Splitting Methods For Solving Multi-Component Transport Model: A Multicomponent Mixture for Hydrogen Plasma

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Abstract. In this paper, we present a splitting algorithm to solve multicomponent transport models. These models are related to plasma simulations, in which we consider the local thermodynamic equilibrium and weakly ionised plasma-mixture models that are used for medical and technical applications in etching processes. These multi-component transport-mixture models can be derived by approximately solving a linearised multi-component Boltzmann equation with an approximation of the collision terms in the mass, momentum and energy equations. The model-equations are nonlinear partial differential equations and they are known as Stefan-Maxwell equations. However, these partial differential equations are delicate to solve and we propose to use noniterative and iterative splitting methods. In the numerical experiments, we see the benefit of the iterative splitting methods, while these methods can relax the nonlinear terms.

Keywords: multi-component model, Boltzmann equation, Chapman-Enskog expansion, Stefan-Maxwell equations, splitting methods, iterative splitting methods.

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

1 Introduction

Understanding normal pressure, room temperature plasma applications is important because of their use in medical and technical processes. The increasing importance of plasma chemistry based on multi-component plasma is a key factor for this trend, for low pressure plasma see [15] and for atmospheric pressure regimes see [19]. Both the influence of the mass transfer in the multi-component mixture and the standard conservation laws have to be improved. Although these improvements are well-known in fusion research—see, for example, the modelling of high ionised plasmas [13]—, only a little work has been done for a weak-ionised plasma in atmospheric pressure regimes.
In this paper, we concentrate on an extension of the multicomponent transport model with respect to the reaction terms, see [18], while we can approximate the collision integrals. The diffusive velocity is simulated by the Stefan-Maxwell problem transport algorithm, see [8]. Based on the nonlinear diffusion term, we have to apply numerical schemes that can solve the Stefan-Maxwell problem. We propose iterative schemes in combination with splitting approaches, which means that we decompose the transport- and reaction-parts, see [14], [16] and [9]. These combinations are efficient and the numerical error can be reduced by the iterative approaches.

The rest of this paper is structured as follows. In section 2 we present our mathematical model. In section 3 we present a simplification of the mathematical model to obtain a computable model. The different solver parts are presented in section 4. The numerical algorithms and examples are given in Section 5. Finally, in Section 6 we summarise our results.

2 Mathematical Model

The starting point for plasma gas mixtures is given in the following reference frame, see also [10], [11] and [17]. We concentrate on the heavy particle description, which is discussed in [18].

The distribution function of the heavy particles are given as:

\[ f_i(x, c_i, t) \]

while \( x \) is the three-dimensional spatial coordinate, \( c_i \) is the velocity of the molecule and \( t \) is the time.

The heavy-particle species distribution are given as:

\[ D_i(f_i) = S_i(f) + C_i(f), \quad i \in I \]

(1)

where \( S_i(f) \) is the scattering source term and given in [10], \( C_i(f) \) is the reactive source term and given in [10]. The differential operator is given as

\[ D_i(f_i) = \frac{\partial}{\partial t} f_i + c_i \cdot \nabla_x f_i + \frac{q_i}{m_i} (E + c_i \times B) \cdot \nabla_{c_i} f_i, \quad i \in I. \]

(2)

Further \( q_i \) is the charge of the \( i \)-th species, \( m_i \) the mass of the \( i \)-th species and \( E, B \) are the electric and magnetic fields, we also assume \( b_i = \frac{q_i}{m_i} (E + c_i \times B) \) is the external force, related to the electro-magnetic field.

In the next step, we apply the Chapman-Enskog expansion, while the zero-th terms correspond to a Maxwellian distribution and we obtain the Euler equations. The first-order perturbed distribution function, where a linearized Boltzmann equation is applied, lead to a Navier-Stokes equation, see [10].

We rewrite the generalized Boltzmann-equation into an Enskog-expansion, see [10]:

\[ D_i(f_i) = \frac{1}{\epsilon} S_i(f) + \epsilon C_i(f), \quad i \in I, \]

(3)

while \( \epsilon \) is a scaling factor, while \( \frac{1}{\epsilon} \) mean, that fast collisions or nonreactive collisions drive the heavy species to the Maxwell equilibrium.
The species distribution functions are given as:
\[ f_i = f_i^0 (1 + \epsilon \phi_i + \mathcal{O} (\epsilon^2)), \ i \in I. \] (4)

### 2.1 Zeroth order approximation

For the equation with powers \( \frac{1}{\epsilon} \) in (3), we have:
\[ S_i(f^0) = 0, \ i \in I, \] (5)
with \( f^0 = (f_i^0)_{i \in I} \) and it follows the Maxwell distribution function.

For the equations with power \( \epsilon^0 \), we obtain the zero-th order macroscopic equations, which are given as the Euler’s equations:

\[
\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{v}) = m_i \omega_i^0, \ i \in I, \tag{6}
\]

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p I) = \sum_{i=1}^I \rho_i \mathbf{b}_i, \tag{7}
\]

\[
\frac{\partial (\frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} + \mathcal{E})}{\partial t} + \nabla \cdot \left( \left( \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} + \mathcal{E} + p \right) \mathbf{v} \right) = \sum_{i=1}^I \rho_i \mathbf{v} \cdot \mathbf{b}_i, \tag{8}
\]
where \( \rho = \sum_{i=1}^I \rho_i \) is the mass density of all species, \( p \) is the thermodynamic pressure. \( \omega_i^0 \) is the zero-th order production rate of species \( i \) with:
\[
\omega_i^0 = \sum_{i \in Q_i} \int C_i(f^0) \, dc_i, \tag{9}
\]
where \( Q_i \) is the set of the quantum internal energy states of \( I \) of species \( i \). The internal energy is given as:
\[
\mathcal{E} = \sum_{i=1}^I \sum_{i \in Q_i} \int \left( \frac{1}{2} m_i (c_i - \mathbf{v}) \cdot (c_i - \mathbf{v}) + E_{ii} \right) f^0_i dc_i, \tag{10}
\]
see [1].

### 2.2 First order approximation

For the first order approximation, a linearized Boltzmann operator around the Maxwellian distribution is used, see [10].

We have a linearized Boltzmann equation, which is given as:
\[
\mathcal{J}_i^S (\phi) = \Phi_i, \ i \in I, \tag{11}
\]
\[
\Phi_i = -d_i (\log f_i^0) + \frac{C_i(f^0)}{f_i^0}, \ i \in I, \tag{12}
\]
with \((\mathcal{J}_i^S)_{i \in I}\) is the linearized Boltzmann operator, see [10].

For the equations with power \(\epsilon^1\), we obtain the first order macroscopic equations, which are given as the macroscopic equations in the Navier-Stokes regime:

\[
\begin{align*}
\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{v}) + \nabla \cdot (\rho_i \mathbf{V}_i) &= m_i \omega_i^0, \quad i \in I, \\
\frac{\partial (\rho \mathbf{V})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + pI) + \nabla \cdot \mathbf{P} &= \sum_{i=1}^I \rho_i \mathbf{b}_i, \\
\frac{\partial (\frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} + \mathcal{E})}{\partial t} + \nabla \cdot \left( \left( \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} + \mathcal{E} + p \right) \mathbf{v} \right) + \nabla \cdot \mathbf{Q} + \mathbf{P} \cdot \mathbf{v} &= \sum_{i=1}^I \rho_i \cdot \mathbf{b}_i (\mathbf{v} + \mathbf{V}_i),
\end{align*}
\]

where we have the following operators:

- The species diffusion velocities \(\mathbf{V}_i\):
  \[
  \rho_i \mathbf{V}_i = m_i \sum_{I \in Q_i} \int (\mathbf{c}_i - \mathbf{v}) f_i^0 \phi_i \, d\mathbf{c}_i, \quad i \in I,
  \]

- The viscous tensor \(\mathbf{P}\):
  \[
  \mathbf{P} = \sum_{i=1}^I \sum_{I \in Q_i} \int m_i (\mathbf{c}_i - \mathbf{v}) \otimes (\mathbf{c}_i - \mathbf{v}) f_i^0 \phi_i \, d\mathbf{c}_i,
  \]

- and the heat flux \(\mathbf{Q}\):
  \[
  \mathbf{Q} = \sum_{i=1}^I \sum_{I \in Q_i} \int \left( \frac{1}{2} m_i (\mathbf{c}_i - \mathbf{v}) \cdot (\mathbf{c}_i - \mathbf{v}) + E_{iI} (\mathbf{c}_i - \mathbf{v}) f_i^0 \phi_i \right) \, d\mathbf{c}_i,
  \]

see [\ref{10}].

\section{Simplified mathematical Model for three species}

This section will present a simplified mathematical model, which concentrates on the first equation of the Navier-Stokes type equations for the heavy species, see Section 2.

We assume that we have \(v = 0\) in a so called isobaric case, see [3].

Then, the Navier-Stokes regime [13]-[15] reduced to a convection-diffusion reaction equation, which are also developed in the works of [18] and [12].

This model considers the mass-transport of a hydrogen plasma. Here, we deal with a hydrogen plasma that is a mixture of \(H, H_2, H_2^+\) particles, means atoms, molecules and ions.
We take into account the dissociation and ionisation reactions, which are given as:
\[
H_2 + e \xrightarrow{\lambda_1} H_2^+ + 2e, \quad (20)
\]
\[
H_2 + e \xrightarrow{\lambda_2} 2H + e, \quad (21)
\]
where the electron temperature is given as \( T_e = 17400 \ [K] \) and the gas temperature values remain constant \( T_h = 600 \ [K] \).

Furthermore, we have \( \lambda_1 = 1.58 \times 10^{-15} T_e^{0.5} \exp\left(\frac{-15.372}{T_e}\right) = 2.082 \times 10^{-13} \) and \( \lambda_2 = 1.413 \times 10^{-15} T_e^2 \exp\left(\frac{-4.48}{T_e}\right) = 4.276 \times 10^{-7} \).

The diffusion coefficients are given in the following formula:
\[
D_{ij} = \frac{3}{16} \frac{f_{ij} k_B^2 T_i T_j}{p_i m_j \Omega_{ij}(1,1)} (T_{ij}), \quad (22)
\]
where the parameters are:
- \( f_{ij} \) is a correction factor of order unity,
- \( m_{ij} = \frac{m_i m_j}{m_i + m_j} \) is the reduced mass,
- \( m_i \) is the mass of species \( i \),
- \( m_j \) is the mass of species \( j \),
- \( p \) is pressure,
- \( T_i, T_j \) is the temperature of the corresponding species, and \( \Omega_{ij}(1,1) \) is a collision integral \( [7] \).

We assume the following binary diffusion parameters for our experiments:
\[
D_{H_2,H^+} = 0.34 \ [cm^2/sec], \quad (23)
\]
\[
D_{H_2,H} = 0.21 \ [cm^2/sec], \quad (24)
\]
\[
D_{H^+,H} = 0.21 \ [cm^2/sec]. \quad (25)
\]

We have used the following Stefan-Maxwell model as a transport model for the gaseous species. The modelling equation is given as:
\[
\partial_t \xi_i + \nabla \cdot N_i = S_i, \ 1 \leq i \leq 3, \quad (26)
\]
\[
\sum_{j=1}^{3} N_j = 0, \quad (27)
\]
\[
\frac{\xi_2 N_1 - \xi_1 N_2}{D_{12}} + \frac{\xi_3 N_1 - \xi_1 N_3}{D_{13}} = -\nabla \xi_1, \quad (28)
\]
\[
\frac{\xi_1 N_2 - \xi_2 N_1}{D_{12}} + \frac{\xi_3 N_2 - \xi_2 N_3}{D_{23}} = -\nabla \xi_2, \quad (29)
\]
where \( \xi_i \) are the mole fractions and \( N_i \) is the molar flux of species \( i \), see \([?]\) and \([4]\). Furthermore, the kinetic term or reaction term \( S_i \) is given as:
\[
S_i = \sum_{j=1}^{3} \lambda_{i,j} \xi_j, \quad (30)
\]
where \( \lambda_{i,j} \) are the reaction-rates. The domain is given as \( \Omega \in \mathbb{R}^d, d \in \mathbb{N}^+ \) with \( \xi_i \in C^2 \).
We decompose the diffusion and the reaction part, and apply the following splitting approach to our problem, we compute \( n = 1, \ldots, N, t_0, t_1, \ldots, t_n \) time-steps: The first step is given as (Diffusion step):

\[
\begin{align*}
\partial_t \tilde{\xi}_i + \nabla \cdot N_i &= 0, \quad 1 \leq i \leq 3, \\
\sum_{j=1}^{3} N_j &= 0, \\
\frac{\tilde{\xi}_2 N_1 - \tilde{\xi}_1 N_2}{D_{12}} + \frac{\tilde{\xi}_3 N_1 - \tilde{\xi}_1 N_3}{D_{13}} &= -\nabla \xi_1, \\
\frac{\tilde{\xi}_1 N_2 - \tilde{\xi}_2 N_1}{D_{12}} + \frac{\tilde{\xi}_3 N_2 - \tilde{\xi}_2 N_3}{D_{23}} &= -\nabla \tilde{\xi}_2, \text{ for } t \in [t^n, t^{n+1}], \\
\tilde{\xi}_i(t^n) &= \xi_i(t^n), \quad i = 1, 2, 3,
\end{align*}
\]  

and the next step is given as (Reaction step):

\[
\begin{align*}
\partial_t \xi_i &= S_i, \quad 1 \leq i \leq 3, \text{ for } t \in [t^n, t^{n+1}], \\
\xi_i(t^n) &= \tilde{\xi}_i(t^{n+1}), \quad i = 1, 2, 3.
\end{align*}
\]

In the following section, we will discuss the different treatments of the sub-problems.

4 Solution of the Transport-Reaction Equation

The transport-reaction equation can be solved in the two parts of the transport part, which is a Stefan-Maxwell equation, and the reaction part, which is a pure ODE.

These two different approaches are discussed in the following schemes:

1. Stefan-Maxwell Problem (Diffusion-part):

   We concentrate on the three component system and solve this system as a linear optimal problem (General Linear Optimal Problem). We deal with:

   \[
   \begin{align*}
   \partial_t \xi_i + \nabla \cdot N_i &= 0, \quad 1 \leq i \leq 3, \\
   \sum_{j=1}^{3} N_j &= 0, \\
   \frac{\xi_2 N_1 - \xi_1 N_2}{D_{12}} + \frac{\xi_3 N_1 - \xi_1 N_3}{D_{13}} &= -\nabla \xi_1, \quad i = 1, 2, 3.
   \end{align*}
   \]

   where the domain is given as \( \Omega \in \mathbb{R}^d, d \in \mathbb{N}^+ \) with \( \xi_i \in C^2 \).
We could reduce this to a simpler model problem as:

\[ \partial_t \xi_i + \nabla \cdot N_i = 0, \quad 1 \leq i \leq 2, \quad (42) \]
\[ \frac{1}{D_{13}} N_1 + \alpha N_1 \xi_2 - \alpha N_2 \xi_1 = -\nabla \xi_1, \quad (43) \]
\[ \frac{1}{D_{23}} N_2 - \beta N_1 \xi_2 + \beta N_2 \xi_1 = -\nabla \xi_2, \quad (44) \]

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

The optimal problem is derived in the following manner. Second, we rewrite the MOR model equation (106) to a set of linearised states \( U_0, U_1, \ldots, U_s \) by using the linear system:

\[ U'_{i+1} = J_i(t) U_{i+1} + \dot{B}(t) v, \quad (45) \]

where \( J_i \) is the Jacobian of \( B(U, t) \) and is given in (106), the control operator is \( \dot{B}(t) = \dot{B}(t) - J_i \), and the system input is \( v = U_i \).

Third, we can now apply the GLCS, using the following notations:

\[ u = U_{i+1}, \quad v = U_i, \quad A_1(t) = J_i(t), \quad A_2(t) = \dot{B}(t). \]

The GLCS is then

\[ \frac{du}{dt} = A_1(t) u + A_2(t) v, \quad (46) \]
\[ \dot{u} = C(t) u + D(t) v, \quad (47) \]
\[ u(0) = u_0, \quad (48) \]

where the time-dependent operators are \( A(t) \in X^n \times X^n, \quad B(t) \in X^n \times X^m, \quad C(t) \in X^p \times X^n, \quad D(t) \in X^p \times X^m, \quad v : X \to X^m \) denotes the system input, \( \dot{u} : X \to X^p \) is the system output and \( u : X \to X^n \) denotes the state vector. Furthermore, \( X \) is an appropriate Banach space; for example, \( U \), a space of continuous or piece-wise continuous functions.

The analytical solution of (46) and (47) is

\[ u(t) = \exp(\int_0^t A_1(s) ds) u_0 + \int_0^t \exp(\int_s^t A_1(\tilde{s}) d\tilde{s}) A_2(s) v(s) ds, \quad (49) \]
\[ \dot{u}(t) = C(t) \exp(\int_0^t A_1(s) ds) u_0 + \int_0^t \exp(\int_s^t A_1(\tilde{s}) d\tilde{s}) A_2(s) v(s) ds + D(t) v(t), \quad (50) \]

where we apply the fast computation of the exponential integral matrices via the Magnus expansion, see [2], [1] and [5], and which is discussed in the following.
2. Kinetic Problem (Reaction-part):
We concentrate on the three component system and we deal with:
\[ \partial_t \xi_i = S_i, \quad 1 \leq i \leq 3, \quad (51) \]
where the domain is given as \( \Omega \in \mathbb{R}^d, d \in \mathbb{N}^+ \) with \( \xi_i \in C^2 \).
We apply the reaction-rates and have the following linear ODE system:
\[ \partial_t \xi = S \xi, \quad (52) \]
where \( \xi = (\xi_1, \xi_2, \xi_3)^t \) and \( S = \begin{pmatrix} \lambda_{1,1} & \lambda_{1,2} & \lambda_{1,3} \\ \lambda_{2,1} & \lambda_{2,2} & \lambda_{2,3} \\ \lambda_{3,1} & \lambda_{3,2} & \lambda_{3,3} \end{pmatrix} \).
We can apply the analytical solution, which is given as:
\[ \xi(t^{n+1}) = \exp(S \Delta t) \xi(t^n), \quad (53) \]
and \( \Delta t = t^{n+1} - t^n \).

5 Numerical Algorithms and Numerical Experiments
In this section, we discuss the different numerical algorithms that are based on splitting approaches and which are to solve the multicomponent transport-reaction equations.
We deal with the following two experiments:
– Pure diffusion problem, here we only apply the Stefan-Maxwell equation.
– Hydrogen Plasma, here we apply the Stefan-Maxwell equation with the reaction equation.

5.1 Pure Diffusion Problem
We concentrate on the three component system:
\[ \partial_t \xi_i + \partial_x N_i = 0, \quad 1 \leq i \leq 3, \quad (54) \]
\[ \sum_{j=1}^{3} N_j = 0, \quad (55) \]
\[ \frac{\xi_2 N_1 - \xi_1 N_2}{D_{12}} + \frac{\xi_3 N_1 - \xi_1 N_3}{D_{13}} = -\partial_x \xi_1, \quad (56) \]
\[ \frac{\xi_1 N_2 - \xi_2 N_1}{D_{12}} + \frac{\xi_3 N_2 - \xi_2 N_3}{D_{23}} = -\partial_x \xi_2, \quad (57) \]
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, semidegenerated Duncan and Toor experiment)
\( D_{12} = 0.0833, D_{13} = 0.680 \) and \( D_{23} = 0.168 \) (asymptotic behavior, Duncan and Toor experiment)

- \( J = 140 \) (spatial grid points)

- The time-step-restriction for the explicit method is given as:
  \[ \Delta t \leq (\Delta x)^2 \max \left\{ \frac{1}{2D_{12}}, \frac{1}{D_{13}}, \frac{1}{D_{23}} \right\} \]

- The spatial domain is \( \Omega = [0, 1] \), the time-domain \( [0, T] = [0, 1] \)

- The initial conditions are:
  1. Uphill example
     \[
     \xi_{1}^i(x) = \begin{cases} 
     0.8 & \text{if } 0 \leq x < 0.25, \\
     1.6(0.75 - x) & \text{if } 0.25 \leq x < 0.75, \\
     0.0 & \text{if } 0.75 \leq x \leq 1.0,
     \end{cases}
     \]
     (58)
     
     \[
     \xi_{2}^i(x) = 0.2, \text{ for all } x \in \Omega = [0, 1],
     \]
     (59)
  2. Diffusion example (asymptotic behavior)
     \[
     \xi_{1}^i(x) = \begin{cases} 
     0.8 \text{ if } 0 \leq x \in 0.5, \\
     0.0 \text{ else,}
     \end{cases}
     \]
     (60)
     
     \[
     \xi_{2}^i(x) = 0.2, \text{ for all } x \in \Omega = [0, 1],
     \]
     (61)

- The boundary conditions are of no-flux type:
  \[
  N_1 = N_2 = N_3 = 0, \text{ on } \partial \Omega \times [0, 1],
  \]
  (62)

We could reduce this to a simpler model problem, as follows:

\[
\partial_t \xi_1 + \partial_x \cdot N_1 = 0, \quad \text{for } 1 \leq i \leq 2,
\]
(63)

\[
\frac{1}{D_{13}} N_1 + \alpha N_1 \xi_2 - \alpha N_2 \xi_1 = -\partial_x \xi_1,
\]
(64)

\[
\frac{1}{D_{23}} N_2 - \beta N_1 \xi_2 + \beta N_2 \xi_1 = -\partial_x \xi_2,
\]
(65)

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

We then rewrite into:

\[
\partial_t \xi_1 + \partial_x \cdot N_1 = 0,
\]
(66)

\[
\partial_t \xi_2 + \partial_x \cdot N_2 = 0,
\]
(67)

\[
\left( \frac{1}{D_{13}} + \alpha \xi_2 - \alpha \xi_1 \right) \left( \frac{1}{D_{23}} + \beta \xi_1 \right) \begin{bmatrix} N_1 \\ N_2 \end{bmatrix} = \begin{bmatrix} -\partial_x \xi_1 \\ -\partial_x \xi_2 \end{bmatrix}
\]
(68)

and we have

\[
\partial_t \xi_1 + \partial_x \cdot N_1 = 0,
\]
(69)

\[
\partial_t \xi_2 + \partial_x \cdot N_2 = 0,
\]
(70)

\[
\begin{bmatrix} N_1 \\ N_2 \end{bmatrix} = \frac{D_{13}D_{23}}{1 + \alpha D_{13} \xi_2 + \beta D_{23} \xi_1} \begin{bmatrix} \frac{1}{D_{23}} + \beta \xi_1 \\ \frac{1}{D_{13}} + \alpha \xi_2 \end{bmatrix} \begin{bmatrix} -\partial_x \xi_1 \\ -\partial_x \xi_2 \end{bmatrix}
\]
(71)
The next step is to apply the semi-discretisation of the partial differential operator \( \frac{\partial}{\partial x} \).

We apply the first differential operator in equation (136) and (137) as a forward upwind scheme, which is given as

\[
\frac{\partial}{\partial x} = \frac{1}{\Delta x} \begin{pmatrix}
-1 & 0 & \ldots & 0 \\
1 & -1 & 0 & \ldots & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & 1 & -1 & 0 & \ldots \\
0 & \ldots & 0 & 1 & -1
\end{pmatrix} \in \mathbb{R}^{(J+1) \times (J+1)}
\]

and we apply the second differential operator in equation (138) as a backward upwind scheme, which is given as

\[
\frac{\partial}{\partial x} = \frac{1}{\Delta x} \begin{pmatrix}
-1 & 1 & 0 & \ldots & 0 \\
0 & -1 & 1 & 0 & \ldots \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \ldots & 0 & -1 & 1 \\
0 & \ldots & 0 & 1 & -1
\end{pmatrix} \in \mathbb{R}^{(J+1) \times (J+1)}
\]

In the next part, we apply the iterative schemes to solve the pure diffusion problem.

**Iterative Scheme in Time for the Pure Diffusion Problem** In this section, we apply a global linearisation of the Stefan-Maxwell equation. Then, we consider the underlying semi-discretised equation with an iterative approach.

We solve the iterative scheme:

\[
\begin{align}
\xi_{1}^{n+1} &= \xi_{1}^{n} - \Delta t \; D_{+} N_{1}^{n}, \\
\xi_{2}^{n+1} &= \xi_{2}^{n} - \Delta t \; D_{+} N_{2}^{n},
\end{align}
\]

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

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

The matrices are given as:

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

\[
A_{j,j} = \frac{1}{D_{13}}, \; j = 0, \ldots, J,
\]

\[
B_{j,j} = -\alpha \xi_{1,j}, \; j = 0, \ldots, J,
\]

\[
C_{j,j} = -\beta \xi_{2,j}, \; j = 0, \ldots, J,
\]

\[
D_{j,j} = \frac{1}{D_{23}} + \beta \xi_{1,j}, \; j = 0, \ldots, J,
\]

\[
A_{i,j} = B_{i,j} = C_{i,j} = D_{i,j} = 0, \; i,j = 0, \ldots, J, \; i \neq J.
\]
which means that the diagonal entries given as for the scale case in equation (138) and the outer-diagonal entries are zero.

The explicit form with time-discretisation is given as:

**Algorithm 1** 1.) Initialisation $n = 0$:

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

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 $\xi_{1,j}^0 = \xi_{1}^n(j\Delta x)$, $\xi_{2,j}^0 = \xi_{2}^n(j\Delta x)$, $j = 0, \ldots, J$ and, given as for the different initialisation, we have:

1. Uphill example

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

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

2. Diffusion example (Asymptotic behavior)

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

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

The inverse matrices are given as:

$$
\tilde{A}, \tilde{B}, \tilde{C}, \tilde{D} \in \mathbb{IR}^{J+1} \times \mathbb{IR}^{J+1},
$$

$$
\tilde{A}_{j,j} = \gamma_j\left(\frac{1}{D_{23}} + \beta \xi_{1,j}^0\right), j = 0, \ldots, J,
$$

$$
B_{j,j} = \gamma_j \alpha \xi_{1,j}^0, j = 0, \ldots, J,
$$

$$
C_{j,j} = \gamma_j \beta \xi_{2,j}^0, j = 0, \ldots, J,
$$

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

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

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

The values of the first and the last grid points of $N$ are zero, which means that $N_{1,0}^0 = N_{1,J}^0 = N_{2,0}^0 = N_{2,J}^0 = 0$ (boundary condition).

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

2.1) Computation of $\xi_1^{n+1}$ and $\xi_2^{n+1}$

$$
\xi_1^{n+1} = \xi_1^n - \Delta t D_{1} N_{1}^n,
$$

$$
\xi_2^{n+1} = \xi_2^n - \Delta t D_{2} N_{2}^n,
$$
2.2) Computation of $N_1^{n+1}$ and $N_2^{n+1}$

$$
\begin{pmatrix}
N_1^{n+1} \\
N_2^{n+1}
\end{pmatrix} = \begin{pmatrix}
\tilde{A} & \tilde{B} \\
\tilde{C} & \tilde{D}
\end{pmatrix}
\begin{pmatrix}
-D_- \xi_1^{n+1} \\
-D_- \xi_2^{n+1}
\end{pmatrix} \tag{97}
$$

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:

$$
\tilde{A}, \tilde{B}, \tilde{C}, \tilde{D} \in \mathbb{R}^{J+1} \times \mathbb{R}^{J+1}, \tag{98}
$$

$$
\tilde{A}_{j,j} = \gamma_j \left( \frac{1}{D_{23}} + \beta \xi_{1,j}^{n+1} \right), \ j = 0, \ldots, J, \tag{99}
$$

$$
B_{j,j} = \gamma_j \alpha \xi_{1,j}^{n+1}, \ j = 0, \ldots, J, \tag{100}
$$

$$
C_{j,j} = \gamma_j \beta \xi_{2,j}^{n+1}, \ j = 0, \ldots, J, \tag{101}
$$

$$
D_{j,j} = \gamma_j \left( \frac{1}{D_{13}} + \alpha \xi_{2,j}^{n+1} \right), \ j = 0, \ldots, J, \tag{102}
$$

$$
\gamma_j = \frac{D_{13}D_{23}}{1 + \alpha D_{13} \xi_{2,j}^{n+1} + \beta D_{23} \xi_{1,j}^{n+1}}, \ j = 0, \ldots, J, \tag{103}
$$

$$
\tilde{A}_{i,j} = \tilde{B}_{i,j} = \tilde{C}_{i,j} = \tilde{D}_{i,j} = 0, \ i, j = 0, \ldots, J, \ i \neq J. \tag{104}
$$

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

3.) Do $n = n + 1$ and then goto 2.)

We have used the following examples:

We test the different schemes and obtain the results shown in Figure 1.

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 5.

Remark 1. The iterative scheme allows us to solve the pure diffusion problem effectively, see also [8]. The improvement can be done with local linearisation in the pure diffusion problem, see also [8] and in the next subsection.

5.2 Hydrogen Plasma: Diffusion-Reaction Problem

In the following section we will discuss the different splitting approaches that are used to solve the diffusion-reaction problem.

We have explicit and implicit versions of the AB and ABA splitting approaches, and also for the iterative splitting approach.
Fig. 1. The figures present the results of the concentration $c_1$, $c_2$ and $c_3$.

In the following, we have used the implicit version of the AB-splitting approach, see Equation (105).

\[
\ldots N^n \rightarrow \xi^n \rightarrow_A \xi^{n+1} \rightarrow_B \xi^{n+1} \rightarrow N^{n+1} \ldots
\]  

(105)

Furthermore, we could also apply a more explicit version of the AB-splitting approach, which allows us to deal with a more parallel idea, see Figure 6.

We concentrate on the three component system with reaction:

\[
\partial_t \xi_i + \partial_x N_i = S_i, \quad 1 \leq i \leq 3,
\]  

(106)

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

(107)

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

(108)

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

(109)

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:

- component 1: $H_2$, component 2: $H_2^+$, component 3: $H$,
- $D_{12} = 0.34$, $D_{13} = 0.21$ and $D_{23} = 0.21$
- Example 1:
  \[
  \lambda_{11} = -4.276 \times 10^{-7}, \quad \lambda_{21} = \lambda_{31} = -\frac{\lambda_{11}}{3},
  \]
  \[
  \lambda_{22} = -2.082 \times 10^{-13}, \quad \lambda_{12} = \lambda_{23} = -\frac{\lambda_{22}}{2},
  \]
  \[
  \lambda_{33} = -4.276 \times 10^{-7}, \quad \lambda_{31} = \lambda_{32} = -\frac{\lambda_{33}}{2}
  \]
Fig. 2. 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 $-\partial_x\xi_2$.

- Example 2:
  \[ \lambda_{11} = -4.276 \times 10^{-2}, \quad \lambda_{21} = \lambda_{31} = -\frac{\lambda_{11}}{2}, \quad \lambda_{22} = -2.082 \times 10^{-8}, \quad \lambda_{12} = \lambda_{23} = -\frac{\lambda_{22}}{2}, \quad \lambda_{33} = -4.276 \times 10^{-8}, \quad \lambda_{31} = \lambda_{32} = -\frac{\lambda_{33}}{2}, \]

- Example 3:
  \[ \lambda_{11} = -4.276 \times 10^{-1}, \quad \lambda_{21} = \lambda_{31} = -\frac{\lambda_{11}}{2}, \quad \lambda_{22} = -2.082 \times 10^{-2}, \quad \lambda_{12} = \lambda_{23} = -\frac{\lambda_{22}}{2}, \quad \lambda_{33} = -4.276 \times 10^{-2}, \quad \lambda_{31} = \lambda_{32} = -\frac{\lambda_{33}}{2}, \]

- $J = 140$ (spatial grid points)

- The time-step-restriction for the explicit method is given as:
  \[ \Delta t \leq (\Delta x)^2 \max \{ \frac{1}{2(D_{12}, D_{13}, D_{23})} \} \]

- The spatial domain is $\Omega = [0, 1]$ and the time-domain is $[0, T] = [0, 1]$

- The initial conditions are:
  1. Example uphill diff. dominant $H_2^+$:
     \[ \xi_1^{in}(x) = \begin{cases} 
     0.8 & \text{if } 0 \leq x < 0.25, \\
     1.6(0.75 - x) & \text{if } 0.25 \leq x < 0.75, \\
     0.0 & \text{if } 0.75 \leq x \leq 1.0, 
     \end{cases} \]
     \[ (110) \]
     \[ \xi_1^{in}(x) = 0.2, \text{ for all } x \in \Omega = [0, 1], \]
     \[ (111) \]
2. Example asymptotic diffusion, dominant $H^+_2$

$$\xi_1^n(x) = \begin{cases} 0.8 & \text{if } 0 \leq x \in 0.5, \\ 0.0 & \text{else}, \end{cases},$$
(112)

$$\xi_2^n(x) = 0.2, \text{ for all } x \in \Omega = [0, 1],$$
(113)

- The boundary conditions are of no-flux type:

$$N_1 = N_2 = N_3 = 0, \text{ on } \partial \Omega \times [0, 1],$$
(114)

We have used the following algorithm, which is given as AB-splitting:

**Algorithm 2 The AB-splitting is given as:**

We start with $\xi_1(0), \xi_2(0)$ and $n = 1$:

- **Step 1: Diffusion Step**

\[
\begin{align*}
\partial_t \tilde{\xi}_1 + \partial_x \cdot N_1 &= 0, \text{ with } t \in [t^n, t^{n+1}], \\
\partial_t \tilde{\xi}_2 + \partial_x \cdot N_2 &= 0, \text{ with } t \in [t^n, t^{n+1}],
\end{align*}
\]

\[
\begin{pmatrix}
N_1 \\
N_2
\end{pmatrix} = \begin{pmatrix}
\frac{D_{13}D_{23}}{1 + \alpha D_{13}\tilde{\xi}_2 + \beta D_{23}\tilde{\xi}_1} \\
\frac{1}{D_{23} + \alpha\tilde{\xi}_2}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
\frac{1}{D_{23}} + \beta \tilde{\xi}_1 & \alpha \tilde{\xi}_1 \\
\beta \tilde{\xi}_2 & \frac{1}{D_{23}} + \alpha \tilde{\xi}_2
\end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
-\partial_x \tilde{\xi}_1 \\
-\partial_x \tilde{\xi}_2
\end{pmatrix}
\end{pmatrix}
\end{pmatrix}
\]
where \( \alpha = \left( \frac{1}{D_{12}} - \frac{1}{D_{13}} \right) \), \( \beta = \left( \frac{1}{D_{12}} - \frac{1}{D_{23}} \right) \) and the initialisation is given as: \( \tilde{\xi}_1(t^n) = \xi_1(t^n), \tilde{\xi}_2(t^n) = \xi_2(t^n) \) (which means from the last second step).

We apply the explicit or implicit methods for the pure diffusion and obtain \( \tilde{\xi}_1(t^{n+1}), \tilde{\xi}_2(t^{n+1}), \tilde{\xi}_3(t^{n+1}) = 1 - \tilde{\xi}_1(t^{n+1}) - \tilde{\xi}_2(t^{n+1}) \).

**Step 2: Reaction Step**

\[
\begin{align*}
\xi_1(t^{n+1}) &= \tilde{\xi}_1(t^{n+1}) + \Delta t(\lambda_{11} - \lambda_{13})\tilde{\xi}_1(t^{n+1}) + \Delta t(\lambda_{12} - \lambda_{13})\tilde{\xi}_2(t^{n+1}) + \lambda_{13}, \\
\xi_2(t^{n+1}) &= \tilde{\xi}_2(t^{n+1}) + \Delta t(\lambda_{21} - \Delta t\lambda_{23})\tilde{\xi}_1(t^{n+1}) + \Delta t(\lambda_{22} - \lambda_{23})\tilde{\xi}_2(t^{n+1}) + \Delta t\lambda_{23}.
\end{align*}
\]

(117)

The solution-vectors are given as

\[
\begin{align*}
\xi_1(t^{n+1}) &= (\xi_{1,0}(t^{n+1}), \ldots, \xi_{1,J}(t^{n+1}))^t, \\
\xi_2(t^{n+1}) &= (\xi_{2,0}(t^{n+1}), \ldots, \xi_{2,J}(t^{n+1}))^t, \\
\xi_3(t^{n+1}) &= (\xi_{3,0}(t^{n+1}), \ldots, \xi_{3,J}(t^{n+1}))^t.
\end{align*}
\]

**Step 3: We go to Step 1 till \( n = N \).**

We have used the following algorithm given as Strang-splitting in two versions, see Algorithm 3 and Algorithm 4. We also explain the ideas of the splitting in Figure 7.
Fig. 5. The figures present the asymptotic diffusion (left hand side) and uphill diffusion (right hand side) in the space-time region.

Algorithm 3 ABA-splitting (Strang-splitting) without updating \( N \) is given as:

We start with \( \xi_1(0), \xi_2(0) \) and \( n = 1 \):

- **Step 1: Predictor Step (updating \( N \))**

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

  where \( \alpha = \left( \frac{1}{D_{13}} - \frac{1}{D_{12}} \right), \beta = \left( \frac{1}{D_{12}} - \frac{1}{D_{23}} \right) \) and the initialisation is given as: \( \tilde{\xi}_1(t^n) = \xi_1(t^n), \tilde{\xi}_2(t^n) = \xi_2(t^n) \) (which means that this is the result of the last computation in step 3).

- **Step 2: Corrector Step (updating \( \xi \))**

  - **Step 2.1: Diffusion Step (with \( \Delta t/2 \))**

    \[
    \partial_t \tilde{\xi}_1 + \partial_x \cdot N_1 = 0, \text{ with } t \in [t^n, t^{n+1/2}],
    \]
    \[
    \partial_t \tilde{\xi}_2 + \partial_x \cdot N_2 = 0, \text{ with } t \in [t^n, t^{n+1/2}],
    \]

    where \( \tilde{\xi}_1(t^n) = \xi_1(t^n), \tilde{\xi}_2(t^n) = \xi_2(t^n) \) and \( N_1, N_2 \) is computed by the Step 1.

    We apply the explicit or implicit methods for the pure diffusion and obtain \( \xi_1(t^{n+1/2}), \xi_2(t^{n+1/2}), \text{ and } \xi_3(t^{n+1/2}) = 1 - \xi_1(t^{n+1/2}) - \xi_2(t^{n+1/2}) \).
Algorithm 4 ABA-splitting (Strang-splitting) with updating

Step 1: Predictor Step (updating $N$)

We start with $\xi_n$.

Step 2.2: Reaction Step (with $\Delta t$)

\[
\hat{\xi}_1(t^{n+1}) = \xi_1(t^{n+1/2}) + \Delta t(\lambda_{11} - \lambda_{13})\xi_1(t^{n+1/2}) + \Delta t(\lambda_{12} - \lambda_{13})\xi_2(t^{n+1}) + \Delta t\lambda_{13},
\]

\[
\hat{\xi}_2(t^{n+1}) = \xi_2(t^{n+1/2}) + \Delta t(\lambda_{21} - \lambda_{23})\xi_1(t^{n+1/2}) + \Delta t(\lambda_{22} - \lambda_{23})\xi_2(t^{n+1}) + \Delta t\lambda_{23}.
\]

(121)

(122)

Step 2.3: Diffusion Step (with $\Delta t/2$)

\[
\partial_t\xi_1 + \partial_x \cdot N_1 = 0, \text{ with } t \in [t^{n+1/2}, t^{n+1}],
\]

\[
\partial_t\xi_2 + \partial_x \cdot N_2 = 0, \text{ with } t \in [t^{n+1/2}, t^{n+1}],
\]

(123)

(124)

where $\xi_1(t^{n+1/2}) = \hat{\xi}_1(t^{n+1}), \xi_2(t^{n+1/2}) = \hat{\xi}_2(t^{n+1})$ and $N_1, N_2$ is given in Step 1 (which means that $N_1(\hat{\xi}_1(t^n)), N_2(\hat{\xi}_2(t^n))$).

We apply the explicit or implicit methods for the pure diffusion and obtain $\xi_1(t^{n+1}), \xi_2(t^{n+1}), \xi_2(t^{n+1}) = 1 - \xi_1(t^{n+1}) - \xi_2(t^{n+1})$.

The solution-vectors are given as

$\xi_1(t^{n+1}) = (\xi_{1,0}(t^{n+1}), \ldots, \xi_{1,J}(t^{n+1}))^T$,

$\xi_2(t^{n+1}) = (\xi_{2,0}(t^{n+1}), \ldots, \xi_{2,J}(t^{n+1}))^T$,

$\xi_3(t^{n+1}) = (\xi_{3,0}(t^{n+1}), \ldots, \xi_{3,J}(t^{n+1}))^T$.

Step 3: We do $n = n + 1$ and go to Step 1 till $n = N$.

Algorithm 4 ABA-splitting (Strang-splitting) with updating $N$ is given as:

We start with $\xi_1(0), \xi_2(0)$ and $n = 1$:

Step 1: Predictor Step (updating $N$)

\[
\begin{pmatrix}
N_1 \\
N_2
\end{pmatrix} = \frac{D_{13}D_{23}}{1 + \alpha D_{13} \xi_2 + \beta D_{23} \xi_1} \begin{pmatrix}
\frac{1}{D_{23}} + \beta \hat{\xi}_1 \\
\beta \xi_2 + \frac{1}{D_{13}} + \alpha \hat{\xi}_2
\end{pmatrix} \begin{pmatrix}
-\partial_x \hat{\xi}_1 \\
-\partial_x \hat{\xi}_2
\end{pmatrix}
\]
where $\alpha = \left(\frac{1}{D_{11}} - \frac{1}{D_{13}}\right)$, $\beta = \left(\frac{1}{D_{12}} - \frac{1}{D_{23}}\right)$ and the initialisation is given as: $\tilde{\xi}_1(t^n) = \xi_1(t^n), \tilde{\xi}_2(t^n) = \xi_2(t^n)$ (which means that this is the result of the last computation in step 3).

- **Step 2: Corrector Step (upating $\xi$)**

  - **Step 2.1: Diffusion Step (with $\Delta t/2$)**
    
    \[
    \partial_t \tilde{\xi}_1 + \partial_x \cdot N_1 = 0, \text{ with } t \in [t^n, t^{n+1/2}], \quad (125)
    \]
    \[
    \partial_t \tilde{\xi}_2 + \partial_x \cdot N_2 = 0, \text{ with } t \in [t^n, t^{n+1/2}], \quad (126)
    \]

    where $\tilde{\xi}_1(t^n) = \xi_1(t^n), \tilde{\xi}_2(t^n) = \xi_2(t^n)$ and $N_1, N_2$ is computed by the Step 1.

    - **Step 2.2: Reaction Step (with $\Delta t/2$)**
      
      \[
      \xi_1(t^{n+1/2}) = \xi_1(t^{n+1/2}) + \Delta t/2(\lambda_{11} - \lambda_{13})\tilde{\xi}_1(t^{n+1/2}) + \Delta t/2\lambda_{12}, \quad (127)
      \]
      \[
      \xi_2(t^{n+1/2}) = \xi_2(t^{n+1/2}) + \Delta t/2(\lambda_{21} - \lambda_{23})\tilde{\xi}_2(t^{n+1/2}) + \Delta t/2\lambda_{22}. \quad (128)
      \]

- **Step 3: Predictor Step (upating $N$)**

\[
\begin{pmatrix}
N_1 \\
N_2
\end{pmatrix}
= \frac{D_{13}D_{23}}{1 + \alpha D_{13}^2 + \beta D_{23}^2 + 1/\alpha} \begin{pmatrix}
\frac{1}{D_{23}} + \beta \xi_1^{n+1/2} & \frac{\alpha \xi_1^{n+1/2}}{1/\alpha} \\
\frac{1}{D_{13}} + \alpha \xi_2^{n+1/2} & \frac{\beta \xi_2^{n+1/2}}{1/\alpha}
\end{pmatrix}
\begin{pmatrix}
-\partial_x \xi_1^{n+1/2} \\
-\partial_x \xi_2^{n+1/2}
\end{pmatrix}
\]

where $\alpha = \left(\frac{1}{D_{11}} - \frac{1}{D_{13}}\right)$, $\beta = \left(\frac{1}{D_{12}} - \frac{1}{D_{23}}\right)$ and the initialisation is given as: $\xi_1^{n+1/2} = \xi_1(t^{n+1/2}), \xi_2^{n+1/2} = \xi_2(t^{n+1/2})$ (which means that this is the result of the last computation in step 2.2).

- **Step 4: Corrector Step (upating $\xi$)**

  - **Step 4.1: Reaction Step (with $\Delta t/2$)**
    
    \[
    \xi_1(t^{n+1}) = \xi_1(t^{n+1/2}) + \Delta t/2(\lambda_{11} - \lambda_{13})\xi_1(t^{n+1/2}) + \Delta t/2\lambda_{12}, \quad (129)
    \]
    \[
    \xi_2(t^{n+1}) = \xi_2(t^{n+1/2}) + \Delta t/2(\lambda_{21} - \lambda_{23})\xi_2(t^{n+1/2}) + \Delta t/2\lambda_{22}. \quad (130)
    \]

  - **Step 4.2: Diffusion Step (with $\Delta t/2$)**
    
    \[
    \partial_t \xi_1 + \partial_x \cdot N_1 = 0, \text{ with } t \in [t^{n+1/2}, t^{n+1}], \quad (131)
    \]
    \[
    \partial_t \xi_2 + \partial_x \cdot N_2 = 0, \text{ with } t \in [t^{n+1/2}, t^{n+1}], \quad (132)
    \]

where $\xi_1(t^{n+1/2}) = \tilde{\xi}_1(t^{n+1}), \xi_2(t^{n+1/2}) = \tilde{\xi}_2(t^{n+1})$ and $N_1, N_2$ is given in the updated Step 3 (which means that $N_1(\xi_1(t^{n+1/2})), N_2(\xi_2(t^{n+1/2}))$).
We apply the explicit or implicit methods for the pure diffusion and obtain \( \xi_1(t^{n+1}), \xi_2(t^{n+1}), \xi_2(t^{n+1}) = 1 - \xi_1(t^{n+1}) - \xi_2(t^{n+1}) \).

The solution-vectors are given as

\[
\begin{align*}
\xi_1(t^{n+1}) &= (\xi_{1,0}(t^{n+1}), \ldots, \xi_{1,J}(t^{n+1}))^t, \\
\xi_2(t^{n+1}) &= (\xi_{2,0}(t^{n+1}), \ldots, \xi_{2,J}(t^{n+1}))^t, \\
\xi_3(t^{n+1}) &= (\xi_{3,0}(t^{n+1}), \ldots, \xi_{3,J}(t^{n+1}))^t,
\end{align*}
\]

- Step 5: We do \( n = n + 1 \) and go to Step 1 till \( n = N \).
We have used the following algorithm, given as an iterative splitting approach, while we solve the diffusion part and perturb over the reaction part:

Algorithm 5 The iterative splitting for reaction (Picard’s fixpoint scheme) is given as:

We start with \( \xi_1(0), \xi_2(0) \) and \( n = 1 \):
- Step 0: Initialisation for \( i = 0 \) with \( \xi_{1,0}(t^{n+1}) = \xi_1(t^n), \xi_{2,0}(t^{n+1}) = \xi_2(t^n) \) and \( N_{1,0}(t^{n+1}) = N_1(t^n), N_{2,0}(t^{n+1}) = N_2(t^n) \).
- Step 1: Iterative step \( i \): Diffusion and Reaction Step (with \( \Delta t \))
  - Step 1.1. Computation of \( \xi_{1,i}^{n+1} \) and \( \xi_{2,i}^{n+1} \)

\[
\xi_{1,i}^{n+1} = \xi_{1,i}^n - \Delta t D \xi_{1,i-1}^n + \\
+ \Delta t \left( \lambda_{11} \xi_{1,i-1}^n + \lambda_{12} \xi_{2,i-1}^n + \lambda_{13}(1 - \xi_{1,i-1}^n - \xi_{2,i-1}^n) \right) \tag{133}
\]

\[
\xi_{2,i}^{n+1} = \xi_{2,i}^n - \Delta t D \xi_{2,i-1}^n + \\
+ \Delta t \left( \lambda_{21} \xi_{1,i-1}^n + \lambda_{22} \xi_{2,i-1}^n + \lambda_{23}(1 - \xi_{1,i-1}^n - \xi_{2,i-1}^n) \right) \tag{134}
\]

- Step 1.2: \( i = i + 1 \) and we go to Step 1 till \( i = I \) (else goto Step 2)
- Step 2. Computation of \( N_{1,i}^{n+1} \) and \( N_{2,i}^{n+1} \)

\[
\left( \begin{array}{c}
N_{1,i}^{n+1} \\
N_{2,i}^{n+1}
\end{array} \right)
= \frac{D_{13}D_{23}}{1 + \alpha D_{13} \xi_{1,i}^{n+1} + \beta D_{23} \xi_{2,i}^{n+1}} \left( \begin{array}{c}
\frac{1}{D_{23}} + \beta \xi_{1,i}^{n+1} \\
\beta \xi_{2,i}^{n+1} + \frac{1}{\beta} \xi_{1,i}^{n+1} + \alpha \xi_{2,i}^{n+1}
\end{array} \right) \left( \begin{array}{c}
-\partial_x \xi_{1,i}^{n+1} \\
-\partial_x \xi_{2,i}^{n+1}
\end{array} \right)
\]  \tag{135}

where \( \alpha = \left( \frac{1}{D_{13}} - \frac{1}{D_{23}} \right) \), \( \beta = \left( \frac{1}{D_{13}} - \frac{1}{D_{23}} \right) \) and the initialisation is given as: \( \xi_{1,i}(t^n) = \xi_1(t^n), \xi_{2,i}(t^n) = \xi_2(t^n) \) (which is the means from the last computation).
- Step 3: \( n = n + 1 \) and we go to Step 0 till \( n = N \).

We apply the explicit or implicit methods for the diffusion-reaction equation and obtain \( \xi_{1,i}(t^{n+1}), \xi_{2,i}(t^{n+1}), \xi_{3,i}(t^{n+1}) = 1 - \xi_{1,i}(t^{n+1}) - \xi_{2,i}(t^{n+1}) \).

Algorithm 6 The iterative splitting for diffusion and reaction (Inner and outer Picard’s fixpoint scheme) is given as:

We start with \( \xi_1(0), \xi_2(0) \) and \( n = 1 \):
- Step 0: Initialisation for \( i, j = 0 \) with \( \xi_{1,0}(t^{n+1}) = \xi_1(t^n), \xi_{2,0}(t^{n+1}) = \xi_2(t^n) \) and \( N_{1,0}(t^{n+1}) = N_1(t^n), N_{2,0}(t^{n+1}) = N_2(t^n) \). We have \( i = j = 1 \) (initialisation of the loops).
- Step 1: Outer Loop (Iterative step \( j \)): Diffusion Step, Computation of \( N_{1,j}^{n+1} \) and \( N_{2,j}^{n+1} \) (with \( \Delta t \))
where the time-space is given as $i$.

- Step 1.1.: Inner Loop (Iterative step $i$): Reaction Step, Computation of $\xi_{1,i}^{n+1}$ and $\xi_{2,i}^{n+1}$

\[
\begin{align*}
\xi_{1,i}^{n+1} & = \xi_{1,i}^n - \Delta tD_N^{1,j-1} + \\
& + \Delta t \left( \lambda_{11}\xi_{1,i-1}^{n+1} + \lambda_{12}\xi_{2,i-1}^{n+1} + \lambda_{13}(1 - \xi_{1,i-1}^{n+1} - \xi_{2,i-1}^{n+1}) \right), \\
\xi_{2,i}^{n+1} & = \xi_{2,i}^n - \Delta tD_N^{2,j-1} + \\
& + \Delta t \left( \lambda_{21}\xi_{1,i-1}^{n+1} + \lambda_{22}\xi_{2,i-1}^{n+1} + \lambda_{23}(1 - \xi_{1,i-1}^{n+1} - \xi_{2,i-1}^{n+1}) \right),
\end{align*}
\]

- Step 1.2.: $i = i + 1$ and we go to Step 1.1. till $i = I \ast j$ (else goto Step 2)

- Step 2. Computation of $N_{1,j}^{n+1}$ and $N_{2,j}^{n+1}$

\[
\begin{align*}
\begin{pmatrix} N_{1,j}^{n+1} \\ N_{2,j}^{n+1} \end{pmatrix} &= \frac{D_{13}D_{23}}{1 + \alpha D_{13}^{n+1} + \beta D_{23}^{n+1}} \\
& \left( \begin{pmatrix} 1 \\ \beta \end{pmatrix}^{n+1} + \alpha \xi_{2,i}^{n+1} \right) \begin{pmatrix} -\partial_x\xi_{1,i}^{n+1} \\ -\partial_x\xi_{2,i}^{n+1} \end{pmatrix},
\end{align*}
\]

where $\alpha = \left( \frac{1}{\tau_{12}} - \frac{1}{\tau_{13}} \right)$, $\beta = \left( \frac{1}{\tau_{12}} - \frac{1}{\tau_{23}} \right)$ and the initialisation is given as: $\xi_{1,i}(t^n) = \xi_{1}(t^n)$, $\xi_{2,i}(t^n) = \xi_{2}(t^n)$ (means from the last computation).

- Step 3: $j = j + 1$ and we go to Step 1 till $j = J$.

- Step 4: $n = n + 1$ and we go to Step 0 till $n = N$.

We apply the explicit or implicit methods for the diffusion-reaction equation and obtain $\xi_{1,i}(t^{n+1}), \xi_{2,i}(t^{n+1}), \xi_{3,i}(t^{n+1}) = 1 - \xi_{1,i}(t^{n+1}) - \xi_{2,i}(t^{n+1}).$

For a run, we assume that $I = J = 2$, which means that we have two iterative loops in the inner and two in the outer. For the convergence threshold, we define the variance between a reference solution and the numerical solutions, given as: Time-averaged mean-square value over time (scan over the time-space):

\[
\sigma_{\xi,\Delta t}^2 = \frac{1}{T} \sum_{i=1}^{N} \Delta t \left( \xi_{\Delta t, \text{Scheme}}(i \Delta t) - \xi_{\Delta t, \text{ref}}(i \Delta t) \right)^2.
\]

\[
\sigma_{\xi,\Delta t}^2 = \frac{1}{T} \sum_{i=1}^{N} \Delta t \left( \xi_{\Delta t, \text{Scheme}}(i \Delta t) - \xi_{\Delta t, \text{ref}}(i \Delta t) \right)^2,
\]

where the time-space is given as $i = 1, \ldots, N$, $\Delta t N = T = 1$.

Furthermore, the vectorial time-averaged means square value is:

\[
\sigma_{\xi,\Delta t}^2 = \frac{1}{T} \sum_{i=1}^{N} \Delta t \left( (\xi_{\Delta t, \text{Scheme}}(i \Delta t) - \xi_{\Delta t, \text{ref}}(i \Delta t))^2 \right),
\]

where the time-space is given as $i = 1, \ldots, N$, $\Delta t N = T = 1$. 

Example 1:
\[ \lambda_{11} = -4.276 \times 10^{-7}, \lambda_{21} = \lambda_{31} = -\frac{\lambda_{11}}{2}, \]
\[ \lambda_{22} = -2.082 \times 10^{-13}, \lambda_{12} = \lambda_{23} = -\frac{\lambda_{22}}{2}, \]
\[ \lambda_{33} = -4.276 \times 10^{-7}, \lambda_{31} = \lambda_{32} = -\frac{\lambda_{33}}{2}. \]
The numerical solutions of the three hydrogen plasma in experiment 1 with the asymptotic diffusion.

Example 2:
\[ \lambda_{11} = -4.276 \times 10^{-7}, \lambda_{21} = \lambda_{31} = -\frac{\lambda_{11}}{2}, \]
\[ \lambda_{22} = -2.082 \times 10^{-13}, \lambda_{12} = \lambda_{23} = -\frac{\lambda_{22}}{2}, \]
\[ \lambda_{33} = -4.276 \times 10^{-7}, \lambda_{31} = \lambda_{32} = -\frac{\lambda_{33}}{2}. \]
The numerical solutions of the three hydrogen plasma in experiment 2 with the asymptotic diffusion.

Example 3:

Fig. 8. The upper left figure presents the concentration of \( x_1 \) at spatial point 0.72, the upper right is the result in the space time region, the lower left figure presents the the 3D plot of the second component and the lower right figure presents all of the components at spatial-point 0.72.

The numerical solutions of the three hydrogen plasma in experiment 1 with the uphill diffusion.

Example 2:
\[ \lambda_{11} = -4.276 \times 10^{-2}, \lambda_{21} = \lambda_{31} = -\frac{\lambda_{11}}{2}, \]
\[ \lambda_{22} = -2.082 \times 10^{-8}, \lambda_{12} = \lambda_{23} = -\frac{\lambda_{22}}{2}, \]
\[ \lambda_{33} = -4.276 \times 10^{-8}, \lambda_{31} = \lambda_{32} = -\frac{\lambda_{33}}{2}. \]
The numerical solutions of the three hydrogen plasma in experiment 2 with the asymptotic diffusion.

The numerical solutions of the three hydrogen plasma in experiment 2 with the uphill diffusion.

Example 3:
Fig. 9. The upper left figure presents the concentration of $x_1$ at spatial point 0.72, the upper right is the result in the space time region, the lower left figure presents the the 3D plot of the second component and the lower right figure presents all of the components at spatial-point 0.72.

$$\lambda_{11} = -4.276 \times 10^{-1}, \lambda_{21} = \lambda_{31} = -\frac{\lambda_{11}}{2},$$
$$\lambda_{22} = -2.082 \times 10^{-2}, \lambda_{12} = \lambda_{23} = -\frac{\lambda_{22}}{2},$$
$$\lambda_{33} = -4.276 \times 10^{-2}, \lambda_{31} = \lambda_{32} = -\frac{\lambda_{33}}{2}$$

The numerical solutions of the three hydrogen plasma in experiment 3 with the asymptotic diffusion \cite{12}

The numerical solutions of the three hydrogen plasma in experiment 3 with the uphill diffusion \cite{13}

In the following, we compare the different splitting methods based on the first example with the uphill diffusion.

We deal with a CFL-grid means and we compare the results to the optimal time- and spatial-grid size. Based on this comparison, we are able to find the convergence-tableau for the explicit methods.

We apply the following errors:

- Scalar for each $\xi_1, \xi_2$:
  - Comparison in Time:
  $$err_{i,j}(x, \Delta t) = \sum_{n=1}^{N} \Delta t |\xi_{i,ref}(x, t_n) - \xi_{i,j}(x, t_n)|, \quad (142)$$
Fig. 10. The upper left figure presents the concentration of $x_1$ at spatial point 0.72, the upper right is the result in the space time region, the lower left figure presents the 3D plot of the second component and the lower right figure presents all of the components at spatial-point 0.72.

where we have the component index $i = 1, 2$ and the method index $j = \{AB, ABA, iter\}$ and $x$ is given as an important spatial point, such as $x = 0.72$. Furthermore, $u_{ref}$ is a reference solution, such as with very small $\Delta t_{ref}$, and $u_j$ is the numerical solution of the method $j$ with $\Delta t = \{\Delta t_{coarse}, \Delta t_{coarse}/2, \Delta t_{coarse}/4, \Delta t_{coarse}/8\}$ and the finest time-step is $\Delta t_{coarse}/16$. In space, we compare to the coarsest grid, which means that we interpolate the finer space solutions to the coarsest grid.

• Comparison in time and space:

$$err_{i,j}(\Delta t) = \sum_{k=1}^{J_{coarse}} \Delta x_{coarse} \sum_{n=1}^{N} \Delta t |\xi_{i,ref}(x_k(\Delta t_{coarse}/16),t_n) - \xi_{i,j}(x_k(\Delta t),t_n)|,$$

where we have the component index $i = 1, 2$ and the method index $j = \{AB, ABA, iter\}$, and $T$ is given as an important time point, such as the end time-point $t = T$. Furthermore, $\xi_{i,ref}$ is a reference solution, such as with very small $\Delta t_{ref}$, and $\xi_{i,j}$ is the numerical solution of the method $j$ with $\Delta t = \{\Delta t_{coarse}, \Delta t_{coarse}/2, \Delta t_{coarse}/4, \Delta t_{coarse}/8\}$ and the finest time-step is $\Delta t_{coarse}/16$. In space, we compare to the coarsest
grid, which means that we interpolate the finer space solutions to the coarsest grid.

Vectorial for $\xi = (\xi_1, \xi_2, \xi_3)^T$:

- Comparison in Time:

$$
err_j(x, \Delta t) = \frac{N}{N} \sum_{n=1}^{N} \Delta t \left( \sum_{i=1}^{3} |\xi_{i,ref}(x, t_n) - \xi_{i,j}(x, t_n)| \right),
$$

(144)

where the method index $j = \{AB, ABA, iter\}$ and $x$ is given as an important spatial point, such as $x = 0.72$. Furthermore, $u_{ref}$ is a reference solution, such as with very small $\Delta t_{ref}$, and $u_j$ is the numerical solution of the method $j$ with $\Delta t = \{\Delta t_{coarse}, \Delta t_{coarse}/2, \Delta t_{coarse}/4, \Delta t_{coarse}/8\}$ and the finest time-step is $\Delta t_{coarse}/16$. In space, we compare to the coarsest grid, which means that we interpolate the finer space solutions to the coarsest grid.

- Comparison in time and space:

$$
err_j(\Delta t) = \\
= \sum_{k=1}^{J_{coarse}} \Delta x_{coarse} \sum_{n=1}^{N} \Delta t \left( \sum_{i=1}^{3} |\xi_{i,ref}(x_k(\Delta t_{coarse}/16), t_n) - \xi_{i,j}(x_k(\Delta t), t_n)| \right),
$$

(145)
where the method index $j = \{AB, ABA, iter\}$ and $T$ is given as an important time point, such as the end time-point $t = T$. Further $u_{\text{ref}}$ is a reference solution, such as with very small $\Delta t_{\text{ref}}$, and $u_j$ is the numerical solution of the method $j$ with $\Delta t = \{\Delta t_{\text{coarse}}, \Delta t_{\text{coarse}}/2, \Delta t_{\text{coarse}}/4, \Delta t_{\text{coarse}}/8\}$ and the finest time-step is $\Delta t_{\text{coarse}}/16$. In space, we compare to the coarsest grid, which means that we interpolate the finer space solutions to the coarsest grid.

Convergence-tableau for the different methods. We have the following CFL-condition:

$$\Delta t \leq \frac{\Delta x^2}{2D_{\text{max}}} \approx \Delta x^2,$$

(146)

where we have $2D_{\text{max}} \approx 1$.

We write in the notation of the grid-points:

$$J^2 \leq N,$$

(147)

where $J$ are the number of spatial grid-points and $N$ is the number of time-points.
Fig. 13. The upper left figure presents the concentration of $x_1$ at spatial point 0.72, the upper right is the result in the space-time region, the lower left figure presents the 3D plot of the second component and the lower right figure presents all of the components at spatial-point 0.72.

We have the following resolutions in Table 1 and Figure 14.

To compare the values only on the coarsest CFL-grid, we have to apply the following approximation:

\[
x_k(\Delta t), k = 0, \ldots, 50,
\]

coarsest spatial grid with time-step $\Delta t$, \hspace{1cm} (148)

\[
x_k(\Delta t/2), k(\Delta t/2) = \lfloor k \sqrt{2} \rfloor = 1, 2, 4, \ldots, 70,
\]

next finer grid with time-step $\Delta t/2$, \hspace{1cm} (149)

\[
x_k(\Delta t/4), k(\Delta t/4) = k 2 = 2, 4, 6, \ldots, 100,
\]

next finer grid with time-step $\Delta t/4$, \hspace{1cm} (150)

\[
x_k(\Delta t/8), k(\Delta t/8) = \lfloor k 2\sqrt{2} \rfloor = 2, 5, 8, \ldots, 140,
\]

next finer grid with time-step $\Delta t/8$, \hspace{1cm} (151)

\[
x_k(\Delta t/16), k(\Delta t/16) = \lfloor k 4 \rfloor = 4, 8, 12, \ldots, 200,
\]

finest grid with time-step $\Delta t/16$, \hspace{1cm} (152)

where $\lfloor x \rfloor = \max\{k \in \mathbb{Z} | k \leq x\}$. 

| Method                  | Spatial-Points | Time-points |
|------------------------|----------------|-------------|
| iter3                  | 190            | 80000       |
| (reference solution)   |                |             |
| iter3, iter2,          | 140            | 40000       |
| AB, ABA                |                |             |
| iter3, iter2,          | 100            | 20000       |
| AB, ABA                |                |             |
| iter3, iter2,          | 70             | 10000       |
| AB, ABA                |                |             |
| iter3, iter2,          | 50             | 5000        |
| AB, ABA                |                |             |

Table 1. The spatial- and time-grid-points related to the reference solution

**Fig. 14.** The optimal spatial-grid (CFL-condition) to the time-steps.

**Remark 2.** We have the following computational times for the Picard’s methods in table 2.

| Example | Computational Time [sec] |
|---------|--------------------------|
| 1       | 6.8736e+03               |
| 2       | 7.3985e+03               |
| 3       | 8.8402e+03               |

Table 2. The computational time of the three experiments with different reaction parameters with \( N_{spatial} = 140 \) number of spatial discretisation points, \( N_{end} = 80000 \) number of time-steps

The convergence results are given in Figure 15. We have the following computational times for the Picard’s methods in table 3. Here, we see the additional work of the iterative methods. We obtain optimal solutions for the iterative methods, while we could extend the time-step. For more detailed computations and smaller time-steps, the non-
Fig. 15. The convergence of the different methods are computed over the full domain and with different time-steps.

| Example | Computational Time [sec] |
|---------|--------------------------|
| AB      | 165.0895 [sec]           |
| ABA     | 262.3892 [sec]           |
| iter2   | 404.9536 [sec]           |
| iter3   | 578.3206 [sec]           |

Table 3. The computational time of the different methods with $N_{\text{spatial}} = 140$ number of spatial discretisation points, $N_{\text{end}} = 80000$ number of time-steps

iterative splitting methods are more effective, while we could obtain at least a second order approach, see also [9].

Remark 3.

6 Conclusions and Discussions

We present the coupled model for a multi-component transport model for reactive plasma. The nonlinear partial differential equations are solved with iterative methods and a combination of splitting approaches. The numerical algorithms are presented and their numerical convergences are shown. Although iterative splitting methods are more time-consuming, they are more accurate than noniterative splitting approaches. The benefits of noniterative methods when we apply explicit schemes include fast computation time and good resolution of space and time space. The implicit behavior of iterative methods allows larger time-steps to be used and they could accelerate the solver process. In the future we aim to study the numerical analysis of the different combined schemes and we will simulate more delicate multicomponent models.

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