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PARTICLE TRANSPORT METHOD FOR CONVECTION-DIFFUSION-REACTION PROBLEMS

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Preface

This study has been carried out between 2003 and 2007 in the Laboratory of Applied Mathematics of the Department of Mathematics and Physics of Lappeenranta University of Technology.

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Olga Shipilova

Abstract

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Convective transport, both pure and combined with diffusion and reaction, can be observed in a wide range of physical and industrial applications, such as heat and mass transfer, crystal growth or biomechanics. The numerical approximation of this class of problems can present substantial difficulties due to regions of high gradients (steep fronts) of the solution, where generation of spurious oscillations or smearing should be precluded. This work is devoted to the development of an efficient numerical technique to deal with pure linear convection and convection-dominated problems in the framework of convection-diffusion-reaction systems.

The particle transport method, developed in this study, is based on using meshless numerical particles which carry out the solution along the characteristics defining the convective transport. The resolution of steep fronts of the solution is controlled by a special spacial adaptivity procedure. The semi-Lagrangian particle transport method uses an Eulerian fixed grid to represent the solution. In the case of convection-diffusion-reaction problems, the method is combined with diffusion and reaction solvers within an operator splitting approach. To transfer the solution from the particle set onto the grid, a fast monotone projection technique is designed.

Our numerical results confirm that the method has a spacial accuracy of the second order and can be faster than typical grid-based methods of the same order; for pure linear convection problems the method demonstrates

optimal linear complexity. The method works on structured and unstructured meshes, demonstrating a high-resolution property in the regions of steep fronts of the solution. Moreover, the particle transport method can be successfully used for the numerical simulation of the real-life problems in, for example, chemical engineering.

Keywords: convection, diffusion, reaction, meshless particles, high-resolution, adaptivity, projection, operator splitting

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Capital letters

$B(L)$	Birth term
$\mathbf{C}$	Vector of moving components of a mixture
D	Diffusion/dispersion coefficient
$D(L)$	Death term
F	Phase ration
G_i	Signal value on the i^{th} element of the grid
G	Crystal growth rate
$K(\mathbf{x}, t)$	Reaction rate function
L	Crystal length
$\mathcal{L}_2$	Space of square integrable functions
M	Number of time steps
N	Number of particles
$\mathcal{N}$	Number of components in a mixture
S	Discontinuity set of the reaction rate function
T	Time interval
$\mathcal{T}$	Set of grid elements (triangulation of the domain)
$\mathbf{X}$	Set of particle coordinates

$\mathbf{X}_g$	Particle vicinity of a node g

Small letters

$f(u, \mathbf{x}, t)$	Source or reaction function
g	Grid's node
h	Width (diameter) of the grid
k	Mass transfer coefficient
n	Number of grid nodes
$n(L, t)$	Population (number) density function
p	Particle
$\mathbf{q}$	Vector of stationary components of a mixture
t	Time variable
$u(\mathbf{x}, t)$	Unknown concentration or mass function
$\mathbf{v}$	Vector of velocity components
$\mathbf{x}$	Vector of space coordinates
$\overline{pg}$	Line through points g and p

Greek letters

Γ	Boundary of computational domain
Ω	Computational domain
ϕ	Monotonic increasing function
τ	Resistance time

Subscripts

i	i^{th} grid element
in	Inflow portion of the domain boundary
m	m^{th} time step
out	Outflow portion of the domain boundary

Superscripts

(m)	Solution at the m^{th} time step
S	Set of grid elements over the discontinuity set of the reaction rate function
$*$	equilibrium
$(*)$	Solution of the convection-reaction subproblem

Abbreviations

1D	One dimensional
2D	Two dimensional
3D	Three dimensional
CDR	Convection-diffusion-reaction
CFL	Courant-Friedrichs-Levy condition
CSD	Crystal size distribution
FD	Finite difference
FE	Finite element

FCT	Flux corrected transport
GDCS	Global Discrete Coordinate System
LED	Local extremum diminishing
MLS	Moving least squares
MM	Meshless method
MOL	Method of lines
ODE	Ordinary differential equation
PBE	Population balance equation
PDE	Partial differential equation
PTM	Particle transport method
round	Round-off operation of a real number
TVD	Total variation diminishing

List of Publications

I. Smolianski A., Shipilova O. and Haario H., "A Fast High-Resolution Algorithm for Linear Convection Problems: Particle Transport Method", *International Journal for Numerical Methods in Engineering*, Vol. 70, 2007, pages 655–684

II. Shipilova O., Haario H. and Smolianski A., "Particle Transport Method for Convection Problems with Reaction and Diffusion", *International Journal for Numerical Methods in Fluids*, Vol. 54, 2007, pages 1215–1238

III. Hatakka H., Shipilova O., Haario H. and Kallas J. "Modeling of Reactive Crystallization: Using Particle Transport Method in Unsteady-State Modeling of Crystal Growth", *Proceedings of the 16th International Symposium on Industrial Crystallization*, Dresden, Germany, September 11-14, 2005, pages 145–150

IV. Hatakka H., Shipilova O., Haario H. and Kallas J. "Using a Meshless Transport Method in Modelling of Reactive Crystallization of Barium Sulphate", *Proceedings of the 12th International Workshop on Industrial Crystallization (BIWIC 2005)*, Halle, Germany, September 7-9, 2005, pages 17–23

V. Shipilova O., Sainio T. and Haario H. "Particle Transport Method for Multicomponent Chromatography Problems", *Journal of Chromatography A* (submitted)

In this thesis, the publications are listed in chronological order of the research development and referred to as *Publication I*, *Publication II*, *Publication III*, *Publication IV* and *Publication V*.

Chapter I

Introduction

One can observe three basic material transfer processes: convection (or advection) caused by external forces, diffusion (or dispersion) due to heterogenic distribution of concentration in material, and reaction. A short list of industrial applications, where the convection-diffusion-reaction (CDR) process can be found, includes crystal growth [51, 99] and metal casting [9] in the iron and steel industry, food processing [1, 87, 91], laser machining [94], biomedical engineering [49, 57] and many others, which indicates a wide range of applicability for the process. Due to the progress of digital computing, mathematical modeling has become a powerful tool in investigating and predicting the behavior of different CDR systems. Consequently, the necessity in proper numerical methods has initiated a specialized current in the field of computational fluid dynamics.

Problems in which convection dominates are of the highest interest for computational treatment. The common feature of this kind of problems, which leads to a number of numerical challenges, is well-known: the profile of the solution (e.g., mass or concentration) might include discontinuities (shocks) or high values of the gradient – in this work, we will call them *singularities* – prescribed initially or developing with time. Modeling of the chromatography separation [26], catalytic convertors and movement of water in dry soils [29] are a few examples where convection-dominated problems may appear. Moreover, the problem of pure convection has to be considered in such areas as the modeling of free interfaces (see, for instance, the volume of fluid method [36, 72] and the level set method [78]) as well as the modeling of multiphase or multicomponent [81, 93] and turbulent [3, 59, 69] flows.

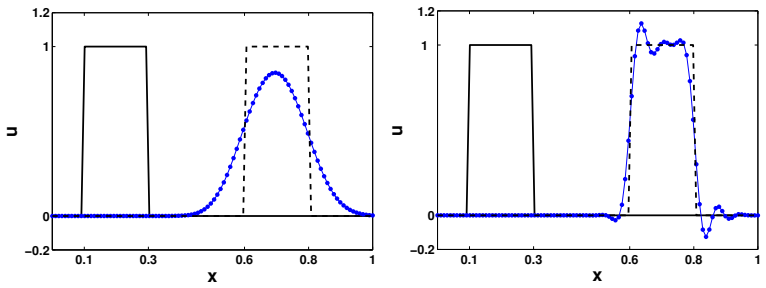
The combination of convection with diffusion can diminish the numerical difficulties due to the smearing nature of a diffusion operator. However, the diffusion coefficient must be "high" enough to influence the solution significantly. In this thesis, the main consideration will be given to the convection problem and its combination with reaction and small diffusion.

1.1 Numerical Methods for CDR Problems

Historically, the first methods applied to problems of mass transfer were methods based on finite differences (FD), which originate from works of I. Newton and J. Lagrange. Being methods of "point approximation" by reformulation of differential equations into algebraic systems, they are quite effective for diffusion and diffusion-dominated problems. However, they might lead to solutions contaminated by excessive smearing of steep fronts in the case of convection domination or pure convection. With creation of the Galerkin theory of a weak problem formulation and a finite element discretization (works of A. Hrennikoff, R. Courant, Rayleigh, W. Ritz) the finite element (FE) methods suggested a new alternative for the approximation of CDR problems. The FE technology is to approximate the solution of the original problem by the solution of a reduced problem, which is easier to resolve. Moreover, the solution is approximated here on a subdomain, e.g. an interval in 1D, a triangle in 2D and a tetrahedron in 3D. In spite of being effective for a wide range of problems, especially, with complex geometry, FE methods may face the development of artificial oscillations in the vicinity of solution singularities for convection-dominated cases. It appears that simply increasing the method accuracy does not lead to an effective scheme for convection problems; artificial smearing produced by a low-order approximation is exchanged by spurious oscillations caused by a high-order discretization, as can be seen in Figure 1.1.

Before discussing numerical tools aimed to diminish numerical errors, such as oscillating and smearing, it is useful first to refer to the classification of numerical methods and consider Eulerian, Lagrangian and mixed Eulerian-Lagrangian groups of schemes.

The main difference between Eulerian and Lagrangian concepts lies in the way how to examine solution changes with respect to a computational grid. The former traces the solution in a fixed point of the domain. Therefore, in this description the computational mesh is fixed. Traditionally,



(a) (b)

Figure 1.1: Contamination of the solution of a linear convection problem by artificial smearing or oscillations: black solid line – initial condition; blue line – solution by a low order method (plot (a)) and by a high order method (plot (b)); black dashed line – the exact solution

the finite difference and finite element methods belong to the class of Eulerian methods (see, for example, the Petrov-Galerkin method [83, 30], the Galerkin/least-squares method [39] and Taylor-Galerkin method [23]). While the explicit Eulerian methods are very attractive for the visualization and interpretation of the solution, they may suffer from the stability constraint on the time and space step size known as the Courant-Friedrichs-Levy (CFL) condition [24]. Since for the convection-dominated problems the discretizations in time and space affect each other essentially, the CFL condition can result here in a small time step that leads to computationally expensive numerical approximations.

In the Lagrangian (characteristics based) methods, the solution of a problem is defined by the movement of fluid particles (infinite small volumes). In this case, physics of the transport problem is directly introduced into the numerical approximation. Hence the main restrictions on time and space steps are eliminated. The convective transport is derived here exactly and tracked either forward or backward along the characteristics (trajectories). Thus, in the mesh-based Lagrangian methods (see, for instance, [32, 85]) a computational grid follows the solution. The main difficulty here is the severe deformation of the computational domain which can appear during the simulation. To avoid excessive distortion of the grid, the procedure of re-meshing, local [33] or global [46], is usually applied. Unfortunately,

for some problems this procedure becomes extremely complex and time consuming. For this reason, the purely mesh-based Lagrangian methods are rarely applied to the convection-dominated transport.

To stress the advantages of Eulerian and Lagrangian approaches and to relax their disadvantages, a number of mixed Eulerian-Lagrangian methods, such as the Eulerian-Lagrangian localized adjoint methods [28], the characteristic Galerkin method [48], the semi-Lagrangian methods [6, 95], have been developed. Here the transport phenomenon is resolved exactly by forward or backward characteristics on a Lagrangian grid while an Eulerian grid is used to protect the scheme from the strong mesh deformation. The connection between Eulerian and Lagrangian grids is accomplished by the procedure of projection. This step (projection between two arbitrary grids) causes the main methodological and technical concern for this class of methods. The principal requirements for a proper projection procedure include good mass conservation and low computational costs. The usual necessity to find a trade-off between these qualitative criteria led to the creation of a number of competitive algorithms. The general way of interpolation between two arbitrary meshes is an $\mathcal{L}_2$-projection, which is by definition mass conserving, but also very time consuming due to an additional integration (see the discussion in [79]). In practice, simpler alternatives based on node-by-node interpolation are used (see, for example, [22] and [65]). Provided that the search for neighbors of a grid node is a fast operation, these projections are computationally quite low-cost. However, the mass conservation property can be lost, which results in a wrong propagation velocity of the solution discontinuities. Thus, the development of an efficient mass-conservative projection is still of high research interest.

1.1.1 Stabilization techniques

One of the classical strategies to preclude spurious oscillations in the vicinity of solution singularities is to stabilize a numerical scheme by an additional viscosity term. This so-called shock-capturing viscosity [97] or stabilizing term [19] acts as diffusion aimed to smooth possible oscillations in regions of singularities. The stabilizing term can be introduced directly into the weak formulation of the problem (see, for example, the streamline upwind/Petrov-Galerkin method [15, 41], the subgrid scale method [38] and the characteristic Galerkin method [25]), and is generally presented by the weighted $\mathcal{L}_2$-product of a certain operator applied to the test function and residual of the equation to be solved. Therefore, the artificial diffusion con-

tributes to the mass matrix of the final algebraic system. The weight is usually estimated from the conditions on stability, convergence and conservation property of a scheme.

Another way to stabilize a numerical scheme is to smooth the solution after each step of the simulation according to the value of artificial viscosity, which generally depends on the second derivative of the solution. The solution can be smoothed either globally over the whole computational domain or, to avoid overdiffusing in regions of the smooth solution, only in the vicinity of singularities, which can be located by the gradient of the solution function (see, for example, [56, 67] and the discussion in [75]). It should be noted that while being more flexible than the previous technique, this method contains a "free" parameter (viscosity).

The stabilization techniques were successfully applied to a wide range of Eulerian, especially high-order, numerical schemes. Unfortunately, artificial viscosity is a solution-dependent term containing a free parameter, which requires experimental tuning. This fact leads to a complication of the whole computational scheme. Moreover, special care should be taken to avoid a downgrade of accuracy in the smooth part of the solution, which may be caused by an excessive numerical diffusion.

1.1.2 Flux corrected transport

J. Boris and D. Book [10] have introduced another concept called Flux Corrected Transport (FCT) for high-resolution schemes. Subsequently, the FCT schemes have entered the more general class of methods satisfying the Total Variation Diminishing (TVD) condition, proposed by A. Harten [34] for one-dimensional problems and extended to multi-dimensional ones as the Local Extremum Diminishing (LED) criteria (see, for example, [45]). These conditions can be reduced to a general principle of non-increasing maxima and non-decreasing minima of the problem solution during the approximation.

The basis of the FCT approach lies in the use of limiters on a numerical flux, which allow a scheme to fulfill the TVD (or LED) condition. The flux limiters can be applied within practically any time-space discretizations (FD or FE). Thus, the accuracy of a resulting FCT (TVD) method depends on the accuracy of the underlying numerical scheme (see, for example, the second order TVD-method based on the Crank-Nicolson scheme in [24]). In addition, the FCT technology allows combining high and low-order accurate

discretizations in such adaptive ways that nonphysical oscillations due to a high-order scheme are suppressed by a low-order scheme, bounded by a flux limiter to avoid extra smearing. A wide range of limiters are presented in literature, for example, the two-parameter minmod, Van Leer and superbee limiters (the full list of limiters can be found, for example, in [60]). From among the high-resolution schemes utilizing flux limiters to satisfy the TVD (LED) criteria, one could mention the Essentially Non-Oscillatory (ENO) schemes [16, 35, 92], the finite-element FCT (FEM-FCT) method [53, 54, 66] and the discontinuous Galerkin (DG) method [7, 47, 52].

The FCT-based methods, the accuracy of which depends on the underlying scheme, give a non-oscillating approximation for convective transport problems. Moreover, the technique works with structured and unstructured grids successfully and can be straightforwardly extended to 3D problems. The main difficulty of the FCT methods is that the limiters depend on the solution nonlinearly, requiring a new estimation at each step of the numerical simulation, which makes the whole numerical scheme more complex.

1.1.3 Space adaptivity

Here, the discussion is switched from the numerical discretization to the spatial decomposition of the computational domain. It is clear that the latter can also be used to improve the resolution of the solution discontinuities by virtue of spacial (mesh) *adaptivity*. The goal of the adaptivity procedure is to refine a computational mesh in regions of singularities, indicated by the gradient or the residual magnitude of the solution [40], or in the regions of the maximum error estimated after each time step [58]. In some cases, singularities are stationary. Hence, the mesh is initially more dense in their vicinity. However, for convective transport it is inherent that high values of the gradient or discontinuities develop or move with time, which requires mesh adaptivity near the singularities during the numerical simulation. From this point of view, adaptivity is similar to the re-meshing procedure needed in free-Lagrangian methods. While the adaptivity procedure is a very powerful tool, it leads to mesh reconstruction, which itself may be rather expensive, especially for the Delaunay triangulation in the 3D case. In addition, the insertion of new nodes implies the necessity of the data projection between the old grid and the new nodes, which can introduce additional errors into the solution and increase the computational time. However, it is worth pointing out that besides adding new computational points adaptivity can also remove them, for example, in the domains

where the solution is smooth. Therefore, the computational time taken by the resolution of the final algebraic system can decrease. The general purpose of the adaptivity procedure can be formulated so as to balance the two main requirements for a numerical scheme: good approximation quality and low computational costs. A number of works have been dedicated to the development of an efficient mesh adaptivity, see e.g. [43, 80, 82, 98].

In light of the construction of an effective adaptive algorithm, the idea to eliminate the traditional mesh-based view of the computational domain seems to be a very promising approach. The mesh-free or the particle concept can significantly simplify the adaptivity procedure, since more relaxed internal connectivity (or even non-connectivity) is inherent to computational meshless sets. The next section is devoted to the meshless (the grid-free) and the particle concepts that are closely related to each other.

1.1.4 Meshless methods

Several decades ago, the meshfree or meshless concept was created in contrast to the mesh-based one, where both a set of computational points (nodes) and an a priori knowledge of their connectivity (mesh) were required. However, meshless methods (MMs) have attracted practical attention only recently. This was caused by the fact that these schemes may be significantly more time-consuming than mesh-based ones due to complex shape functions with a high order of continuity, which demand specially constructed kernels for their evaluation. There are a few monographes and journal papers where authors have made an attempt to unify the constructing principles for MMs and to classify them with respect to their basic properties (see, for example, [14, 62] and [5, 11]). One of the general classifications of MMs is carried out with respect to the form of the partition of unity underlying meshfree interpolants (in analogy with shape functions in FE methods). The most widely used variations are based on smooth kernel functions (i.e. the Gaussian function, the cubic or quadric spline function), the Moving Least Squares (MLS) interpolant, introduced in [55], and its modifications – the MLS Reproducing Kernel interpolant [64] and the Meshfree Wavelet interpolant [61]. Other classifications, based on the choice of the test functions and/or a basic set (intrinsic or extrinsic) for the partition of unity, are presented in literature as well.

The main characteristic of the meshless methods is the absence of a mesh in the classical FE or FD sense. Here, technologies of connectivity are used

that are more relaxed in comparison to the Delaunay triangulation [89] such as the Voronoi diagram [50], the advanced front method [63] or the octree based method [70]. These techniques allow generating sets of particles or, in other words, meshfree computational nodes, to fulfill the requirement of the distribution regularity, which is important for the construction of a mass matrix [74]. At the same time, changes in the particle system during the computations, such as inserting or removing points, do not lead to its complete reconstruction; the connectivity is updated locally in a fully automatic way. Moreover, the use of moving particles may facilitate the application of Lagrangian methods to the transport problems since there is no need in the re-meshing procedure to maintain a sufficient quality of mesh. For these reasons meshless schemes are very suitable for the problems with moving solution discontinuities [4], free-boundary problems and problems in complex geometries, see e.g. [37, 42]. Among numerous MMs, the following methods have widely gained popularity in computational fluid dynamics: the Smooth Particle Hydrodynamics method, formulated initially for astrophysical and quantum mechanics applications [68] and extended later to computational fluid dynamics problems [73]; the Vortex-in-Cell method [21] based on the Lagrangian vorticity-velocity formulation of the government equations and a smoothing kernel function; methods based on Radial Basis Functions, see e.g. [17]. The development of this class of numerical methods is still in progress.

1.1.5 Splitting techniques

The CDR problem may consist of two completely different processes – convection, which is a direct shift in the simplest case, and diffusion, which corresponds to smoothing. Mathematically, the system may turn its type from parabolic to hyperbolic when the diffusion or convection term dominates. Each of these operators requires, in general, different numerical schemes for approximation. Finite difference and finite element numerical methods are traditional solvers for diffusion-dominated problems. However, the sharpness of the solution front induced by the convection domination as well as by reaction might hinder the successful implementation of standard solvers.

Decoupling convection-reaction and diffusion processes from one another can simplify the situation. The most direct way is to split the operators, which is the so-called operator splitting approach [71], and integrate each of them sequentially at each time step. This method has the time error of

the first order, $O(\triangle t)$, which can lead to large magnitudes of the error for operators exhibiting slow and fast timescales. Therefore, the time step size for this kind of problems should be carefully chosen to balance the operators within one time step. The operator splitting approach is used in some mixed Eulerian-Lagrangian schemes for convective transport, for example, in the class of Particles-in-Cell (PIC) methods, which is originally built for problems of computational plasma physics ([8, 76], [44] and references in it). There are few works dedicated to their application within computational fluid dynamics. For example, in [12] and [13] the PIC technology is used to approximate the subsonic and supersonic stream flows, and in [77] the PIC method is applied to the one-dimensional generalized Fisher's equation. Alternatively, splitting (or decomposition) techniques of a higher order can be used, such as the alternating direction implicit method [71, 27], the implicit explicit method [2, 96] and the fractional step θ-method [18]. Here, not only different spacial operators are decoupled, but additionally, each of them is replaced by its additive decomposition.

We have considered some of the most popular techniques suitable for the numerical approximation of the convection-diffusion-reaction process. For each approach, the main advantages and disadvantages have been pointed out, and some of the most representative references have been listed. The investigation of the existing techniques, both Eulerian- and Lagrangian-based, has shown that the creation of a fast high-resolution method suitable for engineering purposes is still an open question in the framework of the numerical analysis of CDR problems. Finally, it is worth noting that many good numerical techniques (for example, the fractional step and marker-particle methods) have been left beyond the scope of the present overview, as they do not allow proper approximation on unstructured grids (which is important for problems with complex geometry and free boundaries) or may be too time-consuming.

1.2 Overview and Aim of the Thesis

This work is dedicated to the development of an efficient numerical technique for pure convection and convection-dominated problems. A new meshless method, the Particle Transport Method (PTM), is presented. The main question is whether it is possible to construct a high-resolution method with optimal complexity utilizing problem properties and existing techniques

such as adaptivity and a meshless base.

The study begins with the pure linear convection problem. Further, the developed particle transport method is extended to convection problems with diffusion and reaction in the framework of the first order operator splitting. After PTM has been verified in classic benchmark tests, the method is applied to problems of chemical engineering, such as chromatographical separation and crystallization.

This thesis is divided into four chapters. Chapter 1 introduces the research field, research problem and objectives of the thesis. Following the introduction, Chapter 2 provides the mathematical formulation of the CDR problem and introduces the particle transport method. Here, questions of method accuracy, complexity and the ability to capture solution singularities are discussed, as well. Chapter 3 is devoted to the practical results of the thesis and fields of the method's application. Chapter 4 contains the discussion, conclusions and possible future research directions. The thesis is concluded with an appendix containing the publications. An overview of the publications is given in Section 1.3.

1.3 Summary of Publications

This thesis contains four publications, two journal papers and two conference papers, and one paper submitted to a journal. The publications can be divided into two parts: *Publication I* and *Publication II* are dedicated to the development and verification of a novel numerical scheme called the Particle Transport Method (PTM), while *Publication III*, *Publication IV* and *Publication V* deal with the applications of the proposed numerical method.

Publication I introduces the particle transport method for solving linear convection problems. The Lagrangian characteristics method combined with the Eulerian representation of the solution on a fixed grid underlies the proposed method. The method utilizes the idea of spacial adaptivity on the basis of a meshless particle set and contains a monotone projection procedure. The set of numerical tests has indicated that PTM is a monotone high-resolution technique, possessing a linear computational complexity. The author of this thesis developed the numerical method based on Anton Smolianski's idea, developed the fast projection algorithm, performed the experiments and wrote the paper.

Publication II is the logical extension of *Publication I* and devoted to convection problems with diffusion and reaction. Here, an operator splitting approach is applied to combine the particle transport method for convection-reaction with an Eulerian scheme, such as the method of lines or the finite element method, for diffusion. The method is experimentally verified with respect to the mass conservation and the resolution of solution singularities for convection-dominated problems. *Publication II* is based on ideas of the author, Anton Smolianski and Heikki Haario, the implementation and experiments were performed by the author. The author extended the approach for the diffusion operator and was the principal author of the publication.

Publication III as well as *Publication IV* are devoted to the engineering application of the particle transport method, namely to the problem of crystallization, where such phenomena as reaction and crystal growth are involved. The particle transport method is applied to resolve the population balance equation, describing the crystal size distribution. The author performed the numerical computations and provided the description of the method, included in the papers.

Publication V is also dedicated to an engineering application of the particle transport method. Here, the problem of multicomponent nonlinear chromatography is considered. The performance of the method, especially with respect to artificial oscillations, computational time, and preservation of the total mass is checked in three cases: ideal chromatography, non-zero axial dispersion, as well as the solution of the equilibrium-dispersive model with numerically generated axial dispersion. The author implemented the particle transport method, performed the error analysis of the obtained results and wrote the paper.

CHAPTER II

Particle Transport Method

This chapter begins with the description of the convection-diffusion-reaction problem. Then, the explicit semi-Lagrangian numerical scheme called the Particle Transport Method (PTM) is introduced. The development of the technique was presented in detail in *Publication I* for linear convection problems and in *Publication II* for full CDR problems. Here, the advantages and restrictions of the proposed method are further discussed.

2.1 Formulation of the Problem

In the Eulerian formulation, the equation governing unsteady convective transport with diffusion and reaction is given as

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = D\triangle u + f(u, \mathbf{x}, t), \qquad \text{in} \quad \Omega \times (0, T),$$

where the unknown solution u is a space- and time-dependent function, $u = u(\mathbf{x}, t)$, and the space variable $\mathbf{x}$ belongs to the domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2$, and the time variable t varies in the interval $[0, T]$. D is a known constant diffusion coefficient. The reaction term, also referred to as a source function in literature, takes the form $f(u, \mathbf{x}, t) = K(\mathbf{x}, t)r(u)$, where reaction rate K may be a (stepwise) discontinuous function of $\mathbf{x}$.

In this work, it is supposed that the velocity field $\mathbf{v}$ is independent of u and divergence free, $\nabla \cdot \mathbf{v} = 0$, and thus the equation under consideration takes

the form

$$\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = D \triangle u + f(u, \mathbf{x}, t), \qquad \text{in} \quad \Omega \times (0, T). \tag{2.1}$$

It is also assumed that the velocity is given *a priori* on the domain Ω. In this case, the value of function u usually describes a physical quantity such as concentration or mass. To resolve Equation (2.1), it should be supplemented by the initial condition

$$u(\mathbf{x}, 0) = u_0(\mathbf{x}) \qquad \text{in} \quad \Omega, \tag{2.2}$$

and boundary conditions

$$\alpha_{in} u(\mathbf{x}, t) + \beta_{in} \frac{\partial u}{\partial n}(\mathbf{x}, t) = u_{in}(\mathbf{x}, t) \qquad \text{on} \quad \Gamma_{in} \times (0, T), \tag{2.3}$$

$$\alpha_{out} u(\mathbf{x}, t) + \beta_{out} \frac{\partial u}{\partial n}(\mathbf{x}, t) = u_{out}(\mathbf{x}, t) \qquad \text{on} \quad \Gamma_{out} \times (0, T). \tag{2.4}$$

Here, α_{in}, α_{out} and β_{in}, β_{out} are nonnegative constants, Γ_{in} and Γ_{out} are the portions of the domain boundary $\Gamma = \partial\Omega$ ($\Gamma_{in} \bigcup \Gamma_{out} = \Gamma$), where the respective inflow and outflow boundary conditions are defined.

As it was mentioned in Chapter 1 and discussed in detail in *Publication II*, the main feature of the presented problem is its ability to change its type from parabolic to hyperbolic when the diffusion or convection term dominates, respectively. This fact leads to a number of numerical challenges caused by the nature of these spacial differential operators.

First, we will address the convective operator and consider a linear convection problem

$$\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = 0 \qquad \text{in} \quad \Omega \times (0, T)\,. \tag{2.5}$$

As a hyperbolic equation, (2.5) needs boundary conditions only on the inflow part of the domain boundary Γ_{in}.

It is a usual procedure to rewrite Equation (2.5) in Lagrangian coordinates as

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u.$$

Thus the l.h.s. of Equation (2.5) is reduced to a total time derivative, which is equal to zero in the pure convection case. Therefore, the solution of the problem is defined by the initial and inflow statements and remains constant during the movement along characteristic curves (or trajectories) which are defined by the ordinary differential equation (ODE)

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}(\mathbf{x}, t). \tag{2.6}$$

This property of the convection equation gives rise to its second fundamental feature in the case of passively convected incompressible flow: the singularities of the solution, such as steep fronts and discontinuities, are determined by the initial and boundary conditions and are not smoothed during the simulation. These properties play the main roles in the construction of all Lagrangian and semi-Lagrangian algorithms for convective transport problems.

In the presence of a non-zero reaction in the r.h.s. of Equation (2.5), the time derivative takes the form

$$\frac{du}{dt} = f(u, \mathbf{x}, t). \tag{2.7}$$

Then, the solution of the convection-reaction problem is given by the integration of the ODE (2.7) along characteristics (2.6). Here, the reaction term becomes an additional source of solution singularities, for example, in the case of different reaction rates K in the computational domain.

The parabolic operator of diffusion, in contrast to convection, implies smoothing of the solution and generally improves the situation for applied numerical techniques. However, in the case of a strong convection domination it does not influence solution singularities significantly.

2.2 Description of the Method

We first list the main points of our approach to solve CDR problem (2.1)–(2.4). We use the operator splitting to separate the convection and diffusion

operators and treat each of them with respect to its properties. Special attention is paid to the resolution of the problem singularities due to initial and boundary conditions as well as reaction, which is done by means of spacial adaptivity. The development and movement of steep fronts and discontinuities is traced by the Lagrangian method based on characteristics combined with a moving system of meshless particles to avoid the strong deformation of a computational mesh. Finally, the solution is saved and visualized on a fixed grid. Hence, a mass conservative and fast projection procedure is needed. The same mesh is used, if diffusion is resolved by a standard mesh-based method, such as the method of lines or the finite element method.

The particle transport method for the convection-diffusion-reaction problem is based on the first order operator splitting approach, decoupling the convection-reaction and diffusion operators at each time interval $[t_{m-1}, t_m]$, $m = 1, ..., M$ on $(0, T)$:

Convection-reaction subproblem

$$\frac{\partial u}{\partial t} + (\mathbf{v} \cdot \bigtriangledown)u = f(u, \mathbf{x}, t) \quad \text{in} \quad \Omega \times [t_{m-1}, t_m], \tag{2.8}$$

$$u(\mathbf{x}, t) = u^{(m-1)}(\mathbf{x}) \quad \text{in} \quad \Omega \times \{t = t_{m-1}\}, \tag{2.9}$$

$$u(\mathbf{x}, t) = u_{in}(\mathbf{x}, t) \quad \text{on} \quad \Gamma_{in} \times (t_{m-1}, t_m). \tag{2.10}$$

The solution of the convection-reaction subproblem $u^{(*)}$ defines the initial condition for the diffusion subproblem.

Diffusion subproblem

$$\frac{\partial u}{\partial t} - D \bigtriangleup u = 0 \quad \text{in} \quad \Omega \times [t_{m-1}, t_m], \tag{2.11}$$

$$u(\mathbf{x}, t) = u^{(*)}(\mathbf{x}) \quad \text{in} \quad \Omega \times \{t = t_{m-1}\}, \tag{2.12}$$

$$u(\mathbf{x}, t) = u_{in}(\mathbf{x}, t) \quad \text{on} \quad \Gamma_{in} \times (t_{m-1}, t_m), \tag{2.13}$$

$$\alpha_{out} u(\mathbf{x}, t) + \beta_{out} \frac{\partial u}{\partial n}(\mathbf{x}, t) = u_{out}(\mathbf{x}, t) \quad \text{on} \quad \Gamma_{out} \times (t_{m-1}, t_m). \tag{2.14}$$

This gives the solution of CDR problem (2.1)–(2.4) at the $m-$th time step, $u^{(m)}$; see [71] for details.

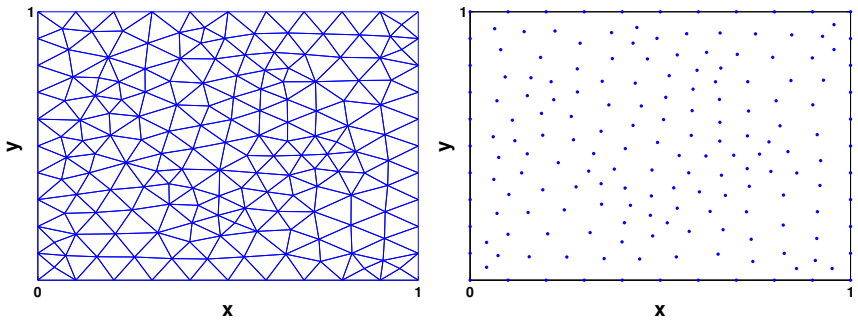


Figure 2.1: The grid (a) and the particle set (b)

In the framework of this decomposition, the linear convective transport is resolved by the Lagrangian method of characteristics while diffusion is integrated by means of an Eulerian FD or FE method. To create a high-resolution technique for convection problems, the concept of meshless numerical particles is applied; here, the only information to be used in the method is Cartesian coordinates of particles. This allows us to develop an effective procedure for spacial adaptivity, which controls the resolution of singularities caused by initial and boundary conditions or by the reaction term.

To simulate a CDR process by means of PTM, one needs both a stationary mesh in the domain, further referred to as *the grid*, and a moving system of particles, further referred to as *the particles*, see Figure 2.1. The convective transport of the solution as well as integration of the reaction term are carried out by the particles. The grid is required to realize three main tasks. First, the grid nodes are used to initialize the particle set. The distribution of the particles is adapted according to the singularities of the problem, the position of which is known either *a priori* from initial conditions or defined by the solution, i.e. by boundary conditions and/or reaction. In addition, the grid may be used to solve the diffusion subproblem. Finally, for multicomponent problems the grid can store data for components of the system, see the chromatography problem in *Publication V*. The use of two different computational sets implies the necessity of information exchange between them. In PTM, it is done by a node-by-node projection procedure based on linear interpolation.

For a more detailed discussion on the particle transport method its main components should be defined:

(i) spacial adaptivity of the particle system;

(ii) solving of the convection-reaction subproblem in the time interval (t_{m-1}, t_m) by the characteristic method on the appropriate particle set

(iii) solving of the diffusion subproblem on the grid or particle set by a standard Eulerian method;

(iv) projection between the particle set and the grid.

These steps are explained below in more detail. In general, the discussion focuses on the 2D case, some possible algorithmic simplifications are presented for 1D problems, as well. The treatment of the 3D case is analogous and can be extended straightforwardly from the 2D case. It should also be pointed out that all grids used in this work consist of triangle elements and are typically unstructured (see Figure 2.1(a) for an example), but again, the extension to quadrilateral grids and mixed (hybrid) grids does not present any difficulty.

2.2.1 Adaptivity procedure

The adaptivity procedure was presented in detail in *Publication I* and *Publication II*. Here it is shortly recalled. We emphasize the questions which were not covered fully in the publications.

The main aim of using spacial adaptivity is to balance between high resolution of singularities and small computational costs. This can be achieved by densifying the particle set, the location of which is initially given by nodes of a sparse grid, in the areas of special interest. These regions are indicated by solution properties such as smoothness and sharpness. Thus, to find the steep fronts of the solution, the absolute value of its gradient can be used. The area of the smooth solution also requires attention in order to avoid artificial smearing by linear interpolation within the projection procedure to be discussed below. This area can be defined by the absolute value of the second derivative of the solution. Using the value of the first or second derivative of the solution, further collectively called *the signal value*,

calculated at each grid element, adaptivity adds more particles in the vicinity of singularities or the smooth solution. The construction of the signal value within the so-called *sharp front* and *smooth* adaptivity was given in *Publication I*.

Provided that the signal value $G = \{G_i\}_{i=1}^{n}$ (n is the number of grid nodes) is computed on the whole computational domain Ω, and its maximum, G_{max}, and mean, G_{mean}, magnitudes are known, the number of new particles on the i-th element to be introduced into the particle system is defined as follows

$$N_{add} = \min\{N_{max} - N_{current}, \text{round}(\phi(G_i))\}, \tag{2.15}$$

where N_{max} is the maximum number of possible added points, $N_{current}$ is the number of particles on the i-th element so far and $\phi(G_i)$ is the monotonic function increasing in the interval $[G_{mean}, G_{max}]$. In this work, a linear function (see Figure 2.2) is always applied

$$\phi(G_i) = \begin{cases} 0\,, \text{ if } G_i \leq G_{mean}, \\ N_{max}\dfrac{G_i - G_{mean}}{G_{max} - G_{mean}}\,, \text{ if } G_{mean} < G_i \leq G_{max}, \\ N_{max}\,, \text{ if } G_i > G_{max}. \end{cases}$$

The maximum number of introduced particles, N_{max}, is defined by a user. Note that N_{max} is between 1 and 10 in all numerical experiments in this work, therefore, N_{add} varies from 0 to 10. The insertion of N_{add} new particles on an element can be implemented in numerous ways, for example, by random generation or uniform distribution at an interval for the 1D case or on triangle medians for 2D triangular elements. In this work, the uniform insertion of new particles has been used to achieve regular distribution of the particles in the vicinity of singularities. In the 2D case, the points are distributed inside the triangle by the barycentric coordinates; the illustration is given in Figure 2.3.

As it was mentioned above, the singularities for passively convected incompressible flow are defined by the initial and inflow boundary conditions as well as by the reaction rate function. Therefore, it is convenient to divide the adaptivity procedure into three general types: initial adaptivity, inflow adaptivity and solution-dependent adaptivity.

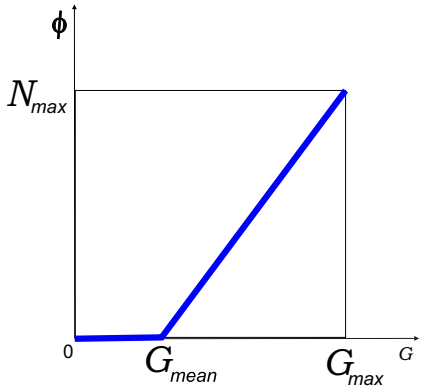


Figure 2.2: Function ϕ defining the number of new particles to be added on an element

Initial adaptivity

The initial adaptivity is used to treat singularities defined by the initial condition function $u_0(\mathbf{x})$, which might be, for example, a step-wise function. In addition, areas of the smooth solution can be adapted at the initial stage. In some cases, a priori knowledge of shocks developing due to the reaction term can be also taken into account by this adaptivity. The information about these singularities can be received from the discontinuity set S of the reaction rate function K,

$$S = \{\mathbf{x} \in \Omega | K \text{ is discontinious at } \mathbf{x}\}.$$

Let $\mathcal{T}^S$ be a set of grid elements lying on the discontinuity curves of the function K. Since $N_{current}$ is zero at the initial stage, by (2.15), the number of particles added by the initial adaptivity on the i-th element is

$$N_{add} = \begin{cases} N_{max}\,, \text{ if } G_i \equiv G_{max} \text{ or } \mathcal{T}_i \in \mathcal{T}^S, \\ \text{round}(\phi(G_i)), \text{ otherwise}\,. \end{cases} \tag{2.16}$$

Additional knowledge on the set S is useful when the singularities due to reaction develop on the discontinuities curves from the beginning of the simulation (a problem of this type will be discussed in the next section), oth-

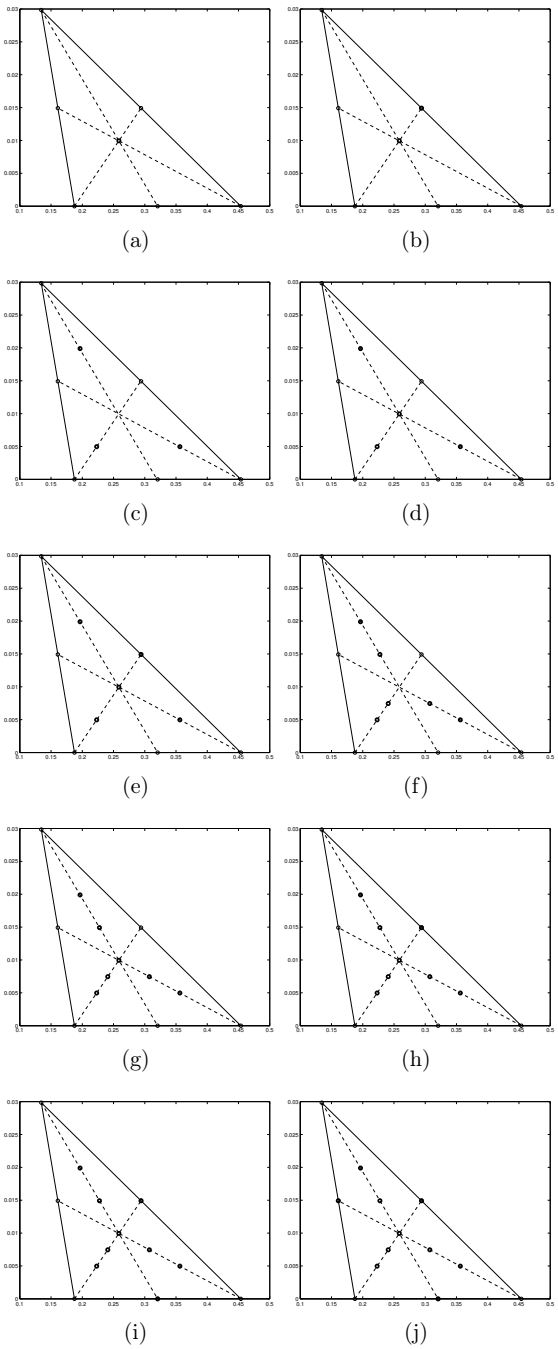


Figure 2.3: Uniform distribution of N_{add} new particles (black circles) introduced on a triangle element, $N_{add} = 1, ..., 10$

erwise it is more effective to adapt these regions by the solution-dependent adaptivity (see, for instance, the numerical examples in *Publication II*).

Thus, initially the generated particle set consists of grid nodes, which can be rather sparse, and points added by the initial adaptivity that makes the system more dense for the singularities and possibly for smooth regions. The function values for the particle set are defined exactly by the initial condition function $u_0(\mathbf{x})$.

Inflow adaptivity

The main purpose of applying the inflow adaptivity is to fill an area which is empty of particles due to their convective transport. The location of this region is defined by the inflow portion Γ_{in} of the domain boundary Γ. Insertion of new particles at this stage is confined by the grid elements occupying the empty area (let $\mathcal{T}_{in}$ denote these elements) and is also influenced by the requirement of good quality for the resolution of singularities. The elements from $\mathcal{T}_{in}$ which are connected with discontinuity set S, so-called, *inflow edges*, $\mathcal{T}_{in}^S$, receive more particles, e.g. N_{max}. Thus the number N_{add} for an element $\mathcal{T}_i$ from $\mathcal{T}_{in}$ is defined as follows

$$N_{add} = \begin{cases} N_{max}\,, \text{ if } G_i \equiv G_{max} \text{ or } \mathcal{T}_i \in \mathcal{T}_{in}^S, \\ \text{round}(\phi(G_i)), \text{ otherwise}\,. \end{cases} \tag{2.17}$$

The inflow adaptivity may also include both sharp and smooth front variations of the algorithm. The value of the solution is defined exactly by the boundary condition function $u_{in}(\mathbf{x}, t)$ for the points entering from the inflow boundary Γ_{in}. The rest of the new particles are, in general, evaluated by projection, which will be discussed bellow. However, for some cases, especially in 1D, it is possible to simplify this procedure by using qualitative information on the problem considered. For example, they can be assigned by the value of the boundary function with the corresponding time-shift, see the wave-packet transport in *Publication I*, or can receive the value of the particle entering at the previous time step, see *Publication V*.

Solution-dependent adaptivity

The solution-dependent adaptivity is closely related to the inflow adaptivity; it is also run during the simulation. This adaptivity influences the particle

distribution after each time step according to the chosen signal value. The main concern at this point is to catch solution singularities, which develop due to the reaction term and can not be localized a priori. Hence, the gradient of the solution is mainly used as a signal value. Here, the number of particles added in the i-th element is given by rule (2.15) and the solution value for them is defined by linear interpolation within the projection procedure.

Finally, it should be emphasized that the adaptivity procedure influences not only the resolution of the problem but also the dimension of the ODE system to be solved at a next time step. However, this does not lead to a significant increase in the total computational time of the method as we have observed in the numerical experiments.

2.2.2 Convection-reaction and diffusion subproblems

For the solution of the CDR problem, a first order operator splitting approach is used to separate convection-reaction from diffusion. The sequence of two subproblems (2.8)–(2.10) and (2.11)–(2.14) is solved at each time step $[t_{m-1}, t_m]$; the approximation of convection-reaction gives an initial estimate for diffusion at t_{m-1}. This allows using the most appropriate solvers for each subproblem.

The convection-reaction subproblem is resolved by the characteristics method, which reduces the PDEs problem to the pair of ODEs (2.6) and (2.7) supplemented by the initial conditions, defined at the beginning of each time step $[t_{m-1}, t_m]$ by the position of the particles, $\mathbf{X}$, and the solution of problem (2.1)–(2.4) in the previous time step.

A wide range of ODE solvers can be applied here; from the simplest Euler method and Runge-Kutta schemes of different orders to implicit or semi-implicit methods for stiff problems. The choice of solver depends on the complexity of a given convection-reaction problem, in particular, the velocity field and the reaction rate, and the required order of accuracy. It is worth noting that even a combination of different schemes (of a low and high order) can be implemented to realize also *temporal* adaptivity for the solution singularities.

For the diffusion subproblem, finite difference or finite element methods on an Eulerian mesh can be successfully applied. In the framework of this thesis the method of lines based on finite difference spacial discretization has been used for 1D problems while the Galerkin finite element method has been

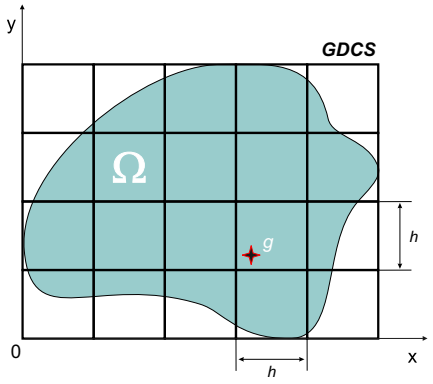


Figure 2.4: Global discrete coordinate system (GDCS)

applied to 2D cases. Since both methods are classic techniques for resolving diffusion problems, the details of the methods are beyond the scope of the present work and can be found, for example, in [90] and [100, 101]. For 1D problems, it is possible to use the particle set for diffusion, as well. The main concern with regard to 2D problems is the effective combination of the solution values given on the particles with those on an Eulerian grid. In the next section, we will discuss these topics.

2.2.3 Projection procedure

In this thesis, a special monotone projection technique has been developed. The procedure is based on node-by-node linear interpolation, which requires two particles in the 1D case and three particles in the 2D case. Thus the interpolation procedure includes a node under the consideration and a so-called *minimal interval* or *minimal triangle* that has to be found.

Any projection procedure can be divided into two principal steps: search and interpolation. The effectiveness of the projection procedure mainly depends on the optimization of the search operation. *Publication I* proposed a search based on an additional Cartesian grid on the domain Ω (the so-called Global Discrete Coordinate System (GDCS)) composed of square cells $h \times h$, where h is the width of the fixed grid, see Figure 2.4. Knowing the GDCS cell for a considered node, g, its neighbors $\mathbf{X}_g$ from the particle set can be easily fixed in the same cell; a minimal triangle is build from these neighbors.

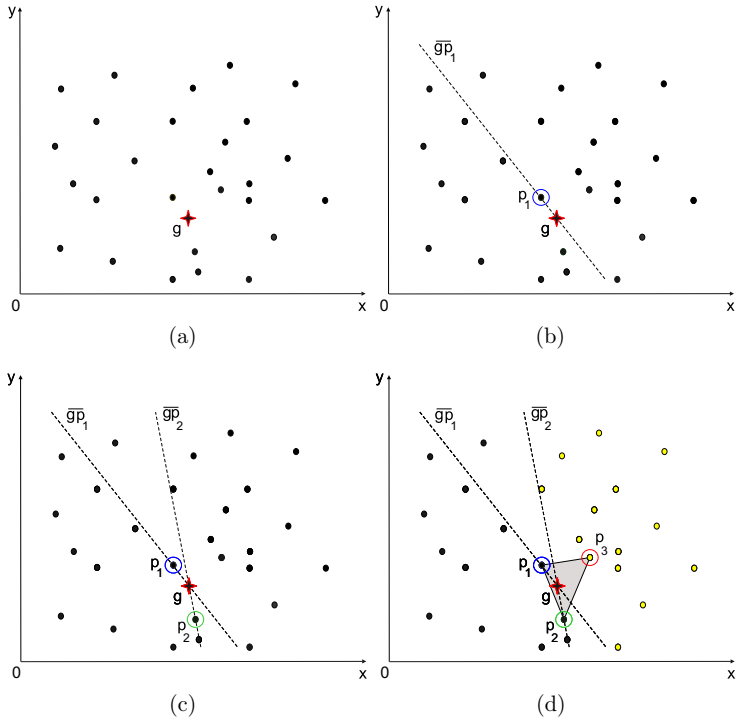


Figure 2.5: The search for a minimal triangle containing a grid node g

The construction of a minimal triangle from $\mathbf{X}_g$ can be realized simply by checking every possible set of three points. Additionally, information of the point set geometry can be used to accelerate the procedure. The first step is then to localize the closest particle p_1 in $\mathbf{X}_g$ to the considered node g, see Figure 2.5(a,b). The second vertex of a minimal triangle is the closest point to g which does not lie on the line through g and p_1, $\overline{gp_1}$, Figure 2.5(c). The last point, p_3, can simply be found from the subset $A \in \mathbf{X}_g$, consisting of points which lie between lines $\overline{gp_1}$ and $\overline{gp_2}$ and belong to the same subspace as the node g with respect to the line $\overline{p_1p_2}$ (see set of yellow points in Figure 2.5(d)).

Since for each grid node the set $\mathbf{X}_g$ is located in GDCS via integer division

of particle coordinates by h, there is no need in the order or connectivity of the particle system, that significantly simplifies the method. Moreover, the amount of operations to form a minimal triangle is not more then $O(1)$, and therefore, the total complexity of the projection procedure from the particle set onto the grid with n nodes is of the order $O(n)$.

2.3 Properties of the Method

In this section the properties of the particle transport method, such as accuracy, quality of singularities capturing and complexity, are discussed. We discuss separately the convection, convection-reaction and convection-diffusion-reaction cases.

2.3.1 Pure convection and convection-reaction

In the pure convection case, the particle transport method is a combination of a simple shift of the particles and adaptivity. If the imposed inflow conditions are zero and the velocity field is constant, the solution of the problem is given exactly by means of transport of the initial condition function on the particle set adapted by the initial adaptivity. In this case, there is, in fact, no need for any time stepping, the problem can be evaluated in one time step equal to the whole interval $[0, T]$.

A more complex velocity field, for example, rotation, as well as time-dependent inflow conditions, for example, a wave-packet function, leads to some restrictions on the step size for time. Here, the inflow adaptivity should be applied at appropriate time moments to catch singularities caused by the inflow condition function. The total temporal accuracy of PTM in this case is determined, in addition, by an ODE solver chosen to resolve the equation of the characteristics. For example, in *Publication I* a Runge-Kutta method of an order from 1 to 3 was used.

Convection and reaction are split at each time step in the particle transport method, where each of the operators is resolved as a system of ODEs defined for the particles. Here, we should distinguish the time step of PTM (in other words, the time step of the operator splitting) and the time step of ODE solvers used for particle transport and reaction. They may be of the same order, however, a complex velocity field and/or reaction term can call for a smaller time increment for the ODEs. This can be done in an automatic way by, for example, the Runge-Kutta method with adaptive time stepping.

In the numerical experiments presented in *Publication I* and *Publication II*, however, particle transport as well as reaction have been resolved with the same time step as the operator splitting. To define the time step size of PTM, two aspects should be taken into account. First, it is a necessity to adapt the particle system during the simulation to treat singularities due to the reaction process. Second, since the operator splitting is of the first order, proper attention should be paid to the comparative rates of the terms. In some real-life applications, for example, chromatography separation, the convection and reaction processes can have significantly different speeds. Hence, the time increment is chosen to balance them within one time step. There are some heuristics for estimating the time increment with respect to the problem parameters, which was discussed in *Publication V* devoted to chromatography problems.

The particle transport method uses an Eulerian grid for the representation of the solution in the case of pure convection and convection-reaction problems. The presence of the projection procedure, used here for the solution visualization only, might lead to an error due to linear interpolation, which, however, does not accumulate. Thus, in the numerical tests (see *sine*-surface convection in *Publication I* and convection-reaction of a Gaussian pulse in *Publication II*), where the projection procedure is implemented, we observe the second order of a spacial accuracy for a smooth solution.

Since adaptivity is applied for the resolution of singularities, and the combination of an exact transport and linear interpolation prevents the development of artificial maxima and minima, the particle transport method may be classified as a high-resolution scheme. The numerical experiments presented in *Publication I* and *Publication II* have confirmed that the method demonstrates high-resolution of singularities, as well as linear complexity ($O(N)+O(n)$) with respect to the number of particles, N, and grid nodes, n.

To demonstrate the ability of the method to resolve singularities of the solution as well as to save mass, we first advert to an experiment of rigid-body rotation presented in *Publication I*. The results of the test show that the movement of a slotted cylinder is approximated without developing artificial oscillations or smearing (see Figure 12 of *Publication I*). In addition, Table 2.1 presents the mass conservation error ε_{mass} with respect to the number of particles, where we change the initial number of particles N (in other words, the density of the grid used to initialize the particle set) or the maximum number of points added on each grid element, N_{max}. The results indicate that the mass conservation error is of the second order with respect

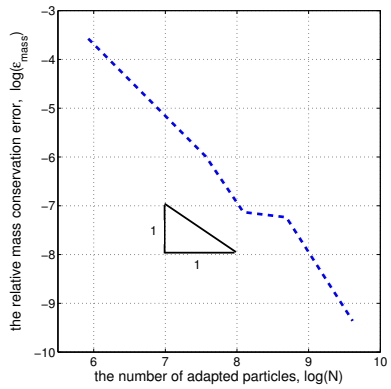


Figure 2.6: The mass conservation error with respect to the number of particles N ($N_{max} = 10$) for the rigid body rotation of a slotted cylinder (logarithmic scale)

to N (see Figure 2.1). Moreover, it can be seen that the error also decreases by increasing N_{max} while keeping the initial number of particles N fixed.

Table 2.1: Rigid body rotation of a slotted cylinder. The mass conservation error with respect to the different initial number of particles N and the different adaptivity parameter N_{max}. The number of grid nodes is fixed as $n = 8401$, one full rotation, $\triangle t = \pi/10$

fixed $N_{max} = 10$			fixed initial $N = 1081$		
initial N	adapted N	ε_{mass}	N_{max}	adapted N	ε_{mass}
148	374	2.8e-02	0	1081	2.8e-02
1081	1930	2.5e-03	2	1269	3.0e-03
2137	3257	8.0e-04	6	1619	4.4e-03
4209	5928	7.2e-04	8	1777	3.8e-03
8401	14691	8.6e-05	10	1930	2.5e-03

Further, in order to discuss effectiveness of PTM with regard to convection-

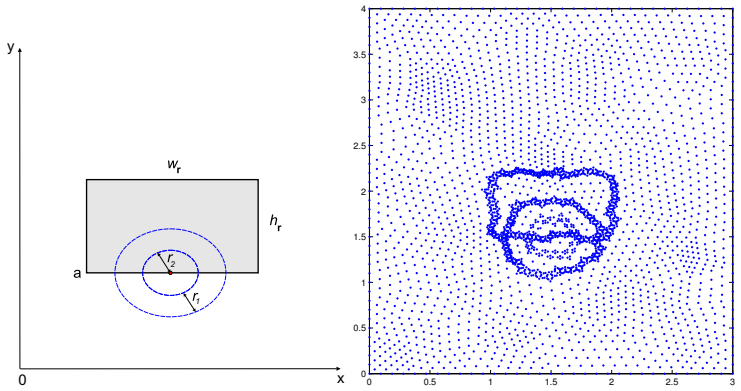


Figure 2.7: Convection-reaction of a prism: (a) – sketch of the initial condition and the reaction rate functions; (b) – initial distribution of the particles

reaction, we consider the rotation of a prism subjected to reaction with different rates in the domain Ω. The initial condition is given as

$$u(\mathbf{x},0) = \begin{cases} 1\,, \text{ if } \mathbf{x} \in D \subset \Omega, \\ 0\,, \text{ otherwise,} \end{cases} \tag{2.18}$$

where $D \subset \Omega$ is a rectangle with a height of $h_r = 0.7$, a width of $w_r = 1.0$ and the bottom left corner $(x_a, y_a) = (1, 1.5)$, see Figure 2.7(a).

The rotation velocity field is

$$\mathbf{v} = \{y - 1.5, -x + 1.5\}.$$

The reaction term is of the first order, $K(\mathbf{x})u(\mathbf{x},t)$, where the rate K is a piecewise constant function in Ω

$$K(\mathbf{x}) = \begin{cases} 1.1\,, \text{ if } \mathbf{x} \in D_1, \\ 0.8\,, \text{ if } \mathbf{x} \in D_2, \\ 0\,, \text{ otherwise.} \end{cases}$$

Here, D_1 is a circle of the radius $r_1 = 0.2$ and D_2 is a ring around D_1 of the width $r_2 = 0.2$. Both regions are centered on the point $(1.5, 1.5)$, see Figure 2.7(a).

Since all possible singularities are defined here by the initial condition function u_0 and the set

$$S = \{\mathbf{x} \in \Omega | (x-1.5)^2+(y-1.5)^2 = r_1^2 \text{ and } (x-1.5)^2+(y-1.5)^2 = (r_1+r_2)^2\},$$

only the initial adaptivity is applied. The distribution of the particles, consisting initially of 2137 points and adapted with $N_{max} = 10$, can be seen in Figure 2.7(b).

The projection procedure is used here only for the visualization, since the reaction term is integrated directly on the particle set. Table 2.2 deals with the mass conservation error ε_{mass} with respect to the initial and adapted number of particles while the number of grid nodes for the visualization is fixed, $n = 8401$. We can conclude that the initial adaptivity results in a non-oscillating solution (see Figure 2.8), which at the same time demonstrates the second order of mass conservation (see Figure 2.9). Here again, we can see a decrease in the error by increasing N_{max} with a fixed initial number of particles; the adapted distribution contains about 2000 particles, which corresponds to the mesh size $h \sim 0.2$ on the given domain.

Table 2.2: Convection-reaction of a prism. The mass conservation error with respect to the different initial number of particles, N, and the different adaptivity parameter N_{max}. The number of grid nodes is fixed as $n = 8401$, one full rotation, $\triangle t = \pi/10$

fixed $N_{max} = 10$			fixed initial $N = 1081$		
initial N	adapted N	ε_{mass}	N_{max}	adapted N	ε_{mass}
148	438	4.1e-02	0	1081	4.64e-02
1081	1804	6.1e-03	2	1293	1.43e-02
2137	3436	4.4e-03	6	1538	1.13e-02
4209	5709	1.4e-03	8	1673	1.10e-02
8401	11096	3.6e-04	10	1804	6.10e-03

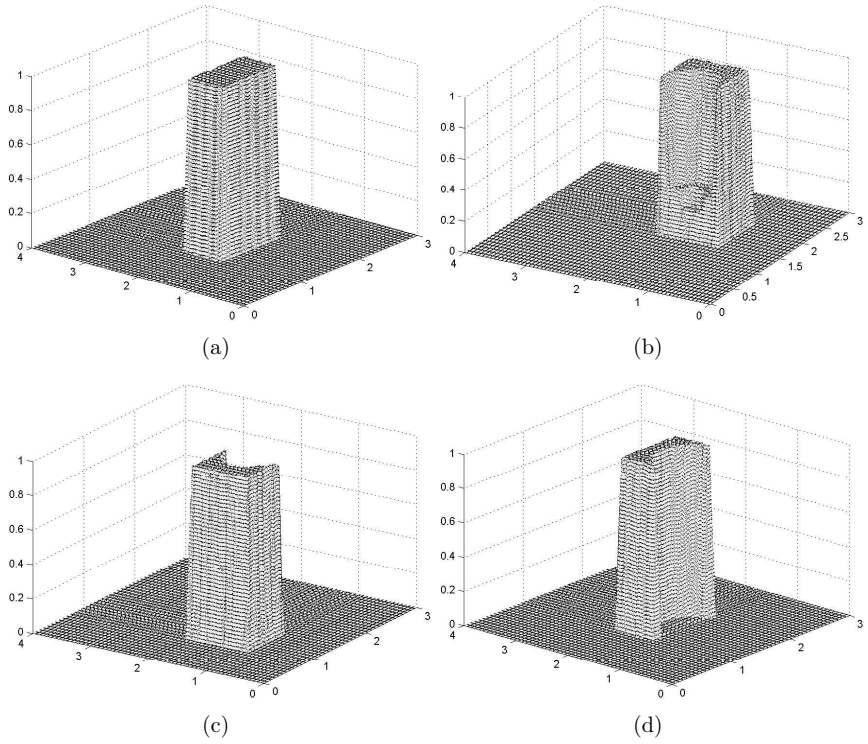


Figure 2.8: Convection-reaction of a prism. The initial number of particles is 1081, $N_{max} = 10$, $\triangle t = \pi/10$. Solution at $t = 0.0$ – (a), $t = 1.5708$ – (b), $t = 3.1416$ – (c), $t = 6.2832$ – (d)

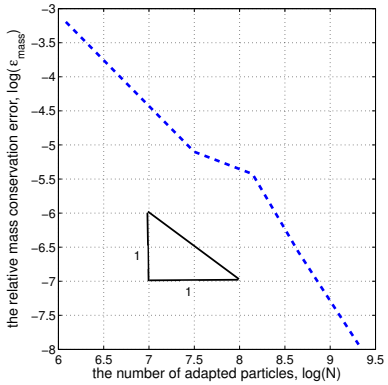


Figure 2.9: The mass conservation error with respect to the number of particles N ($N_{max} = 10$) for convection-reaction of a prism (logarithmic scale)

2.3.2 Convection-diffusion-reaction

In the particle transport method, convection-reaction and diffusion are resolved in the framework of the first order operator splitting. The same consideration as in the convection-reaction case should be given to the time increment of PTM. The time step of ODE solvers for convection and reaction can vary inside the time interval of the operator splitting. For example, in *Publication V* we used the Runge-Kutta method of the fourth order with adaptive time stepping for the reaction term.

The method loses an optimal linear complexity when adding the diffusion subproblem. However, it is still faster than some classical mesh-based methods, such as the method of lines, see *Publication II*. Moreover, adaptivity applied to the convection-reaction subproblem allows high-resolution of the singularities in the case of convection domination (see convection-diffusion of a step function in *Publication I*, mixing of hot and cold fronts and chromatographic separation in *Publication II*).

The diffusion subproblem may be resolved by a suitable discretization based either on the particle set or on the grid. In *Publication II* and *Publication V*, the finite difference discretization in 1D on nonuniform particles (see [88] for details) has been applied in the framework of the method of lines. This

combination avoids interpolation between a stationary uniform grid and the nonuniform particles. Thereby, it eliminates the interpolation error and decreases the computational time. Since all three operators are resolved on the particles, the projection procedure is used here only to visualize the solution.

Use of the standard Galerkin finite element discretization for 2D diffusion requires the grid-function $u^{(*)}$, which gives an initial estimation at the time step $[t_{m-1}, t_m]$. Thus the projection procedure is applied to interpolate the solution from the particle set onto the grid. The main danger here is that the error due to linear interpolation during projection will accumulate with time. This can be avoided by a more dense mesh, but at the cost of increasing the CPU time.

We sum up that the investigation of the PTM properties on test (benchmark) problems has shown that the method is effective in the case of singularities due to reaction which are localized and known *a priori*. Here the initial adaptivity is applied to prevent the contamination of the solution. The initial adaptivity with the smooth signal value is useful in transport of smooth functions with the high second derivative. The comparison with the discontinues Galerkin method in *Publication I* has shown that PTM, reaching the same order of accuracy, can work much faster for convection of a 2D sine-function. In *Publication I*, we have demonstrated that PTM may be more effective for the wave-packet transport than classic high-resolution methods based on flux-limiters. The inflow adaptivity prevents here the non-physical smearing of the singularities caused by boundary conditions. Moreover, it allows us to use a very sparse particle set with comparison to a grid needed for a FCT scheme to receive the same order of accuracy. The solution-dependent adaptivity, which slightly increases computational costs, helps to resolve solution-dependent singularities during the simulation. In *Publication II*, PTM has been compared with the method of lines and the fractional step central and upstream finite difference method. Numerical experiments have confirmed that PTM demonstrates a good accuracy and, at the same time, low computational costs for convection-diffusion-reaction problems. Both structured and unstructured grids can be easily used by the method. Moreover, for the 1D case, PTM can be improved by using the particle set to solve the diffusion subproblem. This is utilized in engineering problems discussed in the next chapter.

CHAPTER III

Applications

In this chapter, we address two topics in chemical engineering which call for an efficient numerical solver of pure and/or convection-dominated problems: crystallization (see *Publication III* and *Publication IV*) and chromatographical separation (see *Publication V*).

3.1 Crystallization

In *Publication III* and *Publication IV*, we apply the particle transport method to the problem of crystallization and precipitation, namely to the problem of crystal size distribution (CSD).

The crystallization operation appears in many industrial applications, such as food and pharmaceutical production, where physical parameters of the crystals (for example, size and form) are of the main importance. The crystal size distribution problem is usually described by the population balance equation (PBE), which includes the formation, growth and breakage of crystals. The general PBE for crystallization with crystal length L as a property coordinate and n as the population (number) density function can be written as follows

$$\frac{\partial n}{\partial t} + G\frac{\partial n}{\partial L} = \frac{n_{in}(L) - n(L,t)}{\tau} + B(L) - D(L).$$

Here, G is the crystal growth rate, the term $\frac{n_{in} - n}{\tau}$ defines the inflow and outflow, τ is the resistance time, $B(L)$ is the birth term and $D(L)$ is the

death term. To simulate the reactive crystallization process, the PBE is supplemented by the equations describing the kinetics of the system, that defines the terms of the crystal birth and death.

According to [20], the numerical methods for solving the PBE can be classified into three main groups: the method of moments, the method of classes and the weighted residuals. The weighted residuals methods were the first ones applied to PBE problems. The solution of the problem is approximated here as a series of trial functions with appropriate coefficients to satisfy the governing equation. The main problem for weighted residuals is to find proper trial functions for the population density function. The method of moments proposed in [84] converts the PDEs of the population balance to ODEs in terms of moments, which, unfortunately, may result in very complex mathematical equations for problems with size-dependent growth terms. The method of classes, also called the discretization sizing technique, transforms the PBE into a discretized population balance in terms of average crystal size classes. The main difficulty here is the appropriate choice of the number of classes, which may lead to a large number of resulting ODEs.

In *Publication III* and *Publication IV*, we consider a reactive crystallization case, where crystals appear in the tank due to kinetics ($B(L)$), i.e. $n_{in}(L,t) \equiv 0$, and vanish from there only due to the outflow, i.e. $D(L) \equiv 0$. We suggest the use of the particle transport method to resolve the population balance equation. In this case, the numerical particles correspond to the classes of crystals, and a priori knowledge on the CSD can be used for the generation of an initial particle set to be adapted in regions of the high gradient during the simulation. Figure 4 in *Publication III* demonstrates that PTM allows resolving the PBE without artificial oscillations that can be observed, for example, in the linear and logarithmic approximations (Figures 2 and 3 in *Publication III*). Further, the proposed technique has been tested on the problem of reactive crystallization of barium sulphate. The results obtained demonstrate a good conformity with the experimental data (see Figures 4 and 5 in *Publication IV*).

3.2 Chromatography

Chromatography is a separation process of a mixture based on the difference between the migration velocities of the components resulting from their different absorption properties. In general, a system of chromatographical

separation consists of a moving (fluid) phase presenting the mixture and a stationary (solid) phase. The fluid phase, injected initially as a concentration pulse, streams through the solid phase column in a way that leads to the separation of mixture components. Mathematically, the chromatographical separation is presented by differential mass balance equations for moving components

$$\frac{\partial \mathbf{C}}{\partial t} + F\frac{\partial \mathbf{q}}{\partial t} + v\frac{\partial \mathbf{C}}{\partial x} = D\frac{\partial^2 \mathbf{C}}{\partial x^2}, \tag{3.1}$$

where $\mathbf{C} = \{C_i\}_{i=1}^{\mathcal{N}}$ is a vector of $\mathcal{N}$ moving components of the mixture, $\mathbf{q} = \{q_i\}_{i=1}^{\mathcal{N}}$ is a vector of stationary components, F is a phase ratio, v is a stream velocity of a moving phase and D is a dispersion coefficient (in general this coefficient can be different for each moving component). Additionally, an algebraic or a differential set of equations describes the mass transfer between the solid and moving phases, i.e. the equilibrium (or adsorption) isotherms. The algebraic form may be written in the so-called equilibrium-dispersive models

$$\mathbf{q} = \mathbf{f}(\mathbf{C}), \tag{3.2}$$

where $\mathbf{f} = \{f_i\}_{i=1}^{\mathcal{N}}$ are non-linear functions of $\mathbf{C}$. The differential description of the isotherm can be written as

$$\frac{\partial \mathbf{q}}{\partial t} = k(\mathbf{q}^* - \mathbf{q}). \tag{3.3}$$

Here, k is the mass transfer coefficient and $\mathbf{q}^*$ denotes the equilibrium term given by (3.2). If the mass transfer coefficient is large enough, the quasi-steady-state solution $\mathbf{q} = \mathbf{q}^*$ of (3.3) coincides with that of (3.2).

There is a large number of works devoted to the different mathematical models of a physical equilibrium. The simplest model is a linear one. Multicomponent systems usually follow the competitive nonlinear equilibrium isotherms (see, for example, [31]), such as the Langmuir

$$q_i = \frac{a_i C_i}{1 + \sum_{i=1}^{\mathcal{N}} b_i C_i}$$

and the Jovanovic isotherm

$$q_i = 1 - \exp\left(-\sum_{i=1}^{\mathcal{N}} b_i C_i\right). \tag{3.4}$$

In general, an isotherm is the source of nonlinearity in the governing differential equations. Moreover, non-linear equilibrium isotherms give rise to steep fronts (shock waves) of the solution, see e.g. Figure 3.1.

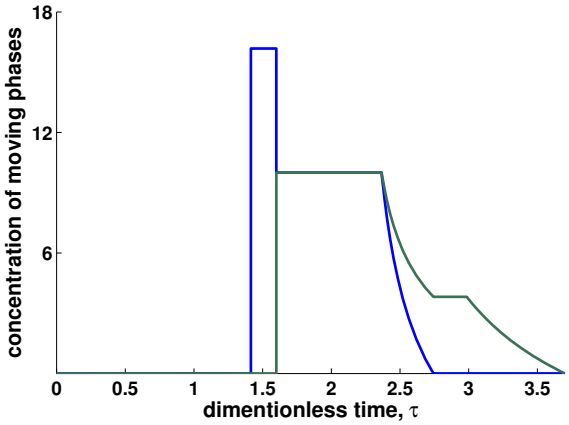


Figure 3.1: Chromatographical separation. The concentration of the moving phases (blue line – C_1, green line – C_2) with respect to the computational time

For ideal chromatography problems, meaning the absence of dispersion (or diffusion), an analytical solution of the governing equations can be obtained in the framework of the equilibrium theory, see e.g. [86]. However, the simulation of a nonlinear nonideal process requires a numerical approach. A number of classical numerical methods, based on both finite differences and finite elements, have been tested for the given problem, such as the orthogonal collocation finite elements method, the method of lines and the Godounov-Rouchon algorithm (for detailed discussion see *Publication V*).

Publication V, continuing the preliminary consideration in *Publication II*, demonstrates the use of the particle transport method for the simulation of

ideal and nonideal nonlinear two-component chromatography described by the reaction-dispersive model with competitive isotherms. A particle set is used here to transport the mobile components. The dispersion subproblem is resolved by means of the method of lines, where the space discretization is implemented by non-uniform finite differences on the same particle set. A stationary grid is needed for storage of the solid phase. To evaluate the mass transfer described by (3.3), the solid phase is projected from the grid onto the particles at each time step. After (3.3) has been integrated, the new values of the solid phase are interpolated back to the storage grid. In order to avoid numerical diffusion due to linear interpolation, the storage grid should be rather dense. However, the numerical experiments have shown that this does not result in a significant increase in computational time since the grid is used only for interpolation, not for integration of a differential equation system (see Tables 1 and 2 and Figures 4 and 7 in *Publication V*). PTM has been tested especially with respect to artificial oscillations, computation time, and preservation of the total mass on two cases: ideal chromatography and non-zero axial dispersion. The shock waves forming with time in both cases are treated by means of the solution-dependent adaptivity that prevents the development of artificial oscillations. On the other hand, the use of the same particle set for the approximation of advection-reaction and dispersion subproblems as well as the use of a dense storage grid for the stationary components allow avoiding spurious smearing of shock waves (see Figure 5 for an ideal case and Figure 6 for a nonideal (advection-dominated) case in *Publication V*).

3.3 Discussion

The particle transport method has been applied and proven to be valid for chemical engineering problems. Here, singularities due to reaction as well as to boundary conditions are not known a priori. Applying the solution-dependent adaptivity and choosing an appropriate time step size allows PTM to obtain better results than some classical methods (such as the method of lines, linear and logarithmic discretization) with respect to the accuracy and computational time, especially in advection-dominated cases. In addition, optimization of the method, required in real-life applications, is also possible: to reduce the computational times, dispersion in the chromatography problem can be approximated artificially by introducing numerical diffusion due to linear interpolation. Considering the crystallization

problem, the particle transport method has optimal linear complexity and can be easily introduced into an existing software for chemical engineering.

Further cases where to apply the particle transport method are continuous and multi-phase chromatography. In addition, the method can be very efficient for reactive crystallization with a size-dependent birth term.

Chapter IV

Conclusions

The main objective of the presented work was to develop numerical methods for convection-diffusion-reaction problems. The domination of the convection term in the CDR system makes its numerical approximation a difficult task due to possible high gradients or discontinuities of the exact solution. The study was initiated with a pure linear convection problem for which a novel numerical technique, the particle transport method, was proposed. Further development has shown that the introduced method is well suited for numerical simulation of linear convective transport including diffusion and reaction.

The main achievement of this study is the construction of a fast high-resolution particle method. The particle transport method (PTM) is a semi-Lagrangian (characteristics based) method which works on meshless particles while using the Eulerian representation of the problem solution on a fixed grid. The approach essentially relies on three basic components: spacial adaptivity, projection and operator splitting. The combination of the exact transport and linear interpolation within the projection procedure allows one to obtain a monotone method with linear computational complexity for pure and reactive convection. The spacial adaptivity, applied at the initial stage as well as during the simulation, enables one to maintain high resolution for the problem singularities (high gradients and discontinuities) without artificial oscillations or smearing. The adaptivity procedure avoids any additional numerical techniques, such as flux limiters and stabilizing viscosity, that would require experimental tuning. The meshless approach is quite advantageous from the viewpoints of both computational reliability

and cost-effectiveness, as the mesh does not have to be reconstructed at each time step and adaptivity can be implemented in an algorithmically simple and inexpensive way.

PTM has a second order accuracy in space, while the temporal accuracy depends on the solver used to perform particle transport. A first order operator splitting approach is employed to combine the different operators of a CDR problem. Thus the whole method has a first order temporal accuracy here. This seems to be sufficient, since the spatial errors usually dominate in problems with singularities and complex velocity fields.

The performance of the proposed computational approach has been assessed in diverse tests and benchmark problems, such as wave transport, rigid-body rotation, mixing of hot and cold fronts, and layered reaction. The numerical tests have shown that the presented technique demonstrates good mass conservation and accuracy with respect to the resolution of the solution singularities while being more effective than some standard mesh-based techniques. It should be pointed out that the applicability of the method is confined to linear convective transport, i.e. the velocity field should be a solution-independent function. However, the particle transport method is useful and effective in a wide range of real-life application problems, such as chromatography and crystallization.

The research, initiated by the presented study, can be continued in two directions: widening of the application area and further algorithmic improvement of the particle transport method. The method can be applied to the solution of such computational fluid dynamics problems as gas bubble dissolution in a viscous flow. Here, the proposed technique can be used for the mass transfer part of the problem as well as for the resolution of the movement of the free interface between gas and liquid fractions, described as convection of a level set function. Some algorithmic improvements are possible in the framework of the adaptivity procedure. In 1D, the diffusion operator has been dealt with both in a Langrangian and Eulerian way. The treatment of the diffusion operator for 2D and 3D cases should be further studied.

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APPENDIX

Publications