Key Factors in Fluid Modelling of Plasmas and Swarms

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In this paper we start with general fluid equations for both ions and electrons in neutral gases, obtained as velocity moments of Boltzmann's equation. Two distinct approximations are required for these exact equations to be of any practical use:
I. The collision transfer terms (right hand side of the fluid equations) must be approximated, and
II. Some closure *ansatz* (hypothesis) is required for the "streaming terms" (left hand side of the fluid equations), to ensure that the number of equations corresponds to the number of unknowns.
For step I, swarm (free diffusion) limit results using, e.g., momentum transfer theory, may be taken over directly to low temperature plasmas, but step II remains problematic, with little guide from swarm physics, and serious doubts about existing assumptions in the plasma literature. We focus on electron fluid equations with closure at the level of momentum and energy balance, which requires an accurate heat flux *ansatz* in order to produce physically meaningful results. The crucial nature of this *ansatz* is illustrated using a simple benchmark calculation for infinite plane parallel geometry, where we show for the first time how periodic spatial structures (Franck-Hertz oscillations) may be generated from fluid equations.

1. Introduction: Kinetic modelling

The Boltzmann kinetic equation for each charged component s of a weakly ionised gas can be written as:

$$(\partial_t + \boldsymbol{c}.\nabla + a^{(s)}.\partial_{\boldsymbol{c}})f^{(s)} = -J(f^{(s)}, f^{(0)}) - \sum_{s'} J(f^{(s)}, f^{(s')}) \qquad (1)$$

where $f^{(s)}(\boldsymbol{r},\boldsymbol{c},t)$ is the phase space distribution function of species s, $\boldsymbol{a}^{(s)} = q^{(s)}/m^{(s)}(\boldsymbol{E} + \boldsymbol{c} \times \boldsymbol{B})$ is the external force per unit mass, and $J(f^{(s)}, f^{(0)})$ and $J(f^{(s)}, f^{(s')})$ denote the collision terms for charge particle-neutral molecule collisions, and charged particle–charged particle interactions respectively. Put in a nutshell, the problem of kinetic theory is to solve equations of the form (1) for $f^{(s)}$ with appropriate boundary and initial conditions. Then we obtain the physical quantities of interest as velocity "moments", starting with the number density,

$$n^{(s)}(\boldsymbol{r}, t) = \int f^{(s)}(\boldsymbol{r}, \boldsymbol{c}, t)\, d\boldsymbol{c} \qquad (2)$$

followed by higher order quantities,

$$\langle \phi(\boldsymbol{c}) \rangle^{(s)} = \frac{1}{n^{(s)}(\boldsymbol{r},t)} \int \phi(\boldsymbol{c}) f^{(s)}(\boldsymbol{r},\boldsymbol{c},t)\, d\boldsymbol{c} \qquad (3)$$

with $\phi(\boldsymbol{c}) = m\boldsymbol{c}, \frac{1}{2} mc^2$,... furnishing the mean velocity $\mathbf{v}^{(s)}$, mean energy $\varepsilon^{(s)}$, and so on.

The current state of affairs in electron and ion kinetic theory has been reviewed by White *et al* [1] and Viehland[2] respectively, for the free diffusion or "swarm" limit, while Winkler [3] has reviewed electron kinetics from the perspective of low temperature plasma physics.

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Note that $f^{(0)}$, the neutral molecule distribution function, is often assumed to be a Maxwellian, but in general it too will be prescribed by the solution of an additional kinetic equation coupled to the hierarchy (1).

For *swarms*, there is generally only one charged component, the fields are externally prescribed and the non-linear term $J(f^{(s)}, f^{(s)})$ is neglected. A hydrodynamic situation usually prevails, and space and time are usually projected out through a density gradient expansion[1].

On the other hand, for low temperature *plasmas*, the fields are determined self-consistently through Maxwell's equations, e.g., Poisson's equation:

$$\nabla.\boldsymbol{E} = \sum_s n^{(s)}(\boldsymbol{r},t) q^{(s)} / \varepsilon_0 \qquad (4)$$

while boundaries and sources usually result in non-hydrodynamic behaviour. This by itself means that the plasma problem is at least an order of magnitude more difficult than the swarm problem from a computational point of view, even when the non-linear terms in Eq. (1) are neglected. When the latter are included, the calculation assumes even more formidable proportions.

It is therefore not surprising that alternative approaches such PIC and Monte Carlo simulations[4] and fluid modelling [5-7] , are favoured. Fluid models are particularly attractive as they offer both computational economy and physical insight, but accuracy and *ad hoc* closure assumptions can be issues[4,5]. In this paper, we outline what we believe are the key factors for successful fluid modelling.

2. Fluid modelling

In the fluid approach one aims at obtaining the physical quantities of interest directly, rather than via the distribution function as in Eqs. (1) and (3). A low order set of moment equations, typically the continuity, momentum balance, and energy balance equations, can be found by taking velocity moment equations of Eq. (1)

with respect to the quantities $\phi(\boldsymbol{c}) = \boldsymbol{1}, m\boldsymbol{c}, \frac{1}{2} m c^2$,... together with some *ansatz* or postulate to close the set. The generic form of the fluid equations thus obtained is

$$\partial_t n + \nabla \cdot n\boldsymbol{v} = C_0 \qquad (5a)$$

$$nm(\partial_t + \boldsymbol{v} \cdot \nabla)\boldsymbol{v} + \nabla \cdot \boldsymbol{P} - nq(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}) = C_1 \qquad (5b)$$

$$n(\partial_t + \boldsymbol{v} \cdot \nabla)(\varepsilon - 1/2 m v^2) + \nabla \cdot \boldsymbol{q} + \boldsymbol{P} : \nabla \boldsymbol{v} = C_3 \qquad (5c)$$

where the collision transfer terms C_i account for all processes: elastic and inelastic collisions, ionisation and attachment, ion-molecule reactions, recombination, and so on. The explicit form depends upon the choice of collision *ansatz*, as explained below. For plasmas, Eqs. (5) are to be solved for each species, in conjunction with Maxwell's equations, for given initial and boundary conditions. For swarms, the fields are externally prescribed. However, the collision terms C_i are the *same* for both cases. Figure 1 shows the steps involved in constructing fluid equations for both swarms and low temperature plasmas.

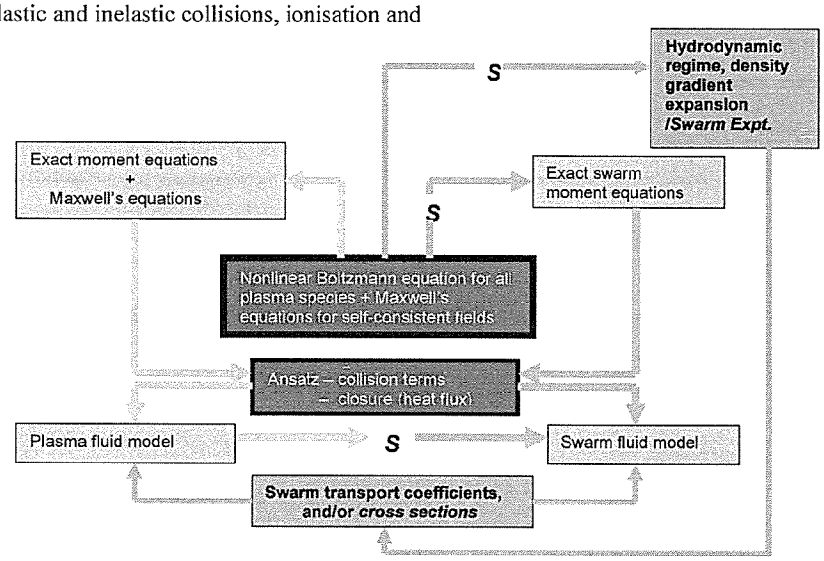

Figure 1. A schematic portrayal of the way in which fluid equations are generated for both plasmas and swarms from their common source, the kinetic equation (1). In the swarm limit *S*, densities are so low that charge particle interactions are negligible.

Starting from the common kinetic equation for each of the ion and electron species, one proceeds through a common set of approximations for the collision terms and closure. In this picture, the resulting plasma fluid equations are consistent with the established results of swarm analysis. In addition, it is legitimate in this scheme to employ measured or theoretically calculated swarm transport coefficients to replace approximate terms in either the swarm or plasma fluid equations, thereby considerably enhancing computational accuracy. On the other hand, purely empirical plasma fluid models generally reproduce neither the swarm fluid equations nor the associated benchmark results and formulas established in the literature over many years. Furthermore, it may be neither logical nor legitimate to try to insert swarm transport coefficients into the empirical fluid equations.
Whichever way one proceeds, the basic difficulty in the fluid approach is that there are always more unknowns than equations, and thus there is a fundamental *closure problem*. There are a number of issues to be addressed:

(i) The collision terms C_i generally involves an infinite number of moments, and must be approximated in some way in order to close the equations. Wannier[8] suggested approximating the collision terms by expressions of the same mathematical *form* as for the constant collision frequency model, effectively eliminating the troublesome unknowns. This procedure, which has come to be known as "momentum transfer theory", has proved very successful in swarm transport theory, where it has been tested and benchmarked for accuracy. It has even been applied recently to unfold cross sections from swarm data – see Fig. 2. It should prove equally successful for low temperature plasmas – after all, collision dynamics is not influenced by either fields or the spatial-temporal behaviour of the system. In the absence of charge-charge interactions, the C_i are defined by the right side of Eqs, (7)-(9) of Ref. 5.

(ii) Both the momentum and energy balance equations (5b,c) contain the pressure tensor $\boldsymbol{P} = nm\langle (\boldsymbol{c}-\boldsymbol{v})(\boldsymbol{c}-\boldsymbol{v}) \rangle$, which has to be found from a higher order moment equation, which in turn contains further unknowns. For light particles such as electrons, however, the tensor can be taken as a scalar at the fluid level of approximation[5], i.e., $\boldsymbol{P} \approx 2/3\, n\varepsilon \boldsymbol{I}$, and there is no closure problem. For heavy particles, however, a

closure *ansatz* will have to be made, using a procedure similar to that for the heat flux vector, described below.

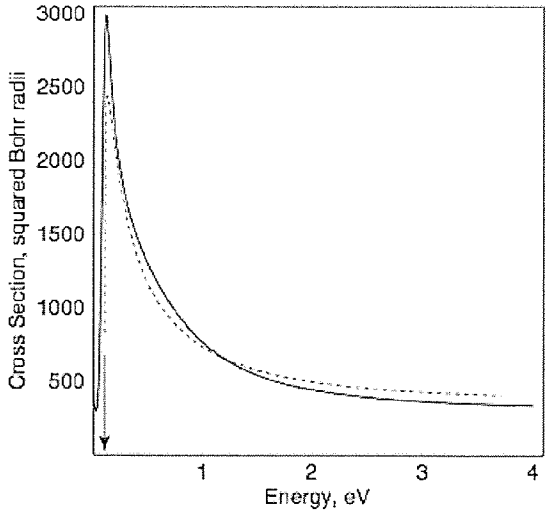

Figure 2. Momentum transfer cross sections for electrons in sodium vapour at T = 803° K, as calculated (a) theoretically from the Fano profile formula (solid curve) and (b) by inverting swarm data using momentum transfer theory (dashed curve) (P. Nicoletopoulos, http://arxiv.org/abs/physics/0307081, 2003). The arrow indicates the thermal energy 3kT/2 = 0.1 eV.

(iii) The energy balance equation (5c) also contains the heat flux term, $\boldsymbol{q} = \frac{1}{2}nm\langle(\boldsymbol{c}-\boldsymbol{v})^2(\boldsymbol{c}-\boldsymbol{v})\rangle$, which must be expressed in terms of lower moments n, $\boldsymbol{v}$, ε if the fluid equations are to be closed. As Surendra and Davie[9] pointed out some time ago, it is unsatisfactory to either neglect $\boldsymbol{q}$, or to use a Fourier type of *ansatz*, $\boldsymbol{q} = -K\nabla\varepsilon$, where K is some constant, and yet this is precisely what continues to be done in the fluid modelling literature[10]. Correct representation of the heat flux is known to be important for analysis of transport properties[3, 5], and thus we have devoted a significant part of our work to addressing this issue. Our strategy has been to aim to find a simple collision model where one can write down an *exact* expression for the heat flux, represented here in functional form as

$$\boldsymbol{q} = Q(n, \boldsymbol{v}, \varepsilon) \qquad (6)$$

and then use this as an *ansatz* for other, more general situations. An explicit form of (6) is given in Eq. (20) of Ref. 5.

The integrity of the fluid equations closed as above can be tested by:

- Ensuring that they reproduce all the well known formulas in the swarm limit: Wannier's energy equation, Tonks' theorem, generalised Einstein relations, and so on
- Benchmarking against exact solutions of the Boltzmann equation for models in simple infinite plane – parallel geometry; including a prototype Franck-Hertz experiment[11]

3. A benchmark model: Franck-Hertz oscillations

We now consider electrons emitted at a steady rate from a source into a neutral gas in the inherently non-hydrodynamic benchmark model of Fig. 3, and use Eq. (20) of Ref. 5 for the heat flux ansatz, which contains an adjustable parameter α. In the asymptotic region far downstream from the source, the fluid equations can be linearised and solved analytically (see Section B of Ref. 5). Here the space-dependence of all quantities is governed by a single exponential e^{Kz}, in which the "wave number" K may be complex when inelastic collisions are significant. This leads to periodic structures which are characteristic of the Franck-Hertz experiment. In the initial study reported here, there is no magnetic field[12] and for simplicity $z_0 = 0$.

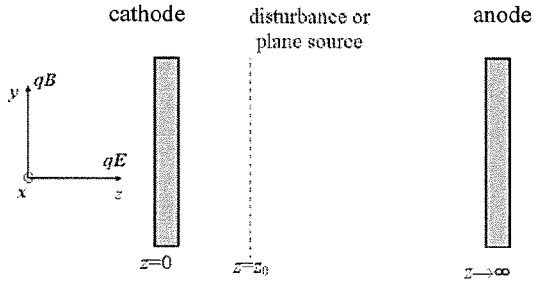

Figure 3. The benchmark plane-parallel geometry model, in which electrons are emitted at a steady rate into a gas.

The cross section model is the one used by Li and collaborators[11] to furnish accurate benchmark solutions of Boltzmann's equation, namely a constant elastic momentum transfer cross section $\sigma_m = 6$ A^2, a constant inelastic cross section $\sigma_I = 0.1$ A^2 above threshold $\varepsilon_I = 2$ eV, a cold gas with atomic mass $M = 4$ a.m.u.

The starting point of our investigation is Eq. (38) of Ref. 5, a cubic equation for K. The solutions shown in Fig. 4 are in reasonable semi-quantitative agreement with the results of precise numerical solution of Boltzmann's equation (see Fig. 4 of Ref 11). It is clear that in the "window" of reduced fields, roughly 0.5 Td < E/N < 10 Td, the real part of K is small, and the imaginary part rises monotonically, implying that periodic structures persist to very large distances downstream from the source, as shown in Fig. 5. Such oscillatory behaviour has been widely studied in the literature in recent times through solutions of the Boltzmann equation[3,11-13], but this is the first time that such behaviour has been produced using a fluid model.

As expected, the heat flux ansatz turns out to be crucial , both qualitatively and quantitatively speaking. To repeat, a Fourier type of *ansatz*, which was already shown to be

inadequate for even the simplest elastic collision model[5] produces no oscillations whatever, and is obviously totally unphysical. Even for the *ansatz* suggested in Ref.5, which is quite adequate for describing elastic collisions, extreme care needs to taken with specification of the parameter α when inelastic collisions are important, as is the case above. Details will be reported in a forthcoming publication (Nicoletopoulos and Robson, in preparation).

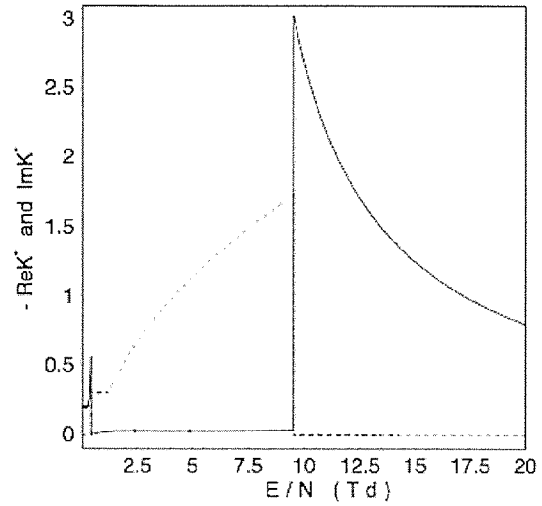

Figure 4. Real (solid line) and imaginary (dashed line) parts of the (normalised) wave number $K^*=K\lambda$, where $\lambda = (\sqrt{2}\, N\, \sigma_0)^{-1}$, $\sigma_0 = 1A^2$, and 1 Td = 1 townsend = 10^{-21} V m^2.

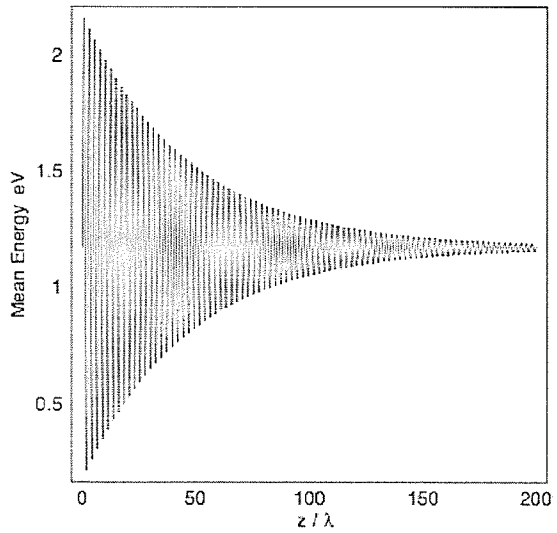

Figure 5. Mean energy at E/N=6.5 Td as a function of normalized distance downstream from the source

4. Concluding remarks and acknowledgment

We have discussed key factors in fluid modelling of swarms and plasmas, both generally and in the context of a deceptively simple-looking benchmark model. We strongly recommend that fluid modellers use collision transfer terms as furnished by momentum transfer theory [5,14-16], or some other systematic method[6]. Particular care needs to be taken with closure through specification of the heat flux, a point which is still not always recognised [7]. We also suggest that any plasma fluid model *must* yield established swarm results in the appropriate limit of low charge densities. After all, if a model cannot reproduce the simplest of I-V characteristics, what hope has it of getting things right in the more complex plasma situation?

Finally, there is a separate set of issues regarding the use of swarm hydrodynamic transport coefficients in plasma fluid models[5], particularly in non-hydrodynamic, space-time varying circumstances, and allowing for the subtleties of non-conservative collisions.

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6. References

(1) R.D. White, K.F. Ness and R.E. Robson, Applied Surf. Sci. 35, 26 (2002)

(2) L.A. Viehland, Comp. Phys. Comm. 142, 7 (2001); See also E.A. Mason and E.W. McDaniel, "The transport properties of ions in gases", (Wiley, New York, 1988)

(3) R. Winkler, Adv. Atom. Mol. Opt. Phys. 43, 20 (2000)

(4) M. Surendra, Plasma Sources Sci. Technol. 4, 56 (1995)

(5) R.E. Robson, R.D. White and Z. Lj. Petrovic, Rev. Mod. Phys. 77, 1303 (2005)

(6) L.A. Viehland and D.E. Goeringer, J. Phys. B 38, 3987 (2005)

(7) G.J.M. Hagelaar and L.C. Pitchford, Plasma Sources Sci. Technol. 14, 722 (2005)

(8) G.H. Wannier, Bell Syst. Tech. J. 32, 170 (1953)

(9) M. Surendra and M. Dalvie, Phys. Rev. E48, 3914 (1993)

(10) J.P. Boeuf and L.C. Pitchford, Phys. Rev. E51, 1376 (1995); J.D. Bukowski, D.B. Graves and P. Vitello, J. Appl. Phys. 80, 2614 (1996); E. Gogolides and H.H. Sawin, J. Appl. Phys. 72, 3971 (1992)

(11) R.E. Robson, B. Li and R.D. White, J. Phys. B 33, 507 (2000)

(12) A kinetic theory analysis of the situation in Fig. 3 for non-zero magnetic field has been given by Li *et al*, Phys. Rev. E 74, 026405 (2006)

(13) G. Petrov and R. Winkler, J. Phys. D30, 53 (1997)

(14) S.B. Vrhovac and Z. Lj. Petrović, Phys. Rev. E 53, 4012 (1996)

(15) E.A. Mason and E.W. McDaniel, *Transport properties of ions in gases* (Wiley, New York, 1988)

(16) R.E. Robson, *Introductory transport theory for charged particles in gases* (World Scientific, Singapore, 2006)