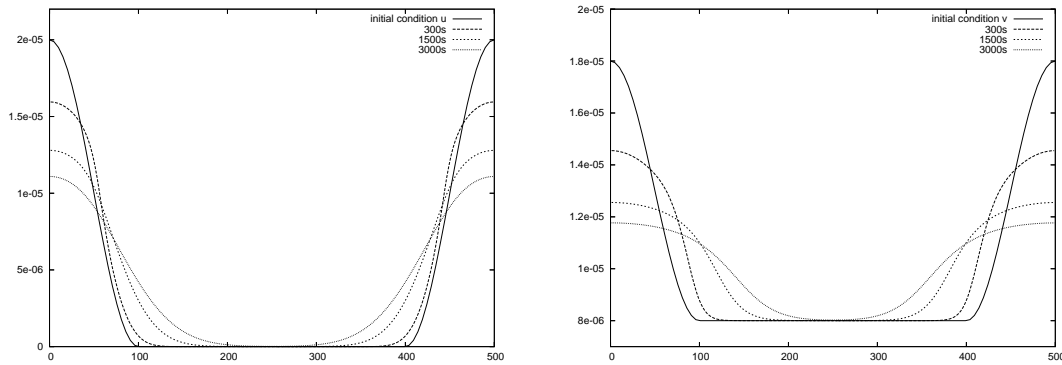This is then the end condition for the next time slice (t_{j-1}, t_j).

Figure 1. Concentration profiles at $t = 0$, 300, 1500 and 3000 seconds.

5. Numerical Example

The numerical code developed to implement the inverse method as outlined in this paper is still in the process of being validated. Some temporary results can however already be given.

We take the following initial condition, $x \in (0, 500)$:

$$u_0(x) = \begin{cases} 10^{-5}(1 + \cos(\frac{\pi x}{100})) + 10^{-10}, & x \le 100 \\ 10^{-10}, & 100 < x < 400 \\ 10^{-5}(1 + \cos(-\frac{\pi(x-500)}{100})) + 10^{-10}, & x \ge 400. \end{cases}$$

$$v_0(x) = \begin{cases} 0.5\,10^{-5}(1 + \cos(\frac{\pi x}{100})) + 8\,10^{-6}, & x \le 100 \\ 8\,10^{-6}, & 100 < x < 400 \\ 0.5\,10^{-5}(1 + \cos(-\frac{\pi(x-500)}{100})) + 8\,10^{-6}, & x \ge 400. \end{cases}$$

We solve the direct problem for diffusion coefficients given by

$$D_{11}(u,v) = 8 \exp\left(-\left((10^5 u - 2)^2/0.2 + (10^5 v - 1.2)^2/0.2\right)\right) + 0.5, \quad D_{12}(u,v) = -10^{-7},$$

$$D_{22}(u,v) = 10 \sin\left(\frac{10^5 v - .8}{1.65 - .8}\frac{\pi}{2}\right) \sin\left(\frac{10^5 u}{4}\frac{\pi}{2}\right) + 0.5, \quad D_{21}(u,v) = -10^{-7},$$

and consider the solution at $t = 300$, 1500 and 3000 seconds as the experimental values u^*, v^*, see Fig. 1. This example resembles the experimental setup, albeit with reduced times (expermental times can be up to 3 hours) to limit the computational time.

For the inverse problem, we consider $\Omega = [0, 4.1\,10^{-5}] \times [.7\,10^{-5}, 1.9\,10^{-5}]$, which we mesh with a 15×15 rectangular grid. This gives us 225 parameters per diffusion coefficient. We will only inversely determine D_{11} and D_{22}, and as starting value for the the inverse algorithm we take a constant profile, $p_i = 0.2$. The results of the inverse method are given in Fig. 2. Only the values that have undergone change from the starting value of $p_i = 0.2$ have been plotted. Those values correspond to the diffusion path of attained concentration values $((u, v) \in \Omega_{\text{sol}})$.

As can be expected, the values at largest concentrations are not well determined as they have little influence on the final diffusion profiles. The closer to the diffusion path, the better the values have been inversely determined. The concentration profiles obtained with the determined parameters are almost indistinguishable from the ones given in Fig. 1.

Further tests are needed, especially to determine the optimal number of parameters and to determine the sensitivity of the method, however these first results already indicate the method is capable of inversely determining multicomponent diffusion coefficients on the diffusion path.
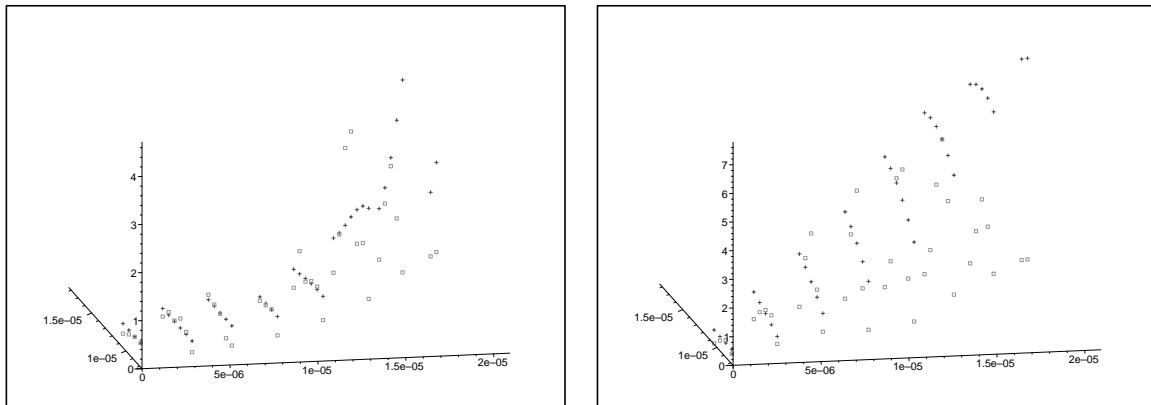
Figure 2. Results of the determined diffusion coefficients. Left: D_{11}, Right: D_{22}. Crosses indicate the exact diffusion coefficient, boxes the determined values.

References

[1] Glicksman M 2000 *Diffusion in Solids* (New York: Wiley)
[2] Barros J, Malengier B, Keer R V and Houbaert Y 2005 *Journal of phase equilibria and diffusion* **26**(5) 417–422
[3] Murakami K, Nishida N, Osamura K, Tomota Y and Suzuki T 2004 *Acta Materialia* **52** 2173–2184
[4] Tai X C and Kärkkäinen T 1995 *Comp. Appl. Mat.* **14** 157–184
[5] Cao H and Pereverzev S V 2006 *Inverse Problems* **22** 2311–2330
[6] Vogel C R 2002 *Computational methods for inverse problems* Frontiers in applied mathematics (USA: Siam) ISBN 0-89871-507-5
[7] Bitterlich S and Knabner P 2004 *Inverse Problems in Science and Engineering* **12**(4) 361
[8] Hanke M and Scherzer O 1999 *SIAM J. Appl. math.* **59**(3) 1012–1027
[9] Lorenzo J B 2006 *Production of High Si-Steel by Hot Dipping and Diffusion Annealing* Ph.D. thesis Ghent University
[10] The Netlib archive URL http://netlib.sandia.gov/master/index.html