Numerical Methods of the Maxwell-Stefan Diffusion Equations and Applications in Plasma and Particle Transport

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Abstract. In this paper, we present a model based on a local thermodynamic equilibrium, weakly ionized plasma-mixture model used for medical and technical applications in etching processes. We consider a simplified model based on the Maxwell-Stefan model, which describe multicomponent diffusive fluxes in the gas mixture. Based on additional conditions to the fluxes, we obtain an irreducible and quasi-positive diffusion matrix. Such problems results into nonlinear diffusion equations, which are more delicate to solve as standard diffusion equations with Fickian’s approach. We propose explicit time-discretisation methods embedded to iterative solvers for the nonlinearities. Such a combination allows to solve the delicate nonlinear differential equations more effective. We present some first ternary component gaseous mixtures and discuss the numerical methods.

Keywords: Maxwell-Stefan approach, Plasma model, Multi-component mixture, explicit discretization schemes, iterative schemes.

AMS subject classifications. 35K25, 35K20, 74S10, 70G65.

1 Introduction

We are motivated to understand the gaseous mixtures of a normal pressure and room temperature plasma. The understanding of normal pressure, room temperature plasma applications is important for applications in medical and technical processes. Since many years, the increasing importance of plasma chemistry based on the multi-component plasma is a key factor to understand the gaseous mixture processes, see for low pressure plasma [7] and for atmospheric pressure regimes [8].

We consider a simplified Maxwell-Stefan diffusion equation to model the gaseous mixture of multicomponent Plasma. While most classical description of the diffusion goes back to the Fickian’s approach, see [5], we apply the modern...
description of the multicomponent diffusion based on the Maxwell-Stefan’s approach, see [6]. The novel approach considers are more detail description of the flux and concentration, which are in deed not only proportional coupled as in the simplified Fickian’s approach. Here, we deal with a inter-species force balance, which allows to model cross-effects, e.g., so-called reverse diffusion (up-hill diffusion in direction of the gradients).

Such a more detailed modeling results in irreducible and quasi-positive diffusion-matrices, which can be reduced by transforming with reductions or transforming with Perron-Frobenius theorems to solvable partial differential equations, see [1].

The obtained system of nonlinear partial differential equations are delicate to solve and numerically, we have taken into account linearisation methods, e.g., iterative fix-point schemes.

The paper is outlined as follows.

In section 2 we present our mathematical model. A possible reduced model for the further approximations is derived in Section 3. In section 4 we discuss the underlying numerical schemes. The first numerical results are presented in Section 5. In the contents, that are given in Section 6 we summarize our results.

2 Mathematical Model

For the full plasma model, we assumes that the neutral particles can be described as fluid dynamical model, where the elastic collision define the dynamics and few inelastic collisions are, among other reasons, responsible for the chemical reactions.

To describe the individual mass densities, as well as the global momentum and the global energy as the dynamical conservation quantities of the system, corresponding conservation equations are derived from Boltzmann equations.

The individual character of each species is considered by mass-conservation equations and the so-called difference equations.

The extension of the non-mixtured multicomponent transport model, [7] is done with respect to the collision integrals related to the right-hand side sources of the conservation laws.

The conservation laws of the neutral elements are given as

\[ \frac{\partial}{\partial t} \rho_s + \frac{\partial}{\partial r} \cdot \rho_s u_s = m_s Q^{(s)}_n, \]
\[ \frac{\partial}{\partial t} \rho u + \frac{\partial}{\partial r} \cdot (P^r + \rho uu) = -Q^{(e)}_m, \]
\[ \frac{\partial}{\partial t} \mathcal{E}_{\text{tot}}^* + \frac{\partial}{\partial r} \cdot (\mathcal{E}_{\text{tot}}^* u + q^* + P^r \cdot u) = -Q^{(e)}_E. \]

where \( \rho_s \) : density of species \( i \), \( \rho = \sum_{i=1}^{N} \rho_i \), \( u \) : velocity, \( \mathcal{E}_{\text{tot}}^* \) : total energy of the neutral particles.
Further the variable $Q^{(s)}_n$ is the collision term of the mass conservation equation, $Q^{(c)}_m$ is the collision term of the momentum conservation equation and $Q^{(c)}_E$ is the collision term of the energy conservation equation.

We derive the collision term with respect to the Chapman-Enskog method, see [3], and achieve for the first derivatives the following results:

$$m_s Q^{(s)}_n = -\nabla \cdot (\rho_i \sum_{j=0}^{n_s} \mathbf{V}_j^i), \quad (1)$$

$$Q^{(c)}_m = -\sum_{i=1}^{n_s} \rho_i F_i \quad (2)$$

$$Q^{(c)}_E = -\sum_{i=1}^{n_s} \rho_i \rho F_i (\mathbf{u} + \sum_{j=0}^{n_s} \mathbf{V}_j^{(j)}), \quad (3)$$

where $i = 1, \ldots, n_s$, $F_i$ is an external force per unit mass (see Boltzmann equation), further the diffusion velocity is given as:

$$\mathbf{V}_i^0 = 0 \quad (4)$$

$$\mathbf{V}_i^1 = -\sum_{j=1}^{N} D_{ij} (d_j + kT \frac{\Delta T}{T}), \quad (5)$$

where $\sum_{i=1}^{N} d_i = 0$, $d_i = \nabla x_i + x_i \frac{\nabla p}{p} - \frac{\rho_i}{\rho} F_i$, $d_i = d_i - \sum_j d_j^*$,

where $x_i = \frac{\alpha_i}{N}$ is the molar fraction of species $i$.

We have an additional constraint based on the mass fraction of each species:

$$\frac{\partial}{\partial t} y_i + \nabla y_i = R_i(y_1, \ldots, y_N), \quad (8)$$

where $y_i$ is the mass fraction of species $i$, $R_i$ is the net production rate of species $i$ due to his reactions.

Remark 1. The full model problem consider a full coupled system of conservation laws and Maxwell-Stefan equations. Each equations are coupled such that the gaseous mixture influences the transport equations and vice versa. In the following, we decouple the equations system and consider only the delicate Maxwell-Stefan equations.

3 Simplified Model with Maxwell-Stefan Diffusion Equations

We discuss in the following a multicomponent gaseous mixture with three species (ternary mixture). The model-problem is discussed in the experiments of Duncan and Toor, see [4].
Here, they studied an ideal gaseous mixture of the following components:

- Hydrogen ($H_2$, first species),
- Nitrogen ($N_2$, second species),
- Carbon dioxide ($CO_2$, third species).

The Maxwell-Stefan equations are given for the three species as (see also [2]):

\[
\frac{\partial_t \xi_i + \nabla \cdot N_i}{3} = 0, \quad 1 \leq i \leq 3, \tag{9}
\]

\[
\sum_{j=1}^{3} N_j = 0, \tag{10}
\]

\[
\frac{\xi_2 N_1 - \xi_1 N_2}{D_{12}} + \frac{\xi_3 N_1 - \xi_1 N_3}{D_{13}} = -\nabla \xi_1, \tag{11}
\]

\[
\frac{\xi_1 N_2 - \xi_2 N_1}{D_{12}} + \frac{\xi_3 N_2 - \xi_2 N_3}{D_{23}} = -\nabla \xi_2, \tag{12}
\]

where the domain is given as $\Omega \in \mathbb{R}^d, d \in \mathbb{N}^+$ with $\xi_i \in C^2$.

For such ternary mixture, we can rewrite the three differential equations (9) and (11)-(12) with the help of the zero-condition (10) into two differential equations, given as:

\[
\frac{\partial_t \xi_i + \nabla \cdot N_i}{2} = 0, \quad 1 \leq i \leq 2, \tag{13}
\]

\[
\frac{1}{D_{13}} N_1 + \alpha N_1 \xi_2 - \alpha N_2 \xi_1 = -\nabla \xi_1, \tag{14}
\]

\[
\frac{1}{D_{23}} N_2 - \beta N_1 \xi_2 + \beta N_2 \xi_1 = -\nabla \xi_2, \tag{15}
\]

where $\alpha = \left(\frac{1}{D_{12}} - \frac{1}{D_{13}}\right)$, $\beta = \left(\frac{1}{D_{12}} - \frac{1}{D_{23}}\right)$.

Further we have the relations:

- Third mole-fraction: $\xi_3 = 1 - \xi_1 - \xi_2$,
- Third molar flux: $N_3 = -N_1 - N_2$.

4 Numerical Methods

In the following, we discuss the numerical methods, which are based on iterative schemes with embedded explicit discretization schemes. We apply the following methods:

- Iterative Scheme in time (Global Linearisation, Matrix Method),
- Iterative Scheme in Time (Local Linearisation with Richardson’s Method).

For the spatial discretization, we apply finite volume or finite difference methods. The underlying time-discretization is based on a first order explicit Euler method.
4.1 Iterative Scheme in time (Global Linearisation, Matrix Method)

We solve the iterative scheme:

\[
\begin{align*}
\xi_1^{n+1} &= \xi_1^n - \Delta t \, D_+ N_1^n, \\
\xi_2^{n+1} &= \xi_2^n - \Delta t \, D_+ N_2^n, \\
\begin{pmatrix} A & B \\
C & D \end{pmatrix} \begin{pmatrix} N_1^{n+1} \\
N_2^{n+1} \end{pmatrix} &= \begin{pmatrix} -D_+ \xi_1^{n+1} \\
-D_+ \xi_2^{n+1} \end{pmatrix}
\end{align*}
\]

for \( j = 0, \ldots, J \), where \( \xi_1^0 = (\xi_{1,0}^0, \ldots, \xi_{1,J}^0)^T \), \( \xi_2^0 = (\xi_{2,0}^0, \ldots, \xi_{2,J}^0)^T \) and \( I_J \in \mathbb{R}^{J+1} \times \mathbb{R}^{J+1} \), \( N_1^n = (N_{1,0}^n, \ldots, N_{1,J}^n)^T \), \( N_2^n = (N_{2,0}^n, \ldots, N_{2,J}^n)^T \) and \( I_J \in \mathbb{R}^{J+1} \times \mathbb{R}^{J+1} \), where \( n = 0, 1, 2, \ldots, N_{end} \) and \( N_{end} \) are the number of time-steps, i.d. \( N_{end} = T/\Delta t \).

The matrices are given as:

\[
A, B, C, D \in \mathbb{R}^{J+1} \times \mathbb{R}^{J+1}, \quad A_{i,j} = \frac{1}{D_{i3}} + \alpha \xi_{2,j}, \quad j = 0, \ldots, J, \\
B_{i,j} = -\alpha \xi_{1,j}, \quad j = 0, \ldots, J, \\
C_{i,j} = -\beta \xi_{2,j}, \quad j = 0, \ldots, J, \\
D_{i,j} = \frac{1}{D_{23}} + \beta \xi_{1,j}, \quad j = 0, \ldots, J, \\
A_{i,j} = B_{i,j} = C_{i,j} = D_{i,j} = 0, \quad i, j = 0, \ldots, J, \quad i \neq J,
\]

means the diagonal entries given as for the scale case in equation (9) and the outer-diagonal entries are zero.

The explicit form with the time-discretization is given as:

\[\begin{pmatrix} N_1^0 \\
N_2^0 \end{pmatrix} = \begin{pmatrix} A & B \\
C & D \end{pmatrix} \begin{pmatrix} -D_+ \xi_1^0 \\
-D_+ \xi_2^0 \end{pmatrix} \]

Algorithm 1 1.) Initialisation \( n = 0 \):

\[
\begin{pmatrix} N_1^0 \\
N_2^0 \end{pmatrix} = \begin{pmatrix} A & B \\
C & D \end{pmatrix} \begin{pmatrix} -D_+ \xi_1^0 \\
-D_+ \xi_2^0 \end{pmatrix}
\]

where \( \xi_1^0 = (\xi_{1,0}^0, \ldots, \xi_{1,J}^0)^T \), \( \xi_2^0 = (\xi_{2,0}^0, \ldots, \xi_{2,J}^0)^T \) and \( \xi_1^0 = \xi_1^0(j \Delta x) \), \( \xi_2^0 = \xi_2^0(j \Delta x) \), \( j = 0, \ldots, J \) and given as for the different initialisations, we have:

1. Uphill example

\[
\xi_1^n(x) = \begin{cases} 0.8 & \text{if } 0 \leq x < 0.25, \\
1.6(0.75 - x) & \text{if } 0.25 \leq x < 0.75, \\
0.0 & \text{if } 0.75 \leq x \leq 1.0,
\end{cases}
\]

\[
\xi_2^n(x) = 0.2, \quad \text{for all } x \in \Omega = [0, 1],
\]

2. Diffusion example (Asymptotic behavior)

\[
\xi_1^n(x) = \begin{cases} 0.8 & \text{if } 0 \leq x \leq 0.5, \\
0.0 & \text{else},
\end{cases}
\]

\[
\xi_2^n(x) = 0.2, \quad \text{for all } x \in \Omega = [0, 1],
\]
The inverse matrices are given as:

\[ \tilde{A}, \tilde{B}, \tilde{C}, \tilde{D} \in \mathbb{R}^{J+1} \times \mathbb{R}^{J+1}, \]

\[ \tilde{A}_{j,j} = \gamma_j (\frac{1}{D_{23}} + \beta \xi_{1,j}^0), \quad j = 0, \ldots, J, \]

\[ B_{j,j} = \gamma_j \alpha \xi_{1,j}^0, \quad j = 0, \ldots, J, \]

\[ C_{j,j} = \gamma_j \beta \xi_{2,j}^0, \quad j = 0, \ldots, J, \]

\[ D_{j,j} = \gamma_j (\frac{1}{D_{13}} + \alpha \xi_{2,j}^0), \quad j = 0, \ldots, J, \]

\[ \gamma_j = \frac{1}{1 + \alpha D_{13} \xi_{2,j}^{n+1} + \beta D_{23} \xi_{1,j}^n}, \quad j = 0, \ldots, J, \]

\[ \tilde{A}_{i,j} = \tilde{B}_{i,j} = \tilde{C}_{i,j} = \tilde{D}_{i,j} = 0, \quad i, j = 0, \ldots, J, i \neq J. \]

Further the values of the first and the last grid points of \( N \) are zero, means

\[ N_0^1 = N_1^1 = N_0^2 = N_2^2 = 0 \] (boundary condition).

2.) Next time-steps (till \( n = N_{\text{end}} \)):

2.1) Computation of \( \xi_{1}^{n+1} \) and \( \xi_{2}^{n+1} \)

\[ \xi_{1}^{n+1} = \xi_{1}^n - \Delta t D_+ N_1^n, \]

\[ \xi_{2}^{n+1} = \xi_{2}^n - \Delta t D_+ N_2^n, \]

2.2) Computation of \( N_1^{n+1} \) and \( N_2^{n+1} \)

\[ \begin{pmatrix} N_1^{n+1} \\ N_2^{n+1} \end{pmatrix} = \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{pmatrix} \begin{pmatrix} -D_{-1} \xi_{1}^{n+1} \\ -D_{-1} \xi_{2}^{n+1} \end{pmatrix}, \]

where \( \xi_{1}^n = (\xi_{1,0}^n, \ldots, \xi_{1,J}^n)^T, \xi_{2}^n = (\xi_{2,0}^n, \ldots, \xi_{2,J}^n)^T \) and the inverse matrices are given as:

\[ \tilde{A}, \tilde{B}, \tilde{C}, \tilde{D} \in \mathbb{R}^{J+1} \times \mathbb{R}^{J+1}, \]

\[ \tilde{A}_{j,j} = \gamma_j (\frac{1}{D_{23}} + \beta \xi_{1,j}^{n+1}), \quad j = 0, \ldots, J, \]

\[ B_{j,j} = \gamma_j \alpha \xi_{1,j}^{n+1}, \quad j = 0, \ldots, J, \]

\[ C_{j,j} = \gamma_j \beta \xi_{2,j}^{n+1}, \quad j = 0, \ldots, J, \]

\[ D_{j,j} = \gamma_j (\frac{1}{D_{13}} + \alpha \xi_{2,j}^{n+1}), \quad j = 0, \ldots, J, \]

\[ \gamma_j = \frac{D_{13} D_{23}}{1 + \alpha D_{13} \xi_{2,j}^{n+1} + \beta D_{23} \xi_{1,j}^n}, \quad j = 0, \ldots, J, \]

\[ \tilde{A}_{i,j} = \tilde{B}_{i,j} = \tilde{C}_{i,j} = \tilde{D}_{i,j} = 0, \quad i, j = 0, \ldots, J, i \neq J. \]

Further the values of the first and the last grid points of \( N \) are zero, means

\[ N_0^n = N_1^n = N_2^n = N_{2,J}^n = 0 \] (boundary condition).

3.) Do \( n = n + 1 \) and goto 2.)
4.2 Iterative Scheme in Time (Local Linearisation with Richardson’s Method)

We solve the iterative scheme given in the Richardson iterative scheme:

\[
\begin{align*}
\xi_1^{n+1,k} &= \xi_1^n - \Delta t \, D_+ N_2^{n+1}, \\
\xi_2^{n+1,k} &= \xi_2^n - \Delta t \, D_+ N_2^{n+1}, \\
(A^{n+1,k-1} B^{n+1,k-1}) (N_1^{n+1}, N_2^{n+1}) &= (-D_+ \xi_1^{n+1,k-1}, -D_+ \xi_2^{n+1,k-1})
\end{align*}
\]

for \( j = 0, \ldots, J \), where \( \xi_1^n = (\xi_1^n, \ldots, \xi_{1,j}^n)^T \), \( \xi_2^n = (\xi_2^n, \ldots, \xi_{2,j}^n)^T \) and \( I_j \in \mathbb{R}^{J+1} \times \mathbb{R}^{J+1} \), \( N_1^n = (N_{1,0}^n, \ldots, N_{1,j}^n)^T \), \( N_2^n = (N_{2,0}^n, \ldots, N_{2,j}^n)^T \) and \( I_J \in \mathbb{R}^{J+1} \times \mathbb{R}^{J+1} \), where \( n = 0, 1, 2, \ldots, N_{end} \) and \( N_{end} \) are the number of time-steps, i.e. \( N_{end} = T/\Delta t \).

Further \( k = 1, 2, \ldots, K \) is the iteration index with where \( \xi_1^{k+1,0} = (\xi_1^{0,0}, \ldots, \xi_{1,j}^{0,0})^T \), \( \xi_2^{k+1,0} = (\xi_2^{0,0}, \ldots, \xi_{2,j}^{0,0})^T \) and \( I_J \in \mathbb{R}^{J+1} \times \mathbb{R}^{J+1} \) is the start solution given with the solution at \( t = t^n \).

The matrices are given as:

\[
\begin{align*}
A^{n+1,k-1}, B^{n+1,k-1}, C^{n+1,k-1}, D^{n+1,k-1} &\in \mathbb{R}^{J+1} \times \mathbb{R}^{J+1}, \\
A_{j,j}^{n+1,k-1} &= \frac{1}{D_{13}} + \alpha \xi_{2,j}^{n+1,k-1}, \; j = 0, \ldots, J, \\
B_{j,j}^{n+1,k-1} &= -\alpha \xi_{1,j}^{n+1,k-1}, \; j = 0, \ldots, J, \\
C_{j,j}^{n+1,k-1} &= -\beta \xi_{2,j}^{n+1,k-1}, \; j = 0, \ldots, J, \\
D_{j,j}^{n+1,k-1} &= \frac{1}{D_{23}} + \beta \xi_{1,j}^{n+1,k-1}, \; j = 0, \ldots, J, \\
A_{i,j}^{n+1,i-1} &= B_{i,j}^{n+1,i-1} = C_{i,j}^{n+1,i-1} = D_{i,j}^{n+1,i-1} = 0, \; i, j = 0, \ldots, J, \; i \neq J
\end{align*}
\]

means the diagonal entries given as for the scale case in equation (55) and the outer-diagonal entries are zero.

The explicit form with the time-discretization is given as:

**Algorithm 2 1.) Initialisation** \( n = 0 \) with an explicit time-step (CFL condition is given):

\[
\begin{align*}
\left[ \begin{array}{c}
N_1^0 \\
N_2^0
\end{array} \right] &= \left[ \begin{array}{c}
\hat{A} \\
\hat{C}
\end{array} \right] \left[ \begin{array}{c}
-\hat{D} \xi_1^0 \xi_2^0 \\
-D_+ \xi_2^0
\end{array} \right]
\end{align*}
\]

where \( \xi_1^0 = (\xi_1^0, \ldots, \xi_{1,j}^0)^T \), \( \xi_2^0 = (\xi_2^0, \ldots, \xi_{2,j}^0)^T \) and \( \xi_1^0 = \xi_1^n(j \Delta x) \), \( \xi_2^0 = \xi_2^n(j \Delta x) \), \( j = 0, \ldots, J \) and given as for the different intialisations, we have:

1. **Uphill example**

\[
\xi_1^{in}(x) = \begin{cases} 
0.8 & \text{if } 0 \leq x < 0.25, \\
1.6(0.75 - x) & \text{if } 0.25 \leq x < 0.75, \\
0.0 & \text{if } 0.75 \leq x \leq 1.0,
\end{cases}
\]

\[
\xi_2^{in}(x) = 0.2, \; \text{for all } x \in \Omega = [0, 1],
\]

2. **Plain example**

\[
\xi_1^{in}(x) = \begin{cases} 
0.8 & \text{if } 0 \leq x < 0.25, \\
1.6(0.75 - x) & \text{if } 0.25 \leq x < 0.75, \\
0.0 & \text{if } 0.75 \leq x \leq 1.0,
\end{cases}
\]

\[
\xi_2^{in}(x) = 0.2, \; \text{for all } x \in \Omega = [0, 1],
\]
2. Diffusion example (Asymptotic behavior)

\[ \xi_1^n(x) = \begin{cases} 0.8 & \text{if } 0 \leq x \leq 0.5, \\ 0.0 & \text{else} \end{cases}, \quad (59) \]

\[ \xi_2^n(x) = 0.2, \text{ for all } x \in \Omega = [0, 1], \quad (60) \]

The inverse matrices are given as:

\[ \tilde{A}, \tilde{B}, \tilde{C}, \tilde{D} \in \mathbb{R}^{J+1}, \quad (61) \]

\[ \tilde{A}_{j,j} = \gamma_j \left( \frac{1}{D_{13}} + \beta \xi_{1,j}^0 \right), \quad j = 0 \ldots, J, \quad (62) \]

\[ B_{j,j} = \gamma_j \alpha \xi_{1,j}^0, \quad j = 0 \ldots, J, \quad (63) \]

\[ C_{j,j} = \gamma_j \beta \xi_{2,j}^0, \quad j = 0 \ldots, J, \quad (64) \]

\[ D_{j,j} = \gamma_j \left( \frac{1}{D_{13}} + \alpha \xi_{2,j}^0 \right), \quad j = 0 \ldots, J, \quad (65) \]

\[ \gamma_j = \frac{D_{13} D_{23}}{1 + \alpha D_{13} \xi_{2,j}^0 + \beta D_{23} \xi_{1,j}^0}, \quad j = 0 \ldots, J, \quad (66) \]

\[ \tilde{A}_{i,j} = \tilde{B}_{i,j} = \tilde{C}_{i,j} = \tilde{D}_{i,j} = 0, \quad i,j = 0 \ldots, J, \quad i \neq J, \quad (67) \]

Further the values of the first and the last grid points of \( N \) are zero, means \( N_{1,0} = N_{1,J} = N_{2,0} = N_{2,J} = 0 \) (boundary condition).

2.) Next timesteps (till \( n = N_{\text{end}} \)) (iterative scheme restricted via the CFL condition based on the previous iterative solutions in the matrices):

2.1) Computation of \( \xi_1^{n+1,J} \) and \( \xi_2^{n+1,J} \)

\[ \xi_1^{n+1,k} = \xi_1^n - \Delta t \, D_4 \, N_1^{n+1}, \quad (68) \]

\[ \xi_2^{n+1,k} = \xi_2^n - \Delta t \, D_2 \, N_2^{n+1}, \quad (69) \]

2.2) Computation of \( N_1^{n+1,k-1} \) and \( N_2^{n+1,k-1} \)

\[ \begin{pmatrix} N_1^{n+1} \\ N_2^{n+1} \end{pmatrix} = \begin{pmatrix} \tilde{A}^{n+1,k-1} & \tilde{B}^{n+1,k-1} \\ \tilde{C}^{n+1,k-1} & \tilde{D}^{n+1,k-1} \end{pmatrix} \begin{pmatrix} -D_4 \xi_1^{n+1,k-1} \\ -D_2 \xi_2^{n+1,k-1} \end{pmatrix} \quad (70) \]

where \( \xi_1^n = (\xi_{1,0}^n, \ldots, \xi_{1,J}^n)^T \), \( \xi_2^n = (\xi_{2,0}^n, \ldots, \xi_{2,J}^n)^T \) and the inverse matrices are given as:

\[ \tilde{A}^{n+1,k-1}, \tilde{B}^{n+1,k-1}, \tilde{C}^{n+1,k-1}, \tilde{D}^{n+1,k-1} \in \mathbb{R}^{J+1}, \quad (71) \]

\[ \tilde{A}_{j,j}^{n+1,k-1} = \gamma_j \left( \frac{1}{D_{13}} + \beta \xi_{1,j}^{n+1,k-1} \right), \quad j = 0 \ldots, J, \quad (72) \]

\[ B_{j,j}^{n+1,k-1} = \gamma_j \alpha \xi_{1,j}^{n+1,k-1}, \quad j = 0 \ldots, J, \quad (73) \]

\[ C_{j,j}^{n+1,k-1} = \gamma_j \beta \xi_{2,j}^{n+1,k-1}, \quad j = 0 \ldots, J, \quad (74) \]

\[ D_{j,j}^{n+1,k-1} = \gamma_j \left( \frac{1}{D_{13}} + \alpha \xi_{2,j}^{n+1,k-1} \right), \quad j = 0 \ldots, J, \quad (75) \]
\[
\gamma_j = \frac{D_{13}D_{23}}{1 + \alpha D_{13}n^{1+k-1} + \beta D_{23}x^{n+1,k-1}}, \ j = 0, \ldots, J, \tag{76}
\]

\[
\hat{A}_{ij}^{n+1,k-1} = \hat{B}_{ij}^{n+1,k-1} = \hat{C}_{ij}^{n+1,k-1} = \hat{D}_{ij}^{n+1,k-1} = 0, \ i, j = 0, \ldots, J, \ i \neq J. \tag{77}
\]

Further the values of the first and the last grid points of \(N\) are zero, means \(N_{1,0}^{n+1} = N_{0,1}^{n+1} = N_{2,0}^{n+1} = N_{2,J}^{n+1} = 0\) (boundary condition).

Further \(k = 1, 2, \ldots, K\) is the iteration index with where \(\xi_{1,0}^{n+1} = (\xi_{1,0}^{n}, \ldots, \xi_{1,J}^{n})^T\), \(\xi_{2,0}^{n+1} = (\xi_{2,0}^{n}, \ldots, \xi_{2,J}^{n})^T\) and \(I_J \in \mathbb{R}^{J+1} \times \mathbb{R}^{J+1}\) is the start solution given with the solution at \(t = t^n\).

3.) Do \(n = n + 1\) and goto 2.)

5 Numerical Experiments

In the following, we concentrate on the following three component system, which is given as:

\[
\partial_t \xi_i + \partial_x N_i = 0, \ 1 \leq i \leq 3, \tag{78}
\]

\[
\sum_{j=1}^{3} N_j = 0, \tag{79}
\]

\[
\frac{\xi_2 N_1 - \xi_1 N_2}{D_{12}} + \frac{\xi_3 N_1 - \xi_1 N_3}{D_{13}} = -\partial_x \xi_1, \tag{80}
\]

\[
\frac{\xi_1 N_2 - \xi_2 N_1}{D_{12}} + \frac{\xi_3 N_2 - \xi_2 N_3}{D_{23}} = -\partial_x \xi_2, \tag{81}
\]

where the domain is given as \(\Omega \in \mathbb{R}^d, \ d \in \mathbb{N}^+\) with \(\xi_i \in C^2\).

The parameters and the initial and boundary conditions are given as:

- \(D_{12} = D_{13} = 0.833\) (means \(\alpha = 0\) and \(D_{23} = 0.168\) (Uphill diffusion, semi-degenerated Duncan and Toor experiment),
- \(D_{12} = 0.0833, D_{13} = 0.680\) and \(D_{23} = 0.168\) (asymptotic behavior, Duncan and Toor experiment, see [4]),
- \(J = 140\) (spatial grid points),
- The time-step-restriction for the explicit method is given as:
  \[
  \Delta t \leq \frac{(\Delta x)^2}{2 \max(D_{12}, D_{13}, D_{23})},
  \]
- The spatial domain is \(\Omega = [0, 1]\), the time-domain \([0, T] = [0, 1]\),
- The initial conditions are:
  1. Uphill example
    \[
    \xi_1^{in}(x) = \begin{cases} 
    0.8 & \text{if } 0 \leq x < 0.25, \\
    1.6(0.75 - x) & \text{if } 0.25 \leq x < 0.75, \\
    0.0 & \text{if } 0.75 \leq x \leq 1.0,
    \end{cases}
    \tag{82}
    \]
    \[
    \xi_2^{in}(x) = 0.2, \text{ for all } x \in \Omega = [0, 1],
    \tag{83}
    \]
2. Diffusion example (Asymptotic behavior)

\[
\xi_1^\text{in}(x) = \begin{cases} 
0.8 & \text{if } 0 \leq x < 0.5, \\
0.0 & \text{else,}
\end{cases} 
\]  
(84)

\[
\xi_2^\text{in}(x) = 0.2, \text{ for all } x \in \Omega = [0, 1].
\]  
(85)

- The boundary conditions are of no-flux type:

\[
N_1 = N_2 = N_3 = 0, \text{ on } \partial \Omega \times [0, 1].
\]  
(86)

We could reduce to a simpler model problem as:

\[
\partial_t \xi_i + \partial_x \cdot N_i = 0, \quad 1 \leq i \leq 2,
\]  
(87)

\[
\frac{1}{D_{13}} N_1 + \alpha N_1 \xi_2 - \alpha N_2 \xi_1 = -\partial_x \xi_1,
\]  
(88)

\[
\frac{1}{D_{23}} N_2 - \beta N_1 \xi_2 + \beta N_2 \xi_1 = -\partial_x \xi_2,
\]  
(89)

where \(\alpha = \left(\frac{1}{D_{12}} - \frac{1}{D_{13}}\right)\), \(\beta = \left(\frac{1}{D_{12}} - \frac{1}{D_{23}}\right)\).

We rewrite into:

\[
\partial_t \xi_1 + \partial_x \cdot N_1 = 0,
\]  
(90)

\[
\partial_t \xi_2 + \partial_x \cdot N_2 = 0,
\]  
(91)

\[
\begin{pmatrix} \frac{1}{D_{13}} + \alpha \xi_2 \\ -\beta \xi_2 \end{pmatrix} + \begin{pmatrix} -\alpha \xi_1 \\ \beta \xi_1 \end{pmatrix} \begin{pmatrix} N_1 \\ N_2 \end{pmatrix} = \begin{pmatrix} -\partial_x \xi_1 \\ -\partial_x \xi_2 \end{pmatrix},
\]  
(92)

and we have

\[
\partial_t \xi_1 + \partial_x \cdot N_1 = 0,
\]  
(93)

\[
\partial_t \xi_2 + \partial_x \cdot N_2 = 0,
\]  
(94)

\[
\begin{pmatrix} N_1 \\ N_2 \end{pmatrix} = \frac{D_{13} D_{23}}{1 + \alpha D_{13} \xi_2 + \beta D_{23} \xi_1} \begin{pmatrix} \frac{1}{D_{23}} + \beta \xi_1 \\ \alpha \xi_1 \end{pmatrix} \begin{pmatrix} -\partial_x \xi_1 \\ -\partial_x \xi_2 \end{pmatrix}.
\]  
(95)

The next step is to apply the semi-discretization of the partial differential operator \(\frac{\partial}{\partial x}\).

We apply the first differential operator in equation (93) and (94) as an forward upwind scheme given as

\[
\frac{\partial}{\partial x} = D_+ = \frac{1}{\Delta x} \cdot \begin{pmatrix} -1 & 0 \ldots & 0 \\ 1 & -1 & 0 \ldots & 0 \\ \vdots & \ldots & \ddots & \vdots \\ 0 & 1 & -1 & 0 \\ 0 \ldots & 0 & 1 & -1 \end{pmatrix} \in \mathbb{R}^{(J+1) \times (J+1)}.
\]  
(96)
and the second differential operator in equation (95) as an backward upwind scheme given as

$$\frac{\partial}{\partial x} = D_- = \frac{1}{\Delta x} \cdot \begin{pmatrix} -1 & 1 & 0 & \cdots & 0 \\ 0 & -1 & 1 & 0 & \cdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -1 & 1 \\ 0 & \cdots & 0 & 0 & -1 \end{pmatrix} \in \mathbb{R}^{(J+1) \times (J+1)}. \quad (97)$$

5.1 Experiments with the Iterative scheme in time (Global Linearisation)

In the first experiments, we test the first iterative scheme (iterative scheme in time (Global Linearisation)). We test the different schemes and obtain the results shown in Figure 1.

![Fig. 1. The figures present the results of the concentration $c_1$, $c_2$ and $c_3$.](image)

The concentration and their fluxes are given in Figure 2.

The full plots in time and space of the concentrations and their fluxes are given in Figure 3.

The space-time regions where $-N2\partial_x \xi_2 \geq 0$ for the uphill diffusion and asymptotic diffusion, given in Figure 4.

Remark 2. The first method applies a global linearization based on the time-steps. All effects are resolved, by the way, we have taken into account the CFL condition. We achieve better results with finer time-steps, e.g., $\Delta t_{CFL}/8$, such that the global linearisation, via the time-step is important.
Fig. 2. The upper figures present the results of the concentration $c_1$ and $-\partial_x \xi_1$. The lower figures presents the results of $c_2$ and $-\partial_x \xi_2$.

5.2 Iterative Schemes in time (Local Linearisation)

In the next series of experiments, we apply the more refined linearization scheme, means the iterative approximation in a single time-step.

We apply the numerical convergence of the schemes with the reference solution of the explicit method by $\Xi_{\text{ref}} = (\xi_1, \xi_2)$ where the time-step is $\Delta t_{CFL}/8$ for this refined solution the error is only marginal.

Based on the reference solution, we deal with the following errors:

$$E_{L_1, \Delta x}(t) = \int_{\Omega} |\Xi_{\text{method}, J, \Delta x}(x, t) - \Xi_{\text{ref}}(x, t)| \, dx$$

$$= \Delta x \sum_{i=1}^{N} |\Xi_{\text{method}, J, \Delta x}(x_i, t) - \Xi_{\text{ref}}(x_i, t)|,$$

where $\text{method, } J$ is the Richardson with $J$ iterative steps and $\Delta t = \Delta t_{CFL}, \Delta t_{CFL}/2, \Delta t_{CFL}/4$. Further $\text{method, } \text{expl}$ is the explicit method with $\Delta t = \Delta t_{CFL}, \Delta t_{CFL}/2, \Delta t_{CFL}/4$.

We apply the different versions of time-steps and iterative steps, a reference solution is obtain with a fine time-step $\Delta t = \Delta t_{CFL}/4$. We see improvements in Figure 5 and the errors in Figure 6.

Remark 3. Here, we see the benefit of large time-steps with $N = 100$ and $K = 800$, means we have only 100 time-steps and 800 iterative steps, which are not
Fig. 3. The figures present the results of the 3d plots in time and space. The upper figures present the results of the concentration $c_1$ and $-\partial_x \xi_1$. The lower figures present the results of $c_2$ and $-\partial_x \xi_2$.

expensive. Therefore we could gain the same results as with many small time-steps $N = 80000$ and only one iterative step $K = 1$. Such that the relaxation method benefits with the iterative cycles and we could enlarge the time-steps.

**Remark 4.** The second method applies a linear linearization based on the iterative approaches in each single time-step. We have the benefit of a relaxation in each local time-step, such that we see a more accurate solution also with larger time-steps than in the global linearization method.

6 Conclusions and Discussions

We present a fluid model based on Maxwell-Stefan diffusion equations. The underlying problems for such a more delicate diffusion matrix is discussed. Based on the nonlinear partial differential equations, we have to apply linearisation approaches. For first test-examples, we achieve more accurate results for a so-called local linearized scheme. In future, we concentrate on the numerical convergence analysis and generalize our results to real-life applications.
Fig. 4. The figures present the asymptotic diffusion (left hand side) and uphill diffusion (right hand side) in the space-time region.

Fig. 5. The figures present the solutions of the different time-step and iterative step of the Richardson-method

References

1. D. Bothe. *On the Maxwell-Stefan equations to multicomponent diffusion.* Progress in Nonlinear Differential Equations and their Applications, P. Guidotti, Chr. Walker et al., eds., Springer, Basel, 60:81-93, 2011.
2. L. Boudin, B. Grec and F. Salvarani. *A Mathematical and Numerical Analysis of the Maxwell-Stefan Diffusion Equations,* Discrete and Continuous Dynamical Systems Series B, 17(5): 1427-1440 2012.
3. S. Chapman and Th.G. Cowling. *The mathematical theory of non-uniform gases: an account of the kinetic theory of viscosity, thermal conduction, and diffusion in gases.* Cambridge University Press, 1990.
4. J.B. Duncan and H.L. Toor. *An experimental study of three component gas diffusion.* AIChE Journal, 8:38-41, 1962.
5. A. Fick. *On liquid diffusion.* Phil. Mag., 10:30-39, 1855.
6. J.C. Maxwell. *On the dynamical theory of gases.* Phil. Trans. R. Soc., 157:49-88, 1866.
7. T.K. Senega and R.P. Brinkmann. *A multi-component transport model for nonequilibrium low-temperature low-pressure plasmas.* J. Phys. D: Appl.Phys., 39, 1606-1618, 2006.
**Fig. 6.** The figures present the errors of the different time-step and iterative step solutions.

8. Y. Tanaka. *Two-temperature chemically non-equilibrium modelling of high-power Ar-N₂ inductively coupled plasmas at atmospheric pressure.* Journal of Physics D: Applied Physics, 37:1190-1205, 2004.