"OVIDIUS" UNIVERSITY OF CONSTANTA
DOCTORAL SCHOOL OF APPLIED SCIENCES
MATHEMATICS DOCTORAL PROGRAM

DOCTORAL THESIS
SUMMARY

DISCRETIZATION AND PRECONDITIONING TECHNIQUES WITH APPLICATIONS TO MULTICOMPONENT DIFFUSION PROBLEMS

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CONSTANŢA, 2014

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Introduction

The mass transfer phenomenon in many real-life and engineering processes often governs the kinetics of the overall process. An accurate modeling of the mass transfer is therefore necessary, opportune and principally possible, particularly in multicomponent systems. For these reasons, multicomponent diffusion has gained a considerably increasing interest during the last decades.

For the description of mutual diffusion in multicomponent systems, two approaches are prevalent in literature[4][19]: generalized Ficks law and the Maxwell-Stefan [13][17] theory. For more details we refer to [2], [10], [11], [15], [20]. It should be noted that, in a multicomponent mixture of chemical species the diffusion of a certain species depends by the concetration gradient of the other species.

As a result of an analysis of the multicomponent mass transfer research, in this thesis we propose:

-to develop a strategy of investigation that emphasizes very clearly the influence of the cross-diffusion coupling and the number of chemical species involved in the process on the convergence rate of the numerical algorithms;

-to develop specific preconditioners for multi-component mass transfer problems, which will be used in connection with the gradient-type and Krylov subspace methods (BICGSTAB and restarted GMRES(m)); the nonlinear algorithm employed in this case is the modified Picard iteration;

-to test multigrid methods for numerical solving of the multicomponent mass transfer problems (both linear and non-linear cases) and modified Picard method (non-linear case);

-to test splitting method for numerical solving of time-dependent multicomponent mass transfer problems.

The general form of partial differential equations of order II, which models the multicomponent mass transfer problems presented in this thesis, is the following

$$\frac{\partial Z_i}{\partial \tau} + \epsilon Peu(y)\frac{\partial Z_i}{\partial x} = \sum_{j=1}^{p}(\epsilon^2 \frac{\partial}{\partial x}(D_{ij}\frac{\partial Z_j}{\partial x}) + \frac{\partial}{\partial y}(D_{ij}\frac{\partial Z_j}{\partial y})) + k_i Z_i,\ i = \overline{1,p},$$

$$(x,y) \in (0,1)\times(0,1),\ \tau \in (0, T_{final}).$$

The unknowns Z_i are the dimensionless concentrations of chemical species. The first term in the right, models the process of mass transfer by diffusion. The functions $D_{ij}(x,y)$ are the multicomponent diffusion Fick coefficients and they express the cross-diffusion coupling of the chemical species involved in the process. The second term in the left sight express the convection process of mass transfer, when the mixture is involved in a flow. Peclet number Pe create a balance between the process of diffusion and of convection. If $Pe \gg 1$ the dominant is the phenomenon of convection. Otherwise, if $Pe \ll 1$ the diffusion

phenomenon becomes dominant. The second term of the right sight represents the reaction term. It express the chemical reactions between species. The term $\frac{\partial Z_i}{\partial \tau}$ express the time dependence of mass transfer. [21]

This thesis is structured in four chapters.

Chapter 1 Preliminaries presents some basic concepts of linear algebra and numerical analysis used throughout the paper.

In **Chapter 2** we approach solving, through numerical methods, the steady state multicomponent diffusion-reaction problems the linear and nonlinear case. These problems are modeled by second-order partial differential equations.

The personal contribution consists of:

-the selection of numerical methods suitable for solving such problems;

-building a preconditioning matrix based on one type of diagonal block, that can be used in the preconditioning techniques for the algebraic systems, obtained from the discretization of the multicomponent diffusion-reaction equations,in order to improve the restarted GMRES and BiCGSTAB methods performances; we made a theoretical analysis of the character of good preconditioner of the proposed matrix ;

-analysis of the influence of the cross-diffusion of chemical species, on the performance of the numerical algorithms used; in the numerical tests we used several sets of values for the parameters of the problem.

In **Chapter 3** we approach solving, through numerical methods, the steady state multicomponent convection-diffusion-reaction problems, the linear and nonlinear case. These problems are modeled by second-order partial differential equations.

The personal contribution consists of:

-the selection of numerical methods suitable for solving such problems;

-building a preconditioning matrix based on one type of diagonal block, that can be used in the preconditioning techniques for the algebraic systems, obtained from the discretization of the multicomponent convection-diffusion-reaction equations,in order to improve the restarted GMRES method performances; in the preconditioning matrix building we considered the influence of the convection term;

-analysis of the influence of the cross-diffusion of chemical species and the convection phenomenon, on the performance of the numerical algorithms used; in the numerical tests we used several sets of values for the parameters of the problem.

In **Chapter 4** we approach solving, through numerical methods, time-dependent multicomponent convection-diffusion problems, the linear case. These problems are modeled by second-order partial differential equations, in which, in addition to the spatial variables derivatives appears the time derivative of order I.

The personal contribution consists of:

-proposal of a spatial operator decomposition in the splitting method used to solve this class of problems;

-determination of sufficient conditions that ensure the stability of the splitting method.

The original results presented in this thesis are contained in the following articles:

- Gh. Juncu, A. Nicola, C. Popa, E. Stroilă, *Preconditioned conjugate gradient and multigrid methods for numerical solution of multicomponent mass transfer equations I. Diffusion-reaction-equations,* Numer. Heat Transfer A 66 (11) pp. 1268-1296, 2014, Impact Factor - 1.80. [7]

- Gh. Juncu, A. Nicola, C. Popa, E. Stroilă, *Preconditioned conjugate gradient and multigrid methods for numerical solution of multicomponent mass transfer equations II. Convection-diffusion-reaction equations,* Numer. Heat Transfer A 66 (11) pp. 1297-1319, 2014, Impact Factor - 1.80. [8]

- E. Stroilă, *Splitting method for multicomponent mass transfer equations,* in Topics in Mathematical Modelling of Life Science Problems - Proceedings of the ninth workshop, Editura Matrix Rom, Bucuresti, pp. 77-91, 2013. [18]

1 Preliminaries

Chapter 1 presents:

- some basic notions and concepts of linear algebra and matrix analysis used throughout this paper: definitions of the canonical scalar product and euclidian norm in $\mathbb{R}^n$, matrices decompositions, spectral proprieties of square matrices, Kronecker product (1.1 Introductory Notions of Matrix Analysis);

- approximation methods of differential operators in the finite differences schemes method that could be applied to multicomponent mass transfer problems (1.2 Finite Differences Scheme) ;

- methods of solving nonlinear discrete problems (1.3 Nonlinear Multigrid Method, 1.4 Modified Picard Method);

- projective iterative methods used for solving systems of linear algebraic equations obtained in a modified Picard method step, or in the case of linear problems: GMRES and BiCGSTAB (1.5 Projective Iterative Methods);

- splitting method used for time-dependent multicomponent mass transfer eqution and conditions of stability of the method (1.6 Splitting Method);
- the concept of preconditioning and general preconditioning techniques of linear algebraic systems (1.7 Overview of Preconditioning Techniques).

2 Steady-State Multicomponent Diffusion-Reaction Problems

The results presented in this chapter are published în [7].

2.1 Problem Formulation

Consider the following isothermal, first-order, complex chemical reaction, taking

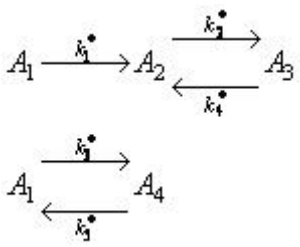

Figure 1: Chemical reaction scheme

place inside a finite slab catalyst pellet with square section. The inter-phase transport resistances are assumed negligibly (the concentrations on the external surface of the catalyst pellet are the same as the bulk values). Considering a homogeneous porous pellet and the total mixture molar concentration constant, the dimensionless steady-state concentrations profiles inside the pellet are given by a second-order partial differential equations system.

$$\sum_{j=1}^{4}\left(\frac{\partial}{\partial x}D_{ij}\frac{\partial Z_j}{\partial x}+\frac{\partial}{\partial y}D_{ij}\frac{\partial Z_j}{\partial y}\right)+R_i=0,\ i=\overline{1,4}, \tag{1}$$

$$(x,y)\in\Omega=(0,1)\times(0,1)$$

where

$$R_1=-k_1Z_1-k_3Z_1+k_5Z_4,\ R_2=k_1Z_1-k_2Z_2+k_4Z_3,$$

$$R_3=k_2Z_2-k_4Z_3,\ R_4=k_3Z_1-k_5Z_4,$$

$Z_i=\frac{A_i}{A_{1b}}$ are the dimensionless concentrations, A_{1b} is the bulk molar concentration of species A_1, $k_i=\frac{k_i^*L^2}{D_{ref}}$ are the dimensionless reaction rate constants,

L is the length of the square section,$D_{ij}(x,y)$ are the multicomponent Fick diffusion coefficients related to D_{ref}. Note that for diffusion-reaction systems the molar average frame can be used. The boundary conditions are

$$Z_1 = 1,\ Z_i = 0,\ i = 2,3,4\ \ (x,y) \in \partial\Omega \tag{2}$$

The mathematical model presented previously represents the nonlinear test problem used in this work. The linear test problem employed in this work is obtained from the non-linear one by considering the multicomponent Fick diffusion coefficients constants.

2.2 Numerical Methods

2.2.1 Problem Discretization

The derivatives of equation (1) were discretized with the central second order accurate finite difference scheme on uniform grids with $N \times N$ points,

$$0 = x_1 < x_2 < ... < x_{N-1} < x_N = 1,\ x_k = (k-1)h;$$

$$0 = y_1 < y_2 < ... < y_{N-1} < y_N = 1,\ y_l = (l-1)h,\ k,l = \overline{0,N},$$

where $h = \frac{1}{(N-1)}$ is the grid step size. The discrete approximation obtained for (1) is

$$\sum_{j=1}^{4}[\frac{D_{ij}^{k+\frac{1}{2},l}(Z_j^{k+1,l} - Z_j^{k,l}) - D_{ij}^{k-\frac{1}{2},l}(Z_j^{k,l} - Z_j^{k-1,l})}{h^2} +$$

$$\frac{D_{ij}^{k,l+\frac{1}{2}}(Z_j^{k,l+1} - Z_j^{k,l}) - D_{ij}^{k,l-\frac{1}{2}}(Z_j^{k,l} - Z_j^{k,l-1})}{h^2}] + R_i^{k,l} = 0,\ i = \overline{1,4} \tag{3}$$

The values of the diffusion coefficients were calculated as arithmetic averages of the grid point values.

The method of calculation of the Fick coefficients values of the grid is presented in this thesis in section 2.1. The derivation formula for the terms $\frac{\partial}{\partial x}D_{ij}(x,y)\frac{\partial Z_j}{\partial x}$ şi $\frac{\partial}{\partial y}D_{ij}(x,y)\frac{\partial Z_j}{\partial y}$ is the following second order aproximation [16] pg. 50:

$$\frac{d}{dx}[a(x)\frac{d}{dx}] \approx \frac{a_{i+\frac{1}{2}}(u_{i+1} + u_i) - a_{i-\frac{1}{2}}(u_i + u_{i-1})}{h^2}. \tag{4}$$

The discrete approximation of the linear test problem is:

$$\sum_{j=1}^{4} D_{ij}\frac{Z_j^{k+1,l} + Z_j^{k-1,l} + Z_j^{k,l+1} + Z_j^{k,l-1} - 4Z_j^{k,l}}{h^2} + R_i^{k,l} = 0,\ i = 1,2,3,4. \tag{5}$$

where $\frac{Z_j^{k+1,l}+Z_j^{k-1,l}+Z_j^{k,l+1}+Z_j^{k,l-1}-4Z_j^{k,l}}{h^2}$ represent the expresion of discrete Laplace operator.). In this case, the multicomponent Fick diffusion coefficients, D_{ij} are constant.

2.2.2 Numerical Algorithms

Two nonlinear algorithms are used in this work: nonlinear multigrid (MG) [1] [9] and modified Picard iteration, [12]. The nonlinear MG algorithm used is the classical Full Approximation Storage (FAS) algorithm [1] [9], suitable for both linear and nonlinear problems.

The structure of the MG cycle is: 1) cycle of type V; 2) two smoothing steps are performed before the coarse grid correction and one after; 3) prolongation by bilinear interpolation for corrections; 4) restriction of residuals by full weighting. Two smoothing algorithms were tested: point Gauss Seidel (PGS) and alternating line Gauss - Seidel (ALGS).

The modified Picard iteration, also called a fixed point method, is given by

$$\begin{aligned} A(Z^m)\delta Z^{m+1} &= b(Z^m) - A(Z^m)Z^m \\ Z^{m+1} &= Z^m + \delta Z^{m+1} \end{aligned} \tag{6}$$

where m is the iteration number $Z^m = [Z_1^m, Z_2^m, Z_3^m, Z_4^m]$, iar Z_0 is the initial estimate. Matrix $A(Z^m)$ is defined by

$$A(Z^m) = \begin{bmatrix} A_{11}^m & A_{12}^m & A_{13}^m & A_{14}^m \\ A_{21}^m & A_{22}^m & A_{23}^m & A_{24}^m \\ A_{31}^m & A_{32}^m & A_{33}^m & A_{34}^m \\ A_{41}^m & A_{42}^m & A_{43}^m & A_{44}^m \end{bmatrix} + \begin{bmatrix} (k_1+k_3)h^2I & 0 & 0 & -k_5h^2I \\ -k_1h^2I & k_2h^2I & -k_4h^2I & 0 \\ 0 & -k_2h^2I & k_4h^2I & 0 \\ -k_3h^2I & 0 & 0 & k_5h^2I \end{bmatrix} \tag{7}$$

where I is the $(N-2)^2 \times (N-2)^2$ identity matrix. The blocks A_{ij}^m are $(N-2)^2 \times (N-2)^2$ penta-diagonal matrices corresponding to the discretization stencil

$$\begin{bmatrix} & CN & \\ CW & CM & CE \\ & CS & \end{bmatrix} \tag{8}$$

$$CM = D_{ij}^{k+\frac{1}{2},l} + D_{ij}^{k-\frac{1}{2},l} + D_{ij}^{k,l+\frac{1}{2}} + D_{ij}^{k,l-\frac{1}{2}}$$

$$CE = -D_{ij}^{k+\frac{1}{2},l},\ CW = -D_{ij}^{k-\frac{1}{2},l},\ CS = -D_{ij}^{k,l-\frac{1}{2}},\ CN = -D_{ij}^{k,l+\frac{1}{2}}$$

and they vary at every iterative step.

The linear solvers employed in the modified Picard iteration are the Matlab R2010b implementations of the preconditioned BICGSTAB and preconditioned restarted GMRES (m), and they are presented in Section 1.5. These algorithms were also used to solve the linear test problem. Codes for the modified Picard method and techniques of preconditioning are our own implementations in Matlab R2010b respectively for MG in FORTRAN 77.

2.2.3 The Preconditioning Techniques

The linear system that should be solved in a Picard step or for the linear test problem can be written as

$$AZ = B \tag{9}$$

where

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix},\ Z = \begin{bmatrix} Z_1 \\ Z_2 \\ Z_3 \\ Z_4 \end{bmatrix},\ B = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}.$$

A_{ij} blocks are $(N-2)^2 \times (N-2)^2$ square matrices and A_{ii} blocks, $i = \overline{1,4}$ are symmetric and positive definite matrices. The classic construction method of a preconditioning matrix for (9) is based on a Choleski decomposition, complete or incomplete of the diagonal blocks:

$$A_{ii} = C_i C_i^T + R_i,\ i = \overline{1,4} \tag{10}$$

(if $R_i = 0,\ i = \overline{1,4}$ we refer to a complete decomposition, otherwise we refer to the incomplete case [14] [16]).

Block-diagonal Jacobi preconditioning techniques are quite good, but needs four Choleski decompositions, complete or incomplete, of diagonal blocks, which gets high costs from the computational point of view in the practical applications.

We proposed a block preconditioning method for the system (9), which uses the same matrix for any diagonal block.

Thus, after the discretization of the equations (1) the blocks A_{ij} have the structure

$$A_{11} = D_{11}\Delta_0 + (k_1+k_3)h^2 I;\ A_{12} = D_{12}\Delta_0;\ A_{13} = D_{13}\Delta_0;\ A_{14} = D_{14}\Delta_0 - k_5 h^2 I;$$

$$A_{21} = D_{21}\Delta_0 - k_1 h^2 I;\ A_{22} = D_{22}\Delta_0 + k_2 h^2 I;\ A_{23} = D_{23}\Delta_0 - k_4 h^2 I;\ A_{24} = D_{24}\Delta_0;$$

$$A_{31} = D_{31}\Delta_0;\ A_{32} = D_{32}\Delta_0 - k_2 h^2 I;\ A_{33} = D_{33}\Delta_0 + k_4 h^2 I;\ A_{34} = D_{34}\Delta_0; \tag{11}$$

$$A_{41} = D_{41}\Delta_0 - k_3 h^2 I;\ A_{42} = D_{42}\Delta_0;\ A_{43} = D_{43}\Delta_0;\ A_{44} = D_{44}\Delta_0 + k_5 h^2 I.$$

where I is the $(N-2)^2 \times (N-2)^2$ unitary matrix and Δ_0 correspond to the 5-point stencil nite difference discretization of the equation $-\Delta z = 0$ with the same condition on the boundary $\partial\Omega$ with respect to Z_1, $z = 1$ (see (2)). Matrix Δ_0 is symmetric and positive definite.

We define

$$\tilde{\Delta}_0 = \Delta_0 + h^2 I. \tag{12}$$

By construction $\tilde{\Delta}_0$ is a symmetric and positive definite matrix ($\langle\tilde{\Delta}_0 x, x\rangle = \langle\Delta_0 x, x\rangle + h^2\|x\|^2 > 0, \forall x \neq 0$) and admits a Choleski decomposition (for R=0 the decomposition is complety, otherwise is incomplete)

$$\tilde{\Delta}_0 = CC^T + R. \tag{13}$$

According to these considerations we propose as preconditioner the matrix

$$\begin{aligned} P &= \begin{bmatrix} \tilde{\Delta}_0 & 0 & 0 & 0 \\ 0 & \tilde{\Delta}_0 & 0 & 0 \\ 0 & 0 & \tilde{\Delta}_0 & 0 \\ 0 & 0 & 0 & \tilde{\Delta}_0 \end{bmatrix} = \\ &= \begin{bmatrix} C & 0 & 0 & 0 \\ 0 & C & 0 & 0 \\ 0 & 0 & C & 0 \\ 0 & 0 & 0 & C \end{bmatrix} \begin{bmatrix} C^T & 0 & 0 & 0 \\ 0 & C^T & 0 & 0 \\ 0 & 0 & C^T & 0 \\ 0 & 0 & 0 & C^T \end{bmatrix} = \Gamma \cdot \Gamma^T \end{aligned} \tag{14}$$

in the following three cases
- right preconditioning

$$AU = B \Leftrightarrow \tilde{A}_1\tilde{U}_1 = \tilde{B}_1,\ \tilde{A}_1 = AP^{-1},\ \tilde{U}_1 = PU,\ \tilde{B}_1 = B \tag{15}$$

-left preconditioning

$$AU = B \Leftrightarrow \tilde{A}_2\tilde{U}_2 = \tilde{B}_2,\ \tilde{A}_2 = P^{-1}A,\ \tilde{U}_2 = U,\ \tilde{B}_2 = P^{-1}B \tag{16}$$

- split preconditioning

$$AU = B \Leftrightarrow \tilde{A}_3\tilde{U}_3 = \tilde{B}_3,\ \tilde{A}_3 = \Gamma^{-1}A\Gamma^{-T},\ \tilde{U}_3 = \Gamma^T U,\ \tilde{B}_3 = \Gamma^{-1}B \tag{17}$$

Comments on spectra of the preconditioned matrices

From relations (11) the system's matrix A could be written

$$\begin{bmatrix} D_{11}\Delta_0 & D_{12}\Delta_0 & D_{13}\Delta_0 & D_{14}\Delta_0 \\ D_{21}\Delta_0 & D_{22}\Delta_0 & D_{23}\Delta_0 & D_{24}\Delta_0 \\ D_{31}\Delta_0 & D_{32}\Delta_0 & D_{33}\Delta_0 & D_{34}\Delta_0 \\ D_{41}\Delta_0 & D_{42}\Delta_0 & D_{43}\Delta_0 & D_{44}\Delta_0 \end{bmatrix} + \begin{bmatrix} (k_1+k_3)h^2I & 0 & 0 & -k_5h^2I \\ -k_1h^2I & k_2h^2I & -k_4h^2I & 0 \\ 0 & -k_2h^2I & k_4h^2I & 0 \\ -k_3h^2I & 0 & 0 & k_5h^2I \end{bmatrix} \tag{18}$$

where I is the $(N-2)^2 \times (N-2)^2$ unitary matrix and

$$D = \begin{bmatrix} D_{11} & D_{12} & D_{13} & D_{14} \\ D_{21} & D_{22} & D_{23} & D_{24} \\ D_{31} & D_{32} & D_{33} & D_{34} \\ D_{41} & D_{42} & D_{43} & D_{44} \end{bmatrix},\ \aleph = h^2 \begin{bmatrix} (k_1+k_3) & 0 & 0 & -k_5 \\ -k_1 & k_2 & -k_4 & 0 \\ 0 & -k_2 & k_4 & 0 \\ -k_3 & 0 & 0 & k_5 \end{bmatrix} \tag{19}$$

are the diffusion, respectively reaction coefficients matrices. If ($\otimes$) denotes the Kronecker product of two matrices (see Section 1.1), relation (18) could be written

$$A = (D \otimes \Delta_0) + (\aleph \otimes I). \tag{20}$$

From relation (14) we obtain

$$P^{-1} = \begin{bmatrix} \tilde{\Delta}_0^{-1} & 0 & 0 & 0 \\ 0 & \tilde{\Delta}_0^{-1} & 0 & 0 \\ 0 & 0 & \tilde{\Delta}_0^{-1} & 0 \\ 0 & 0 & 0 & \tilde{\Delta}_0^{-1} \end{bmatrix} = I_4 \otimes \tilde{\Delta}_0^{-1} \tag{21}$$

where I_4 is the 4×4 unitary matrix.

$$\tilde{A}_1 = AP^{-1} = [(D \otimes \Delta_0) + (\aleph \otimes I)](I_4 \otimes \tilde{\Delta}_0^{-1}) = (D \otimes \Delta_0 \tilde{\Delta}_0^{-1}) + (\aleph \otimes \tilde{\Delta}_0^{-1}). \tag{22}$$

If the two matrices $D \otimes \Delta_0 \tilde{\Delta}_0^{-1}$ and $\aleph \otimes \tilde{\Delta}_0^{-1}$ were symmetric, according to Weyls theorem (see Section 1.1) we would get some information about the eigenvalues of their sum, i.e. $\tilde{A}_1$. But, unfortunately this is not the case for general problems and the only information we can get are concerned with the spectra of the matrices $D \otimes \Delta_0 \tilde{\Delta}_0^{-1}$ and $\aleph \otimes \tilde{\Delta}_0^{-1}$ separately.

We obtain

$$\sigma(D \otimes \Delta_0 \tilde{\Delta}_0^{-1}) = \{\frac{\lambda d_i}{\lambda + h^2},\ \lambda \in \sigma(\Delta_0),\ i = 1, 2, 3, 4\}, \tag{23}$$

$$\sigma(\aleph \otimes \tilde{\Delta}_0^{-1}) = \{\frac{\alpha_i}{\lambda + h^2},\ \lambda \in \sigma(\Delta_0),\ i = 1, 2, 3, 4\}, \tag{24}$$

where $\sigma(D)$, $\sigma(\aleph)$ represents the D and $\aleph$ spectra,

$$\sigma(D) = \{d_1, d_2, d_3, d_4\},\ \sigma(\aleph) = \{\alpha_1, \alpha_2, \alpha_3, \alpha_4\}. \tag{25}$$

The eigenvalues of $\aleph$ can be calculated directly

$$\sigma(\aleph) = \{0, h^2(k_2 + k_4), h^2 x_1, h^2 x_2\} \tag{26}$$

where x_1, x_2 are the real solutions of the equation

$$x^2 - (k_1 + k_2 + k_5)x + k_1 k_5 = 0. \tag{27}$$

Spectral properties for the blocks of the split preconditioning matrix

Definition 1. *For a nonsingular $n \times n$ matrix S we define the spectral condition number [6] by*

$$cond_2(S) = \sqrt{\frac{\lambda_{max}(S^T S)}{\lambda_{min}(S^T S)}}, \tag{28}$$

where $\lambda_{max}(S^TS) \geq \lambda_{min}(S^TS) > 0$ *are the extreme eigenvalues of the symmetric and positive definite matrix* S^TS.. *If* S *is itself symmetric and positive definite then*

$$cond_2(S) = \frac{\lambda_{max}(S)}{\lambda_{min}(S)}. \tag{29}$$

Definition 2. *Two symmetric and positive definite matrices* S, T *are spectrally equivalent if ([3]) there exist positive constants* α_1, α_2 *independent on the dimension* n *such that*

$$\alpha_1 \leq \frac{\langle Sx, x\rangle}{\langle Tx, x\rangle} \leq \alpha_2, \ \forall x \in \mathbb{R}^n, x \neq 0, \tag{30}$$

where $\langle \cdot, \cdot \rangle$, $\| \cdot \|$ *will denote the scalar product and the Euclidean norm.*

Proposition 1. *[6], [14] Let* S, T *be spectrally equivalent as in (30) and*

$$T = QQ^T \tag{31}$$

a Cholesky decomposition of T. *Then*

$$cond_2(Q^{-1}SQ^{-T}) \leq \frac{\alpha_2}{\alpha_1}, \tag{32}$$

i.e., T *is a good preconditioner for* S. *Moreover this result is independent on the decomposition (31).*

We prove spectral equivalence relations as (30) for $S = A_{ij}$ and $T = \tilde{\Delta}_0 = CC^T$. From Proposition 1 and (11), the spectral condition number of the matrix $C^{-1}A_{ii}C^{-T}$ satisfies

$$cond_2(C^{-1}A_{ii}C^{-T}) \leq \frac{\alpha_2}{\alpha_1}, \tag{33}$$

where
$\alpha_1 = \min\{\min_{1\leq i\leq 4} D_{ii}, (k_1 + k_3), k_2, k_4, k_5\}$, $\alpha_2 = \max\{\max_{1\leq i\leq 4} D_{ii}, (k_1 + k_3), k_2, k_4, k_5\}$.

Let now

$$B = d\Delta_0 - kh^2I = d\Delta_0 - kh^2I = d\tilde{\Delta}_0 - (k + d)h^2I, \tag{34}$$

where $d \in \{D_{ij}, i, j = \overline{1,4}, i \neq j\}$, $k \in \{0, k_i, i = \overline{1,5}\}$ with appropriate combinations (see (11)), be a generic notation for one of the off-diagonal blocks A_{ij}, $i, j = \overline{1,4}$, $i \neq j$. Using again the relation (32) and considering $\lambda_{min}(\Delta_0) = ch^2$ [5] with c independent of h we obtain

$$cond_2(C^{-1}A_{ij}C^{-T}) \leq \gamma, \tag{35}$$

with $\gamma = \frac{\max\{d,k\}(c+1)}{dc-k} > 0$ independent of N.

The conclusion is that for both, diagonal and off-diagonal preconditioned blocks, we obtain a mesh independent condition number.

2.3 Numerical Results

The main objective of the present work is to analyze the influence of cross-diffusion coupling on the numerical performances of the numerical algorithms. In order to achieve this objective, we considered, for each sets of parameters, the following four structures for the multi-component Fick diffusion matrix:

$$\begin{bmatrix} D_{11} & 0 & 0 & 0 \\ 0 & D_{22} & 0 & 0 \\ 0 & 0 & D_{33} & 0 \\ 0 & 0 & 0 & D_{44} \end{bmatrix}, \begin{bmatrix} D_{11} & D_{12} & 0 & 0 \\ D_{21} & D_{22} & 0 & 0 \\ 0 & 0 & D_{33} & 0 \\ 0 & 0 & 0 & D_{44} \end{bmatrix}, \begin{bmatrix} D_{11} & D_{12} & D_{13} & 0 \\ D_{21} & D_{22} & D_{23} & 0 \\ D_{31} & D_{32} & D_{33} & 0 \\ 0 & 0 & 0 & D_{44} \end{bmatrix},$$

$$(a) \qquad (b) \qquad (c)$$

$$\begin{bmatrix} D_{11} & D_{12} & D_{13} & D_{14} \\ D_{21} & D_{22} & D_{23} & D_{24} \\ D_{31} & D_{32} & D_{33} & D_{34} \\ D_{41} & D_{42} & D_{43} & D_{44} \end{bmatrix}, \tag{36}$$

$$(d)$$

In case (a) there is no cross-diffusion coupling. The species interact only through the chemical reactions. For cases (b) to (d) the cross-diffusion coupling increases progressively, from two species interaction (case (b)) to all species interaction (case (d)). In the next paragraphs of this section, for brevity, the case (a) will be symbolized by CPL1, case (b) by CPL2, case (c) by CPL3 and case (d) by CPL4. In these cases, for the linear problem, cross-diffusion constantes are selected from the Fick coefficients matrices presented in Appendix A of the thesis. For the non-linear problem, the values of the Stefan-Maxwell coefficients used to calculate the Fick coefficients are presented in Appendix B of the thesis.

The performances of the numerical algorithms are monitored by the average reduction factor, $\bar{\rho}$, and the efficiency, τ:

$$\tau = \frac{W}{|ln\bar{\rho}|}, \tag{37}$$

$$\bar{\rho} = (\frac{\|res_i\|}{\|res_0\|})^{\frac{1}{i}}, \tag{38}$$

where $res_i = \|b_i - A_i Z_i\|$ is the residue after i iterations, $\|\cdot\|$ euclidean vectorial norm, W (the work) is the number of arithmetic operations per grid point and iteration step.

In Sections 2.3.1 şi 2.3.2 we present the numerical results of the tests and an analysis of them.

2.4 Conclusions

In this work we have analysed the numerical performances of the MG and modified Picard preconditioned conjugated gradient methods for solving steady state, linear / non-linear multicomponent diffusion - reaction equations in two space dimensions. Different sets of Stefan-Maxwell / Fick diffusion coefficient matrices and dimensionless chemical reaction rate constants were used. In this work we have analysed the numerical performances of the MG and modified Picard preconditioned conjugated gradient methods for solving steady state, linear / non-linear multicomponent diffusion-reaction equations in two space dimensions. Different sets of Stefan-Maxwell / Fick diffusion coefficient matrices and dimensionless chemical reaction rate constants were used.

The numerical experiments presented in the previous section can be summarized as follows:

-for the linear test problem, the influence of cross-diffusion coupling on the convergence rate and efficiency of the numerical algorithms depend on: (1) the smoothing algorithm for the MG method; (2) the preconditioner and the algorithm for the preconditioned conjugated gradient methods; the increase in the cross-diffusion coupling decreases the convergence rate and the efficiency; the decrease is negligible for MG-ALGS and GMRES (m) preconditioned with CC (complete Choleski decomposition case), relatively significant for BICGSTAB preconditioned with CC, GMRES (m) preconditioned with IC (incomplete Choleski decomposition case) and MG PGS and significant for the BICGSTAB preconditioned with IC, non-preconditioned GMRES (m) and BICGSTAB;

-for the non-linear test problem the influence of cross diffusion coupling on the convergence rate and efficiency of the numerical algorithms is less evident; for a given mesh and parameters value, the cross-diffusion coupling does not influence significantly $\bar{\rho}$ and τ; the key parameter seems to be the dilution ratio, Z_{5b}; high values of the dilution ratio decreases significantly the Fick cross-diffusion coefficients and implicitly their influence on the numerical performances of the algorithms.

3 Steady-State Multicomponent Convection-Diffusion-Reaction Problems

The results presented în this chapter are published in [8].

3.1 Problem Formulation

Consider the steady, 2D, laminar flow of an incompressible fluid inside a slot of thickness d in which the following isothermal, first order, complex chemical

reaction, takes place. Considering the density of the mixture constant, the

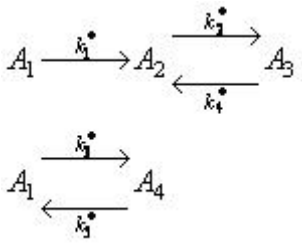

Figure 2: Chemical reaction scheme

dimensionless steady state concentrations profiles are given by a second-order partial differential equations system

$$\epsilon Peu(y)\frac{\partial Z_i}{\partial x} = \sum_{j=1}^{4}(\epsilon^2\frac{\partial}{\partial x}D_{ij}\frac{\partial Z_j}{\partial x} + \frac{\partial}{\partial y}D_{ij}\frac{\partial Z_j}{\partial y}) + R_i,\ i = \overline{1,4}, \tag{39}$$

$$(x,y) \in \Omega = (0,1)\times(0,1)$$

where

$$u(y) = -\frac{1}{2}(y^2 - y),\ \epsilon = \frac{d}{L},\ Pe = \frac{U_0 d}{D_{ref}},$$

$$R_1 = -k_1Z_1 - k_3Z_1 + k_5Z_4,\ R_2 = k_1Z_1 - k_2Z_2 + k_4Z_3,$$

$$R_3 = k_2Z_2 - k_4Z_3,\ R_4 = k_3Z_1 - k_5Z_4,$$

$Z_i = \frac{A_i}{A_{1b}}$ are the dimensionless mass concentrations, A_{1b} is the mass concentration of species A_1 at the channel inlet, i.e. $x = 0$, d is the slot thickness, $k_i = \frac{k_i^* d^2}{D_{ref}}$ are the non - dimensional reaction rate constants, L is the length of the channel, Pe is the Peclet number, U_0 is the constant rate of the uniform flow, $D_{ij}(x,y)$ are the multicomponent Fick diffusion coefficients in the mass average frame related to D_{ref}.

The boundary conditions are:

$$x = 0,\ Z_1 = 1,\ Z_i = 0,\ i = 2,3,4,$$

$$\begin{aligned} x &= 1,\ J_i = 0,\ i = \overline{1,4}, \\ y &= 0,\ J_i = 0,\ i = \overline{1,4}, \\ y &= 1,\ J_i = 0,\ i = \overline{1,4}, \end{aligned} \tag{40}$$

where

$$J_i = \sum_{j=1}^{4} D_{ij}\frac{\partial Z_j}{\partial x},\ or\ J_i = \sum_{j=1}^{4} D_{ij}\frac{\partial Z_j}{\partial y},\ i = \overline{1,4}, \tag{41}$$

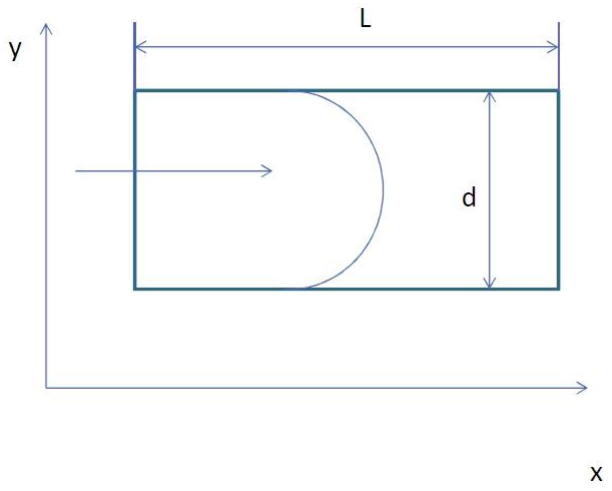

Figure 3: Schematic representation of the problem domain

is the mass diffusion flux of the ith species with respect to the mass average velocity.

The mathematical model previously descriebed represents the non-linear test problem. The liniar test problem is obtained from the non-linear one by considering the multicomponent Fick diffusion coefficients constants.

3.2 Numerical Methods

3.2.1 Problem Discretization

The spatial derivatives of equation (39) were discretized with the upwind finite difference scheme on uniform grids with $N \times N$ points,

$$0 = x_1 < x_2 < ... < x_{N-1} < x_N = 1,\ x_k = (k-1)h;$$

$$0 = y_1 < y_2 < ... < y_{N-1} < y_N = 1,\ y_l = (l-1)h,\ k,l = \overline{0,N},$$

where $h = \frac{1}{(N-1)}$ is the grid step size. The discrete approximation obtained for equations (39) is

$$\begin{aligned}
&\tfrac{\epsilon Peu(y_l)-|\epsilon Peu(y_l)|}{2}\tfrac{Z_i^{k+1,l}-Z_i^{k,l}}{h} + \tfrac{\epsilon Peu(y_l)+|\epsilon Peu(y_l)|}{2}\tfrac{Z_i^{k,l}-Z_i^{k-1,l}}{h} = \\
&= \textstyle\sum_{j=1}^{4}\big[\epsilon^2\tfrac{D_{ij}^{k+\frac{1}{2},l}(Z_j^{k+1,l}-Z_j^{k,l})-D_{ij}^{k-\frac{1}{2},l}(Z_j^{k,l}-Z_j^{k-1,l})}{h^2} + \\
&+\tfrac{D_{ij}^{k,l+\frac{1}{2}}(Z_j^{k,l+1}-Z_j^{k,l})-D_{ij}^{k,l-\frac{1}{2}}(Z_j^{k,l}-Z_j^{k,l-1})}{h^2}\big] + R_i^{k,l},\ i = \overline{1,4}
\end{aligned} \tag{42}$$

The values of the diffusion coefficients were calculated as arithmetic averages of the grid point values.

The method of calculation of the Fick coefficients values of the grid is presented in this thesis in section 3.1.

For the linear test problems, the multicomponent Fick diffusion coefficients, D_{ij}, are constant. The discrete approximation obtained in this case is:

$$\frac{\epsilon Peu(y_l)-|\epsilon Peu(y_l)|}{2}\frac{Z_i^{k+1,l}-Z_i^{k,l}}{h}+\frac{\epsilon Peu(y_l)+|\epsilon Peu(y_l)|}{2}\frac{Z_i^{k,l}-Z_i^{k-1,l}}{h}=$$
$$=\sum_{j=1}^{4}D_{ij}\frac{\epsilon^2 Z_j^{k+1,l}+Z_j^{k,l+1}+\epsilon^2 Z_j^{k-1,l}+Z_j^{k,l-1}-(2+2\epsilon^2)Z_j^{k,l}}{h^2}+R_i^{k,l},\ i=\overline{1,4} \quad (43)$$

For both nonlinear and linear problems, the flux boundary conditions were discretized with the central second order accurate scheme considering that the solution can be symmetrically extrapolated with one grid point outside the boundary.

3.2.2 Numerical Algorithms

We used the same nonlinear algorithms nonlinear multigrid (MG)[1] [9] and modified Picard iteration, [12]. The point Gauss Seidel is not a good smoothing algorithm for convection diffusion equations,[1] [9]. For this reason, the only smoothing algorithm employed in this work is the alternating line Gauss Seidel (ALGS) method. The nonlinear MG algorithm used is the classical Full Approximation Storage (FAS) algorithm,[1] [9].

The structure of the MG cycle is: 1) cycle of type V; 2) smoothing by ALGS; 3) two smoothing steps are performed before the coarse grid correction and one after; 4) prolongation by bilinear interpolation for corrections; 5) restriction of residuals by full weighting.

The modified Picard iteration, also called a fixed point method, for the problem (39) is given by

$$A(Z^m)\delta Z^{m+1}=b(Z^m)-A(Z^m)Z^m \quad (44)$$
$$Z^{m+1}=Z^m+\delta Z^{m+1}$$

where m is the iteration number $Z^m=[Z_1^m,Z_2^m,Z_3^m,Z_4^m]$, iar Z_0 is the initial estimate. Matrix $A(Z^m)$ is defined by

$$A(Z^m)=\begin{bmatrix} A_{11}^m & A_{12}^m & A_{13}^m & A_{14}^m \\ A_{21}^m & A_{22}^m & A_{23}^m & A_{24}^m \\ A_{31}^m & A_{32}^m & A_{33}^m & A_{34}^m \\ A_{41}^m & A_{42}^m & A_{43}^m & A_{44}^m \end{bmatrix}+\begin{bmatrix} (k_1+k_3)h^2I & 0 & 0 & -k_5h^2I \\ -k_1h^2I & k_2h^2I & -k_4h^2I & 0 \\ 0 & -k_2h^2I & k_4h^2I & 0 \\ -k_3h^2I & 0 & 0 & k_5h^2I \end{bmatrix} \quad (45)$$

where I is the $N(N-1)\times N(N-1)$ identity matrix. The blocks A_{ii}^m are $N(N-1)\times N(N-1)$ penta-diagonal matrices corresponding to the discretization stencil

$$\begin{bmatrix} & CN & \\ CW & CM & CE \\ & CS & \end{bmatrix} \quad (46)$$

$$CM = \epsilon^2 D_{ij}^{k+\frac{1}{2},l} + \epsilon^2 D_{ij}^{k-\frac{1}{2},l} + D_{ij}^{k,l+\frac{1}{2}} + D_{ij}^{k,l-\frac{1}{2}} + h|\epsilon Peu(y_l)|$$

$$CE = -\epsilon^2 D_{ij}^{k+\frac{1}{2},l} + h\frac{\epsilon Peu(y_l) - |\epsilon Peu(y_l)|}{2}$$

$$CW = -\epsilon^2 D_{ij}^{k-\frac{1}{2},l} - h\frac{\epsilon Peu(y_l) + |\epsilon Peu(y_l)|}{2}$$

$$CS = -D_{ij}^{k,l-\frac{1}{2}},\ CN = -D_{ij}^{k,l+\frac{1}{2}},$$

while the blocks $A_{ij}^m,\ i \neq j$ are $N(N-1) \times N(N-1)$ penta-diagonal matrices corresponding to the discretization stencil

$$CM = \epsilon^2 D_{ij}^{k+\frac{1}{2},l} + \epsilon^2 D_{ij}^{k-\frac{1}{2},l} + D_{ij}^{k,l+\frac{1}{2}} + D_{ij}^{k,l-\frac{1}{2}}$$

$$CE = -\epsilon^2 D_{ij}^{k+\frac{1}{2},l},\ CW = -\epsilon^2 D_{ij}^{k-\frac{1}{2},l}$$

$$CS = -D_{ij}^{k,l-\frac{1}{2}},\ CN = -D_{ij}^{k,l+\frac{1}{2}}$$

and they vary at every iterative step.

The linear solvers employed in the modified Picard iteration are the Matlab R2010b implementations of the preconditioned BICGSTAB and preconditioned restarted GMRES (m), and they are presented in Section 1.5. These algorithms were also used to solve the linear test problem. Codes for the modified Picard method and techniques of preconditioning are our own implementations in Matlab R2010b, respectively for MG in FORTRAN 77.

3.2.3 The Preconditioning Techniques

The linear system that should be solved in a Picard step or for the linear test problem can be written as

$$AZ = B \tag{47}$$

where

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix},\ Z = \begin{bmatrix} Z_1 \\ Z_2 \\ Z_3 \\ Z_4 \end{bmatrix},\ B = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}.$$

A_{ij} blocks are $N(N-1) \times N(N-1)$ square matrices and A_{ii} blocks, $i = \overline{1,4}$ are no more symmetric and positive definite matrices. The classic construction method of a preconditioning matrix for (47) is based on a LU decomposition, complete or incomplete of the diagonal blocks:

$$A_{ii} = L_i U_i + R_i,\ i = \overline{1,4} \tag{48}$$

(if $R_i = 0,\ i = \overline{1,4}$ we refer to a complete decomposition, otherwise we refer to the incomplete case [14] [16]).

We proposed a block preconditioning method for the system (47) which uses the same matrix for any diagonal block. We consider Δ_0 matrix that correspond to the 5-point stencil finite difference discretization of the equation

$$-(\epsilon^2\frac{\partial^2 z}{\partial x^2}+\frac{\partial^2 z}{\partial y^2})+\epsilon Peu(y)\frac{\partial z}{\partial x}=0 \tag{49}$$

with the same boundary conditions with respect to Z_1. We define the following preconditioning matrix

$$\begin{aligned} P &= \begin{bmatrix} \tilde{\Delta}_0 & 0 & 0 & 0 \\ 0 & \tilde{\Delta}_0 & 0 & 0 \\ 0 & 0 & \tilde{\Delta}_0 & 0 \\ 0 & 0 & 0 & \tilde{\Delta}_0 \end{bmatrix} = \\ &= \begin{bmatrix} L & 0 & 0 & 0 \\ 0 & L & 0 & 0 \\ 0 & 0 & L & 0 \\ 0 & 0 & 0 & L \end{bmatrix} \begin{bmatrix} U & 0 & 0 & 0 \\ 0 & U & 0 & 0 \\ 0 & 0 & U & 0 \\ 0 & 0 & 0 & U \end{bmatrix} \end{aligned} \tag{50}$$

where $\tilde{\Delta}_0 = \Delta_0 + h^2 I$.

3.3 Numerical Results

The main objective of the present work is to analyze the influence of cross-diffusion coupling on the numerical performances of the numerical algorithms. In order to achieve this objective, we considered, for each sets of parameters, the same four structures for the multi-component Fick diffusion matrix as in the case of diffusion-reaction problem. We symbolized these cases by CPL1 (case (a)), CPL2 (case (b)), CPL3 (case (c)) and by CPL4 (case (d)). In these cases, for the linear problem, cross-diffusion constantes are selected from the Fick coefficients matrices presented in Appendix A of the thesis. For the non-linear problem, the values of the Stefan-Maxwell coefficients used to calculate the Fick coefficients are presented in Appendix B of the thesis. The performances of the numerical algorithms are monitored by the average reduction factor, $\bar{\rho}$, and the efficiency, τ:

$$\tau = \frac{W}{|ln\bar{\rho}|}, \tag{51}$$

$$\bar{\rho} = (\frac{\|res_i\|}{\|res_0\|})^{\frac{1}{i}}, \tag{52}$$

where $res_i = \|b_i - A_i Z_i\|$ is the residue after i iterations, $\|\cdot\|$ euclidean vectorial norm, W (the work) is the number of arithmetic operations per grid point and iteration step.

In Sections 3.3.1 şi 3.3.2 we present the numerical results of the tests and an analysis of them.

3.4 Conclusions

This work continues our previous study and analyses the numerical performances of the MG and modified Picard preconditioned GMRES methods for solving steady-state, linear / non-linear multicomponent convection-diffusion-reaction equations in two space dimensions.

The numerical experiments presented in the previous section can be summarized as follows:

-for the linear test problem, the influence of cross-diffusion coupling on the convergence rate and efficiency of the preconditioned GMRES (m) depend on the values of the Pe numbers; for high values of the Pe numbers, i.e. $Pe = 10^4$, the influence of the cross-diffusion coupling on the convergence rate and efficiency is not very significant; for moderate Pe number values, i.e. $Pe = 100$, the cross-diffusion coupling influences the convergence rate and the efficiency of the preconditioned GMRES (m); the convergence rate of MG-ALGS is less sensitive to the influence of cross-diffusion coupling and Pe number values compared to the preconditioned GMRES (m);

-for the non-linear test problem the influence of cross-diffusion coupling on the convergence rate and efficiency of the numerical algorithms is more complex; the cross-diffusion coupling does not practically influence the convergence rate of the modified Picard iteration; however, the efficiency of the modified Picard iteration decreases with the increase in the cross-diffusion coupling only for the set B2 of the Stefan-Maxwell diffusion coefficients; the convergence rate and efficiency of the MG algorithm depend on the cross-diffusion coupling; the increase in the dilution ratio increases the convergence rate and efficiency of both numerical algorithms; however, its effect is less significant compared to the diffusion-reaction equations;

-for both linear and non-linear test problems, the increase in Pe decreases the effects of cross-diffusion coupling on the numerical performances of the algorithms. For high and very high values of the Pe number, the convection is the dominant mechanism from both physical and numerical points of view.

4 Time-Dependent Multicomponent Linear Convection-Diffusion Problems

4.1 Problem Formulation

In this chapter we approach solving, through numerical methods, time-dependent multicomponent convection-diffusion problems, the linear case. These problems are modeled by second-order partial differential equations, in which, in addition to the spatial variables derivatives appears the time derivative of order I. We considered as test problem a partial differential equations system that models a time-dependent linear multicomponent convection-diffusion problem with cu $p = 2, 3, 4$ chemical species:

$$\frac{\partial Z_i}{\partial \tau} + \epsilon Peu(y)\frac{\partial Z_i}{\partial x} = \sum_{j=1}^{p} D_{ij}(\epsilon^2 \frac{\partial^2 Z_j}{\partial x^2} + \frac{\partial^2 Z_j}{\partial y^2}),\ i = \overline{1,p}, \tag{53}$$

$$(x, y) \in (0, 1) \times (0, 1),\ \tau \in (0, T_{final})$$

unde

- Z_i dimensionless mass concentration of the chemical species i ,
- D_{ij} Fick diffusion coefficients,
- $\epsilon = \frac{d}{L}$, $Pe = \frac{U_0 d}{D_{11}}$, $\tau = \frac{tD_{11}}{d^2}$
- $u(y) = -\frac{1}{2}(y^2 - y)$.

Boundary conditions of the problem are:

$$x = 0,\ Z_i = 0, i = \overline{1,p}$$

$$x = 1,\ J_i = 0, i = \overline{1,p}$$

$$y = 0,\ Z_i = A_i sin(C_i x)(1 + \omega_i sin(\alpha_i \tau)),\ x \leq X < 1$$

$$Z_i = 0\ \ X \leq x \leq 1,\ i = \overline{1,p}$$

$$y = 1,\ Z_i = 0,\ i = \overline{1,p}$$

where $J_i = \sum_{i=1}^{p} D_{ij}\frac{\partial Z_j}{\partial x}$ mass diffusion flux of the ith chemical species respect to the mass average velocity. Initial conditions are:

$$\tau = 0,\ y = 0,\ Z_i = A_i sin(C_i x)(1 + \omega_i sin(\alpha_i \tau)),\ x \leq X < 1$$

şi în rest $Z_i = 0,\ \overline{1,p}$.

4.2 Numerical Results

4.2.1 Problem Discretization

The spatial derivatives of equations (53) were discretized with the central second order accurate finite scheme on uniform grids with $N \times N$ points

$$0 = x_1 < x_2 < ... < x_{N-1} < x_N = 1,\ x_k = (k-1)h;$$

$$0 = y_1 < y_2 < ... < y_{N-1} < y_N = 1,\ y_l = (l-1)h,\ k, l = \overline{0, N},$$

where $h = \frac{1}{(N-1)}$ is the grid step size. The discret approximation is

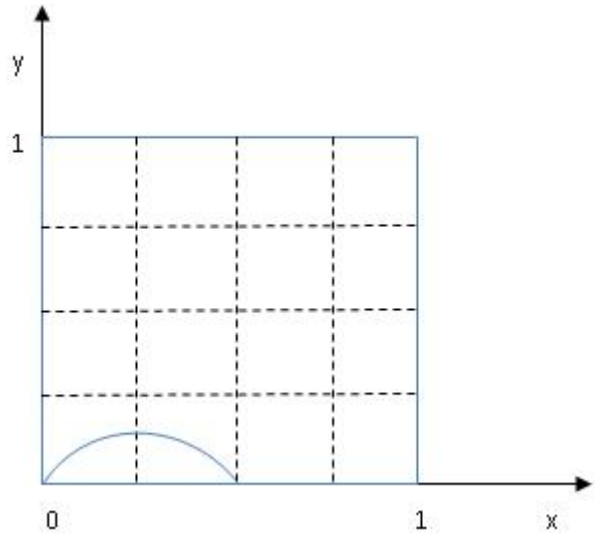

Figure 4: Domain Discretization

$$\frac{\partial Z_i^{k,l}}{\partial \tau} + \epsilon Peu^{k,l} \frac{Z_i^{k+1,l} - Z_i^{k-1,l}}{2h} -$$

$$- \sum_{j=1}^{p} D_{ij} (\epsilon^2 \frac{Z_j^{k+1,l} - 2Z_j^{k,l} + Z_j^{k-1,l}}{h^2} + \frac{Z_j^{k,l+1} - 2Z_j^{k,l} + Z_j^{k,l-1}}{h^2}) = 0,\ i = \overline{1, p} \tag{54}$$

For the case of three chemical species we obtain the following algebrical system

$$\begin{aligned}
\frac{\partial Z_1}{\partial \tau} + \Lambda_h Z_1 &= D_{11}\Delta_h Z_1 + D_{12}\Delta_h Z_2 + D_{13}\Delta_h Z_3 \\
\frac{\partial Z_2}{\partial \tau} + \Lambda_h Z_2 &= D_{21}\Delta_h Z_1 + D_{22}\Delta_h Z_2 + D_{23}\Delta_h Z_3 \\
\frac{\partial Z_3}{\partial \tau} + \Lambda_h Z_3 &= D_{31}\Delta_h Z_1 + D_{32}\Delta_h Z_2 + D_{33}\Delta_h Z_3
\end{aligned} \tag{55}$$

where Δ_h is a symmetric and positive definite matrix and we may suppose that Λ_h is skew-symmetric ($\Lambda_h = -\Lambda_h^T$) for central finite differences discretizations.[3]

4.2.2 Numerical Algoritms

In order to apply the splitting method to the problem (53) we proposed a algebraic decomposition of the discretization matrix of the spatial variables in a sum of two upper/lower triangular matrices.

$$\begin{bmatrix} D_{11}\Delta_h - \Lambda_h & D_{12}\Delta_h & D_{13}\Delta_h \\ D_{21}\Delta_h & D_{22}\Delta_h - \Lambda_h & D_{23}\Delta_h \\ D_{31}\Delta_h & D_{32}\Delta_h & D_{33}\Delta_h - \Lambda_h \end{bmatrix} =$$

$$\begin{bmatrix} \frac{1}{2}(D_{11}\Delta_h - \Lambda_h) & D_{12}\Delta_h & D_{13}\Delta_h \\ 0 & \frac{1}{2}(D_{22}\Delta_h - \Lambda_h) & D_{23}\Delta_h \\ 0 & 0 & \frac{1}{2}(D_{33}\Delta_h - \Lambda_h) \end{bmatrix} +$$

$$\begin{bmatrix} \frac{1}{2}(D_{11}\Delta_h - \Lambda_h) & 0 & 0 \\ D_{21}\Delta_h & \frac{1}{2}(D_{22}\Delta_h - \Lambda_h) & 0 \\ D_{31}\Delta_h & D_{32}\Delta_h & \frac{1}{2}(D_{33}\Delta_h - \Lambda_h) \end{bmatrix}, \tag{56}$$

To ensure the stability of time integration scheme and of the splitting method also, the two block triangular matrices should be positive definite. The advantage of using this decomposition is that algebraic systems that shoud be solved are block triangular.

4.3 Positive Definiteness Analysis of Block Triangular Matrices Classes

Because we want to solve multicomponent convection-diffusion problems with 3 or 4 chemical species we tried to determine the positive definiteness of 3×3 or 4×4 block triangular matrices classes to ensure the stability of splitting method.

The results prezented in this section are published in [18].

4.3.1 Positive Definiteness of a Class of 3×3 Block Real Matrices

Proposition 2. *Let us suppose that for a 3×3 real matrix*

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & 0 & a_{33} \end{bmatrix} \tag{57}$$

there exist a, b, c, d, e, f positive real numbers with the properties

$$|a_{12}| < 2\sqrt{ab}, \quad |a_{13}| < 2\sqrt{cd}, \quad |a_{23}| < 2\sqrt{ef}, \tag{58}$$

and

$$a+c\leq a_{11},\quad b+e\leq a_{22},\quad d+f\leq a_{33}. \tag{59}$$

Then, A from (57) is positive definite.

Let A be a $3n\times 3n$ real matrix of the form

$$A=\begin{bmatrix} \alpha\Delta^* & \gamma_1\Delta & \gamma_2\Delta \\ 0 & \beta_1\Delta^*+\delta_1\Delta & \gamma_3\Delta \\ 0 & 0 & \beta_2\Delta^*+\delta_2\Delta \end{bmatrix} \tag{60}$$

where Δ^* and Δ are $n\times n$ blocks, Δ is symmetric and positive definite and $\alpha,\beta_1,\beta_2,\delta_1,\delta_2,\gamma_1,\gamma_2,\gamma_3$ are positive real numbers.

Proposition 3. *If $\Delta^*=\Delta$ and Δ a symmetric and positive definite matrix then matrix A from (60) is positive definite if there exist a,b,c,d,e,f positive real numbers with the properties*

$$|\gamma_1|<2\sqrt{ab},\quad |\gamma_2|<2\sqrt{cd},\quad |\gamma_3|<2\sqrt{ef},$$

and

$$a+c\leq\alpha,\quad b+e\leq\beta_1+\delta_1,\quad d+f\leq\beta_2+\delta_2. \tag{61}$$

Proposition 4. *If there exists a positive real number C such that*

$$\Delta=C(\Delta^*+(\Delta^*)^T) \tag{62}$$

then the matrix A from (60) is positive definite if there exist a,b,c,d,e,f positive real numbers with the properties

$$|\gamma_1|<2\sqrt{ab},\quad |\gamma_2|<2\sqrt{cd},\quad |\gamma_3|<2\sqrt{ef},$$

and

$$a+c\leq\frac{\alpha}{2C},\quad b+e\leq(\frac{\beta_1}{2C}+\delta_1),\quad d+f\leq(\frac{\beta_2}{2C}+\delta_2). \tag{63}$$

4.3.2 Positive Definiteness of a Class of 4×4 Block Real Matrices

Proposition 5. *Let us suppose that for a real matrix*

$$A=\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22} & a_{23} & a_{24} \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & 0 & a_{44} \end{bmatrix} \tag{64}$$

there exist a,b,c,d,e,f,g,h,i,j,k,l positive real numbers with the properties

$$|a_{12}|<2\sqrt{ab},\quad |a_{13}|<2\sqrt{cd},\quad |a_{14}|<2\sqrt{ef},\quad |a_{23}|<2\sqrt{gh},$$
$$|a_{24}|<2\sqrt{ij},\quad |a_{34}|<2\sqrt{kl},\quad a+c+e\leq a_{11},$$

$$b+g+i\leq a_{22},\quad d+h+k\leq a_{33},\quad f+j+l\leq a_{44}. \tag{65}$$

Then, the matrix A from (64) is positive definite.

Let now A be a $4n \times 4n$ real matrix of the form

$$A = \begin{bmatrix} \alpha\Delta^* & \gamma_1\Delta & \gamma_2\Delta & \gamma_3\Delta \\ 0 & \beta_1\Delta^* + \delta_1\Delta & \gamma_4\Delta & \gamma_5\Delta \\ 0 & 0 & \beta_2\Delta^* + \delta_2\Delta & \gamma_6\Delta \\ 0 & 0 & 0 & \beta_3\Delta^* + \delta_3\Delta \end{bmatrix} \tag{66}$$

where Δ^* and Δ are $n \times n$ blocks, Δ is a symmetric and positive definite matrix and $\alpha, \beta_1, \beta_2, \beta_3, \delta_1, \delta_2, \delta_3, \gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_5, \gamma_6$ are positive real numbers.

Proposition 6. *If $\Delta^* = \Delta$ and Δ is a symmetric and pozitive definite matrix then matrix A from (66) is positive definite if there exist $a, b, c, d, e, f, g, h, i, j, k, l$ positive real numbers with the properties*

$$|\gamma_1| < 2\sqrt{ab}, \quad |\gamma_2| < 2\sqrt{cd}, \quad |\gamma_3| < 2\sqrt{ef}, \quad |\gamma_4| < 2\sqrt{gh},$$
$$|\gamma_5| < 2\sqrt{ij}, \quad |\gamma_6| < 2\sqrt{kl}, \quad a + c + e \leq \alpha,$$

$$b + g + i \leq \beta_1 + \delta_1, \quad d + h + k \leq \beta_2 + \delta_2, \quad f + j + l \leq \beta_3 + \delta_3. \tag{67}$$

Proposition 7. *If there exists a positive real number C such that*

$$\Delta = C(\Delta^* + (\Delta^*)^T)$$

then the matrix A from (66) is positive definite if there exist $a, b, c, d, e, f, g, h, i, j, k, l$ positive real numbers with the properties

$$|\gamma_1| < 2\sqrt{ab}, \quad |\gamma_2| < 2\sqrt{cd}, \quad |\gamma_3| < 2\sqrt{ef}, \quad |\gamma_4| < 2\sqrt{gh},$$
$$|\gamma_5| < 2\sqrt{ij}, \quad |\gamma_6| < 2\sqrt{kl}, \quad a + c + e \leq \frac{\alpha}{2C},$$

$$b + g + i \leq \frac{\beta_1}{2C} + \delta_1, \quad d + h + k \leq \frac{\beta_2}{2C} + \delta_2, \quad f + j + l \leq \frac{\beta_3}{2C} + \delta_3. \tag{68}$$

We make the notations

$$\Delta_h^* = \frac{1}{2}(D_{11}\Delta_h - \Lambda_h)$$
$$\alpha = \beta_1 = \beta_2 = \beta_3$$
$$\delta_1 = \frac{1}{2}(D_{22} - D_{11}) \quad \delta_2 = \frac{1}{2}(D_{33} - D_{11}) \quad \delta_3 = \frac{1}{2}(D_{44} - D_{11})$$
$$\gamma_1 = D_{12} \quad \gamma_2 = D_{13} \quad \gamma_3 = D_{14} \quad \gamma_4 = D_{23} \quad \gamma_5 = D_{24} \quad \gamma_6 = D_{34}.$$

The upper triangular matrix from the relation (60) becames the upper matrix of the decomposition (56). These presented propositions remain valid for lower triangular matrices. We found a way to verify the positive definiteness of the matrix obtained in the splitting method for the linear time-dependent multicomponent convection-diffusion problems.

4.4 Conclusions

We present the splitting method as a method that could be used to solve the linear time-dependent multicomponent convection-diffusion problems. We propose a decomposition of the spatial operator thus the algebraic systems matrices obtained in a numerical time integration step are upper/lower triangular matrices.

We propose a strategy to verify the positive definiteness of $2n \times 2n$, $3n \times 3n$ or $4n \times 4n$ real triangular matrices classes that ensure the stability of the splitting method.

Final conclusions and future developments

In this thesis we approached solving of multicomponent mass transfer problems. These problems are modeled by second-order partial differential equations.

For selecting the appropriate numerical methods to solve the problems, we classified the problems in the following classes:

- steady-state multicomponent diffusion-reaction equations, non-linear and linear cases;
- steady-state multicomponent convection-diffusion-reaction equations, non-linear and linear cases;
- time-dependent multicomponent convection-diffusion equations, linear case.

Numerical methods for nonlinear problems in case of the first two classes are the algorithms nonlinear multigrid (MG) and modified Picard. In the case of linear problems the solvers are the iterative methods restarted GMRES (m) and BiCGSTAB. We made an analysis of the influence of cross-diffusion coupling of the chemical species on the numerical performances of the algorithms used. We also made an analysis of the influence of the convection process in the case of convection-diffusion-reaction equations.The numerical tests we used several sets of values for the parameters of the problem.

We proposed, for the diffusion-reaction problems and also for diffusion-convection-reaction problems, a preconditioner, based on one type of diagonal block , that can be used within the preconditioning techniques to improve performance of the iterative algorithms: restarted GMRES and BiCGSTAB. We analyzed, from the theoretical point of view the character of good preconditioner of the proposed matrix in case of the diffusion-reaction problem.

In the class of time-dependent multicomponent convection-diffusion problems, linear case, are characterized the convection-diffusion processes evolving in time.

To solve these problems we have selected the splitting method. Within this method, we have proposed a spatial operator decomposition, thus the obtained algebraic systems matrices are upper/ lower triangular. We determined sufficient conditions that ensure the stability of the method in the case of problems with 3 or 4 chemical species.

As future concerns we want to apply the splitting method to solve the time-dependent multicomponent convection-diffusion problems, linear case, for the case with 3 or 4 species and we want to analyze the influence of cross-diffusion of chemical species and of the convection process on the performances of the splitting method.

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