DISCRETE AND CONTINUOUS
DYNAMICAL SYSTEMS–SERIES B
Volume **4**, Number **4**, November **2004**

Website: http://AIMsciences.org

pp. **961–982**

ON THE L^2-MOMENT CLOSURE OF TRANSPORT EQUATIONS: THE CATTANEO APPROXIMATION

T. Hillen

Department of Mathematical and Statistical Sciences
University of Alberta
Edmonton, AB, T6G 2G1, Canada

(Communicated by Yanping Lin)

Abstract. We consider the moment-closure approach to transport equations which arise in Mathematical Biology. We show that the negative L^2-norm is an entropy in the sense of thermodynamics, and it satisfies an H-theorem. With an L^2-norm minimization procedure we formally close the moment hierarchy for the first two moments. The closure leads to semilinear Cattaneo systems, which are closely related to damped wave equations. In the linear case we derive estimates for the accuracy of this moment approximation. The method is used to study reaction-transport models and transport models for chemosensitive movement. With this method also order one perturbations of the turning kernel can be treated - in extension of an earlier theory on the parabolic limit of transport equations (Hillen and Othmer 2000). Moreover, this closure procedure allows us to derive appropriate boundary conditions for the Cattaneo approximation. Finally, we illustrate that the Cattaneo system is the gradient flow of a weighted Dirichlet integral and we show simulations.

The moment closure for higher order moments and for general transport models will be studied in a second paper.

1. **Introduction.** Flagellated bacteria show a very distinct movement behavior. They move with an almost constant speed (run), then they stop to choose a new direction (tumble) and continue to move. The tumbling intervals are short compared to the mean run times. This movement pattern can be modeled by a *velocity jump process* or *transport equation* (Stroock [35], Othmer, Dunbar, and Alt [27]). The characteristic parameters are mean runtime, turning distribution and mean speed. In Hillen and Othmer [20] a transport model (1) has been studied systematically with respect to different forms of biases and possible limit equations (of reaction-advection-diffusion type).

In this paper and in a following paper (Part II [18]) we present an L^2-moment closure procedure for transport equations in biology. In this paper we focus on the simplest nontrivial case: the Cattaneo closure (second-moment approximation). This case alone is of particular interest in biological modeling and it has been used to analyse pattern formation in populations of slime molds *Dictyostelium discoideum*, and bacteria *Salmonella typhimurium* and *Eschirichia coli* in [9], [10], [33]. A nonlinear reaction-Cattaneo model has been studied in detail in [15], where a Lyapunov function was constructed to show that solutions converge to steady

1991 *Mathematics Subject Classification.* 92B05, 45K05, 35L65.
Key words and phrases. Moment Closure, Transport Equations, Cattaneo System.

states.
In Part II [18] we treat the general case for general turning kernel, and arbitrary number of moments.

1.1. **Transport Equations.** Let $p(t,x,v)$ denote the population density at time $t \geq 0$ at spatial position $x \in \mathbb{R}^n$ with velocity $v \in \mathbb{R}^n$. Most important are space dimensions of $n = 1, 2, 3$, the theory, however, works for all $n \in \mathbb{N}$. We assume that individuals choose any movement direction with bounded speed. We denote the set of possible velocities as V, where we assume $V \subset \mathbb{R}^n$ is bounded and symmetric (i.e. $v \in V \Rightarrow -v \in V$). Then the linear transport model reads

$$\frac{\partial}{\partial t}p(t,x,v) + v \cdot \nabla p(t,x,v) = -\mu p(t,x,v) + \mu \int_V T(v,v')p(t,x,v')dv', \qquad (1)$$

where μ is the turning rate or turning frequency, hence $\tau = \frac{1}{\mu}$ is the mean run time, and $T(v,v')$ is the probability kernel for the new velocity v given the previous velocity was v'. Of course

$$\int T(v,v')dv = 1$$

to ensure particle conservation.

If cell proliferation, death and other interactions were included, then we obtain *reaction-transport models*, or *resting-phase transport models*. The resting-phase transport models are important if birth events are correlated to resting phases of the "mothers". That case is studied in detail in [19]. Here we assume that resting is not so important for the overall dynamics and we model birth-death with a reaction-transport equation of the form as used by Hadeler (see the review article [14]):

$$p_t + v \cdot \nabla p = -\mu p + \mu \int T(v,v')p(t,x,v')dv' + f(v,p,m^0), \qquad (2)$$

where the total population density is denoted by

$$m^0(t,x) = \int_V p(t,x,v)\, dv. \qquad (3)$$

In the *isotropic* case the nonlinearity f depends only on the total population density m^0.

Transport equations appear in physics as models for dilute gases, i.e. Boltzmann equations, in neutron transport theory, in models for radiation transport, and in semiconductor theory (for references to the physical literature see also [17]). In the cases of gases and neutrons, reorientation results from collisions of two particles, hence the right-hand side of the transport equation (2) is quadratic in p ([7]). In some cases collisions are modeled with respect to a background Maxwellian distribution, then the model equations are linear. In case of radiation transport the right-hand side of (2) consists of a linear absorbing term and the Planck function, which describes emission of radiation. In physical applications some quantities are conserved, among these are energy, momentum and mass. In biological applications the only conserved quantity is the total particle number (in absence of birth or death). Bellomo and co-workers [3, 4] developed a theory to generalize the Boltzmann equation to biological systems. Internal state variables of the underlying species are included. A quadratic scattering term is derived based on the assumption that binary particle interactions dominate. Depending on the application these include transmission of an infection or of a parasite, predator-prey

interactions, or competition for nutrients. Our model (2) falls into the class studied in [4] and Hilbert- and Chapman-Enskog approximations can be derived. The moment closure method presented here differs from the Hilbert method, and from the Chapman-Enskog method as it is not based on an asymptotic expansion, it is based on energy minimization.

1.2. **The Moment Closure Method.** One common feature in understanding the dynamic properties of reaction-transport equations and of Boltzmann equations are *moment methods*. By multiplying (1) with powers of v and integrating them, we can derive an infinite sequence of equations for the v-moments of p. As a matter of fact, in the equation for the n–th moment the $(n+1)$–st moment appears. To close the equations for the first n moments one needs to approximate the $(n+1)$–moment. This "closure problem" is well known and widely discussed in transport theory. Most authors use *ad hoc* arguments or projection methods to close the moment system (see e.g. [1], [29], [32]). Here we present a theory for closing the moment equations, which is based on a minimization principle.

For Boltzmann equations the closure problem has also been treated in the theory of *Extended Thermodynamics* (see e.g. Müller and Ruggeri [25]). The physical entropy is maximized under the constraint of fixed first n moments. One assumes that the $(n+1)$–st moment of the minimizer approximates the $(n+1)$–st moment of the true solution. This gives the desired closure. It appears that theories for a large number of moments can approximate steep gradients and shocks [25].
The most important first-moment approximations to the Boltzmann equation are the Euler equations and the Navier-Stokes equations ([25]). Here the Cattaneo system (17) ranges at the same level as the Euler equations.
The Cattaneo system of heat transport also appears in the theory of extended thermodynamics. There it is part of the 13-moment model. It extends the Navier-Stokes-Fourier model if some terms, which might have the same order in magnitude than other remaining terms, in the 13 moment system are neglected, (see Müller and Ruggeri [25] for details). Hence in that context, the Cattaneo model is not useful.

Ringhofer *et al.* [32] study moment systems for the semiconductor Boltzmann equation. They use orthogonal projections of expansions in terms of Hermite polynomials. The closed system forms a Galerkin approximation to the transport equation. Ringhofer *et al.* derive a numerical method and, given appropriate scaling of space and time, they prove error estimates. As pointed out in [32], the expansion in Hermite polynomials together with an orthogonal projection is equivalent to Levermore's procedure of moment closure [24] and also to entropy maximization used in *Extended Thermodynamics*.

The method presented here is different in many ways. First of all, we use a different entropy (the negative L^2-norm), secondly there is only one conserved quantity (the total population size), whereas, in physical context, mass, momentum and energy are conserved. This difference leads to different properties of the turning operator (called $\mathcal{L}$ in this paper). Finally, the nonlinearities are quite different. Here we are interested in particle interaction, birth- or death-events and in oriented movement of self propelling particles.

The method presented here is also different from Fourier-series truncation. In one space dimension, for example, the Fourier transform $\hat{p}(\sigma)$ of a distribution $p(v)$

can be expressed by the moments

$$\hat{p}(\sigma) = \sum_{j=1}^{\infty} \frac{(i\sigma)^j}{j!}\mu_j,$$

where $\mu_j = \int v^j p(v)dv$ denotes the j-th moment. A moment approximation could be achieved by

$$\hat{p}_N(\sigma) = \sum_{j=1}^{N} \frac{(i\sigma)^j}{j!}\mu_j,$$

where all higher moments are set to zero, in contrast to the L^2-closure method presented here (see e.g. formula (16) and Part II [18]).

In the context studied here, the negative $L^2(V)$-norm can be seen as an entropy as defined in thermodynamics. We close the moment system by minimizing the L^2-norm under the constraint of fixed first n-moments. This minimization flattens oscillations, details and high oscillations: high frequencies in space and time will be smoothed out and the global structure of the solution will be emphasized. In this paper we introduce this minimization procedure and we close the system for the first two moments (total population density and population flux). The closed system is a Cattaneo system, which is well known in heat transport theory (see the next section). We show estimates for the accuracy of this approximation. Finally we apply this method to the transport equation for chemosensitive movement and to reaction- transport equations. In Part II [18] we generalize this approach to close the moment system at any order and we discuss the 3-moment closure in more detail.

1.3. **Cattaneo's Law.** The Cattaneo system has the following form

$$\begin{array}{rcl} u_t + \nabla \cdot v & = & 0 \\ \tau v_t + d\nabla u + v & = & 0, \end{array} \tag{4}$$

where $u(t,x) \in \mathbb{R}$ and $v(t,x) \in \mathbb{R}^n$ are functions of space $x \in \Omega \subset \mathbb{R}^n$ and time $t \geq 0$. The diffusion constant d and the time constant τ are positive. There are two interpretations of this system. First, it appears to describe heat transport with finite speed, or heat transport in media with memory ([22, 12]). In that case u is the temperature and v is the heat flux. Second, the Cattaneo system can be seen as a generalization of a correlated random walk ([14]). Then u is the population density and v is the population flux. The Cattaneo law (second equation in (4)) was introduced by Cattaneo [6] to describe heat transport with finite speed. For $\tau = 0$ Cattaneo's law becomes Fourier's law. For $\tau \neq 0$ the flux is not directly proportional to the temperature gradient, it adapts with a time constant of τ.

The Cattaneo system directly leads to a damped wave equation

$$\tau u_{tt} + u_t = D\Delta u,$$

which, for $\tau \to 0$, formally converges to the heat equation (see the review article of Joseph and Preziosi [22] on heat transport or Hillen [15] on the Cattaneo system). In Section 6.1 we show that the Cattaneo law appears as gradient flux of an exponentially weighted Dirichlet integral.

The connections of the Cattaneo system to biological applications was first noticed by Hadeler [13]. In more than one space dimension there is no random walk which leads directly to the Cattaneo system. In [26] it is claimed that such a random walk exists, but the arguments are incomplete. Hence, it was long unclear

how the n-dimensional Cattaneo model is related to the n-dimensional transport equation. The moment closure procedure presented here establishes a formal relation between these models. The Cattaneo model is a moment approximation to the transport equation, and we show that the error can be controlled (Theorem 3.6). The closure theory gives a new understanding of the role of the Cattaneo system in biological applications. Moreover, the relevant parameters are now related to the individual movement behavior of the underlying species.

The results of this paper are based on my habilitation thesis [16], which is unpublished. The method for the Cattaneo closure has been mentioned in the review article [17] and it has been used in [9] to describe aggregations in bacteria and slime molds. Here we present the whole theory and also the proofs for the approximation properties which have not been published elsewhere.

1.4. **Velocity Moments.** We consider the equations of the first two velocity moments (m^0, m^1) of p, where m^0 is defined by (3) and the higher moments of p are denoted by $m^1 = (m_1, \dots, m_n)$ and $m^2 = (m_{ij})_{ij}$, where the coefficients are

$$m_i(t,x) = \int_V v_i p(t,x,v)\, dv, \qquad i = 1, \dots, n \tag{5}$$

$$m_{ij}(t,x) = \int_V v_i v_j\, p(t,x,v)\, dv, \qquad i,j = 1, \dots, n. \tag{6}$$

For constant turn-angle distribution $T(v, v')$ we will show that the negative of the $L^2(V)$-norm is an entropy for (1). We minimize the $L^2(V)$-norm under the constraint of fixed moments m^0 and m^1. Then we assume that the second moment $m^2(u_{\min})$ of the minimizer $u_{\min}$ approximates the second moment $m^2(p)$. This leads to a closed hyperbolic system (17) for an approximate density M^0 and an approximate flow M^1. Since the resulting system is known from heat transport theory as the Cattaneo system we call it *Cattaneo approximation* to (m^0, m^1). We derive an error estimate for $(m^0, m^1) - (M^0, M^1)$ in $L^2(\mathbb{R}^n)$ in Theorem 3.6. This estimate motivates the use of Cattaneo systems as models for the movement of microorganisms like bacteria or amoeba (see [9]).

The approximation method presented here can also be interpreted in the sense that minimizing the $L^2(V)$-norm minimizes oscillations (see Remark 2.1). Qualitatively the approximate solution is smoother than the true solution. High frequencies are damped and envelopes of the particle distribution are formed.

It turns out that the minimizer is the orthogonal projection of p onto the $n+1$-dimensional subspace of $L^2(V)$ spanned by the functions $1, v_1, \dots, v_n$. Schnitzer [33] derived a Cattaneo model for chemosensitive movement ((5.12) in [33]) with the *ad hoc* assumption that the density can be expanded as $p = p^0(t,x) + v \cdot p^1(t,x)$. The minimizing procedure developed here gives a justification of his ansatz.

Since our estimates are valid for all times (in the linear case) the Cattaneo model can be used to approximate the transport model for all times whereas the parabolic approximations are valid for large times only (see the discussion in Section 6).

In the context of the moment closure method presented here the Cattaneo approximation is the first nontrivial approximation to the transport process. If we fix the zero's moment m^0 only and minimize the $L^2(V)$-norm then the minimizer is simply the mean density with respect to velocity v. The one-moment closure does not depend on v and t and it is an equilibrium distribution (see Remark 2.3). Generalizations to higher closure levels, general sets of velocities V and general kernel T are given in [18].

In the case of one spatial dimension with only two velocities $\pm s$, the even moments are proportional to the zero–moment and the odd moments are proportional to the first moment. Hence the first two moment equations are closed by itself and the 1-D Cattaneo system is equivalent to the 1-D transport equation ([27, 13]).

Applications to chemosensitive movement and to reaction transport equations appear at the end of this article. In case of chemosensitive movement we use our method to close the first moment equations and obtain a *Cattaneo system for chemosensitive movement*. Then we consider appropriate scaling of speed and turning rate (parabolic limit) to arrive at the well known and well studied Patlak-Keller-Segel equations (PKS-equations) [23]. In this framework we are able to handle order one perturbations of the turning rate due to chemical cues. This was not possible in the framework of parabolic scaling, as illustrated in [20].

The paper is organized as follows: In Section 2 we present the minimizing principle for the linear transport equation (1) for equally distributed turn-angle distribution $T(v, v')$ =const. We calculate the minimizer $u_{\min}$ which motivates the Cattaneo approximation (17) for (M^0, M^1). We show that the moment closure method presented here can be used to find appropriate boundary conditions for the Cattaneo system on bounded domains. In Section 3 we consider the $L^2(V)$-norm of the true solution p and compare it to the norm of the minimizer $u_{\min}$ (Theorem 3.2). An $L^2(\mathbb{R}^n)$–estimate is derived for $(m^0, m^1) - (M^0, M^1)$ in Theorem 3.6. In Section 4 we generalize the moment closure method to nonlinear reaction-transport equations (2), again with equally distributed kernel T. A nonlinear Cattaneo system (41) follows, which has been studied in detail in [15]. In Section 5 we introduce a prototype model for chemosensitive movement based on a transport equation (1). We show that under natural assumptions the 2-moment approximation is a Cattaneo model for chemosensitive movement (49) which was used in [9] to model biological pattern formation. In the discussion section (Section 6) we show that the Cattaneo system is the minimizing flux of a weighted Dirichlet integral. Finally we show simulations of the Cattaneo model for chemosensitive movement, which have been developed in collaboration with Y. Dolak [9].

2. **A Minimization Principle.** We consider a transport equation which corresponds to a velocity jump process with fixed speed, but variable direction (*Pearson walk*). In this case $V = sS^{n-1}$ with $s > 0$ and we denote $\omega = |V| = s^{n-1}\omega_0$, where $\omega_0 = |S^{n-1}|$. The turn-angle distribution is assumed to be constant $T(v, v') = \frac{1}{\omega}$. The method developed here will be generalized to more general kernel T and more general velocity sets V in [18]

The initial value problem for the linear transport equation reads

$$p_t + v \cdot \nabla p = \mu \left(\frac{m^0}{\omega} - p \right), \tag{7}$$

$$p(0, x, v) = \varphi_0(x, v). \tag{8}$$

The shift operator $\Phi := -v \cdot \nabla$ on $L^2(\mathbb{R}^n \times V)$ with domain

$$\mathcal{D}(\Phi) = \{\phi \in L^2(\mathbb{R}^n \times V) : \phi(., v) \in H^1(\mathbb{R}^n)\}$$

is skew-adjoint. Hence it generates a strongly continuous unitary group on $L^2(\mathbb{R}^n \times V)$ (see e.g. Pazy [30]: Stones Theorem). The right-hand side of (7) is bounded,

therefore the linear transport equation (7) defines a strongly continuous solution group on $L^2(\mathbb{R}^n \times V)$. For $\varphi_0 \in \mathcal{D}(\Phi)$ solutions $p(t,x,v)$ exist in

$$\mathcal{X} = C^1([0,\infty), L^2(\mathbb{R}^n \times V)) \cap C([0,\infty), \mathcal{D}(\Phi)). \tag{9}$$

A detailed existence theory on transport and reaction-transport equations of the above type on bounded domains is given in Schwetlick [34].

Later we will use the L^2-norm to carry out the moment closure. Hence in this context it is natural to work in L^2 spaces. For other applications the L^1-theory is preferred, since the total particle number is preserved by the linear transport equation.

To derive the equations for the first two moments m^0 and m^1 we integrate (7) over V to obtain the conservation law

$$m_t^0 + \nabla \cdot m^1 = 0. \tag{10}$$

Multiplication of (7) with v and integration gives

$$\int v p_t \, dv = -\int v(v \cdot \nabla) p \, dv + \mu \frac{m^0}{\omega} \int v \, dv - \mu \int v p \, dv.$$

¿From the symmetry of $V = sS^{n-1}$ it follows that $\int v dv = 0$. Hence

$$m_t^1 + \nabla \cdot m^2 = -\mu m^1. \tag{11}$$

To close this system of two-moment equations (10) and (11) we want to replace $m^2(p)$. We derive a function $u_{\min}(t,x,v)$ which minimizes the $L^2(V)$ norm under the constraint that $u_{\min}$ has the same first moments m^0 and m^1 as p has. We will show in (25) that this norm is an entropy in the sense of thermodynamics. Once we have such a function $u_{\min}$ we replace $m^2(p)$ by $m^2(u_{\min})$.

We introduce Lagrangian multipliers $\Lambda^0 \in \mathbb{R}$ and $\Lambda^1 = (\Lambda_1, \ldots, \Lambda_n) \in \mathbb{R}^n$ and define

$$H(u) := \frac{1}{2} \int_V u^2 dv - \Lambda^0 \left(\int_V u dv - m^0 \right) - \Lambda^1 \cdot \left(\int_V v u dv - m^1 \right).$$

The Euler-Lagrange equation (first variation) of $H(u)$ reads $u - \Lambda^0 - \Lambda^1 \cdot v = 0$, which gives

$$u = \Lambda^0 + \Lambda^1 \cdot v. \tag{12}$$

We use the constraints to determine Λ^0 and Λ^1:

1. $$m^0 = \int_V u \, dv = \int_V \Lambda^0 \, dv + \int_V v \cdot \Lambda^1 \, dv.$$
   We have $\int_V v \, dv \cdot \Lambda^1 = 0$ hence
   $$\Lambda_0 = \frac{m^0}{\omega}. \tag{13}$$
2. $$m^1 = \int_V v u \, dv = \int_V v \Lambda^0 dv + \int_V v(\Lambda^1 \cdot v) dv$$
   The first integral vanishes. To evaluate the second integral note that
   $$\int_{S^{n-1}} \sigma \sigma^T \, d\sigma = \frac{\omega_0}{n} I,$$

where I denotes the $n \times n$ identity matrix. Hence

$$\int_V vv^T \, dv = \int_{S^{n-1}} (s\sigma)(s\sigma)^T s^{n-1} d\sigma = \omega \frac{s^2}{n} I. \tag{14}$$

It follows that Λ^1 is given by

$$\Lambda^1 = \frac{n}{\omega s^2} m^1.$$

Then from (12) we get an explicit representation of the minimizer

$$u_{\min}(t,x,v) = \frac{1}{\omega}\left(m^0(t,x) + \frac{n}{s^2}(v \cdot m^1(t,x))\right). \tag{15}$$

Remark 2.1.

1. Let $\langle 1, v_1, \ldots, v_n \rangle \subset L^2(V)$ denote the subspace generated by the constant functions and linear functions. Let Π denote the orthogonal projection to this subspace
$$\Pi\phi(v) = \frac{1}{\omega}\int \phi(v')dv' + \frac{n}{\omega s^2}\int v'\phi(v')dv' \cdot v.$$
It turns out that the minimizer $u_{\min}$ in (15) satisfies $u_{\min} = \Pi p$ for each $(t,x) \in \mathbb{R}^+ \times \mathbb{R}^n$.
2. If we minimize the functional
$$H_a(u) := \frac{1}{2}\int_V (u-a)^2 dv - \Lambda^0\left(\int_V u dv - m^0\right) - \Lambda^1 \cdot \left(\int_V vu dv - m^1\right),$$
for some arbitrary $a \in \mathbb{R}$ with the same constraints as above we arrive at the same minimizer (15). For fixed $a \in \mathbb{R}$ the norm $\|u(t,x,.) - a\|_2$ is a measure of the oscillation around the level a. Hence $u_{\min}$ minimizes oscillations with respect to every given level.
3. The previous remark gives us a key to understand the biological significance of the minimization procedure. The minimization procedure acts on the v-dependence and x and t appear only as parameters. Hence $u_{\min}$ also minimizes
$$\|u(t,x,.) - m^0(t,x)\|_2,$$
which is the variance in the velocity distribution. This means that this form of moment closure is appropriate for species that tend to minimize the variance in movement velocity. This could occur through next neighbor correlations.
4. The extremum $u_{\min}$ is indeed a minimum, since the second variation of H is $\delta^2 H(u) = 1 > 0$.

To finally derive the moment closure we consider the second moment of the minimizer $u_{\min}$:

$$\begin{aligned} m^2(u_{\min}) &= \int_V vv^T \, u_{\min}(t,x,v) dv \\ &= \frac{1}{\omega}\int_V vv^T \, m^0 \, dv + \frac{n}{\omega s^2}\int_V (vv^T)v \, dv \cdot m^1 \\ &= \frac{s^2}{n} m^0 \, I, \end{aligned} \tag{16}$$

where (14) has been used, and because the tensor $(\int_V v_i v_j v_k \, dv)_{ijk}$ vanishes (see the following Lemma).

Lemma 2.2. *For all vectors $a, b, c \in \mathbb{R}^n$ we have*

$$\int_V (v \cdot a)(v \cdot b)(v \cdot c) dv = 0.$$

Proof: Using the divergence theorem on the ball $B_s(0) \in \mathbb{R}^n$ gives

$$\begin{aligned}
\int_V (v \cdot a)(v \cdot b)(v \cdot c) dv &= \int_V v \cdot (a(v \cdot b)(v \cdot c)) dv \\
&= s \int_{B_s(0)} \nabla_v \cdot (a(v \cdot b)(v \cdot c)) dW \\
&= s \left((a \cdot b)c \cdot \int_{B_s(0)} v dW + (a \cdot c)b \cdot \int_{B_s(0)} v dW \right) \\
&= 0,
\end{aligned}$$

where dv describes the surface element on V and dW the volume element on $B_s(0)$. □

We have chosen $u_{\min}$ such that $m^0(u_{\min}) = m^0(p)$ and $m^1(u_{\min}) = m^1(p)$. Now we close the system of the first two moments (10), (11) by assuming that $m^2(u_{\min}) \approx m^2(p)$. Then, replacing m^2 in (11) together with (10) gives a linear Cattaneo system

$$\begin{aligned}
M^0_t + \nabla \cdot M^1 &= 0, \\
M^1_t + \tfrac{s^2}{n} \nabla M^0 &= -\mu M^1,
\end{aligned} \tag{17}$$

with initial conditions

$$M^0(0, .) = m^0(0, .), \quad M^1(0, .) = m^1(0, .). \tag{18}$$

We introduce capital letters to distinguish between the moments (m^0, m^1) of p and the solutions (M^0, M^1) of the Cattaneo system (17). Of course, if $m^2(u_{\min}) \neq m^2(p)$ then $(M^0, M^1) \neq (m^0, m^1)$. In the next Section we consider errors between $u_{\min}$ and p and between (M^0, M^1) and (m^0, m^1).

Remark 2.3. The minimizer $u_{\min}(t, x, v)$ given by (15) is the first nontrivial approximation to $p(t, x, v)$ in the following sense: If we only fix the first moment m^0 then minimizing the $L^2(V)$-norm leads to

$$u^*_{\min}(t, x, v) = \frac{1}{\omega} m^0(t, x).$$

Then $u^*_{\min}$ is the projection of p onto the space of functions constant in v. Then the first moment of this minimizer $u^*_{\min}$ vanishes and it follows from the conservation law (10) that the corresponding moment closure is simply

$$M^0_t = 0.$$

To develop a sequence of approximating functions $(u^*_{\min}, u_{\min}, \dots)$ one can derive equations for higher moments and fix more and more moments in the minimizing procedure. We will do this in [18].

In [15] the Cattaneo system has been studied in $L^2(\Omega)$ with homogeneous Dirichlet or Neumann boundary conditions. Existence of solutions was shown using Stones theorem for skew-adjoint generators (see Pazy [30]). The same argument applies

on an unbounded domain. Using a simple scaling of the space coordinates the generator of the Cattaneo system (17) has the form

$$G := \begin{pmatrix} 0 & -\partial_1 & \cdots & -\partial_n \\ -\partial_1 & 0 & & \\ \vdots & & \ddots & \\ -\partial_n & & & 0 \end{pmatrix}$$

with domain

$$\mathcal{D}(G) := \{(\varphi^0, \ldots, \varphi^n) \in L^2(\mathbb{R}^n)^{n+1} : \ \partial_i\varphi^0, \partial_i\varphi^i \in L^2(\mathbb{R}^n), \ i = 1, \ldots, n\}$$

The operator G is skew adjoint. Therefore it is dissipative, the spectrum belongs to the imaginary axis and it generates a unitary group on $(L^2(\mathbb{R}^n))^{n+1}$. Since the Cattaneo approximation (17) is linear we have global existence:

Lemma 2.4. *For each $(\varphi^0, \varphi^i, i = 1, \ldots, n) \in \mathcal{D}(G)$ there exists a unique global solution (M^0, M^1) of (17) with*

$$(M^0, M^1) \in C^1((-\infty, \infty), L^2(\mathbb{R}^n)^{n+1}) \cap C^0((-\infty, \infty), \mathcal{D}(G)),$$

with $M^0(0) = \varphi^0$ and $M_i(0) = \varphi^i$, $i = 1, \ldots, n$.

2.1. **Boundary Conditions.** The use of this method for bounded domains with boundary conditions has to be considered carefully. It is not obvious, how boundary conditions for transport models translate into boundary conditions of the Cattaneo approximation. We will give two examples for a bounded domain $\Omega \in \mathbb{R}^n$ with smooth boundary $\partial\Omega$. For $x \in \partial\Omega$ we denote the outer normal by $\eta(x)$. We assume V is symmetric with respect to $SO(n)$ and at each $x \in \partial\Omega$ we split V into inward and outward pointing velocities:

$$V^-(x) := \{v \in V : \ v \cdot \eta(x) < 0\}, \quad V^+(x) := \{v \in V : \ v \cdot \eta(x) \geq 0\}.$$

a) Dirichlet boundary conditions: The homogeneous Dirichlet boundary condition for the transport equation (7) reads

$$p(t, x, v) = 0, \quad \forall\, x \in \partial\Omega, \, v \in V^-(x).$$

We stipulate that the energy minimizer $u_{\min}$ constructed in (15) satisfies the same boundary condition

$$m^0(t, x) + \frac{n}{s^2} v \cdot m^1(t, x) = 0, \quad \forall\, x \in \partial\Omega, \, v \in V^-(x).$$

We integrate this boundary condition along V^- and obtain

$$m^0 = \frac{n}{s^2} \frac{2\kappa_V}{\omega} \, \eta \cdot m^1, \quad \text{with} \quad \kappa_V := \int_{\{v \in V : v^1 \geq 0\}} v \, dv \cdot e_1, \tag{19}$$

where e_1 denotes the first unit vector in an orthonormal basis of $\mathbb{R}^n$ and $\omega = |V|$ as usual. Hence the Dirichlet boundary conditions of the Cattaneo approximation are given by

$$M^0 = \frac{n}{s^2} \frac{2\kappa_V}{\omega} \, \eta \cdot M^1. \tag{20}$$

This condition has been suggested by Hadeler [13] and it has been used in [15] for a nonlinear Cattaneo system. It is remarkable that the Dirichlet condition appears in form of a Robin condition for the Cattaneo system. Note that in the parabolic scaling of $s \to \infty, \mu \to \infty$ with $s^2/\mu < \infty$ the homogeneous Dirichlet boundary

condition $M^0 = 0$ follows.

b) Neumann boundary conditions: General reflection boundary conditions for the transport model (7) have the following form:

$$p(t,x,v) = \int_{V^+} B(v,v')p(t,x,v')dv', \quad \forall\, v \in V^-,$$

with a nonnegative symmetric kernel B with $\int_{V^-} B(v,v')dv = \int_{V^+} B(v,v')dv' = 1$. We assume the same boundary condition to hold for the minimizer $u_{\min}$, which leads to

$$\frac{1}{\omega}\left(m^0 + \frac{n}{s^2} v \cdot m^1\right) = \int_{V^+} B(v,v')\frac{1}{\omega}\left(m^0 + \frac{n}{s^2} v' \cdot m^1\right) dv', \quad \forall\, v \in V^-,$$

hence

$$v \cdot m^1 = \int_{V^+} B(v,v') v'\, dv' \cdot m^1, \quad \forall\, v \in V^-. \tag{21}$$

In case of pure physical reflection an outgoing velocity $v' \in V^+$ is reflected into the incoming velocity $v = r(v') := v' - 2(\eta \cdot v')\eta$. In this case the kernel B is given by

$$B(v,v') = \delta_0(v - r(v')),\ v' \in V^+, v \in V^-.$$

Condition (21) reduces to

$$v \cdot m^1 = (v - 2(\eta \cdot v)\eta) \cdot m^1, \quad \forall\, v \in V^-$$

Since on V^- we have $\eta \cdot v \neq 0$ it follows that

$$\eta \cdot m^1 = 0, \quad \text{on} \quad \partial\Omega.$$

Hence the corresponding Neumann boundary condition for the Cattaneo approximation reads

$$\eta \cdot M^1 = 0. \tag{22}$$

Also this boundary condition has been suggested by Hadeler [13].

3. **Error Estimates.**

3.1. **Estimate of u_{min} Versus p.** The $L^2(V)$-norm of the minimizer (15) is

$$\begin{aligned}
\|u_{\min}(t,x,.)\|_2^2 &= \frac{1}{\omega^2}\int_V \left(m^0 + \frac{n}{s^2}(v \cdot m^1)\right)^2 dv \\
&= \frac{1}{\omega^2}\int_V \left((m^0)^2 + 2m^0\frac{n}{s^2}(v \cdot m^1) + \frac{n^2}{s^4}(v \cdot m^1)^2\right) dv \\
&= \frac{1}{\omega^2}\left(\omega(m^0)^2 + \frac{n^2\omega s^2}{s^4 n} m^1 \cdot m^1\right), \\
&= \frac{1}{\omega}\left((m^0)^2 + \frac{n}{s^2}(m^1)^2\right),
\end{aligned} \tag{23}$$

which of course is the L^2 norm of p restricted to the subspace $\langle 1, v_1, \ldots, v_n\rangle$ (see Remark 2.1).

For the L^2-norm of p we have

$$\begin{aligned}
\frac{d}{dt}\|p(t,x,.)\|_2^2 &= 2\int_V p p_t\, dv \\
&= -2\int_V p(v \cdot \nabla)p\, dv - 2\mu\int_V p^2 dv + 2\mu\int_V p\frac{m^0}{\omega} dv,
\end{aligned}$$

which leads to the balance equation

$$\frac{d}{dt}\|p(t,x,.)\|_2^2 + \nabla \cdot F(p) = -2\mu\|p(t,x,.)\|_2^2 + \frac{2\mu}{\omega}(m^0)^2(t,x) \tag{24}$$

with energy flow

$$F(p) = \int_V v\, p^2 dv.$$

Moreover, the negative $L^2(V)$-norm satisfies an H-Theorem, i.e., it is an entropy for equation (7):

Proposition 3.1.

$$\frac{d}{dt}\|p(t,x,.)\|_2^2 + \nabla \cdot F(p) \leq 0. \tag{25}$$

Proof: The right-hand side of (24) can be written as

$$\begin{aligned} -2\mu\|p(t,x,.)\|_2^2 + \frac{2\mu}{\omega}(m^0)^2 &= 2\mu\left(-\int_V p^2 dv + \frac{1}{\omega}\left(\int_V p\, dv\right)^2\right) \\ &= -2\mu\int_V \left(p - \frac{m^0}{\omega}\right)^2 dv \\ &\leq 0. \end{aligned}$$

□

We denote the square of the L^2-norm on $\mathbb{R}^n \times V$ by

$$\mathcal{E}(p) := \int_{\mathbb{R}^n} \|p(t,x,.)\|_2^2 dx$$

and we abbreviate

$$\mathcal{E}^0 = \int_{\mathbb{R}^n}\int_V p(0,x,v)^2 dv\, dx.$$

Theorem 3.2. *Let $p(t,x,v) \in \mathcal{X}$ denote the solution of* (7), (8) *and let $u_{min}(t,x,v)$ denote the minimizer constructed in* (15). *Then for all $t \geq 0$*

$$0 \leq \mathcal{E}(p(t)) - \mathcal{E}(u_{min}(t)) \leq e^{-2\mu t}\mathcal{E}^0 + \frac{1}{\omega}\left(\sup_{0\leq\vartheta\leq t}\|m^0(\vartheta,.)\|_2^2\left(1-e^{-2\mu t}\right) - \|m^0(t,.)\|_2^2\right). \tag{26}$$

Proof: If we integrate the balance equation (24) over $\mathbb{R}^n$ we observe that

$$\frac{d}{dt}\mathcal{E}(p) = -2\mu\mathcal{E}(p) + \frac{2\mu}{\omega}\|m^0(t,.)\|_2^2. \tag{27}$$

Hence

$$\mathcal{E}(p)(t) = e^{-2\mu t}\mathcal{E}^0 + \frac{2\mu}{\omega}\int_0^t e^{-2\mu(t-\vartheta)}\|m^0(\vartheta,.)\|_2^2 d\vartheta \tag{28}$$

Since $u_{\min}$ is a minimizer we have $\|u_{\min}(t,x,.)\|_2 \leq \|p(t,x,.)\|_2$. From (23) we obtain

$$\mathcal{E}(u_{\min}) = \frac{1}{\omega}\left(\|m^0(t,.)\|_2^2 + \frac{n}{s^2}\|m^1(t,.)\|_2^2\right).$$

Then with (28) it follows that

$$0 \leq \mathcal{E}(p) - \mathcal{E}(u) = (I) + (II) + (III)$$

with

$$\begin{aligned}(I) &:= e^{-2\mu t}\mathcal{E}^0\\ (II) &:= \frac{1}{\omega}\left(2\mu\int_0^t e^{-2\mu(t-\vartheta)}\|m^0(\vartheta,.)\|_2^2 d\vartheta - \|m^0(t,.)\|_2^2\right)\\ (III) &:= -\frac{n}{\omega s^2}\|m^1(t,.)\|_2^2.\end{aligned}$$

The first term (I) tends to zero exponentially for $t\to\infty$. The third term (III) is non-positive. We consider the second term (II) in more detail. For this let $y(t) := \|m^0(t,.)\|_2^2$.

$$\begin{aligned}2\mu\int_0^t e^{-2\mu(t-s)}y(s)ds &\le \Big(\sup_{0\le\vartheta\le t} y(\vartheta)\Big)2\mu\int_0^t e^{-2\mu(t-s)}ds\\ &= \Big(\sup_{0\le\vartheta\le t} y(\vartheta)\Big)\left(1-e^{-2\mu t}\right)\end{aligned}$$

Putting all this together we arrive at (26). □

Remark 3.3. 1. The right-hand side of (26) is bounded by

$$\mathcal{E}^0 + \frac{1}{\omega}\sup_{0\le\vartheta\le t}\|m^0(\vartheta,.)\|_2^2.$$

If in addition we know that $\|m^0(t,.)\|_2$ is not decreasing in time, then the right-hand side converges to zero for $t\to\infty$.

2. It follows from (25) and from (27) that $\mathcal{E}(p)$ tends to zero in $L^2(\mathbb{R}^n\times V)$ for $t\to\infty$. Hence solutions converge to zero, which is expected by a dissipative system on the whole of $\mathbb{R}^n$.

3.2. **Estimates of the True Moments** (m^0, m^1) **Versus the Solution of the Cattaneo System** (M^0, M^1)**.** We define

$$r := m^0 - M^0 \quad\text{and}\quad q := m^1 - M^1.$$

¿From the moment equations (10), (11) and from the Cattaneo system (17) it follows that

$$r_t + \nabla\cdot q = 0, \tag{29}$$

$$q_t + \mu q + \frac{s^2}{n}\nabla r = \nabla\cdot(m^2(u) - m^2(p)), \tag{30}$$

$$r(0,.) = 0, \qquad q(0,.) = 0. \tag{31}$$

Integration of the first equation (29) gives $\frac{d}{dt}\int r dx = 0$, hence due to the initial conditions (31) it follows that

$$\int_{\mathbb{R}^n}(m^0 - M^0)(t,x)dx = 0. \tag{32}$$

Integration of the second equation (30) gives $\frac{d}{dt}\int q dx = -\mu\int q dx$ then from the initial conditions (31) it follows that

$$\int_{\mathbb{R}^n}(m^1 - M^1)(t,x)dx = 0. \tag{33}$$

We aim to estimate r and q, in terms of $m^2(u) - m^2(p)$. For this we define another energy

$$\mathsf{e}_s(r,q) := \frac{1}{2}\int_{\mathbb{R}^n} r^2 + \frac{n}{s^2}\,q^2\,dx, \tag{34}$$

which is the L^2- norm in space, where the speed s appears as a parameter.

Lemma 3.4. *Solutions (r,q) of (29)-(31) satisfy the energy estimate*

$$\mathsf{e}_s(r(t,.),q(t,.)) \le \frac{n^2}{2\mu s^2}\sum_{i,j=1}^n \int_0^t \int_{\mathbb{R}^n} e^{-\mu(t-\vartheta)}\Big(\partial_j(m_{ij}(u)-m_{ij}(p))\Big)^2 dx d\vartheta.$$

Proof: We differentiate the energy with respect to time. With Young's inequality we get

$$\begin{aligned}
\frac{d}{dt}\mathsf{e}_s(r,q) &= \int r r_t + \frac{n}{s^2} q\cdot q_t\, dx \\
&= \int -r\nabla\cdot q + \frac{n}{s^2} q\cdot\left(-\mu q - \frac{s^2}{n}\nabla r + \nabla\cdot(m^2(u)-m^2(p))\right) dx \\
&= -\mu\int \frac{n}{s^2} q^2\, dx + \int \frac{n}{s^2}\, q\cdot(\nabla\cdot(m^2(u)-m^2(p)))dx \\
&\le -\mu\int \frac{n}{s^2} q^2\, dx + \frac{\mu}{2}\int \frac{n}{s^2} q^2\, dx + \frac{n}{2\mu}\sum_{i,j=1}^n \int \frac{n}{s^2}\Big(\partial_i(m_{ji}(u)-m_{ji}(p))\Big)^2 dx \\
&\le -\mu\,\mathsf{e}_s(r,q) + \frac{n^2}{2\mu s^2}\sum_{i,j=1}^n \int \Big(\partial_i(m_{ji}(u)-m_{ji}(p))\Big)^2 dx.
\end{aligned}$$

With Gronwall's Lemma the assertion follows. □

Lemma 3.5. *For all $(t,x)\in[0,\infty)\times\mathbb{R}^n$ and all $i,j=1,\dots,n$ we have*

$$\begin{aligned}
|(m^2(u)-m^2(p))(t,x)|_2 &\le b_n s^2 |m^0(t,x)|, \\
|D_\alpha\,(m^2(u)-m^2(p))(t,x)|_2 &\le b_n s^2 |D_\alpha\, m^0(t,x)|,
\end{aligned}$$

where D_α denotes partial derivative with respect to $\alpha\in\{t,x_1,\dots,x_n\}$ and the constant b_n is given in (37).

Proof: Remember that $m_{ij}(u)=\frac{s^2}{n}\delta_{ij}\,m^0=\frac{s^2}{n}\delta_{ij}\int_V p(t,x,v)dv$, hence we can write

$$m_{ij}(u)-m_{ij}(p)=\int B^{ij}_{n,v}p(t,x,v)dv,$$

with the $n\times n$ matrix

$$B_{n,v}:=\frac{s^2}{n}I_n - vv^T,$$

with entries

$$b_{ij}:=B^{ij}_{n,v}=\frac{s^2}{n}\delta_{ij}-v_iv_j.$$

If $i=j$ then $b_{ii}=\frac{s^2}{n}-(v^i)^2$. Since $s=|v|\ge(v^i)^2$ we have $\frac{s^2}{n}-s^2\le b_{ii}\le\frac{s^2}{n}$. Hence

$$|b_{ii}|\le s^2,\ \text{for}\ \ n=1,\quad\text{and}\quad |b_{ii}|\le s^2\frac{n-1}{n},\ \text{for}\ n\ge 2. \tag{35}$$

If $i\neq j$ then $b_{ij}=-v_iv_j$. Since $-\frac{1}{2}((v_i)^2+(v_j)^2)\le v_iv_j\le\frac{1}{2}((v_i)^2+(v_j)^2)$ it follows that

$$|b_{ij}|\le\frac{s^2}{2}. \tag{36}$$

For now we denote the vector-norms in $\mathbb{R}^n$ by $|.|_2$ and $|.|_\infty$. Then we have for $n\ge 2$ that

$$|B_{n,v}|_2\le\sqrt{n}|B_{n,v}|_\infty\le\sqrt{n}(n-1)\frac{n+2}{2n}\ s^2=:b_ns^2 \tag{37}$$

and the same estimate $|B_{n,v}| \le b_n s^2$ with $b_n = 1$ for $n = 1$. Then for each vector $\zeta \in \mathbb{R}^n$ we have

$$\begin{aligned} |(m^2(u) - m^2(p))(t,x)\zeta|_2 &= \left| \int B_{n,v} \zeta p \, dv \right|_2 \\ &\le b_n s^2 \left| \zeta \int_V p(t,x,v) dv \right|_2 \\ &= b_n s^2 |m^0(t,x)| \, |\zeta|_2. \end{aligned}$$

The same lines apply for $D_\alpha(m^2(u) - m^2(p))$. □

Together with Lemma 3.4 we arrive at the following result:

Theorem 3.6. *The solution* (r,q) *of* (29)-(31) *satisfies for each* $t \ge 0$

$$\mathsf{e}_s(r(t,.),q(t,.)) \le n^2 b_n^2 \frac{s^2}{2\mu} \|\nabla_x m^0\|^2_{L^2([0,t]\times\mathbb{R}^n)}. \tag{38}$$

Remark 3.7.
1. Here the L^2 norm of the differences in the first two moments is estimated by the norm of ∇m^0. If the gradient of m^0 is small, we obtain a good approximation. Some experimental setups for bacteria are designed for shallow gradients (see e.g. Chen *et al.* [8]). Patlak [29] derived the classical PKS-model for chemosensitive movement under the assumption, that on an average distance traveled by particles between turns, the change in particle distribution – hence $\|\nabla m^0\|$ – is small.
2. In contrast to parabolic approximations the estimate (38) is valid for all times $t \ge 0$. This motivates us to use the Cattaneo model for short time periods and parabolic models for longer times periods and for asymptotics (see also [9]).

4. **The Nonlinear Case: Reaction Transport Equations.** Here we consider the nonlinear reaction transport equation:

$$p_t + v \cdot \nabla p = \mu\Big(\frac{m^0}{\omega} - p\Big) + f(v,p,m^0), \tag{39}$$

where f describes birth, death and interaction of particles. We choose f such that the reaction transport equation (39) admits a solution semigroup in $L^2(\mathbb{R}^n \times V)$. This certainly is the case if f is continuous and linearly bounded in p. Again we formulate the equations for the first moments m^0, m^1 and m^2.

$$\begin{aligned} m^0_t + \nabla \cdot m^1 &= g \\ m^1_t + \nabla \cdot m^2 &= -\mu m^1 + h \end{aligned}$$

with the v-moments of f

$$g(t,x) = \int_V f(v,p,m^0)\, dv, \qquad h(t,x) = \int_V v\, f(v,p,m^0)\, dv.$$

To find an appropriate expression for m^2, we again minimize the $L^2(V)$-norm with the same constraints as in the previous sections. Hence we continue with the minimum given in (15). Again the second moment of the minimizer $u_{\min}$ is given by (16) and a semilinear Cattaneo system follows

$$\begin{aligned} M^0_t + \nabla \cdot M^1 &= G \\ M^1_t + \tfrac{s^2}{n} \nabla M^0 &= -\mu M^1 + H, \end{aligned} \tag{40}$$

where now

$$G(t,x) = \int_V f(v,U,M^0)\,dv, \qquad H(t,x) = \int_V v\, f(v,U,M^0)\,dv,$$

with

$$U = \frac{1}{\omega}\Big(M^0 + \frac{n}{s^2}(v\cdot M^1)\Big).$$

In case of reactions, which are independent of the actual velocity, $f = f(m^0)$, we have

$$H = \int_V v f(M^0)dv = 0 \quad \text{and} \quad G = \int_V f(M^0)dv = \omega\, f(M^0).$$

Then a semilinear Cattaneo system follows which has been studied qualitatively in [15]:

$$\begin{array}{rcl} M^0_t + \nabla\cdot M^1 &=& \omega f(M^0) \\ M^1_t + \frac{s^2}{n}\nabla M^0 &=& -\mu M^1. \end{array} \tag{41}$$

5. **Transport Equations for Chemosensitive Movement.** The two independent parameters in the general velocity jump process (1) are the turning rate μ and the distribution kernel T, which describe the probability of changing from velocity v' to velocity v. In the case of bacterial chemotaxis bacteria can significantly change their turning rate in response to external stimuli, but they do not change their turn angle distribution ([5]). Hence we modify the turning rate to derive a model for chemosensitive movement. As in the 1-D model (see the review [17]), the turning rate should depend on the velocity v, on the concentration of the external signal S, and on its gradient ∇S

$$\mu = \mu(v, S, \nabla S).$$

It is, however, clear that bacteria are too small to measure concentration gradients along their body axis. They measure gradients while moving through them. Then the turning rate depends not directly on ∇S but on the directional derivative

$$\delta_v S := S_t + v\cdot\nabla S.$$

This assumption has also been used by Alt [2] and by Grünbaum [11] (To see that $\delta_v S$ is the correct term consider a Taylor series expansion of the difference in the signal concentrations at (x,t) and at $(x+v\Delta t, t+\Delta t)$ for a small time increment Δt). If the chemical concentration equilibrates fast compared to the movement of the species then $S(t,x)$ would be close to equilibrium in each time step and we can assume $\delta_v S = v\cdot\nabla S$. This quasi-steady state assumption for the signal has been used e.g. by Jäger and Luckhaus [21] for the PKS-model. Here we continue to consider the full characteristic derivative $\delta_v S$. It will turn out that in the parabolic scaling the S_t-term is of lower order and it vanishes for the parabolic limit equation. We assume

$$\mu = \mu(S, \delta_v S). \tag{42}$$

We choose a kernel $K(v,v')$ in such a way that the total particle number is preserved. This can be achieved with $K(v,v') = \mu(S,\delta_{v'}S)T(v,v')$ with $\int_V T(v,v')dv = 1$. Then the transport equation for chemosensitive movement reads

$$p_t + v\cdot\nabla p = -\mu(S,\delta_v S)\,p(v) + \int_V \mu(S,\delta_{v'}S)\,T(v,v')\,p(v')dv'. \tag{43}$$

Restricted to 1-D with two speeds $\pm s$ the 1-D model considered in [17] follows.

To become more specific and to have an explicit prototype we consider

$$\mu(S, \delta_v S) = \mu_0(1 - \alpha(S)\delta_v S) \tag{44}$$

with some constant $\mu_0 > 0$ and an appropriate function $\alpha(S)$. We will write α instead of $\alpha(S)$ throughout the following calculations. If we assume moreover that $T(v, v') = 1/\omega$, then a prototype model for chemosensitive movement reads

$$p_t + v \cdot \nabla p = -\mu_0(1 - \alpha\delta_v S)\, p(v) + \frac{\mu_0}{\omega} \int_V (1 - \alpha\delta_{v'} S)\, p(v')\, dv'. \tag{45}$$

5.1. **A Cattaneo Model for Chemosensitive Movement.** Using the notation of the moments m^0 and m^1 we can write (45) equivalently as

$$p_t + v \cdot \nabla p = -\mu_0 \left(1 - \alpha(S_t + v \cdot \nabla S)\right) p(v) + \frac{\mu_0}{\omega} \left(m^0 - \alpha m^0 S_t - \alpha m^1 \cdot \nabla S\right). \tag{46}$$

To derive the equations for the first two moments we integrate (46) and obtain

$$m^0_t + \nabla \cdot m^1 = 0. \tag{47}$$

Multiplication of (46) with v and integration gives

$$m^1_t + \nabla \cdot m^2 = -\mu_0(1 - \alpha S_t)m^1 + \mu_0 \alpha \nabla S \cdot\ m^2. \tag{48}$$

Again with (16) the corresponding Cattaneo system for chemosensitive movement reads

$$\begin{array}{rcl} M^0_t + \nabla \cdot M^1 & = & 0 \\ M^1_t + \frac{s^2}{n} \nabla M^0 & = & -\mu_0(1 - \alpha S_t)M^1 + \frac{s^2}{n} \mu_0 \alpha \nabla S\, M^0. \end{array} \tag{49}$$

To obtain a parabolic limit we divide the second equation of (49) by μ_0 and consider the limit of

$$\mu_0, s \to \infty, \quad \alpha \to 0, \quad \frac{s^2}{\mu_0 n} \to D < \infty, \quad \mu_0 \alpha \to \chi < \infty.$$

Note that χ depends on S via $\alpha(S)$. We divide the second equation of (49) by μ_0 and in the above limit the S_t-term vanishes. Formally, the second equation of (49) becomes

$$M^1 = -D\nabla M^0 + D\chi(S)M^0 \nabla S. \tag{50}$$

Hence the limiting equation is the Patlak-Keller-Segel model:

$$M^0_t = D\nabla(\nabla M^0 - \chi(S)M^0 \nabla S). \tag{51}$$

Remark 5.1.

1. The prototype chemotaxis model (45) leads to the well-known Keller-Segel model in two steps: First closure of the first two-moment equations to get the Cattaneo approximation (49), and then passing to the parabolic limit for fast speeds and large turning rates.
2. As shown by Patlak [29] or Alt [2] and also in [20] one can directly scale the transport equation to derive the parabolic limit (51). If we use the expression for M^1 in (50) to calculate the minimizer u given in (15) we arrive at an *ad hoc* assumption which was made by Patlak or Alt. In the framework of moment closure the assumption of Patlak and Alt can be justified *a posteriori*.

5.2. **A Chemotaxis Model with Density Control.** In [28] a parabolic chemotaxis model with density control mechanism is introduced and investigated. The density control leads to the effect that at high population densities the chemotaxis is turned off and pure diffusion dominates. Solutions exist globally and no blow-up occurs. The model in [28] can be constructed from a transport equation via a corresponding Cattaneo approximation. We consider a turning rate of the form

$$\mu(S, \delta_v S) := \mu_0 \left(1 - \frac{n}{s^2}\beta(m^0)\chi(S)\delta_v S\right),$$

where $\beta(m^0)$ is a density dependent sensitivity. The function β is assumed to have a zero at some $m^* > 0$ and $\beta(m) > 0$ for $0 < m < m^*$ (see the details in [28]). With turning kernel $T(v, v') := \omega^{-1}\mu(S, \delta_{v'} S)$ the moment closure procedure leads to a *Cattaneo model for chemosensitive movement with density control*

$$\begin{aligned} M^0_t + \nabla \cdot M^1 &= 0 \\ M^1_t + \tfrac{s^2}{n}\nabla M^0 &= -\mu_0 \left(1 - \tfrac{n}{s^2}\beta(M^0)\chi(S)S_t\right) M^1 + \beta(M^0)\chi(S)\, M^0\, \nabla S. \end{aligned} \tag{52}$$

The parabolic limit of this equation is the model which was studied in [28]. The Cattaneo model for chemosensitive movement (52) was used in [9] to model aggregations in *Dictyostelium discoideum*, in *Eschirichia coli*, and *Salmonella typhimurium*. In [9] also a second-order numerical scheme is given.

6. **Discussion.** The Cattaneo model was introduced in 1948 by C. Cattaneo into heat transport theory. It was later used to model heat transport with finite speed. Since the early 1990's the Cattaneo model was discussed related to biological applications. In one space dimension the Cattaneo model is equivalent to a transport equation. But this is not true for 2 or more space dimensions. Even worse - in two or more dimensions there is no random walk which would lead directly to the Cattaneo model (the result in [26] is not convincing). It appears that kinetic models and Cattaneo models in higher dimensions are two types of models for similar processes and it was long unclear how these models were related.

With the moment closure procedure presented here a relation is established. The Cattaneo model is a closed moment system of a kinetic equation. We find that the negative L^2 norm is an entropy and we describe an algorithm to derive the Cattaneo model. In addition, the closure method is used to derive the "correct" boundary conditions for the Cattaneo model. Moreover we show that the Cattaneo approximation is good for shallow gradients.

Since the closure problem is well known in transport theory there are a large number of arguments based on expansions, projections, scaling properties, or logical insight to close the first two-moment equations for m^0 and m^1. Here, minimizing an appropriate energy motivates the choice of the approximation to the second moment $m^2(p)$. This method is directly generalizable to equations for arbitrarily high moments $(m^0, m^1, \ldots, m^k)$. We will present this in another paper [18].

The Cattaneo approximation developed here gives a new model for applications which can be used to understand the behavior of biological systems for short times without using the full transport equation. It is well known that at large times the transport equation and the Cattaneo system behave as their parabolic limit. This explains the success of reaction diffusion equations in mathematical biology. However, there is no doubt that for small or intermediate values of time the diffusion model is inaccurate. For those time ranges the Cattaneo approximation helps to

understand the dynamic behavior of the biological system. The relevant parameters of the Cattaneo approximation can be estimated directly from experiments.

6.1. **Memory Effects.** Gurtin and Pipkin ([12]) show that the Cattaneo system appears if the medium under consideration "remembers" its history with exponentially decay backwards in time. This interpretation can be extended to the following fact:

Lemma 6.1. *The Cattaneo system* (17) *is the minimizing flux of the exponentially weighted Dirichlet integral*

$$J(u) := \frac{D}{2\tau} \int_0^t \int_\Omega e^{-\frac{1}{\tau}(t-s)} |\nabla u|^2 dx ds.$$

Proof: The minimizing flux of J is given by the solution of

$$u_t = -\nabla j$$

with

$$j = \frac{D}{\tau} \int_0^t e^{-\frac{1}{\tau}(t-s)} \nabla u \, ds.$$

Hence j satisfies the Cattaneo law:

$$\tau j_t = -j + D\nabla u.$$

□

6.2. **Numerical Simulations.** For illustration purposes we show some numerical simulations of the Cattaneo model for chemosensitive movement with density control (52).

In Figures 1 and 2 we consider an interval of length $l = 1$ with homogeneous Neumann boundary conditions (22) and we assume that the species move with constant speed $\gamma = 0.2$. The turning rates $\mu^\pm$ are density dependent as discussed in Section 5.2:

$$\mu^\pm(S, \nabla S, u^+ + u^-) = \left(\frac{\gamma^2}{2D} \mp \beta(u^+ + u^-)\chi(S)\nabla S \right)^+,$$

with effective diffusion coefficient $D = 0.036$. The superscript + indicates to take the positive part. The density-sensitivity function β and the chemotactic sensitivity χ are given as $\beta(u) = 1 - u$ and $\chi(S) = 1/(1 + S)$. The parameters for the signal equation are of the form $\tau = 1, \alpha = 4 \cdot 10^{-6}$ and the reproduction term is $f(S, u^+ + u^-) = -aS + u^+ + u^-$. For simulations we use a Godunov-scheme (see also [17]). In Fig. 1 we show the long-time behavior in absence of signal degradation ($a = 0$), whereas in Fig. 2 we assume that there is a small decay rate of $a = 0.001$. The initial conditions in both runs are random perturbations of 0.3% of the constant level $u^\pm = 0.3$ and S is assumed to be initially constant at a low level of $S_0 = 0.5$.

The simulation in Fig. 1 shows transient patterns, which eventually decays to the homogeneous steady state. This is in good agreement with observations on bacteria as shown by Tyson *et al.* [36]. The second simulation (with decay of S) shows the same initial patterns, which eventually coarsen, and a global pattern remains. The transient behavior in Fig.1 can be explained by a linear stability

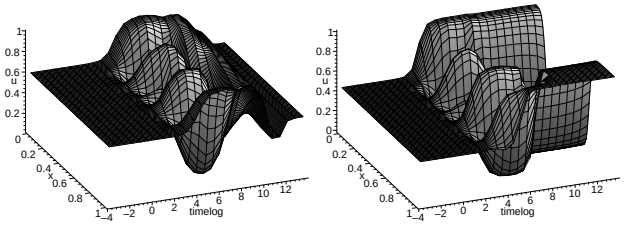

FIGURE 1. Long-time evolution of the total particle density $u = u^+ + u^-$ in a time-logarithmic plot without degradation of S (left) and with degradation of S (right).

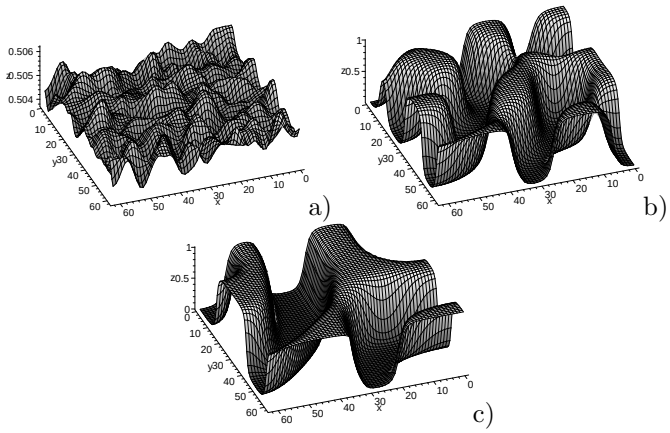

FIGURE 2. Typical time evolution. Particle density shown for a) $t = 1$, b) $t = 150$, and c) $t = 500$.

analysis of homogeneous solutions. For $a \neq 0$ a stationary homogeneous solution $(\bar{u}^+, \bar{u}^-, \bar{S})$ with $\bar{u}^+ = \bar{u}^-$ is linearly unstable, if

$$\gamma(\pi^2\alpha + a) < 2\bar{u}^+\beta(2\bar{u}^+)\chi(\bar{S}). \tag{53}$$

The chemotactic sensitivity $\chi(S)$ has been chosen to converge to 0 as $S \to \infty$. Hence in the beginning of the simulation of Fig.1 the homogeneous solution is linearly unstable, whereas later, when S increases drastically, the chemotaxis term fades out, the diffusion dominates, and the homogeneous steady state becomes linearly stable.

In two space dimensions we developed a numerical scheme for the Cattaneo model for chemosensitive movement (52) in [9]. The algorithm is based on a Lax-Wendroff scheme. Here a typical time evolution is shown for randomly chosen initial data with constant χ and $\beta = 1 - u$:

In Figure 2 one clearly observes merging local maxima and coarsening of the pattern. The dynamics of these patterns and the underlying bifurcations are currently being investigated [31].

REFERENCES

[1] W. Alt. Biased random walk model for chemotaxis and related diffusion approximation. *J. Math. Biology*, 9:147–177, 1980.

[2] W. Alt. Singular perturbation of differential integral equations describing biased random walks. *J. reine angew. Math.*, 322:15–41, 1981.

[3] L. Arlotti, N. Bellomo, and E. De Angelis. Generalized kinetic (Boltzmann) models: mathematical structures and applications. *Math. Mod. Meth. Appl. Sci.*, 12:567–592, 2002.

[4] N. Bellomo and A. Bellouquid. From a class of kinetic models to the macroscopic equations for multicellular systems in biology. *Discrete and Cont. Dyn. Syst. Series B*, 2003. submitted.

[5] H.C. Berg. *Random Walks in Biology*. Princeton University Press, 1983.

[6] C. Cattaneo. Sulla conduzione de calore. *Atti del Semin. Mat. e Fis. Univ. Modena*, 3:83–101, 1948.

[7] C. Cercignani, R. Illner, and M. Pulvirenti. *The Mathematical Theory of Diluted Gases*. Springer, New York, 1994.

[8] K.C. Chen, R.M. Ford, and P.T. Cummings. Perturbation expansion of Alt's cell balance equations reduces to Segel's 1d equation for shallow chemoattractant gradients. *SIAM J. Appl. Math.*, 59(1):35–57, 1999.

[9] Y. Dolak and T. Hillen. Cattaneo models for chemotaxis, numerical solution and pattern formation. *J. Math. Biol.*, 46(2):153–170, 2003.

[10] R.M. Ford and D.A. Lauffenburger. Measurement of bacterial random motility and chemotaxis coefficients: II. application of single cell based mathematical model. *Biotechnol. Bioeng.*, 37:661–672, 1991.

[11] D. Grünbaum. Advection-diffusion equations for internal state-mediated random walks. *SIAM J. Appl. Math.*, 61:43–73, 2001.

[12] M.E. Gurtin and A.C. Pipkin. A general theory of heat conduction with finite wave speed. *Arch. Rational Mech. Anal.*, 31:113–126, 1968.

[13] K.P. Hadeler. Reaction telegraph equations and random walk systems. In S.J. van Strien and S.M. Verduyn Lunel, editors, *Stochastic and Spatial Structures of Dynamical Systems*. Royal Academy of the Netherlands, 1995.

[14] K.P. Hadeler. Reaction transport systems. In V. Capasso and O. Diekmann, editors, *Mathematics inspired by biology*, pages 95–150. CIME Letures 1997, Florence, Springer, 1998.

[15] T. Hillen. Qualitative analysis of semilinear Cattaneo systems. *Math. Models Meth. Appl. Sci.*, 8(3):507–519, 1998.

[16] T. Hillen. *Transport Equations and Chemosensitive Movement*. University of Tübingen, 2001. Habilitation thesis.

[17] T. Hillen. Hyperbolic models for chemosensitive movement. *Math. Models Methods Appl. Sci.*, 12(7):1007–1034, 2002.

[18] T. Hillen. On the L^2-closure of transport equations: The general case. *Discrete and Cont. Dyn. Syst. Series B*, 2003. accepted.

[19] T. Hillen. Transport equations with resting phases. *Europ. J. Appl. Math.*, 14(5):613–636, 2003.

[20] T. Hillen and H.G. Othmer. The diffusion limit of transport equations derived from velocity jump processes. *SIAM J. Appl. Math.*, 61(3):751–775, 2000.

[21] W. Jäger and S. Luckhaus. On explosions of solutions to a system of partial differential equations modelling chemotaxis. *Trans. AMS*, 329:819–824, 1992.

[22] D.D. Joseph and L. Preziosi. Heat waves. *Reviews of Modern Physics*, 61:41–73, 1988.

[23] E.F. Keller and L.A. Segel. Initiation of slime mold aggregation viewed as an instability. *J. Theor. Biology*, 26:399–415, 1970.

[24] C.D. Levermore. Moment closure hierarchies for kinetic theories. *J. Stat. Phys.*, 83:1021–1065, 1996.

[25] I. Müller and T. Ruggeri. *Rational Extended Thermodynamics*. Springer, New, York, 2nd edition, 1998.

[26] E. Orsingher. A planar random motion governed by the two dimensional telegraph equation. *J. Appl. Prob.*, 23:385–397, 1986.

[27] H.G. Othmer, S.R. Dunbar, and W. Alt. Models of dispersal in biological systems. *J. Math. Biol.*, 26:263–298, 1988.

[28] K. Painter and T. Hillen. Volume-filling and quorum-sensing in models for chemosensitive movement. *Canadian Appl. Math. Quart.*, 10:501–543, 2002.

[29] C. S. Patlak. Random walk with persistence and external bias. *Bull. Math. Biophys.*, 15:311–338, 1953.
[30] A. Pazy. *Semigroups of Linear Operators and Applications to Partial Differential Equations*. Springer, New York, 1983.
[31] A. Potapov and T. Hillen. Metastability in chemotaxis models. *J. Dynamics Diff. Eq.*, 2003. submitted.
[32] C. Ringhofer, C. Schmeiser, and A. Zwirchmayr. Moment methods for the semiconductor Boltzmann equation on bounded position domains. *SIAM J. Num. Ana.*, 39(3):1078–1095, 2001.
[33] M.J. Schnitzer. Theory of continuum random walks and applications to chemotaxis. *Physical Rev. E*, 48:2553–2568, 1993.
[34] H. Schwetlick. *Reaktions-Transportgleichungen*. PhD thesis, Uni. Tübingen, 1998.
[35] D.W. Stroock. Some stochastic processes which arise from a model of the motion of a bacterium. *Probab. Theory Rel. Fields*, 28:305–315, 1974.
[36] R. Tyson, S.R. Lubkin, and J.D. Murray. A minimal mechanism for bacterial pattern formation. *Proc. R. Soc. London B*, 266:299–304, 1999.

Received June 2003; revised November 2003; final version April 2004.

E-mail address: thillen@ualberta.ca