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An Overview of Different Models described by Diffusion-Convection-Reaction Equations

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Abstract

Many physical phenomena can be formulated in terms of partial differential equations (PDEs). For this reason it is important to have an overview over typical classes of PDEs. In this thesis, we focus on one special class of PDEs, namely diffusion-convection-reaction equations. Diffusion-convection-reaction equations describe physical phenomena where particles, energy or other physical quantities are transferred inside a physical system. The diffusive part in a diffusion-convection-reaction equation describes a quantity that is undergoing diffusion, i.e., the quantity is "spreading out" from a location at which there is a higher concentration of that quantity. The convective term in diffusion-convection-reaction equations models the movement of the quantity of interest due to a given velocity field. By adding a reaction term, chemical reactions in which substances are transformed into each other can be modeled. Diffusion-convection-reaction equations occur in many different areas such as physics, chemistry or life sciences. In this Bachelor thesis, we will derive suitable mathematical models from physical principles or other considerations. These models can be described by diffusion-convection-reaction equations.

Zusammenfassung

Viele physikalische Gesetze lassen sich mithilfe von partiellen Differentialgleichungen (PDEs) formulieren. Aus diesem Grund ist es wichtig, einen Überblick über typische Klassen von PDEs zu haben. In dieser Bakkalaureatsarbeit steht die Klasse der Diffusions-Konvektions-Reaktionsgleichungen im Fokus. Diffusions-Konvektions-Reaktionsgleichungen beschreiben physikalische Phänomene, in welchen Partikel, Energie oder andere physikalische Größen in einem physikalischen System transportiert werden. Der Diffusionsanteil in Diffusions-Konvektions-Reaktionsgleichungen beschreibt Objekte die einem Diffusionsprozess ausgesetzt sind, d.h. das Objekt breitet sich von einem Ort höherer Konzentration aus zu Orten mit niedrigerer Konzentration des Objekts. Der konvektive Ausdruck modelliert die Bewegung des Objekts. Durch Hinzufügen eines Reaktionsterms können chemische Reaktionen, wo chemische Substanzen ineinander umgewandelt werden, beschrieben werden. Außerdem können viele Problemstellungen von anderen Wissenschaftszweigen, wie z.B. Populationsmodelle oder der Personenfluss modelliert werden. In dieser Bakkalaureatsarbeit leiten wir sämtliche mathematische Modelle aus physikalischen Prinzipen oder anderen Überlegungen her. Diese Modelle können mithilfe von Diffusions-Konvektions-Reaktionsgleichungen beschrieben werden.

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Chapter 1

Introduction

1.1 Motivation

Many processes are dependent on heat or temperature such as metal forming or reaction processes. To have a better understanding of such processes it would be necessary to describe the behaviour of heat or temperature.

Another issue which has gained very much interest since the last few decades is the pollution of our environment. Because environmental pollution affects the health of an animate being in a negative way it would be very interesting to know how certain pollutants behave or, more general, how chemical substances react in our eco-system.

One can also ask: Can the behavior of animate beings be modelled mathematically e.g. to predict the livestock in a certain area or to evacuate people in case of fire?

The answer to these thoughts are "Convection-Diffusion-Reaction equations". With the help of this kind of equations problems like those above can be modelled.
In this thesis ideas will be provided to describe such problems mentioned above.

1.2 Notation

In this thesis the following operators will appear frequently:

Definition 1.1. *(Gradient)*
Let $A \subseteq \mathbb{R}^n$ be an open domain, $f : A \to \mathbb{R}$, $x = (x_1, \dots, x_n) \in A$ and $k \in \{1, \dots, n\}$. The functional f is called partially differentiable with respect to (w.r.t.) x_k in x if the following limit exists:

$$\lim_{t \to 0} \frac{f(x_1, \dots, x_{k-1}, x_k + t, x_{k+1} \dots, x_n) - f(x)}{t} =: \frac{\partial f}{\partial x_k}(x) := \partial_{x_k} f(x)$$

The function $\frac{\partial f}{\partial x_k}(x)$ *is called partial derivative of* f *with respect to* x_k.

If there exist all partial derivatives in x *then* f *is called partially differentiable in* x *and* $(\frac{\partial f}{\partial x_1}(x), \ldots, \frac{\partial f}{\partial x_n}(x))^T$ *is called the* gradient *of* f *in* x.
Notations: grad $f(x)$ *or* $\nabla f(x)$

Definition 1.2. *(Divergence)*
Let $A \subseteq \mathbb{R}^3$ *be an open domain and let* $F : A \to \mathbb{R}^3$ *be a sufficiently smooth vector field.*
Then the divergence *of* F *is defined as:*

$$\nabla \cdot F := \operatorname{div}(F) := \sum_{i=1}^{3} \frac{\partial F_i}{\partial x_i}$$

Definition 1.3. *(Laplacian)*
Let $A \subseteq \mathbb{R}^3$ *be an open domain and let* $F : A \to \mathbb{R}$ *be a sufficiently smooth scalar field.*
Then the Laplacian *of* F *is defined as:*

$$\Delta F := \nabla^2(F) := \operatorname{div}(\text{grad } F) := \nabla \cdot (\nabla F) := \sum_{i=1}^{3} \frac{\partial^2 F}{\partial x_i^2}$$

Definition 1.4. *Let* $M \subseteq \mathbb{R}^d$, $d \in \{1, 2, 3\}$ *be an arbitrary set. Throughout this thesis we say that a property* P *holds* almost everywhere *or* for almost all $x \in M$ *iff there are only countably many elements in* M *for which* P *does not hold.*
Notation: $\dot{\forall}$

1.3 Prototype

A generic example of a diffusion-convection-reaction equation is given by

$$\frac{\partial u}{\partial t} - \operatorname{div}(a(u)\nabla u) + b(u) \cdot \nabla u + c(u) = f \tag{1.1}$$

where a denotes the diffusion term, b denotes the convection term and c the reaction term. The right hand side f describes ”sources” or ”sinks” of u which is the variable of interest. All terms may depend on u. In this case the differential equation is nonlinear.

Remark 1.5. *Note that (1.1) is an example of an instationary equation. In the stationary case the term* $\frac{\partial u}{\partial t}$ *vanishes.*

Chapter 2

Derivation of thermodynamic equations

In this chapter we derive the thermodynamic equations. First, we derive the general heat conduction and heat transport equation based on the physical law of conservation of energy, then this equation will be reduced to some specific cases. For all these cases a homogeneous material is assumed.
Before we start with the mathematical theory it would be helpful to introduce the physical quantities that are used and the required physical laws:

Physical quantity	Unit	Description
c	$\frac{J}{kg \cdot K}$	specific heat capacity
ρ	$\frac{kg}{m^3}$	mass density
$\Lambda = (\lambda_{ij})_{i,j=\overline{1,3}}$	$\frac{W}{m \cdot K}$	heat conductivity
q		proportionality factor of a chemical reaction
σ	$\frac{W}{m^2}$	heat flow

Remark 2.1. *The entries in Λ describe the conductivity of a certain material and are determined experimentally.*
The heat conduction tensor Λ is symmetric, i.e.,

$$\Lambda(x) = \Lambda^T(x) \qquad \dot{\forall} x \in \Omega$$

and uniformly elliptic, i.e.,

$$\exists \underline{\lambda}, \overline{\lambda} = const. > 0 : \underline{\lambda} ||\xi||^2_{\mathbb{R}^3} \leq (\Lambda(x)\xi, \xi)_{\mathbb{R}^3} \leq \overline{\lambda} ||\xi||^2_{\mathbb{R}^3} \qquad \xi = (\xi_1, \xi_2, \xi_3)^T \in \mathbb{R}^3, \ \dot{\forall} x \in \Omega.$$

If the considered material is isotropic then

$$\Lambda(x) = \lambda(x) I$$

where I is the identity matrix.

Additionally, the following physical laws are needed to derive the heat conduction and heat transport equation:

1. *Fourier's first law of conduction*: $\sigma = -\Lambda \nabla u$
   This law says that the heat flow is equal to the product of the heat conductivity Λ and the negative temperature gradient $-\nabla u$. The negative gradient $-\nabla u$ denotes the direction of the steepest descent of the temperature, which means that heat flows from regions of high temperature to low temperature.

2. *Law of conservation of energy*:
   This law says that the total energy of an isolated system remains constant, i.e., energy can be neither created nor destroyed, but one form of energy can be transformed into another form of energy.

2.1 Preliminaries

The following results will be useful for the derivation of the heat conduction and heat transport theorem:

Theorem 2.2. *Let $f, g : [a, b] \to \mathbb{R}$ be continuous and $g \geq 0$.*
Then there exists $\xi \in [a, b]$ with:

$$\int_a^b f(x)g(x)dx = f(\xi) \int_a^b g(x)dx.$$

This theorem is called the mean value theorem of integral calculus and a proof can be found in [5] (Theorem 7.19).

The theorem of Gauss is also needed to derive the thermodynamic equations:

Theorem 2.3. *Let $\Omega \subset \mathbb{R}^n$ be a compact domain with sufficiently smooth boundary $\partial\Omega$, n the outer normal vector on $\partial\Omega$ and let F be a continuously differentiable vector field on Ω. Then*

$$\int_\Omega \operatorname{div}(F)dx = \int_{\partial\Omega} F \cdot n \, dS_x.$$

For a proof of Theorem 2.2 see [7] (Theorem 3.5.5)

The third important theorem to derive the heat conduction and heat transport equation is Reynolds transport theorem [12]:

Theorem 2.4. *Let $t_0 \in (T_1, T_2)$ where (T_1, T_2) is the time interval where the particles are considered and t_0 is a fixed reference point in time. Let $G(t_0) \subset \Omega(t_0)$ be a bounded domain with Lipschitz smooth boundary and $\overline{G(t_0)} \subset \Omega(t_0)$. Let*

$$v : Q \to \mathbb{R}^d \text{ and } F : Q \to \mathbb{R}$$

be continuously differentiable with $Q := \{(x,t) \in \mathbb{R}^{d+1} : x \in \Omega(t), t \in (T_1, T_2)\}$. Let $\mathcal{F}(t) := \int_{G(t)} F(x,t)dx$ with $G(t) := \{\varphi(X,t) : X \in G(t_0)\}$.
Then $\mathcal{F}$ is well defined, continuously differentiable within an interval $(t_1, t_2) \subset (T_1, T_2)$ and

$$\frac{d\mathcal{F}}{dt}(t) = \int_{G(t)} [\frac{\partial F}{\partial t}(x,t) + \text{div}_x(Fv)(x,t)]dx$$

holds, where

$$\text{div}_x(Fv) = \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(Fv_i) = (\nabla_x F) \cdot v + \text{div}_x(v)F$$

2.2 Derivation of the heat conduction and heat transport equation

Consider a moving medium, e.g., a specific fluid. In order to obtain a temperature field, we have to take into account the heat conduction, the heat transport due to the moving physical particles and the possibly additionally produced heat (external or internal due to, e.g., chemical reactions).

For that purpose consider an arbitrary Lipschitz domain $G(t) \subset \bar{\Omega} \subset \mathbb{R}^3$ moving through a velocity field $v = \vec{v}(x,t) = (v_1(x,t), v_2(x,t), v_3(x,t))^T$ during a time interval $\Delta t = [t_1, t_2] \subseteq [0, T]$ where $t_1 = t - \frac{\Delta t}{2}, t_2 = t + \frac{\Delta t}{2}$

With the physical law of conservation of energy we get the informal equation

-	Amount of energy, which flow out on $\partial G(t)$ during the time interval Δt	+	Amount of energy produced in $G(t)$ during the time interval Δt	=	Difference in the amount of heat in $G(t)$ between time t_1 and time t_2	.

Interpreting this scheme mathematically, we obtain the balance equation

$$-\int_{t_1}^{t_2} \int_{\partial G(t)} \sigma(x,t) \cdot n(x) dS_x dt + \int_{t_1}^{t_2} \int_{G(t)} [f(x,t) - qu(x,t)]dxdt = \int_{G(t_2)} c\rho u(x,t_2) - \int_{G(t_1)} c\rho u(x,t_1) \quad (2.1)$$

of the heat conduction and heat transport problem.
Together with Fourier's first law of conduction, $\sigma(x,t) = -\Lambda(x,t)\nabla u(x,t)$, the equation can be rewritten as

$$\int_{t_1}^{t_2}\int_{\partial G}(\Lambda(x,t)\nabla u(x,t))\cdot n(x)dS_x dt + \int_{t_1}^{t_2}\int_{G(t)}[f(x,t) - q(x,t)u(x,t)]dxdt = \int_{G(t_2)} c(x)\rho(x)u(x,t_2) - \int_{G(t_1)} c(x)\rho(x)u(x,t_1). \quad (2.2)$$

Now we introduce the function

$$W(t) := \int_{G(t)} c(x)\rho(x)u(x,t)dx = \int_{G(t)} w(x,t)dx, \quad (2.3)$$

which denotes the amount of heat in G(t) at time t.

We make the following assumptions:

Assumption 1.

1. $\Lambda\nabla u, c\rho u \in C^1(G(t))$,
   $f, qu \in C(G(t))$.
2. c, ρ are const.
3. the fluid is incompressible, i.e., $\mathrm{div}_x(v) = 0$.

Under Assumption 1(1), the limit $\lim\limits_{\Delta t\to 0}\frac{1}{\Delta t}$ (2.2) exists and (2.2) can be simplified to

$$\int_{\partial G(t)} \Lambda(x,t)\nabla u(x,t)\cdot n(x)dS_x + \int_{G(t)}[f(x,t) - q(x,t)u(x,t)]dx = \frac{d}{dt}W(t). \quad (2.4)$$

With Gauss' theorem we get in the left hand side

$$\int_{\partial G} \Lambda(x,t)\nabla u(x,t)\cdot n(x)dS_x = \int_{G(t)} \mathrm{div}(\Lambda(x,t)\nabla u(x,t))dx \quad (2.5)$$

and with the help of Reynolds' transport theorem on the right hand side

$$\frac{d}{dt}W(t) = \int_{G(t)}[\frac{\partial w}{\partial t}(x,t) + \mathrm{div}_x(w\vec{v})(x,t)]dx. \quad (2.6)$$

By Assumption 1(2) it follows from (2.6) together with (2.3) that

$$\frac{d}{dt}W(t) = \int_{G(t)}[c\rho\frac{\partial u}{\partial t}(x,t) + c\rho\cdot\mathrm{div}_x(u\vec{v})(x,t)]dx. \quad (2.7)$$

Assumption 1(3) yields that $\mathrm{div}_x(u\vec{v}) = v_1\frac{\partial u_1}{\partial x_1} + v_2\frac{\partial u_2}{\partial x_2} + v_3\frac{\partial u_3}{\partial x_3} + u\cdot\underbrace{\mathrm{div}_x v}_{=0} = v\cdot\nabla u$.

Before we go further consider the following theorem:

Lemma 2.5. *Let* $\Omega \subset \mathbb{R}^3$ *be open,* $g \in C(\Omega)$*, and suppose that*

$$\int_G g(x)dx = 0$$

for all $G \subset \Omega$.
Then

$$g(x) = 0 \qquad \forall x \in \Omega.$$

Proof. Suppose there exists an $x \in \Omega$ such that

$$g(x) \neq 0$$
$$W.l.o.g : g(x) > 0$$

Due to continuity there exists a set $U_x \subset \Omega$ of x with

$$g(\xi) > 0 \qquad \forall \xi \in U_x.$$

Then with the choice $G = U_x$, we get

$$\int_{G=U_x} g(\xi)\, d\xi > 0,$$

which is the desired contradiction. □

Now by applying Lemma 2.5 to $g(x) := c\rho \frac{\partial u}{\partial t}(x,t) - \mathrm{div}_x(\Lambda \nabla u)(x,t) + c\rho v \cdot \nabla u(x,t) + qu(x,t) - f(x,t)$ for a fixed t we immediately obtain the differential form of the heat conduction and heat transport equation

$$c\rho \frac{\partial u}{\partial t}(x,t) - \mathrm{div}_x(\Lambda \nabla u)(x,t) + c\rho v \cdot \nabla u(x,t) + qu(x,t) = f(x,t) \text{ in } Q_T = \Omega \times (0,T). \tag{2.8}$$

Remark 2.6. *Note that (2.8) is of the form (1.1).*

Now the corresponding heat conduction and heat transport problem in a divergence free and continuously differentiable velocity field can be formulated as initial-boundary value problem as follows:

Find: Temperature field $u \in \mathcal{X} := C^{2,1}(Q_T) \cap C(\overline{Q}_T) \cap C^1((\Omega \cup \Gamma_2 \cup \Gamma_3) \times (0,T))$

$$c\rho \frac{\partial u}{\partial t}(x,t) - \mathrm{div}_x(\Lambda \nabla u)(x,t) + c\rho v \cdot \nabla u(x,t) + qu(x,t) = f(x,t) \text{ in } Q_T = \Omega \times (0,T)$$

with bounday conditions

$$\begin{aligned} u(x,t) &= g_1(x,t)\ \forall (x,t) \in \Gamma_1 \times (0,T) \\ -\frac{\partial u}{\partial N}(x,t) &= g_2(x,t)\ \forall (x,t) \in \Gamma_2 \times (0,T) \\ -\frac{\partial u}{\partial N}(x,t) &= \alpha(u(x,t) - g_3(x,t))\ \forall (x,t) \in \Gamma_3 \times (0,T) \end{aligned}$$

and inital condition

$$u(x,0) = u_0(x)\ \forall x \in \overline{\Omega}$$

Remark 2.7. *The term* $\frac{\partial u}{\partial N}(x,t) := (\Lambda \nabla u)(x,t) \cdot n(x)$ *is called conormal derivative.*

Remark 2.8. *The term* $q(x,t)u(x,t)$ *is a reaction term which occurs often to model chemical reactions.*

Remark 2.9. *If* $v = 0$ *we obtain from* (2.8) *the unsteady heat conduction equation*

$$c\rho \frac{\partial u}{\partial t}(x,t) - \mathrm{div}_x(\Lambda \nabla u)(x,t) + qu(x,t) = f(x,t) \text{ in } Q_T = \Omega \times (0,T)$$

Chapter 3

Dispersal of Pollutants

In this chapter a description of how the dispersal of pollutants can be mathematically modelled by convection and diffusion will be given. This chapter is based on [6].

This can be done with the help of Fick's first law. It postulates that flow goes from regions of high concentration to regions of low concentration. It can be formally written as:

$$J = -D\nabla c \tag{3.1}$$

where

Physical quantity	Unit	Description
J	$\frac{mol}{m^2 \cdot s}$	Diffusion flow
D	$\frac{m^2}{s}$	Diffusion matrix (respectively: coefficient)
c	$\frac{mol}{m^3}$	Concentration
x	m	Position

Remark 3.1. *Diffusion is a natural physical process to compensate for concentration differences. Molecules or atoms move from regions of high concentration to regions of low concentration.*
The media in which the diffusion process in this chapter happens is air which is assumed to be homogeneous and isotropic. So, D is usually assumed to be constant.
The entries in D will be experimentally defined.

For better understanding consider the following simplified situation:
Assume there is an industrial plant emitting noxious fumes. Also suppose that the plant emits a very concentrated batch of these offensive fumes for a few minutes and then stops. A mile away there is a beautiful house you would like to buy. Assume that the wind is blowing in the direction of that house. Now you can ask yourself, what the maximum concentration of the fumes will be at the house you would like to buy.
There are two processes at work here: convection and diffusion. To simplify this illustration further suppose the wind has fixed velocity v and the density of the fumes can

be described by a distribution given by $c_0(x)$ at time $t = 0$.

From this introductory example, if the inner production of pollutants is ignored, the following balance equation, a convection-diffusion equation can be deduced:
For this purpose let $\Omega \subset \mathbb{R}^2$ be sufficiently large at a fixed height above the earth's surface such that the noxius concentration vanishes on the boundary and let G(t) be an arbitrary subdomain of Ω in the noxious fume cone. Then the flow leaving $G(t)$ through the boundary during a time interval (t_1, t_2) must be equal to the difference of the concentration in t_1 and t_2,

$$\int_{G(t_2)} c(x,t_2)dx - \int_{G(t_1)} c(x,t_1)dx = -\int_{t_1}^{t_2} \int_{\partial G(t)} J(x,t) \cdot \vec{n}(x)\, dS_x dt$$

With Fick's law of diffusion (3.1) we obtain

$$\int_{G(t_2)} c(x,t_2)dx - \int_{G(t_1)} c(x,t_1)dx = \int_{t_1}^{t_2} \int_{\partial G(t)} D(x,t)\nabla c(x,t) \cdot \vec{n}(x)\, dS_x dt.$$

Finally with Gauss' theorem (Theorem 2.3), the transport theorem (Theorem 2.4) and Theorem 2.5 we obtain analogously to the derivation of the heat conduction and heat transport equation in Chapter 2 the differential form

$$\frac{\partial c}{\partial t}(x,t) - \mathrm{div}_x(D\nabla c)(x,t) + \mathrm{div}_x(\vec{v}c)(x,t) = 0 \qquad \forall x \in \Omega\ \forall t \in (0,T). \tag{3.2}$$

Remark 3.2. *Note that (3.2) is of the form (1.1).*

As already mentioned above the considered domain Ω is chosen sufficiently large such that the concentraction c can be assumed to vanish on the boundary. Finally we can formulate the problem to get the distribution of the concentration c in the domain Ω.

Find: Concentration field $c \in \mathcal{X} := C^{2,1}(Q_T) \cap C(\overline{Q}_T)$

$$\frac{\partial c}{\partial t}(x,t) - \mathrm{div}_x(D\nabla c)(x,t) + \mathrm{div}_x(\vec{v}c)(x,t) = 0 \text{ in } Q_T = \Omega \times (0,T)$$

with bounday conditions

$$c(x,t) = 0 \qquad \forall (x,t) \in \partial\Omega \times (0,T)$$

and inital value

$$c(x,0) = c_0(x) \qquad \forall x \in \overline{\Omega}$$

A very interesting special case is obtained if diffusion is ignored and a horizontal wind velocity is assumed. For further simplicity the direction of the wind is assumed to be fixed, say in the x-direction $\vec{v} = (V(x), 0, 0)$. Then (3.2) reduces to the convection-equation

$$\frac{\partial c}{\partial t} + \frac{\partial (Vc)}{\partial x} = 0. \tag{3.3}$$

Additionally the concentration at $t = 0$ is

$$c(x, 0) = c_0(x), \qquad x \in \mathbb{R}.$$

To solve (3.3) we rewrite it in the form:

$$\frac{\partial c}{\partial t} + V\frac{\partial c}{\partial x} = -\frac{\partial V}{\partial x}c =: f \qquad \forall (x,t) \in Q_T \tag{3.4}$$

and assume that V is continuously differentiable.

It can be observed that $(V, 1)$ is a direction field in $\mathbb{R}^2$. The left hand side of (3.4) defines the directional derivative in (x, t) in the direction $(V, 1)$:

$$\frac{\partial c}{\partial t} + V\frac{\partial c}{\partial x} = (V, 1) \cdot \nabla_{(x,t)}c = \frac{d}{d(V,1)}c$$

where $\frac{d}{d(V,1)}c$ denotes the total derivative.

This idea results in a solution finding process: Suppose we have a curve C with tangent $(V, 1)$. For this purpose let C be parameterised as $C := \{(x(r), t(r)), r > 0\}$.
Then

$$\begin{aligned} &\frac{d}{dr}t(r) = 1 \\ &\frac{d}{dr}x(r) = V(x(r)). \end{aligned} \tag{3.5}$$

Theorem 3.3. *Let c(x, t) be a solution of (3.3) and (x(r), t(r)) defined as in (3.5). Then z(r):= c(x(r),t(r)) solves*

$$\frac{d}{dr}z(r) = -\frac{\partial V}{\partial x}(x(r))z(r) \qquad \text{on } C. \tag{3.6}$$

Proof.

$$\begin{aligned} \frac{dz}{dr} = \frac{d}{dr}c(x(r), t(r)) &= (\nabla_{(x,t)}c)(x(r), t(r)).(x'(r), t'(r)) \\ &= (\nabla_{(x,t)}c)(x(r), t(r)).(V(x(r)), 1) \\ &= -\frac{\partial V}{\partial x}(x(r))c(x(r), t(r)) \\ &= -\frac{\partial V}{\partial x}(x(r))z(r) \end{aligned}$$

□

With these preliminaries we can solve (3.3) with the "Method of characteristics for PDEs" in two steps.

Definition 3.4. *The set of curves (x(r), t(r)) defined as in (3.5) are called* charac-teristic curves *for (3.3).*

First we have to solve the equations in (3.5).
The first equation in (3.5) has the solution $t(r) = r + k$, where k denotes a constant. Using the initial condition $t(0) = 0$, we get $t(r) = r$.
In this specific case we have only the equation

$$\frac{d}{dt}x = V(x) \qquad \text{on } C$$

with the initial condition

$$x(0) = x_0$$

to solve. Denote the solution of the IVP above by $x(t; x_0)$, which determines a unique curve passing through the point $(x_0, 0)$.

Second, if we are given $c(x, t)$ as a solution of (3.3), then

$$\frac{d}{dr}c(x(r), t(r)) = -\frac{\partial V}{\partial x}(x(r))c(x(r), t(r)) \text{ on } C$$

which is equal to

$$\frac{d}{dt}c(x(t; x_0), t) = -\frac{\partial V}{\partial x}(x(t; x_0))c(x(t; x_0), t)$$

or

$$\frac{d}{dt}ln(c(x(t; x_0), t)) = -\frac{\partial V}{\partial x}(x(t; x_0)) \tag{3.7}$$

From (3.7) it follows that

$$c(x(t; x_0), t) = c_0(x_0)\text{exp}[-\int_0^t \frac{\partial V}{\partial x}(x(s; x_0))\, ds]$$

is a solution of (3.3).

Remark 3.5. *The "Method of characteristics" can be generalized and applied to all types of partial differential equations of first order and this method is also applicable for equations of higher dimensions. See [9].*

Chapter 4

Chemical reactions

This chapter is based on [11] and [4].
In this chapter we will look at irreversible competitive-consecutive chemical reactions of the form

$$\begin{aligned} A + B &\xrightarrow{k_1} R, \\ B + R &\xrightarrow{k_2} S \end{aligned} \tag{4.1}$$

in a domain $\Omega := [0,1]\times[0,1]$, where A and B are completely segregated reactants with concentrations a and b, respectively, R and S denote the desired product and the waste, with the concentrations r and s, respectively. The parameters k_1 and k_2 represent the reaction rates, i.e., the speeds the reactions take place. Competitive means that a substance reacts simultaneously and gives two different products whereas consecutive means that the product of a reaction is the initial material for another reaction.
The goal of this chapter is to derive a suitable mathematical model for this type of reactions.

For this purpose, we assume that the change of product in time corresponds to the number of collisions between two molecules, multiplied by the probability that a reaction happens between these molecules in case of a collision. For discrete time steps we obtain for our system (4.1) for the concentraction differences

$$\begin{aligned} \Delta a &= -k_1 ab\Delta t \\ \Delta b &= -k_1 ab\Delta t - k_2 br\Delta t \\ \Delta r &= k_1 ab\Delta t - k_2 br\Delta t \\ \Delta s &= k_2 br\Delta t \end{aligned}$$

with $k_1 = q_1 p_1$ and $k_2 = q_2 p_2$ where $q_1 ab\Delta t$ and $q_1 br\Delta t$ denote the number of collisions in Δt and p_1, p_2 represent the probabilities that a reaction happens in case of a collision.

Dividing that system by Δt and with $\Delta t \to 0$ we finally get the system of differential equations

$$\begin{aligned}
\frac{\partial a}{\partial t} &= -k_1 ab \\
\frac{\partial b}{\partial t} &= -k_1 ab - k_2 br \\
\frac{\partial r}{\partial t} &= k_1 ab - k_2 br \\
\frac{\partial s}{\partial t} &= k_2 br
\end{aligned}$$

for (4.1).
If we consider these reaction processes in a velocity field we can add a convection term $u \cdot \nabla c$, furthermore if we also account diffusion of the reactants, we can add another additional term, a diffusion term $\mathcal{P}^{-1}\Delta c$ to the system of differential equations above. Then we obtain

$$\frac{\partial c}{\partial t} - \mathcal{P}^{-1}\Delta c + u \cdot \nabla c + k(c) = 0 \tag{4.2}$$

for a chemical system of the form (4.1) where

$$c := \begin{pmatrix} a \\ b \\ r \\ s \end{pmatrix}$$

and a non-linear reaction term

$$k(c) := \begin{pmatrix} -k_1 ab \\ -k_1 ab - k_2 br \\ k_1 ab - k_2 br \\ k_2 br \end{pmatrix}$$

occurs. The parameter $\mathcal{P}$ is called Péclet number which is the ratio of the rate of advection of the concentraction to the rate of diffusion of the concentration. The Péclet number is a dimensionless parameter.

Remark 4.1. *Note that (4.2) is of the form (1.1).*

Since the reactants are segregated at the beginning we can choose the initial conditions for (4.2) in a specific way. The fluid motion takes place in a square box. We assume that the sides $x = 0$ and $x = 1$ are identified with one another such that fluid escaping from the unit square through one side reenters through the other. The same holds for the sides $y = 0$ and $y = 1$. Then we can assume periodic boundary conditions.

Now we can formulate the problem to get the concentraction field c of the reactants in the domain Ω in the time interval $(0, T)$.

Find: Concentration field $c \in \mathcal{X} := C^{2,1}(Q_T) \cap C(\overline{Q}_T)$

$$\frac{\partial c}{\partial t}(x,t) - \mathcal{P}^{-1}\Delta c(x,t) + u \cdot \nabla c(x,t) + k(c(x,t)) = 0 \text{ in } Q_T = \Omega \times (0,T)$$

with inital values

$$\begin{aligned} a(x,y,0) &= \begin{cases} a_0(x,y) & 0 \le x < \frac{1}{2} \\ 0 & \frac{1}{2} \le x < 1 \end{cases} \\ b(x,y,0) &= \begin{cases} 0 & 0 \le x < \frac{1}{2} \\ b_0(x,y) & \frac{1}{2} \le x < 1 \end{cases} \\ r(x,y,0) &= 0 \\ s(x,y,0) &= 0 \\ \forall (x,y) &\in \overline{\Omega} \end{aligned}$$

and periodic boundary conditions

$$\begin{aligned} c(0,y,t) &= c(1,y,t) \qquad \forall (y,t) \in [0,1] \times (0,T) \\ c(x,0,t) &= c(x,1,t) \qquad \forall (x,t) \in [0,1] \times (0,T). \end{aligned}$$

Remark 4.2. *The considerations above can be adapted to reversible chemical reactions, i.e., to chemical reactions of the form*

$$A + B \underset{k_1^-}{\overset{k_1^+}{\rightleftharpoons}} R,$$

$$B + R \underset{k_2^-}{\overset{k_2^+}{\rightleftharpoons}} S.$$

Then we get a similar system of differential equations.

Chapter 5

Population models

This chapter is based on [14].

In this chapter we will have a look at a special application of reaction-diffusion equations, namely deterministic and continuous population models.

Population models are very important in ecology and economy e.g. to describe predator-prey and competition interactions. The population can be affected by certain processes such as birth, death, movement to another position, etc.

Before we can start with the population models let us define population.

Definition 5.1. *(Population)*
A group of elements, individuals, or units that share one or more characteristics from which data can be gathered and analysed is called a population. The total of all populations is called a universe.

Throughout this chapter let $u(t)$ be the population number of a certain species at time $t \geq 0$.

5.1 Population of one species

Exponential growth model

In the exponential growth model we have that the growth rate depends on the size of the population. As an introductory illustration consider the discrete case. For this purpose let u_t be the size of a certain population at time t and let u_{t+1} be the size of the population at the next time step $t+1$. Additionally let a be the effective growth rate of the population and Δt be the time step between t and $t+1$. The variable a is typically a positive number.
Then we get

$$u_{t+1} = (1 + a\Delta t)u_t.$$

If we do some further steps we get

$$\begin{aligned} u_1 &= (1 + a\Delta t)u_0 \\ u_2 &= (1 + a\Delta t)u_1 = (1 + a\Delta t)(1 + a\Delta t)u_0 \\ u_3 &= (1 + a\Delta t)u_2 = (1 + a\Delta t)(1 + a\Delta t)(1 + a\Delta t)u_0 \\ &\dots \end{aligned}$$

We observe that we obtain for the considered population the formula

$$u_t = (1 + a\Delta t)^t u_0$$

after t time-steps.
The exponential growth can be graphically illustrated:

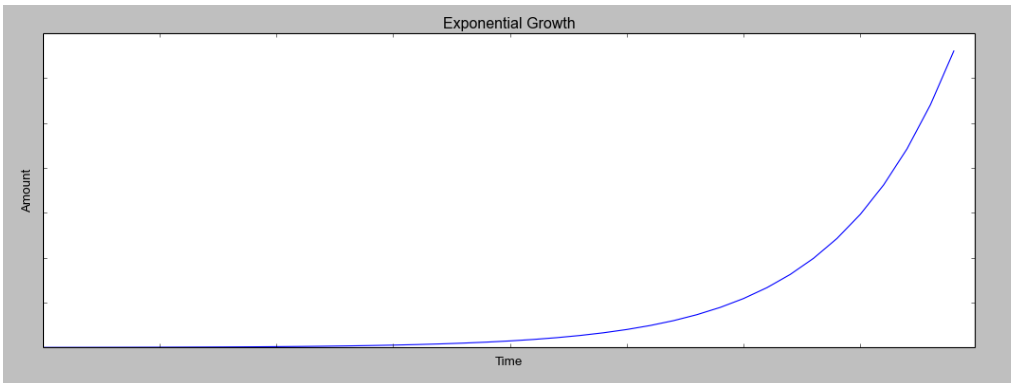

Figure 5.1: Exponential growth function

The equation

$$u_{t+1} = u_t + a\Delta t u_t$$

is equivalent to

$$u_{t+1} - u_t = a\Delta t u_t.$$

Now by dividing this equation by Δt and with $\lim\limits_{\Delta t \to 0}$, we obtain the ordinary differential equation

$$\frac{du}{dt} = au \qquad \text{with } t > 0,\ u(0) = u_0. \tag{5.1}$$

Remark 5.2. *Note that (5.1) is of the form (1.1). In (5.1) only the reaction term does not vanish.*

Examples for processes which can be modelled with exponential growth are world population, water consumption all over the world, debits.

Solutions of (5.1) model unlimited exponential growth. This case does not represent the reality because unlimited environmental resources are assumed in this case.

To get a more realistic model, a self-limiting term can be introduced. This leads to the logistic-growth model.

Logistic-growth model

The differential equation of this model can be stated as

$$\frac{du}{dt} = u(a - bu) \qquad \text{with } t > 0,\ u(0) = u_0 \tag{5.2}$$

where $b > 0$ is a measure of the environment capacity.

Now let us solve equation (5.2). This can be done by separation of variables. The we get

$$\frac{1}{u(a - bu)} du = dt. \tag{5.3}$$

With the partial fraction decomposition we obtain

$$\frac{1}{u(a - bu)} = \frac{1}{au} + \frac{b}{(a - bu)a} = \frac{1}{a}(\frac{1}{u} + \frac{b}{(a - bu)}).$$

Now by bringing the a to the left hand side (5.3) changes to

$$a\ dt = \frac{1}{u}\frac{b}{(a - bu)}du.$$

Integrating both sides we get

$$at + \tilde{C} = ln(\frac{u}{(a - bu)}).$$

By applying the exponential function and computing the reciprocal and setting $\tilde{C}^{-1} := C$ we obtain

$$u(t) = \frac{a}{Ce^{-at} + b}. \tag{5.4}$$

When we integrate the initial value $u(0) = u_0$ (5.4) changes to the solution of the differential equation

$$u(t) = \frac{au_0}{(a - u_0 b)e^{-at} + bu_0}.$$

It can be observed that $u(t)$ converges to $\frac{a}{b}$ as $t \to \infty$.

5.2 Population of two species

In this section let $v(t)$ be the size of a second population. In a logistic-growth approach we get

$$\frac{du}{dt} = u(a_1 - b_1 u)$$
$$\frac{dv}{dt} = v(a_2 - c_2 v)$$

for $t > 0$.

The terms $b_1 \geq 0$ and $c_2 \geq 0$ are called the intraspecific competition constants. In this situation, the populations are evolving independently from each other. When the species are interacting, we add competition terms proportional to the population numbers and obtain

$$\frac{du}{dt} = u(a_1 - b_1 u - c_1 v)$$
$$\frac{dv}{dt} = v(a_2 - c_2 v - b_2 u)$$

for $t > 0$.
The newly introduced coefficients c_1 and b_2 model inter-specific competition or benefit, depending on their sign.

Predator-prey model

Suppose that $c_1 > 0$ and $b_2 < 0$. In this case the growth rate of u decreases and the growth rate of v increases. Hence v represents the predator species and u is the prey.

An interesting predator-prey model is obtained when the intraspecific competition vanishes, i.e., $b_1 = c_2 = 0$. For this setting we get

$$\begin{aligned}\frac{du}{dt} &= u(a_1 - c_1 v)\\ \frac{dv}{dt} &= -v(\alpha - \beta u)\end{aligned} \tag{5.5}$$

for $t > 0$.
In this special case $\alpha := -a_2 > 0$ and $\beta := -b_2 > 0$.
This assumption means that the predator species will become extinct in the absence of the prey, because then $dv/dt = -\alpha v$. This system is well-known as Lotka-Volterra

model.
Now we will derive a first integral F of that system, i.e., a function such that

$$\frac{d}{dt}F(u(t), v(t)) = 0 \tag{5.6}$$

for all solutions (u, v) of the system (5.5). This means that the solution is time independent or in a steady-state.
First multiply the first equation with β, the second equation with c_1 and add the two obtained equations, so we get

$$\beta\frac{du}{dt} + c_1\frac{dv}{dt} = \beta u(a_1 - c_1 v) - vc_1(\alpha - \beta u). \tag{5.7}$$

By multiplying $\frac{\alpha}{u}$ to the first equation in (5.5) and $\frac{a_1}{v}$ to the second equation in (5.5) and then adding these equations again we get

$$\frac{\alpha}{u}\frac{du}{dt} = \alpha(a_1 - c_1 v)$$

and

$$\frac{a_1}{v}\frac{dv}{dt} = -a_1(\alpha - \beta u).$$

If we add these two equations and then subtract that sum from (5.7) we obtain the equation

$$c_1\frac{dv}{dt} - \frac{a_1}{v}\frac{dv}{dt} + \beta\frac{du}{dt} - \frac{\alpha}{u}\frac{du}{dt} = 0.$$

Finally integrating over t will result in

$$F(u, v) = c_1 v - a_1 ln(v) + \beta u - \alpha ln(u) = const.$$

or

$$F(u, v) = c_1 v + \beta u - ln(u^\alpha v^{a_1}) = const. \tag{5.8}$$

With this first integral we can find non-constant solutions of the predator-prey system above in the following way:
Given the initial populations $u(0), v(0)$ we can compute the constant $F(u(0), v(0))$ in (5.8). Equation (5.6) yields that $F(u(t), v(t)) = F(u(0), v(0))$. Thus, given one of the populations u or v at time t, it is possible to deduce the other from equation (5.8).

Competition model

Now $c_1 > 0$ and $b_2 > 0$. The growth rates of both species decrease. This can be interpreted that both species are competing for the resources which could be food or living space.

Mutualistic (symbiotic) model

Finally consider the case $c_1 < 0$ and $b_2 < 0$. Both growth rates increase which means that the species benefit from each other.

So far we have considered populations which are spatially homogeneous. In a spatially heterogeneous environment, the population density will depend on space. In the next considerations it is assumed that populations tend to move to regions with smaller number density. For single-species populations $u(x,t) \in \mathbb{R}$ the equation

$$u_t - d\Delta u = uf(x,u), \qquad \text{with } x \in \Omega, t > 0, u(x,0) = u_0$$

for a bounded domain $\Omega \subset \mathbb{R}^n$ can be deduced.

For multiple species we get vector-valued equations of the form

$$u_t - \Delta(Du) = g(x,u), \qquad \text{with } x \in \Omega, t > 0, u(x,0) = u_0$$

where $u \in \mathbb{R}^m$ is a vector-valued function, $D = diag(d_1, \dots d_m)$ is a diagonal matrix with constant coefficients and $g = (g_i) : \Omega \times \mathbb{R}^m \to \mathbb{R}^m$ $(m > 1)$.

Remark 5.3. *Just a few notes on the boundary values of the population models. Dirichlet and Neumann boundary conditions on $\partial\Omega$ are justified.*
In case of spatially homogeneous models, often homogeneous Dirichlet boundary conditions $u = 0$ are taken which should express a hostile area at the boundary but also homogeneous Neumann boundary conditions $\nabla u \cdot \vec{n}$ are taken which means that no migration occurs.

Chapter 6

Pedestrian flow models

6.1 Preliminaries

In this chapter we will look at another application of "diffusion-convection-reaction equations", the flow of large crowds of pedestrians since this topic is likely to become very important. This issue has aroused interest of many scientists especially in the last three decades.
Before we go further in this topic, first recall the well known physical law of conservation of mass which says that for any system closed to all transfers of matter and energy, the mass remains the same over time.
Next, we will take a look at the Lagrangian and Eulerian specification of the flow field.

Lagrangian specification of a flow field:
The Lagrangian specification of a flow field is a way of looking at fluid motion where the observer follows an individual particle through space and time. Considering each position of an individual particle through time gives the pathline of that particle. This can be seen as sitting in a boat and following a particle down a river.

To formalize the previous statement let for this purpose $(T_1, T_2) \subset \mathbb{R}$ the time interval, in which die movement of the fluid is traced. Let $\Omega(t) \subset \mathbb{R}$ be the domain at time $t \in (T_1, T_2)$ and let $t_0 \in [T_1, T_2]$ a fixed reference time point and let $X \in \Omega(t_0)$ the space-coordinate of a fluid particle at time t_0.
Then the pathline of a fluid particle can be written as bijective map

$$\begin{aligned} \varphi : \Omega(t_0) \times (T_1, T_2) \to \Omega(t), \\ (X, t) \mapsto \varphi(X, t) \end{aligned}$$

where $(X, t) \in \Omega(t_0) \times (T_1, T_2)$ are the so-called Lagrangian coordinates. In the Lagrangian specification of a flow field position $\hat{x}$, velocity $\hat{v}$ and acceleration $\hat{a}$ are given by φ and the derivatives of it, which means that

$$\begin{aligned}\hat{x}(X,t) &= \varphi(X,t),\\ \hat{v}(X,t) &= \frac{\partial\varphi(X,t)}{\partial t},\\ \hat{a}(X,t) &= \frac{\partial^2\varphi(X,t)}{\partial t^2}.\end{aligned}$$

Eulerian specification of a flow field:

The Eulerian specification of a flow field is a way of looking at fluid motion that focuses on specific locations in space through which the fluid flow as time passes. This can be seen as sitting on a bank and measuring the velocity of the particles passing through a fixed location.

This informal description can be formalized. For this purpose let (T_1, T_2) be as in the Lagrangian specification, $(x,t) \in Q := \{(x,t) \in \mathbb{R}^{d+1} : x \in \Omega(t), t \in (T_1,T_2)\}$ and $v = v(x,t)$ the velocity of a fluid particle at location x and time t.

$(x,t) \in \Omega(t) \times (T_1, T_2)$ denotes the so-called Euler coordinates.

For the velocity we obtain

$$v(x,t) = \hat{v}(X,t) = \frac{\partial\varphi}{\partial t}(X,t)$$

where $x = \hat{x} = \varphi(X,t)$.

For the acceleration we get

$$a(x,t) = \hat{a}(X,t) = \frac{\partial^2\varphi}{\partial t^2}(X,t) = \frac{\partial}{\partial t}[\frac{\partial\varphi}{\partial t}(X,t)] = \frac{\partial}{\partial t}v(\varphi(X,t),t) =$$
$$\sum_{i=1}^{d}\frac{\partial v}{\partial x_i}(x,t)\frac{\partial\varphi_i}{\partial t}(X,t) + \frac{\partial v}{\partial t}(x,t) = \sum_{i=1}^{d}\frac{\partial v}{\partial x_i}(x,t)\frac{\partial v_i}{\partial t}(x,t) + \frac{\partial v}{\partial t}(x,t).$$

Thus, summing up gives

$$a(x,t) = v(x,t)\cdot\nabla v(x,t) + \frac{\partial v}{\partial t}(x,t) := \frac{dv}{dt}$$

where $\frac{d}{dt} = \frac{\partial}{\partial t} + v\cdot\nabla$ is called the material or total derivative.

To obtain the pathline $\varphi(X,t)$ of a particle with Lagrangian space coordinate X for a given velocity field $v : \Omega(t) \times (T_1, T_2) \to \mathbb{R}^d$ we have to solve the initial value problem

$$\begin{aligned}\frac{dx}{dt} &= v(x,t),\\ x(t_0) &= X\end{aligned}$$

There are two distinct approaches to model crowd flow.
The first one is treating pedestrians as discrete individuals. In this case pedestrians are treated as granular analogue or it is assumed that pedestrians try to optimize their immediate local behavior or it is assumed that pedestrians try to move along predefined globally determined paths. This philosophy provides flexibility and is well-suited for small crowds and both, Lagrangian and Eulerian specification is used.

The second approach treats the crowd as a whole. In this case crowds are either treated as a fluid or a continuum responding to local influences or the individuals of the crowd try to optimize their behaviour to reach non-local goals. For this second philosophy the point of view has been restricted mainly to Eulerian specification and this philosophy is used to model big crowds where different motion of individuals is not important.

Both philosophies are justified and should be seen as complementing each other.

6.2 Macroscopic pedestrian models

This section is based on [8] and [3].

In this section we use the second approach to model pedestrian flow where each member of the crowd tries to move in such a way as to optimize their behaviour to reach a non-local goal. Throughout this chapter we assume that the behaviour of the pedestrians is goal directed which means that each individual has a well-defined goal at a known location. Also assume further that crowds behave rationally. For a justification of the last assumption see [13].

6.2.1 Pedestrians of a single type

At first we will describe the flow of pedestrians of a single type in terms of two qualities. These qualities are:

1. density ρ of the flow which is the expected number of individuals located whithin a certain area of space at a given time t and location (x, y)
2. velocity $\vec{V} = (u, v)$ of the flow which is the expected velocity of individuals at a given time t and location (x, y), but the velocity should also consider the pedestrians attitude to adapt their path choice to the crowd density they estimate to find along this path.

For the next considerations let $z := (x, y)$ and $\Omega(t) := \{z = \varphi(X, t) : X \in \Omega(t_0)\}$ be a domain of a fixed amount of pedestrians at time $t \in (t_A, t_E) \subset (T_1, T_2) \subset \mathbb{R}$ where

(t_A, t_E) is the domain of interest. Because of conservation of mass M in a certain region of pedestrians we can say that

$$\frac{dM}{dt}(t) = 0 \text{ with } M(t) = \int_{\Omega(t)} \rho(z,t)dz$$

where $\rho(z,t)$ is the mass density of the flow at position z at time t.
Due to the transport theorem (Theorem 2.4) it follows that

$$0 = \frac{dM}{dt}(t) = \int_{\Omega(t)} [\frac{\partial \rho}{\partial t}(z,t) + \text{div}_z(\rho\vec{V})(z,t)]dz.$$

By applying Theorem 2.5. to $f(z) := \frac{\partial \rho}{\partial t}(z,t) + \text{div}_z(\rho\vec{V})(z,t)$ we obtain the so-called continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) = 0 \text{ in } \Omega(t) \tag{6.1}$$

for a fixed t.

To proceed further the following hypotheses about pedestrian motion are necessary:

Hypothesis 1. The walking speed of pedestrians is determined solely by the density of the surrounding pedestrian flow and the behavioural characterisitics of the pedestrians.

So the velocity components are given by

$$u = f(\rho)\hat{\phi}_x$$
$$v = f(\rho)\hat{\phi}_y$$

where $f(\rho)$ is the speed and $\hat{\phi}_x$ and $\hat{\phi}_y$ are the cosines of the angles between the moving direction and the x-, and y-coordinate axes respectively. This is a standard hypothesis for modeling crowds where the density can be rather high, but not extreme and is similar to Greenshields model of vehicular flow which assumes a linear correspondence between velocity and density

$$f(\rho) = A - B\rho$$

with A and B positive constants where A represents the free flow speed and A/B represents the jam density. For the entire model description see [15]

Hypothesis 2. Pedestrians have a common sense of the task (called potential) they face to reach their common destination such that any two individuals at different locations having the same potential would see no advantage to either of exchanging places.

This means that there is no perceived advantage of moving along a line of constant potential. So, the motion of any pedestrian is in the direction perpendicular to the

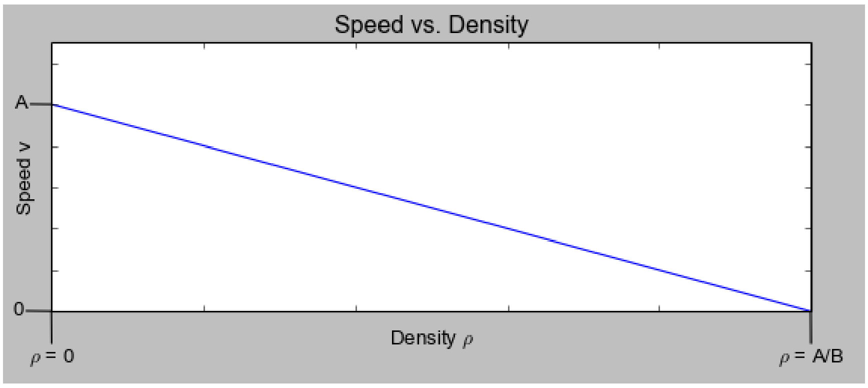

Figure 6.1: Speed vs. Density

potential, that is, in the direction for which

$$\hat{\phi}_x = \frac{-\frac{\partial \phi}{\partial x}}{\sqrt{(\frac{\partial \phi}{\partial x})^2 + (\frac{\partial \phi}{\partial y})^2}}$$

$$\hat{\phi}_x = \frac{-\frac{\partial \phi}{\partial y}}{\sqrt{(\frac{\partial \phi}{\partial x})^2 + (\frac{\partial \phi}{\partial y})^2}}$$

where ϕ is the potential.
This hypothesis is not suitable for vehicular flow but is appropriate for pedestrian flow. Even for crowds for which it is not applicable it is a good approximation.

Hypothesis 3. Pedestrians would like to minimize their travel time, but temper this behaviour to avoid extremely high densities. This tempering is assumed to be "separable", such that pedestrians minimize the product of their travel time and a function of the density.

This hypothesis means that any two pedestrians which are on a given potential must both be at the same new potential as each other at some later time. So, the distance between potentials must be proportional to pedestrian speed irrespective of the initial position of a pedestrian. Because of this we can write

$$\frac{1}{\sqrt{(\frac{\partial \phi}{\partial x})^2 + (\frac{\partial \phi}{\partial y})^2}} = g(\rho)\sqrt{u^2 + v^2}$$

where ϕ has been scaled appropriately and $g(\rho)$ is a factor to allow for discomfort at very high densities in accordance with Hypothesis 3.

Combining the equations we had so far results in

$$-\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho g(\rho) f^2(\rho)\frac{\partial \phi}{\partial x}) + \frac{\partial}{\partial y}(\rho g(\rho) f^2(\rho)\frac{\partial \phi}{\partial y}) = 0 \qquad (6.2)$$

for the continuity equation and

$$g(\rho)f(\rho) = \frac{1}{\sqrt{(\frac{\partial \phi}{\partial x})^2 + (\frac{\partial \phi}{\partial y})^2}}. \tag{6.3}$$

The model introduced here is a special case of the model introduced in [3]. In this paper the authors start from

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho v(\rho)(\nu(z) + \mathcal{I}(\rho))) = 0$$

with initial condition

$$\rho(0, z) = \rho_0(z)$$

where $\nu(z)$ denotes the desired direction of the pedestrian and $\mathcal{I}(\rho(t))$ describes the deviation from $\nu(z)$ due to the density at time t at point $z := (x, y)$. So the vector $\nu(z) + \mathcal{I}(\rho(t))$ can be interpreted as the direction that an individual located at z follows. This means that an individual at position z at time t is assumed to move in the direction $\nu(z) + \mathcal{I}(\rho(t))$. Note here that if $\mathcal{I} = 0$ it can be assumed that the paths followed by the pedestrians are chosen a priori, independently of the density ρ.
If we define $v(\rho) := f^2(\rho), \nu(z) := 0$ and $\mathcal{I}(\rho) := -\nabla \phi g(\rho)$ we get equation (6.2) where ϕ denotes the solution to the eikonal equation $|\nabla \phi| = \frac{1}{g(\rho)f(\rho)}$.

Remark 6.1. *Boundary conditions for* (6.2) *and* (6.3) *are given by specifying* ρ *which is generally specified on those open boundaries that correspond to entrances. Note that the speed* $f(\rho)$ *and the flow* $\rho f(\rho)$ *depend only on* ρ.

Remark 6.2. *The model introduced above is sufficient for the vast majority of situations. To cover some special cases it would be necessary to introduce some additional hypotheses.*

Another frequently used choice of $\mathcal{I}(\rho)$ is $\mathcal{I}(\rho) = -\varepsilon \frac{\nabla(\rho * \eta)}{\sqrt{1 + \|\nabla(\rho * \eta)\|}}$ where the convolution $(\rho * \eta)$ with a fixed mollifier η denotes an average of the crowd density in a neighbourhood of x, where the diameter of the neighbourhood is specified by the mollifier η and ε is a positive scaling parameter. With this setting $\mathcal{I}(\rho)$ states that individuals deviate from the optimal path trying to avoid entering regions with higher densities.

Remark 6.3. *Note that with the setting* $\mathcal{I}(\rho) = -\varepsilon \frac{\nabla(\rho * \eta)}{\sqrt{1 + \|\nabla(\rho * \eta)\|}}$*, (6.2) and (6.4) are of the form (1.1).*

As a motivating example for these thoughts about pedestrian flow modelling, we consider the evacuation of a room. The goal in this example is to minimize the evacuation time.

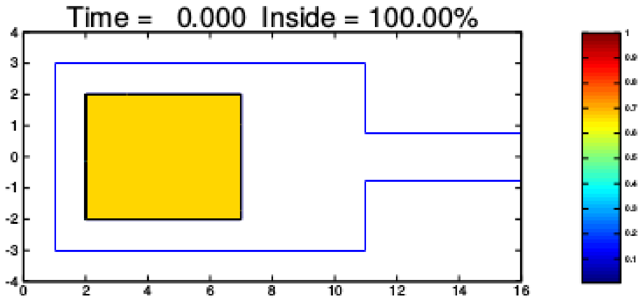

Figure 6.2: Initial datum and room geometry (taken from [3])

Consider a room as in Figure 6.2 the yellow square denoting the crowd and some fixed parameters. In this example written in terms of the model introduced in [3] the function $\mathcal{I}(\rho)$ is set to $-\varepsilon\frac{\nabla(\rho*\eta)}{\sqrt{1+\|\nabla(\rho*\eta)\|}}$. For more details about the choice of the parameters see [3].

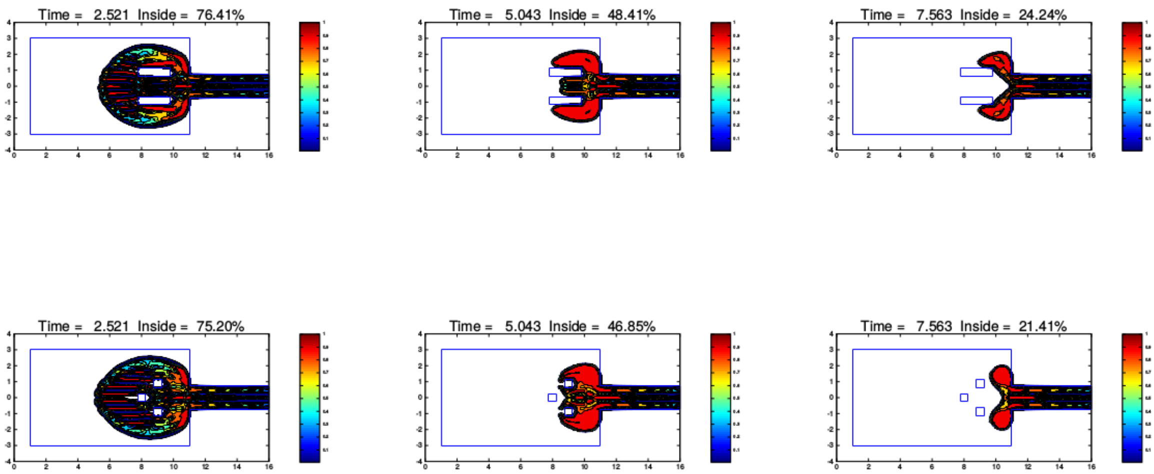

Figure 6.3: Crowd guided with two columns (first line) and 3 columns (second line) (taken from [3])

The first line in Figure 6.3 shows the crowd escaping the room guided by 2 symmetrically arranged columns. Before the bottleneck, three lanes merge into one.
In the second line in Figure 6.3, three columns guide the crowd out of the room.
Note that in each case there is a massive congestion at the exit.

In the first line in Figure 6.4 the crowd merges from 7 lanes before the bottleneck to 4 in beween it. We also see that the individuals that do not pass through the bottleneck

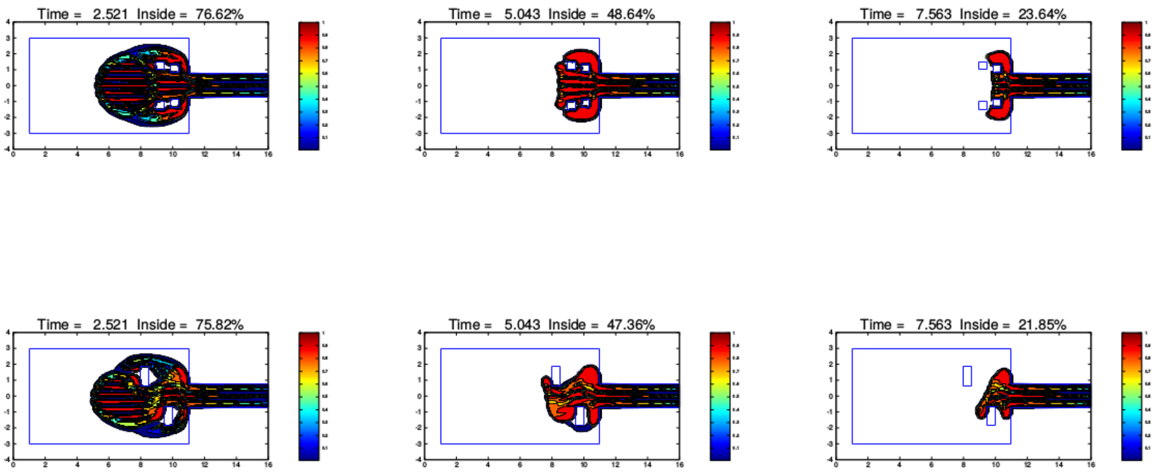

Figure 6.4: Crowd guided with four columns (first line) and 2 asymmetric columns (second line) (taken from [3])

are penalized by the high density at the door jambs.
Observe that in the second line in Figure 6.4 the asymmetrical layout of the columns avoids lane formation.

6.2.2 Pedestrians of multiple type

So far we have considered only pedestrians of a single type, but generally it is the case that crowds consist of pedestrians of multiple types. Fortunately, there are many correspondences to the situation where a crowd consists only of pedestrians of a single type. There are also three hypotheses which have to be made and only the first one differs from the single pedestrian case above widely:

Hypothesis 4. The speed of pedestrians of a single type in multiple type flow is still determined by the function $f(\rho)$ but now ρ is the total density rather than the density of a single pedestrian type.

This hypothesis might be surprising, although it is very accurate. A justification of this behaviour is given in [1]. This paper says that pedestrian crowds form into bands as they pass through each other such that any pedestrian is walking amongst pedestrians of the same type at the combined density, see Figure 6.5. There are time delays at the entry and the exit which are negligible if these delays are small in comparison to the crossing time. An interesting special case arises if the destinations of two pedestrian types are the same, but the walking characteristics are different. The slower moving crowd adjusts such that the faster crowd can pass freely if the densities of the moving crowds are similar. But in this special case the hypothesis also holds.

For more than two different types of pedestrians this hypothesis also holds but this case is more complicated since there are bands within bands which must be taken into account.

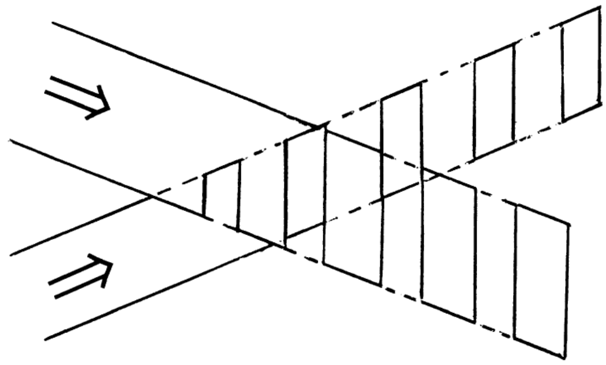

Figure 6.5: Representation of how two flows pass through one another (taken from [8])

Hypothesis 5. A potential field exists for each pedestrian type such that pedestrians move at right angles to lines of constant potential.

Hypothesis 6. Pedestrians try to minimize their travel time, but temper this behaviour to avoid extremely high densities.

The latter two hypotheses can be interpreted in a similar way as in the case with only one type of pedestrian.

For further discussion of the differential equation let $\rho_i f_i(\rho)$ the flow of a particular pedestrian type $i = 1, \dots, N$ where ρ_i is the density of pedestrians of a particular type, N is the number of different pedestrian types, $f_i(\rho)$ is a specified function of total pedestrian density for pedestrians of type i and

$$\rho = \sum_{i=1}^{N} \rho_i.$$

Then for each pedestrian type we obtain the equation

$$-\frac{\partial \rho_i}{\partial t} + \frac{\partial}{\partial x}(\rho_i g(\rho) f_i^2(\rho) \frac{\partial \phi_i}{\partial x}) + \frac{\partial}{\partial y}(\rho_i g(\rho) f_i^2(\rho) \frac{\partial \phi_i}{\partial y}) = 0 \tag{6.4}$$

and

$$g(\rho) f_i(\rho) = \frac{1}{\sqrt{(\frac{\partial \phi_i}{\partial x})^2 + (\frac{\partial \phi_i}{\partial y})^2}} \tag{6.5}$$

for $i = 1, \dots, N$. In these equations ϕ_i corresponds to the potential for type i of pedestrians moving over the (x, y) floor plane.
With the corresponding definitions as in the case of a single pedestrian type we can fit equations (6.4) and (6.5) into the model in [3].

6.3 Microscopic pedestrian models

This section is based on paper [2], [10].

Here in this section we look at the microscopic pedestrian model. Based on a lattice approach we will derive the corresponding mean-field PDE[1] with Taylor expansion up to second order.

Throughout this section let us consider two groups of individuals, blue individuals moving from right to left and red individuals moving from left to right. For our purpose let $\Omega = [-L_x, L_x] \times [-L_y, L_y] \subseteq \mathbb{R}^2$ with $L_y << L_x$ be a domain which corresponds to a corridor and is partitioned into an equidistant grid of mesh size h, i.e., $(x_i, y_j) = (ih, jh), i \in \{0, \dots, N\}$ and $j \in \{0, \dots, M\}, N, M \in \mathbb{N}$ denotes a grid point which can be occupied by an either blue or red individual. The probability that a red individual is at position (x_i, y_j) at time t is given by

$$r_{i,j}(t) = P(\text{red individual is at position } (x_i, y_j) \text{ at time t}).$$

The probability for a blue individual is defined analogously. The probabilities depend on the transition rates which are defined by

$$\begin{aligned}
\mathcal{T}_r^{\{i,j\}\to\{i+1,j\}} &= (1 - \rho_{i+1,j})(1 + \alpha r_{i+2,j}),\\
\mathcal{T}_r^{\{i,j\}\to\{i,j-1\}} &= (1 - \rho_{i,j-1})(\gamma_0 + \gamma_1 b_{i+1,j}),\\
\mathcal{T}_r^{\{i,j\}\to\{i,j+1\}} &= (1 - \rho_{i,j+1})(\gamma_0 + \gamma_2 b_{i+1,j}),
\end{aligned} \tag{6.6}$$

where $\mathcal{T}_r^{\{i,j\}\to\{i+1,j\}}$ denotes the transition rate that a red individual moves from the discrete position (x_i, y_j) to (x_{i+1}, y_j). The factor $(1 - \rho)$ in (6.6) with $\rho = r + b$ corresponds to size exclusion, i.e., an individual cannot move to a point which is occupied by another individual. The parameters $\gamma_0, \gamma_1, \gamma_2$ can only take values between 0 and 1, 0 and 1 included. The parameter $\gamma_0 > 0$ denotes diffusion in y-direction, if $\gamma_0 = 0$, individuals only step aside if approached by another individual in opposite direction. If $\gamma_1 > \gamma_2$ then a red individual moves to the right when a blue individual approaches, therefore $\gamma_2 > \gamma_1$ means moving to the left side. If the parameter $0 \leq \alpha \leq \frac{1}{2}$ is positive, then the probability of moving in the walking direction is increased if the individual at (x_{i+2}, y_j) is moving in the same direction.
We can now deduce the final equation for the probability to find a red individual at a discrete point in time t_{k+1} at position (x_i, y_j), which is

$$\begin{aligned}
r_{i,j}(t_{k+1}) = &r_{i,j}(t_k) + \mathcal{T}_r^{\{i-1,j\}\to\{i,j\}} r_{i-1,j}(t_k)\\
&+ \mathcal{T}_r^{\{i,j+1\}\to\{i,j\}} r_{i,j+1}(t_k) + \mathcal{T}_r^{\{i,j-1\}\to\{i,j\}} r_{i,j-1}(t_k)\\
&- (\mathcal{T}_r^{\{i,j\}\to\{i+1,j\}} + \mathcal{T}_r^{\{i,j\}\to\{i,j-1\}} + \mathcal{T}_r^{\{i,j\}\to\{i,j+1\}}) r_{i,j}(t_k)
\end{aligned} \tag{6.7}$$

[1] simply put, in the derivation of mean-field models the effect of a large number of individuals on a single individual is approximated by a single averaging effect, the so called mean-field

or, in words,

Probability to find a red individual at position (x_i, y_j)	=	Probability that a red individual moves from position (x_{i-1}, y_j) forward	+	Probability that particles located above or below jump down or up	-	Probability that an individual at (x_i, y_j) moves forward or steps aside	.

Of course, these thoughts are analogous for blue individuals. In this case we obtain for the transition rates

$$\begin{aligned} \mathcal{T}_b^{\{i,j\}\to\{i-1,j\}} &= (1-\rho_{i-1,j})(1+\alpha b_{i-2,j}), \\ \mathcal{T}_b^{\{i,j\}\to\{i,j+1\}} &= (1-\rho_{i,j+1})(\gamma_0+\gamma_1 r_{i-1,j}), \\ \mathcal{T}_b^{\{i,j\}\to\{i,j-1\}} &= (1-\rho_{i,j-1})(\gamma_0+\gamma_2 r_{i-1,j}), \end{aligned} \tag{6.8}$$

and for the probability to find a blue individual at position (x_i, y_j) at a discrete point in time t_{k+1} the equation

$$\begin{aligned} b_{i,j}(t_{k+1}) =& b_{i,j}(t_k) + \mathcal{T}_b^{\{i+1,j\}\to\{i,j\}} b_{i+1,j}(t_k) \\ &+ \mathcal{T}_b^{\{i,j-1\}\to\{i,j\}} b_{i,j-1}(t_k) + \mathcal{T}_b^{\{i,j+1\}\to\{i,j\}} b_{i,j+1}(t_k) \\ &- (\mathcal{T}_b^{\{i,j\}\to\{i-1,j\}} + \mathcal{T}_b^{\{i,j\}\to\{i,j+1\}} + \mathcal{T}_b^{\{i,j\}\to\{i,j-1\}}) b_{i,j}(t_k). \end{aligned} \tag{6.9}$$

After performing a Taylor expansion with the help of computer algebra techniques up to second order, see [10], we get

$$\begin{aligned} \partial_t r &= -\nabla \cdot J_r, \\ \partial_t b &= -\nabla \cdot J_b, \end{aligned} \tag{6.10}$$

where

$$J_r := \begin{pmatrix} (1-\rho)(1+\alpha r)r + \frac{h}{2}(\partial_x(r(1-\rho)(1+\alpha r)) - 2((1-\rho)\partial_x r)) \\ -(\gamma_1-\gamma_2)(1-\rho)br - \frac{h}{2}((\gamma_1+\gamma_2)((1-\rho)\partial_y(rb) + br\partial_y\rho) \\ +2\gamma_0((1-\rho)\partial_y r + r\partial_y\rho) + 2(\gamma_1-\gamma_2)(1-\rho)r\partial_x b) \end{pmatrix} \tag{6.11}$$

and

$$J_b := \begin{pmatrix} -(1-\rho)(1+\alpha r)b + \frac{h}{2}(\partial_x(b(1-\rho)(1+\alpha b)) - 2((1-\rho)\partial_x b)) \\ (\gamma_1-\gamma_2)(1-\rho)br - \frac{h}{2}((\gamma_1+\gamma_2)((1-\rho)\partial_y(rb) + br\partial_y\rho) \\ +2\gamma_0((1-\rho)\partial_y b + b\partial_y\rho) + 2(\gamma_1-\gamma_2)(1-\rho)b\partial_x r) \end{pmatrix} \tag{6.12}$$

denote the fluxes for r and b, respectively.

Setting $\alpha = 0, \gamma := \gamma_1 = \gamma_2$, the fluxes simplifiy to

$$J_r := \begin{pmatrix} (1-\rho)r + \frac{h}{2}(\partial_x(r(1-\rho)) - 2((1-\rho)\partial_x r)) \\ -\frac{h}{2}((2\gamma)((1-\rho)\partial_y(rb) + br\partial_y\rho) + 2\gamma_0((1-\rho)\partial_y r + r\partial_y\rho)) \end{pmatrix} \tag{6.13}$$

and

$$J_b := \begin{pmatrix} -(1-\rho)b + \frac{h}{2}(\partial_x(b(1-\rho)) - 2((1-\rho)\partial_x b)) \\ -\frac{h}{2}((2\gamma)((1-\rho)\partial_y(rb) + br\partial_y\rho) + 2\gamma_0((1-\rho)\partial_y b + b\partial_y\rho)) \end{pmatrix}. \tag{6.14}$$

Now we simplify the fluxes further by substituting ρ with $b+r$. In the next line, we do this for (6.13). The case (6.14) is analogous. Performing the announced substitution, the first component in (6.13) changes to

$$(1-\rho)r + \frac{h}{2}(\partial_x(r(1-b-r)) - 2((1-b-r)\partial_x r)).$$

Applying the product rule leads to the expression

$$(1-\rho)r + \frac{h}{2}(\partial_x r - b\partial_x r - r\partial_x r - r\partial_x b - r\partial_x r - 2\partial_x r + 2b\partial_x r + 2r\partial_x r).$$

By adding and subtracting the terms, we finally get

$$(1-\rho)r + \frac{h}{2}(-\partial_x r - r\partial_x b + b\partial_x r)$$

or

$$(1-\rho)r + \frac{h}{2}((b-1)\partial_x r - r\partial_x b).$$

The second component can be rewritten under the assumptions above to

$$-\frac{h}{2}(2\gamma((1-b-r)\partial_y(rb) + br\partial_y(b+r)) + 2\gamma_0((1-b-r)\partial_y r + r\partial_y(b+r)).$$

Computing the derivatives and expanding the terms gives

$$-\frac{h}{2}(2\gamma(1-b)b\partial_y r - 2\gamma rb\partial_y r + 2\gamma(1-b)r\partial_y b - 2\gamma r^2\partial_b + 2\gamma br\partial_y b + 2\gamma br\partial_y r$$
$$+2\gamma_0(1-b)\partial_y r - 2\gamma_0 r\partial_y r + 2\gamma_0 r\partial_y b + 2\gamma_0 r\partial_y r).$$

This expression can be further simplified by cancelling certain terms and by factoring $\partial_y r$ and $\partial_y b$ out to

$$-\frac{h}{2}((2\gamma(1-b)b + 2\gamma_0(1-b))\partial_y r + (2\gamma(1-r)r + 2\gamma_0 r)\partial_y b.$$

Doing the analogous steps in (6.14) leads to the nicer representation

$$\begin{pmatrix} \partial_t r \\ \partial_t b \end{pmatrix} = \begin{pmatrix} \nabla & 0 \\ 0 & \nabla \end{pmatrix} \cdot \left(A(r,b) \begin{pmatrix} \nabla r \\ \nabla b \end{pmatrix} + \begin{pmatrix} (1-\rho)r\nabla V_r \\ (1-\rho)b\nabla V_b \end{pmatrix} \right) \tag{6.15}$$

of (6.10) where A(r,b) is the diffusion matrix given by

$$A(r,b) = \frac{h}{2}\begin{pmatrix} (1-b) & 0 & r & 0 \\ 0 & 2\gamma(1-b)b + 2\gamma_0(1-b) & 0 & 2\gamma(1-r)r + 2\gamma_0 r \\ b & 0 & (1-r) & 0 \\ 0 & 2\gamma(1-b)b + 2\gamma_0(b) & 0 & 2\gamma(1-r)r + 2\gamma_0(1-r) \end{pmatrix}$$

and $V_r(x,y) = x$ and $V_b(x,y) = -x$ denotes the motion of the red and blue individuals to the right and left, respectively.
Since pedestrians cannot penetrate the walls, the boundary conditions on top and bottom are set to no flux boundary conditions. At the entrance and the exit of the corridor, i.e., $x = \pm L_x$, periodic boundary conditions are assumed.

Remark 6.4. *Note that (6.15) is of the form (1.1).*

The following example which is taken from [2], shows the numerical results of the microscopic flow model described above.
In the first part of the example we will look at the simplified model (6.15), i.e., $\alpha = 0$, so the probability of moving in the walking direction is not increased if the individual in front is moving into the same direction and $\gamma := \gamma_1 = \gamma_2$, so the individuals are stepping aside if another individual approaches, but there is no preference of an individual stepping aside to the right or stepping aside to the left with respect to their moving direction. Figure 6.6 shows the initial value r_0 with a small perturbation of a

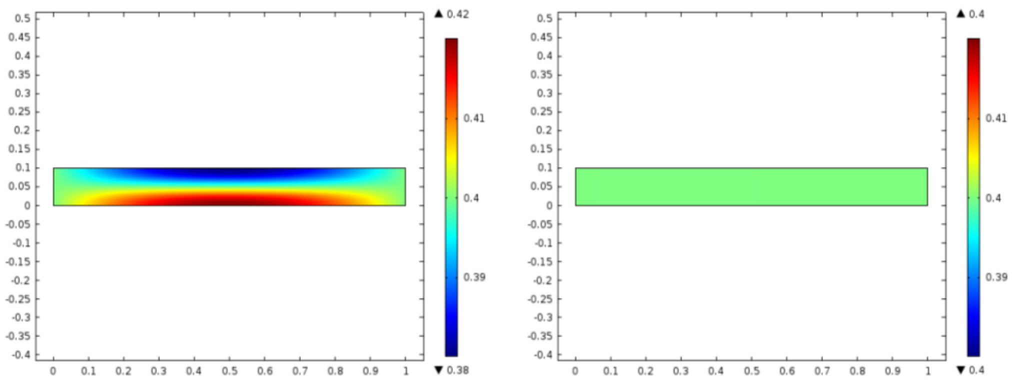

Figure 6.6: Density of red individuals is returning to the constant stationary state (right) after inital perturbation (left) (taken from [2])

stationary state in the left picture, and the solution r_T of the system (6.15) at time $T = 5$ in the right picture.

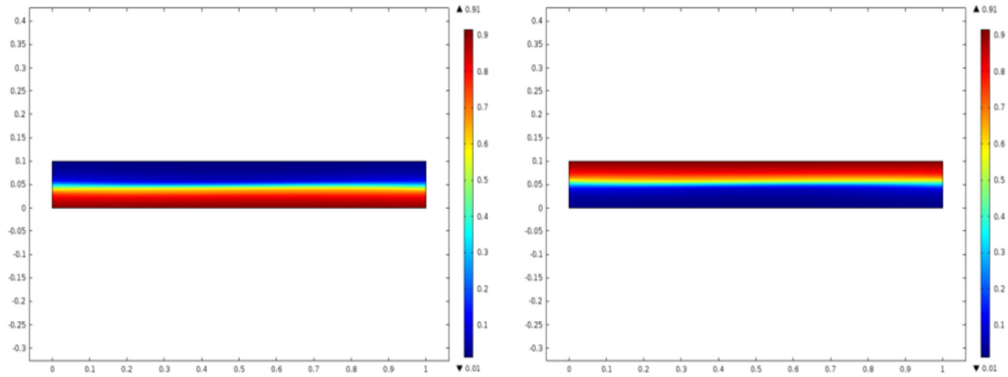

Figure 6.7: Density of red individuals in the left picture and of blue individuals in the right picture at time $T = 5$ forming lanes (taken from [2])

In the second example, system (6.10) is modelled. In Figure 6.7 we can observe lane formation assuming that $\gamma_1 > \gamma_2$ which means that an individual prefers to make a step aside to the right with respect to their moving direction.

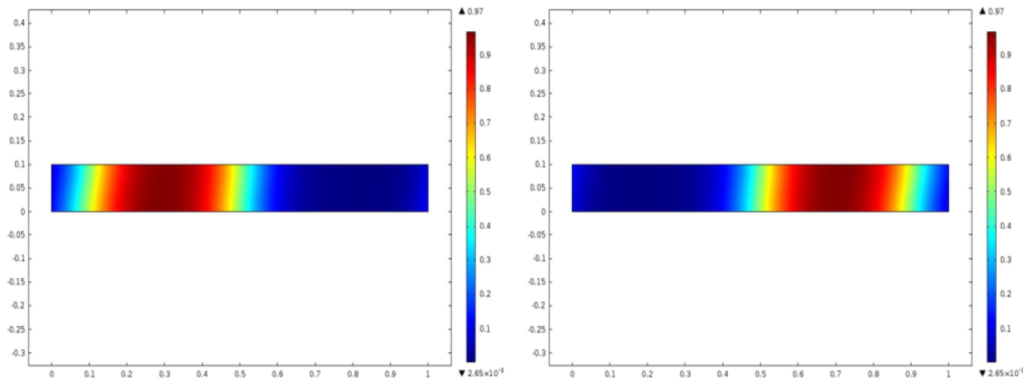

Figure 6.8: Congestion in the red (left) and blue (right) individual density result in a deadlock (taken from [2])

The third example shows the well-known phenomenon of a jam. Jams happen if the initial masses are high compared to the diffusion coefficients $\gamma_1 - \gamma_2$ and γ_0. This case results in a frozen configuration, i.e., the individuals are unable to walk in their moving direction further as depicted in Figure 6.8.

Chapter 7

Conclusion

As we have seen, diffusion-convection-reaction equations are a powerful class of partial differential equations to model a lot of different problems in various kinds of sciences for example physics, chemistry, biology. In this thesis, we first derived the thermodynamic equations and gave a formulation of the problem to find a temperature field. Then we saw that environmental pollution can be modelled in terms of a diffusion-convection-reaction equation. Under some circumstances this equation simplifies and can even be solved analytically. In the subsequent chapter we considered irreversible competitive-consecutive chemical reactions and derived a model to calculate the concentration differences of the reactants in time. Next we looked at population models and discovered different models with either one or two species. The last chapter of the thesis was devoted to pedestrian flow models. There are two types of models, the macroscopic flow model and the microscopic flow model. Both models have their justification. The first one treats the crowd as a whole in order to understand the overall behaviour of these crowds whereas the second one is often more suitable for small crowds. We have seen that it is very often the case that a diffusion-convection-reaction equation cannot be solved analytically. In such cases the only possibility to get an approximate solution is by applying numerical methods, such as the Finite Element Method, which is beyond the scope of this thesis. In order to get correct solutions with the help of numerical methods, it must be ensured that the underlying model is suitable.

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