Chapter 4

Applications

4.1 Lecture 8: Conservation laws and application of finite volume methods

4.1.1 Introduction

In the following lecture, we deal with conservation laws which we met in many physical applications, e.g. fluid dynamics, mass conservation, transport problems, etc.

In the novel applications of multicomponent transport, e.g. applied in plasma modelling, we deal with such mass conserved equations.

4.1.2 Plasma Modelling: Mass transfer and exchange for Multicomponent Problems

We assume to model the ionized plasma as an underlying media in the chamber with mobile and immobile phases. Here transport in the plasma with gaseous species contain of mobile and immobile concentrations, [128]. For such a homogenous plasma, we applied our expertise in modeling multiphase transport through a porous medium.

To amplify the modeling of the gaseous flow to the gas chamber which is filled with ionized plasma, we deal with the so-called far-field model based on a porous media. Here the plasma can be modeled as a continuous flow [93], that has mobile and immobile phases, see [**?**].

We assume a near vacuum and a diffusion-dominated process, derived from the Knudsen diffusion, [**?**]. In such viscous flow regimes, we deal with small Knudsen

Numbers and a pressure of nearly zero.

In Figure 4.1, the gas chamber of the CVD apparatus is shown, which is done with a porous media.

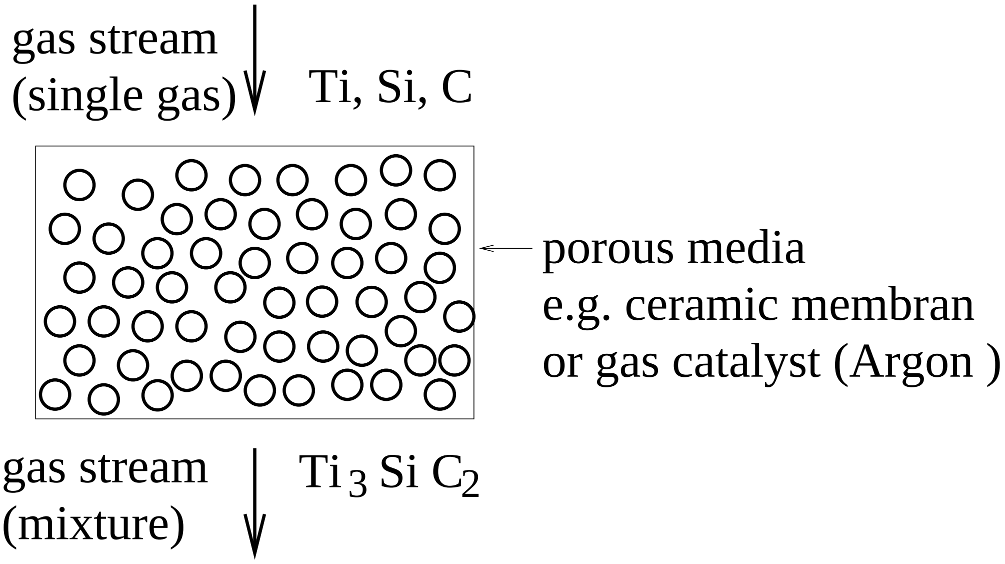

Figure 4.1: Gas chamber of the CVD apparatus.

In Figure 4.2, the mobile and immobile phases of the gas concentration are shown in the macroscopic scale of the porous media.

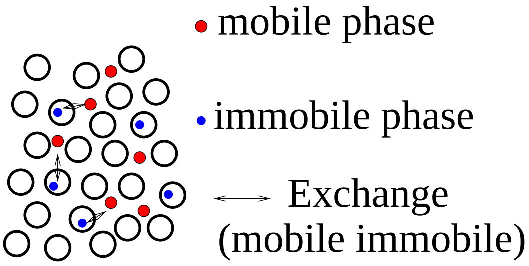

Figure 4.2: Mobile and immobile phase.

In Figure 4.3, the mobile and adsorbed phases of the gas concentration are shown in the macroscopic scale of the porous media.

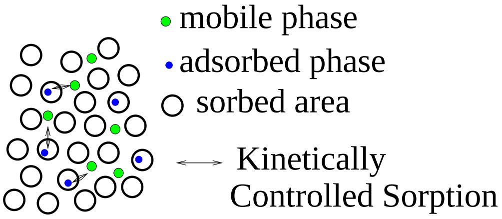

Figure 4.3: Mobile-adsorbed phase.

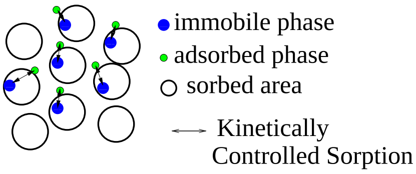

Figure 4.4: Immobile-adsorbed phase.

In the following we present the transport model for the multicomponent problem with the embedded multiple phases.

$$\phi \partial_t c_i^L + \nabla \cdot (\mathbf{v} c_i^L - D^{e(i)} \nabla c_i^L) = g(-c_i^L + c_{i,im}^L) + k_\alpha(-c_i^L + c_{i,ad}^L \\ -\lambda_{i,i} \phi c_i^L + \sum_{k=k(i)} \lambda_{i,k} \phi c_k^L + \tilde{Q}_i, \tag{4.1}$$

$$\phi \partial_t c_{i,im}^L = g(c_i^L - c_{i,im}^L) + k_\alpha(c_{i,im,ad}^L - c_{i,im}^L) \\ -\lambda_{i,i} \phi c_{i,im}^L + \sum_{k=k(i)} \lambda_{i,k} \phi c_{k,im}^L + \tilde{Q}_{i,im}, \tag{4.2}$$

$$\phi \partial_t c_{i,ad}^L = k_\alpha(c_i^L - c_{i,ad}^L) - \lambda_{i,i} \phi c_{i,ad}^L + \sum_{k=k(i)} \lambda_{i,k} \phi c_{k,ad}^L + \tilde{Q}_{i,ad}, \tag{4.3}$$

$$\phi \partial_t c_{i,im,ad}^L = k_\alpha(c_{i,im}^L - c_{i,im,ad}^L) - \lambda_{i,i} \phi c_{i,im,ad}^L \\ + \sum_{k=k(i)} \lambda_{i,k} \phi c_{k,im,ad}^L + \tilde{Q}_{i,im,ad}, \tag{4.4}$$

ϕ : effective porosity $[-]$,
c_i^L : concentration of the ith gaseous species in the plasma chamber
$c_{i,im}^L$: concentration of the ith gaseous species in the immobile zones of the plasma chamber $[mol/cm^3]$,
$\mathbf{v}$: velocity in the plasma chamber $[cm/nsec]]$,
$D^{e(i)}$: element-specific diffusions-dispersions tensor $[cm^2/nsec]]$,
$\lambda_{i,i}$: decay constant of the ith species $[1/nsec]]$,
$\tilde{Q}_i$: source term of the ith species $[mol/(cm^3 nsec)]$,
g : exchange rate between the mobile and immobile concentration $[1/nsec]$,
k_α : exchange rate between the mobile and adsorbed concentration or immobile and immobile adsorbed concentration (kinitic controlled sorption) $[1/nsec]$,

with $i = 1, \dots, M$ and M denotes the number of components.

The parameters in equation (4.1) are further described, see also [70].
The effective porosity is denoted by ϕ and declares the portion of the porosities of the aquifer, that is filled with plasma, and we assume a nearly fluid phase. The transport term is indicated by the Darcy velocity $\mathbf{v}$, that presents the flow-direction and the absolute value of the plasma flux. The velocity field is divergence-free. The decay constant of the ith species is denoted by λ_i. Thereby does $k(i)$ denote the indices of the other species.

4.1.3 Motivation to the discretization schemes

To discretize such equations, methods are designed, that taken into account the conservation laws, see [127] and [55]. We deal with finite volume methods as a discretisation method which is well suited for the numerical simulations of such mass conserved equations.

It is extensively used in several engineering fields, such as fluid mechanics, heat and mass transfer or petroleum engineering. Some features are equal to the Finite Element methods as arbitrary geometries, using structured or unstructured meshes and robust schemes. An additional feature is the local conservativity on the numerical fluxes, that is the numerical flux conserved from one discretisation cell to its neighbor.

This makes the finite volume scheme attractive, when modelling problems for which the flux is of importance. The finite volume method is locally conservative because it is based on a balance, i.e. a local balance is written on each discretisation cell (called often "control volume").

Therefore an integral formulation of the fluxes over the boundary of the control volumes is obtained.

For example the mass balance between inflow and outflow in the finite control volume:

$$\sum_{j \in in(i)} v n_j u_j = \sum_{k \in out(i)} v n_k u_k \ , \tag{4.5}$$

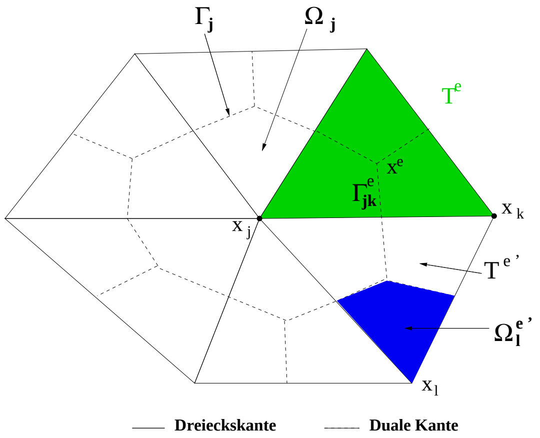

Figure 4.5: Triangulation of the Finite-Volume Method.

4.1.4 Example for the introduction

We consider the linear transport equation

$$u_t + div(v\ u) = 0 \ , \ x \in I\!R^2 \ t \in I\!R^+ \tag{4.6}$$

$$u(x,0) = u_0(x) \ , \ x \in I\!R^2 \ , \tag{4.7}$$

where $u, v \in C^1(I\!R^2, I\!R^+)$ and $u_0 \in L^\infty(I\!R^2)$.

$\mathcal{T}$ is a mesh of $I\!R^2$ consisting polynomial bounded convex subsets of $I\!R^2$ and $K \in \mathcal{T}$ a control volume.

We integrate 4.6 over K and yield the balance equation over K :

$$\int_K u_t \ dx \ + \int_{\partial K} v \ n_K \ u \ d\gamma = 0 \ , \ t \in I\!R^+, \tag{4.8}$$

where n_K denotes the normal vector of ∂K.

The semi-discretisation by implicit Euler scheme yields :

$$\frac{1}{\Delta t}\int_K (u^{n+1}-u^n)\,dx \;+\; \int_{\partial K} v^{n+1}\,n_K\,u^{n+1}\,d\gamma = 0\;, \qquad \forall\, n\in I\!N\;,\;\forall\, K\in\mathcal{T} \tag{4.9}$$

where n_K denotes the normal vector of ∂K.

The full discretisation of the equation 4.6 is given by

$$\frac{m(K)}{\Delta t}\,(u^{n+1}-u^n) \;+\; \sum_{\sigma\in\epsilon_K} F^{n+1}_{K,\sigma} = 0\;, \qquad \forall\, n\in I\!N\;,\;\forall\, K\in\mathcal{T} \tag{4.10}$$

where $m(K)$ is the measure of the control volume K, $u^0_K = \int_K\; u_0\;dx$.

We decide the flux with the upwinding :

$$F^{n+1}_{K,\sigma} = \begin{cases} v^{n+1}_{K,\sigma}\;u^{n+1}_K & \text{if } v^{n+1}_{K,\sigma}\geq 0 \\ v^{n+1}_{K,\sigma}\;u^{n+1}_L & \text{if } v^{n+1}_{K,\sigma} < 0 \end{cases} \tag{4.11}$$

where $v^{n+1}_{K,\sigma} = \int_\sigma\; v^{n+1}\;n_{K,\sigma}\;d\gamma$.

4.1.5 One-dimensional elliptic-equation (ordinary differential equation)

We introduce the one-dimensional elliptic problem and the error-estimates for the finite volume methods.

4.1.5.1 A finite volume method for the Dirichlet problem

We consider the following differential equation :

$$-u_{xx}(x) = f(x)\;,\; x\in(0,1) \tag{4.12}$$

$$u(0) = 0\;,\; u(1) = 0\;, \tag{4.13}$$

where $f\in C([0,1], I\!R)$

The equation could be written in convervative form :

$div(F) = f$ with $F = -u_x$

Definition 4.1 *Admissible one-dimensional mesh :*
An admissible one-dimensional mesh of $(0,1)$*, denoted by* $\mathcal{T}$ *is given by a family* $(K_i)_{i=1,\dots,N}, N \in I\!N$ *such that* $K_i = (x_{i-1/2}, x_{i+1/2})$ *and a family* $(x_i)_{i=0,\dots,N+1}$ *such that*

$x_0 = x_{1/2} = 0 < x_1 < x_{3/2} < \dots < x_{i-1/2} < x_i < x_{i+1/2} < \dots < x_N < x_{N+1/2} = x_{N+1} = 1$

we have $h_i = m(K_i) = x_{i+1/2} - x_{i-1/2}$.

The discrete unknown are denoted by $u_i, i = 1,\dots,N$ are approximations of u in the cell K_i.

The equation 4.12 is integrated over each cell K_i and yields

$$-u_x(x_{i+1/2}) + u_x(x_{i-1/2}) = \int_{K_i} f(x)\,dx\ ,\ i = 1,\dots N \tag{4.14}$$

The approximations of $-u_x(x_{i+1/2})$ is given with the differential quotient :

$$F_{i+1/2} = -\frac{u_{i+1} - u_i}{h_{i+1/2}} \tag{4.15}$$

where $h_{i+1/2} = x_{i+1} - x_i$.

The linear equation-system is written as :

$$Au = b \tag{4.16}$$

where $u = (u_1,\dots,u_N)^T$ and $b = (b_1,\dots,b_N)^T$.

We have the expression :

$$(Au)_i = \frac{1}{h_i}\left(-\frac{u_{i+1} - u_i}{h_{i+1/2}} + \frac{u_i - u_{i-1}}{h_{i-1/2}}\right) \tag{4.17}$$

$$b_i = \frac{1}{h_i}\int_{K_i} f(x)\,dx \tag{4.18}$$

where $i = 1,\dots,N$.

4.1.5.2 Convergence theorem and error-estimates for the Dirichlet problem

The finite volume error-estimates for the one-dimensional elliptic problem is given as

Theorem 4.2 *Let* $f \in C([0,1], I\!R)$ *and let* $u \in C^2([0,1], I\!R)$ *be the unique solution of problem 4.12.*

Let $\mathcal{T} = (K_i)_{i=1,\ldots,N}$ *be an admissible in the sense of definition 4.1. Then there exists a unique vector* $u = (u_1, \ldots, u_N)^T \in I\!R^N$ *solution to 4.16 and there exists* $C \geq 0$*, only depending on* u*, such that*

$$\sum_{i=0}^{N} \frac{(e_{i+1} - e_i)^2}{h_{i+1/2}} \leq C^2 h^2 \tag{4.19}$$

and $|e_i| \leq Ch$ *,* $\forall i = \{1, \ldots, N\}$
with $e_0 = e_N = 0$ *;* $e_i = u(x_i) - u_i$ *,* $\forall i = \{1, \ldots, N\}$*.*

Proof 4.3 *See the proof in [55].*