FINITE SPEED TRANSPORT

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ABSTRACT

Effective finite transport speeds are crucial to many situations of great industrial and medical importance. Traditional finite speed transport models are critically reviewed and new models are introduced. It is concluded that realistic finite speed models with constant coefficients cannot be local in space and are either local in phase-space or non local in space; models with time-dependent coefficients are also considered.

1. INTRODUCTION

The short time behaviour of many transport phenomena of great industrial and medical importance (Klossika et al., 1996; Kumar and Mitra, 1999; Chen et al., 2004; Banerjee et al., 2005; Dumett et al., 2005; Itina et al., 2005) reveals the existence of an effective finite upper bound for transport speed. Traditional nineteenth century macroscopic models (Landau and Lifschitz, 1987) cannot be used to model such transport phenomena because these models are all based on parabolic differential equations (Sommerfeld, 1978) and, thus, allow infinite speed transport. The standard way out of this difficulty is to replace these models by other, still macroscopic ones, in which transport is now described by hyperbolic differential equations; these new models are usually based either on Cattaneo's seminal work (Cattaneo, 1948) or on the more modern extended thermodynamics framework (Müller and Ruggeri, 1993; Jou et al., 1996). It is however well known that these new macroscopic finite speed models suffer from theoretical inconsistencies (Israel, 1987; Müller and Ruggeri, 1993) and have been at least partially invalidated by experiments on shock waves in gas (Israel, 1987).

The aim of this contribution is to review the shortcomings of these models and to propose alternative solutions. For simplicity sake, the discussion is restricted to matter transport. We consider strict finite speed microscopic models based on Markov stochastic processes. These models are local in phase-space and describe transport through a so called Kolmogorov (or Fokker-Planck) equation. Explicit computations show that the finite speed effects of these diffusions cannot be captured by effective macroscopic local models with constant coefficients. This striking conclusion extends to more general microscopic finite speed transport models based on Boltzmann like equations.

One is thus left with the following alternatives. Strict finite speed can be enforced, either in finite speed microscopic models, which can be chosen as local in phase space, or in non local macroscopic models (Balescu, 1997; Dunkel, Talkner and Hänggi, 2007). Another solution is to enforce an effective apparent finite speed on the time behaviour on the experimentally relevant macroscopic fields only; this can be done by introducing time-dependent transport coefficients (Debbasch and Rivet, 2007) in purely macroscopic effective models.

2. NINETEENTH CENTURY MODELS

The macroscopic nineteenth century models describe the instantaneous state of a system by a collection of time- and space-dependent fields (temperature, particle or mass density, velocity, ...) and model transport phenomena by assuming a local linear relation between the fluxes and the gradient of these fields (Landau and Lifschitz, 1987). These relations, when used in conjunction with equations of motion, lead to parabolic macroscopic transport equations which allow finite speed transport. Standard examples are Fourier and Fick laws, which lead to the standard heat and diffusion equations. Note that the Navier-Stokes equation is another example, obtained by modelling momentum transport through viscous stresses proportional to velocity gradients. In all cases, the coefficients linking the fluxes to the gradients are taken as constants.

The remainder of this article is devoted to understanding how these models should be modified to take into account finite speed effects. Having this task in mind, let us here recall that traditional nineteenth century transport models can be given a microscopic justification, at least when dealing with dilute gases. Indeed, the dynamics of dilute gases is traditionally described by Boltzmann equation (Huang, 1987), which fixes the time evolution of the so-called one particle distribution in phase-space. This equation can be solved approximately by the Chapman-Enskog method in near equilibrium situations where all macroscopic fields vary on typical length and time scales much greater than the mean free path and the mean collision time of the gaz particles (Chapman and Cowling, 1970; Huang, 1987). The expansion is controlled by a single small parameter ε and it turns out that macroscopic fields corresponding to such a solution obey, at least at first order in ε, the standard proportionality laws between fluxes and gradients.

The problem of finding alternatives to these laws has thus two aspects. One is to find macroscopic models which correctly take into account finite speed effects; the other is to link these alternative macroscopic models to already existing or new microscopic models. These to aspects are discussed below.

3. ALTERNATIVE LOCAL MACROSCOPIC MODELS

All models used in the literature originate with Cattaneo's seminal work (Cattaneo, 1948). Cattaneo adresses heat transport and suggests to convert the parabolic heat equation into a hyperbolic telegraph equation by adding to the traditional parabolic equation a contribution proportional to the second time derivative of the temperature. This idea has later been developed and expanded by various authors into what is currently known as the extended thermodynamics framework (Müller and Ruggeri, 1993; Jou et al., 1996). The qualificative "extended" is used because the framework suggests that undesired parabolic character of the traditional 19th century models comes from the fact that these models do not retain enough macroscopic fields to describe the instantaneous state of a system. Indeed, extended thermodynamics shows that choosing judiciously the number of retained macroscopic fields and the constitutive relations between these fields automatically leads to hyperbolic macroscopic differential equations. Cattaneo's proposal now appears as a simplification of the simplest extended thermodynamical model of diffusion (Müller and Ruggeri, 1993).

The just described extension of traditional models has, at least for dilute gases, a microscopic interpretation. Grad (1949) has indeed suggested an original expansion method for solving approximately the Boltzmann equation and truncations of this method at different orders deliver, at the macroscopic level, the various extended thermodynamics theories of dilute gases; the number of macroscopic fields retained by each of these theories depends on the order of the associated truncation of the Grad expansion; the simplest extended thermodynamics theory of dilute gases (Müller and Ruggeri, 1993) uses 13 macroscopic fields to describe a single constituent gaz (instead of the 5 retained by the standard 19th century description), the second simplest theory retains 20 fields.

The extended thermodynamics framework and the associated Grad expansion undoubtedly offer interesting models of finite speed transport phenomena. But they also present serious shortcomings. On a purely practical side, the rather large number of macroscopic field retained by all extended thermodynamical theories to model even the simplest systems certainly does not make the theories particularly easy to use. But there are more fundamental problems. The first one is related to the fact that the Grad expansion, unlike the Chapman Enskog one, does not contain any small parameter. The order at which the Grad expansion is truncated thus seems rather arbitrary, as does therefore the number of macroscopic fields in which an extended thermodynamical theory encodes the state of the system. One might thus imagine that the predictions of these theories get better and better as the number of retained fields is increased. Unfortunately, this does not seem to be the case, and some predictions even appear to diverge (Müller and Ruggeri, 1993) with the number of fields (or, if one prefers, with the order at which the Grad expansion is truncated). Finally, experiments performed on shock waves in Argon for Mach numbers up to at least 10 appear, not only to contradict the existing extended thermodynamical theories, but rather to support traditional 19th century models (Israel, 1987).

Thus, extended thermodynamics theories do model finite speed transport, but they do not appear to do so in a realistic and conceptually consistent manner. As far as their status is concerned, both traditional parabolic and modern extended thermodynamics models are macroscopic and local, and they use constant transport coefficients. It thus seems logical to relax at least one of this characteristics to try and build finite speed transport models.

4. MICROSCOPIC MODELS WITH BOUNDED SPEED

4.1 The models

For simplicity sake, we now restrict the discussion to matter transport *i.e.* diffusion and consider the simplest case where the diffusing particles do not interact with each other. The simplest microscopic diffusion models of non interacting particles are stochastic Markov process in the one particle phase space. A standard example is the Langevin model (Reif, 1965), where the momentum of the diffusing particle undergoes an Ornstein-Uhlenbeck process with constant friction and noise coefficients. This model does not bound particle velocities. There are two equivalent ways of modifying the Langevin equation to obtain a process with strictly bounded velocities. The first one consists in modifying the equation of motion obeyed by the particle momentum; this practically amounts to allowing the friction and noise coefficients to become momentum dependent; the inconvenience of this approach is that this momentum dependence cannot be chosen arbitrarily, and that imposing bounded velocities does not transcribe into simple intuitive relations obeyed by both coefficients. The other method is to change variable and replace momentum by another vector, say $\mathbf{u}$, with arbitrary prescribed dynamics, the bound on velocities being enforced by the very definition of momentum in terms of the new variable $\mathbf{u}$. One of the easiest implementation of this idea is the following class of stochastic differential equations:

$$\left\{ \begin{array}{rcl} d\mathbf{x}_t &=& c_m\ \phi(\mathbf{u}^2)\mathbf{u}dt \\ & & \\ d\mathbf{u}_t &=& -\alpha(\mathbf{u})\mathbf{u}dt + \sqrt{2D(\mathbf{u})}d\mathbf{B}_t \end{array} \right. \tag{1}$$

where ϕ is any sufficiently regular function which map $\mathbb{R}^+$ unto $(0;1)$. (so that $\mid \phi(\mathbf{u}^2) \mid \leq 1$ for all $\mathbf{u} \in \mathbb{R}^3$). The maximum velocity c_m and the coefficients α and D can be chosen arbitrarily to best describe the physics one is interested in. These models are directly inspired by the Relativistic Ornstein-Uhlenbeck process (Debbasch et al., 1997) and several of its generalizations (Debbasch, 2004; Chevalier and Debbasch, 2007b; Franchi and Le Jan, 2007; Dunkel and Hänggi, 2005). These have been introduced to model diffusions of relativistic point masses for which $c_m = c$, the velocity of light in vacuo; the choice $\phi(\mathbf{u}^2) =$

$1/\gamma(\mathbf{u}^2)$ with $\gamma(\mathbf{u}^2) = \sqrt{\mathbf{u}^2 + 1}$ is natural in this context, provided there is no gravitation.

The simplest choice of phase-space is $\mathbb{R}^6 = \{(\mathbf{x}, \mathbf{u})\}$ equipped with the Lebesgue measure $d^3x d^3u$ and (1), interpreted in the Stratonovich sense, leads to the following transport equation for the one particle distribution f :

$$\partial_t f + \partial_{\mathbf{x}} \cdot \left(c_m\ \phi(\mathbf{u}^2)\mathbf{u} f\right) - \partial_{\mathbf{u}} \cdot (\alpha(\mathbf{u})\mathbf{u} f) = \partial_{\mathbf{uu}}(D(\mathbf{u})f). \quad (2)$$

This equation is called a Kolmogorov (sometimes Fokker-Planck) equation. It shows that the model is local in the one particle phase-space. Suppose now for example that one wishes to describe a situation where the moving particle diffuses through its interactions with a fluid in thermal equilibrium and that these interactions thermalize the particle with the fluid. The simplest model is obtained by choosing a constant noise coefficient D_0 and the condition that the (unnormalized) Maxwell distribution :

$$f_M(\mathbf{u}) = \exp\Big(-\frac{m c_m^2}{2k_B T}\psi(\mathbf{u}^2)\Big), \quad (3)$$

with $\psi(\mathbf{u}^2) = \left(\phi(\mathbf{u}^2)\right)^2 \mathbf{u}^2$, be a solution of (2) reads :

$$\frac{\alpha(\mathbf{u})}{D_0} = \frac{m c_m^2}{k_B T}\psi'(\mathbf{u}^2), \quad (4)$$

where k_B is the Boltzmann's constant. This last equation is a fluctuation dissipation relation and generalizes the standard Langevin result to this finite speed diffusion process. Similar relations can naturally be obtained in the relativistic context (see for example Debbasch et al. (1997); Chevalier and Debbasch (2007a) for fluctuation dissipation relations obeyed by relativistic cosmological diffusions). Note also that models of this kind can easily be extended to include all sorts of transport phenomena in fluids; this can be done by introducing a generalized Boltzmann equation where the role played by velocities in the standard equation is now played by other variables whose definitions ensure that all velocities remain bounded; the relativistic Boltzmann equation (Israel, 1987) is constructed in this manner and can serve as an example of how to implement this general procedure.

4.2 Their large scale, macroscopic behaviour

The large scale behaviour of models of type (1) with $\phi(\mathbf{u}^2) = 1/\gamma(\mathbf{u}^2) = 1/\sqrt{\mathbf{u}^2+1}$ was first investigated in Debbasch and Rivet (1998) by a Chapman-Enskog expansion. The most recent and thorough contribution is Angst and Franchi (2007), where the large scale dynamics is assimilated with the asymptotic time behaviour of the stochastic processes (1). The striking conclusions obtained both in Debbasch and Rivet (1998) and Angst and Franchi (2007) is that, for sufficiently regular functions α and D, the law of the processes always coincide, up to a multiplicative constant, with the law of a Brownian motion; the associated particle density then obeys the standard diffusion equation, which is parabolic and does not bound transport speeds. Note that the same kind of conclusion was obtained long ago on the relativistic Boltzmann equation (Israel, 1987). In fact, this equation bounds all velocities by the velocity of light in vacuo, but the hydrodynamical equations obtained from the relativistic Boltzmann equation through a Chapman-Enskog expansion allow transport at infinite speed.

The above conclusion is perhaps surprising, but physically meaningful and actually intuitive. Indeed, macroscopic finite speed effects are known to be short time effects, and it thus makes sense that an effective long time dynamics is unable to reproduce these effects. The root of the difficulty one encounters in trying to build macroscopic models of finite speed macroscopic effects in transport is precisely that the only regime for which we know how to isolate an effective large scale, macroscopic dynamics from the the small scale one is the long time regime, where effective finite speed effects are not expected to play any significant role.

5. POSSIBLE MODELS OF FINITE SPEED EFFECTS IN TRANSPORT PHENOMENA

5.1 Strict finite speed models

Local microscopic models can enforce strict finite speed and be local in phase space. This double advantage comes with the price of having to deal, not with macroscopic experimentally accessible fields, but typically with distribution functions in phase space.

It seems the only method to enforce strict finite speed at the macroscopic level is through non local models (Balescu, 1997; Dunkel, Talkner and Hänggi, 2007). The standard heat equation is typically replaced by an equation of the form :

$$\partial_t T = \int K(t-t', \mathbf{x}-\mathbf{x}')T(t', \mathbf{x}')d^3x' \quad (5)$$

where the choice of the Kernel K ensures finite speed transport. An equation of this type involves only a macroscopic field (the temperature) but presents the technical shortcoming of not being a differential, but rather an integro-differential equation. This difficulty can be somewhat alleviated if one considers models which are local in Fourier space (Maruani, 2008); the simplest example is a matter diffusion model where the time- and space-Fourier transform $\hat{\mathbf{j}}(\omega, \mathbf{k})$ of the particle current is linked to the Fourier transform $-\mathbf{k}^2\hat{n}(\omega, \mathbf{k})$ of the particle density gradient by an equation of the form:

$$\hat{\mathbf{j}}(\omega, \mathbf{k}) = -\chi(\omega, \mathbf{k})\mathbf{k}^2\hat{n}(\omega, \mathbf{k}) \quad (6)$$

in which the function χ can be chosen to ensure finite speed transport.

5.2 Effective finite speed models

Consider for example the usual Langevin diffusion model. As already stated, this model does not bound velocities. Suppose now one considers an initial phase space distribution of the form :

$$f_0(\mathbf{x}, \mathbf{v}) = n_0(\mathbf{x})\Big(\frac{m}{2\pi k_B T_0}\Big)^{\frac{3}{2}} \exp\Big(-\frac{m v^2}{2k_B T_0}\Big), \quad (7)$$

where T_0 is an initial temperature. The simplicity of the Langevin model permits an exact computation of the time evolution of this density, and thus, of all macroscopic fields. It is found (Debbasch and Rivet, 2007) that the particle current $\mathbf{j}$ and the particle density n obey at all times the exact proportionality relation :

$$\mathbf{j}(t, \mathbf{x}) = -\chi(t)\nabla_x n, \quad (8)$$

with a time-dependent diffusion coefficient $\chi(t)$ given by :

$$\chi(t) = \frac{k_B T_e}{m\alpha}(1 - e^{-\alpha t})\Big(1 - \frac{(T_e - T_0)}{T_e}e^{-\alpha t}\Big). \quad (9)$$

Here, T_e is the temperature of the surrounding fluid, which is not necessarily identical to the initial temperature T_0 of the diffusing particles.

Equations (8) and (9) imply that, for an initially point-like spatial distribution of diffusion particles, the standard relation $< r^2 >= \frac{k_B T_e}{m\alpha} t$ for the variance of the particle position is replaced by :

$$< r^2 >= \frac{k_B T_e}{m\alpha} \left(t - \frac{(1 - e^{-2\alpha t})}{2\alpha} - \frac{T_e - T_0}{T_e} \frac{(1 - 2e^{-\alpha t} + e^{-2\alpha t})}{\alpha} \right), \tag{10}$$

which scales as $\frac{k_B T_0}{m} t^2$ rather than $\frac{k_B T_e}{m\alpha} t$ for 'small t' (*i.e.* $\alpha t \ll 1$). Consequently, the effective diffusion speed $\frac{d}{dt}\sqrt{< r^2 >}$ remains finite even for arbitrarily small values of t.

This result suggests that macroscopic finite speed effects in transport phenomena may be modelled by purely macroscopic local models with time-dependent transport coefficients.

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