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The Steady State Townsend Experiment: Comparison of Boltzmann Equation and Diffusion Equation Analysis*

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Abstract

A general solution of the diffusion equation corresponding to an idealised swarm experiment in infinite plane–parallel electrode geometry is given and the result is then specialised to the steady state Townsend experiment. The role of the 'dispersion relation' generated by the diffusion equation is discussed, and the physical meaning of its two zeros explored. It is found that the smaller zero generally allows adequate representation of the electron density distribution downstream of the source, but the larger zero must be found from the full Boltzmann eigenvalue equation in order that the upstream region be represented even qualitatively correctly. The results of a numerical calculation for electrons in water vapour are presented. The procedure adopted by Tagashira *et al.* (1994) to obviate this difficulty is discussed.

1. Introduction

In this paper, we wish to analyse the steady state Townsend (SST) experiment, which may be idealised by the infinite plane–parallel electrode geometry shown in Fig. 1. The source at $z = z_0$ emits electrons continuously into a gas in equilibrium filling the region between the electrodes. These electrons are accelerated by an external electrostatic field to energies sufficiently high so that ionisation of molecules may occur in collisions. Eventually, a steady state is reached where the electrons drift and diffuse away from the source at the same rate at which they are created at the source. We wish to analyse the density profile $n(z)$ of electrons both downstream and upstream from the source.

Thomas (1969) postulated the existence of an 'equilibrium region' downstream from the source where the number density has a simple exponential growth rate

$$n(z) \sim \mathrm{e}^{K(z-z_0)}, \tag{1}$$

where K is a constant. If equation (1) is substituted into the diffusion equation [Huxley and Crompton (1974); see equation (3) below with the r.h.s. set equal to zero, away from the source], there results a quadratic in K with solutions

$$K = K_{\pm} \equiv \frac{W}{2D} \pm \left\{ \left[\frac{W}{2D} \right]^2 - \frac{\nu_{\mathrm{I}}}{D} \right\}^{\frac{1}{2}}, \tag{2}$$

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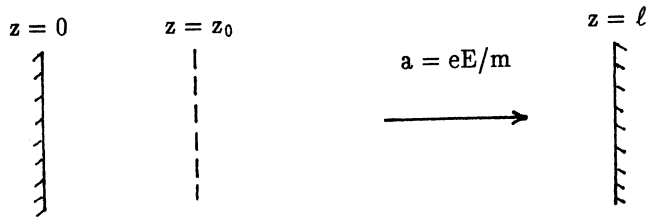

Fig. 1. Idealised experimental arrangement in which an infinite plane source at $z = z_0$ lies between infinite plane electrodes at $z = 0$, and ℓ, the gap being occupied by a neutral gas of number density n_0 and temperature T_0.

where W, D and ν_I denote the electron drift velocity, longitudinal diffusion coefficient and ionisation rate respectively. *Both* roots play a role for finite geometry, as we demonstrate in this paper, although in the limit of infinite geometry, only K_- enters the expression for $n(z)$ *downstream* from the source. A similar conclusion was reached by Thomas (1969) and Tagashira *et al.* (1977) on the basis of a 'physical argument' and K_- is identified with α_T, Townsend's ionisation coefficient. On the other hand, *upstream* from the source, for infinite geometry, the density profile decays exponentially at a rate governed by the larger root K_+, according to the solution of the diffusion equation. This is discussed in Section 2. This is in accord with the results of Standish (1989) and Tagashira (1985, 1991).

An examination starting from Boltzmann's equation is also given, and this could be expected to yield a more accurate description, especially in the case of large gradients, where the diffusion equation breaks down. The corresponding analysis is, of course, much more difficult (Standish 1989; Kondo and Tagashira 1990; Robson 1991; Sugawara *et al.* 1994), but certain key factors quickly emerge. Thus, it turns out that in this picture there are two *sets* of eigenvalues of a certain operator, $\{K_\mu^{(-)}\}$ and $\{K_\mu^{(+)}\}$, where $\mu = 0, 1, 2, \ldots$ is an index defining the order within the respective sets, which determine the steady state density profile. For infinite geometry, the smaller set, and in particular the fundamental member $K_0^{(-)}$, controls the downstream behaviour, while $K_0^{(+)}$ controls the profile upstream of the source.

We shall show in Section 3 that while $K_- \approx K_0^{(-)}$, and therefore the diffusion equation can reasonably be expected to describe the downstream profile, $K_0^{(+)}$, differs substantially from K_+ in general, and therefore it is hopeless to try to model the upstream behaviour using the diffusion equation.

Tagashira *et al.* (1994) have tried to come to terms with this problem by postulating different transport quantities W, D and ν_I in regions upstream and downstream from the source. However, we believe that, while such an *ad hoc* remedy is interesting, it is unsatisfactory in principle, and that the best way of dealing with the upstream region is to bring to bear the full Boltzmann equation eigenvalue analysis. This aspect, along with certain other physical arguments which point to the inherent failure of the diffusion equation in the upstream region, are discussed in Section 4. A numerical example is given for electrons in water vapour.

2. Diffusion Equation Analysis

(2a) Solution for Pulsed Source

We consider for simplicity an idealised swarm experiment conducted in the plane-parallel electrode geometry shown in Fig. 1. A planar source at $z = z_0$ emits charged particles of charge e and mass m into a gas confined by infinite plane electrodes at $z = 0$ and $z = \ell$. The particles drift, diffuse and react with the gas molecules at rates governed by the drift velocity W, longitudinal diffusion coefficient D and reaction rate ν_I respectively, in response to an external electrostatic force $a = eE/m$ per unit mass, and a gradient in number density $n(z, t)$ of the particles. The latter gradient arises from a combination of the effects of source and boundaries. There is only one spatial variable z, directed normal to the electrodes, to consider in this ideal arrangement, with all properties assumed to be uniform in the x, y directions.

In this paper, we first analyse the problem phenomenologically, using the diffusion equation

$$(\partial_t + L)n = S(z, t)\,, \tag{3}$$

where

$$L = -D\partial_z^2 + W\partial_z - \nu_I \tag{4}$$

and $S(z, t)$ is the source strength at position z and time t. If the source is localised as shown in Fig. 1 and σ particles are emitted in a pulse at $t = t_0$, then

$$S(z, t) = \sigma\delta(z - z_0)\,\delta(t - t_0)\,. \tag{5}$$

Other modes of source operation can be dealt with by integrating the solution over z_0 and/or t_0 as appropriate. Boundary conditions corresponding to perfectly absorbing electrodes are assumed, i.e.

$$n(0, t) = 0 = n(\ell, t)\,. \tag{6}$$

It is important to note in the context of the present discussion that the parameters D, W and ν_I are the same everywhere; in particular there is no distinction between regions upstream and downstream of the source.

The diffusion equation analysis presented in this section is really a weak-gradient theory, a point which should be borne in mind when considering the upstream region in the SST experiment discussed below.

The form of the solution of (3) for the source function (5) and boundary conditions (6) is given by

$$n(z, t) = \frac{\sigma}{2\ell}\,\Theta(t - t_0) \sum_{j=-\infty}^{\infty} e^{\Omega(\lambda + ik_j)(t-t_0) + \lambda(z-z_0)}\left[e^{-ik_j(z-z_0)} - e^{-ik_j(z+z_0)}\right], \tag{7}$$

where

$$\Omega(K) \equiv \nu_I - WK + DK^2\,, \tag{8}$$

$$\lambda \equiv W/2D\,, \qquad k_j \equiv j\pi/\ell \quad (j = 1, 2, \ldots)\,, \tag{9,10}$$

and $\Theta(t-t_0)$ is the unit step function.

(2b) Application to Steady State Townsend Experiment

In the SST experiment, the source in Fig. 1 emits electrons at a constant rate into the gas and the field is sufficiently strong so that ionisation is appreciable. Eventually a steady state is reached, where there is a balance between creation at the source and by ionisation and a loss by drift and diffusion. The corresponding density profile can be found by integrating the pulsed-source solution (7) over all t_0, and then taking the limit $t \to \infty$. The Poisson summation theorem (Robson 1985) may be used and we find after much algebra the following long-time asymptotic expression for the density:

$$\begin{aligned} n_\infty(z) &= \frac{\sigma}{2D\lambda} \sum_{j=-\infty}^{\infty} \mathrm{e}^{\lambda(z-z_0)}[\mathrm{e}^{-\lambda'|2j\ell+z-z_0|} - \mathrm{e}^{-\lambda'|2j\ell+z+z_0|}] \\ &= \frac{\sigma}{2D\lambda'} \mathrm{e}^{\lambda(z-z_0)}\{\mathrm{e}^{-\lambda'|z-z_0|} - \mathrm{e}^{-\lambda'(z+z_0)} + B[\mathrm{e}^{\lambda'(z-z_0)} + \mathrm{e}^{-\lambda'(z-z_0)} \\ &\qquad - \mathrm{e}^{\lambda'(z-z_0)} - \mathrm{e}^{-\lambda'(z+z_0)}]\}\,, \end{aligned} \tag{11}$$

where

$$\lambda' \equiv (\lambda^2 - \nu_1/D)^{\frac{1}{2}}\,, \qquad B \equiv (\mathrm{e}^{2\lambda'\ell} - 1)^{-1}\,. \tag{12, 13}$$

The two zeros of $\Omega(K)$ are given by (2) and may also be written as

$$K_\pm = \lambda \pm \lambda'\,. \tag{14}$$

These figure prominently in the following discussion.

Downstream from the source, $z > z_0$, and (11) gives

$$n_\infty(z) = \frac{\sigma}{2D\lambda'}[\mathrm{e}^{K_-(z-z_0)}(1 - \mathrm{e}^{-2\lambda' z_0})(1 - B) + B\mathrm{e}^{K_+(z-z_o)}(1 - \mathrm{e}^{2\lambda' z_0})]\,. \tag{15}$$

Obviously both zeros $K_\pm$ contribute for finite geometry. However, for an unbounded medium, $\ell \to \infty$, $B \to 0$ and (15) reduces to a simple exponential form

$$n_\infty(z) \sim \mathrm{e}^{K_-(z-z_0)}\,. \tag{16}$$

On this basis, we would like to identify

$$\alpha_\mathrm{T} = K_- \tag{17}$$

as the Townsend primary ionisation coefficient. Clearly only the smallest zero K_- of $\Omega(K) = 0$ contributes for infinite geometry. This result follows directly from the general expression (15), without appealing to any 'physical' arguments (Thomas 1969; Tagashira *et al.* 1977). Equation (15) also demonstrates however

that *both* zeros $K_\pm$ must be retained for finite geometry, downstream of the source.

Now consider regions $z < z_0$ *upstream* from the source, also in the limit $\ell \to \infty$. Equation (11) becomes

$$n_\infty(z) = \frac{\sigma}{2D\lambda'} e^{-\lambda|z-z_0|}[e^{-\lambda'|z-z_0|} - e^{-\lambda'(z+z_0)}], \tag{18}$$

and if the source is far from the boundary at $z = 0$, we have

$$n_\infty(z) \sim e^{-K_+|z-z_0|} \tag{19}$$

in the neighbourhood of that source and upstream from it. That is, the largest zero K_+ of $\Omega(K) = 0$ controls the upstream behaviour. Again, this result is in accordance with other studies (Standish 1989; Tagashira 1985, 1991), but follows from the general expression for finite geometry in a natural way.

Finally, we emphasise that other experiments could be analysed using equation (7). For example, for the time-of-flight (TOF) experiment, which can be modelled as a pulse of swarm particles injected into an infinite gas, the density profile reduces to the familar travelling pulse for $z \gg z_0$:

$$n(z, t) = \frac{\sigma\Theta(t-t_0)}{[4\pi D(t-t_0)]^{\frac{1}{2}}} \exp\left(\nu_I(t-t_0) - \frac{[z - z_0 - W(t-t_0)]^2}{4D(t-t_0)}\right). \tag{20}$$

For later reference, we note from (8) that the following identities hold:

$$\nu_I = \Omega(0), \quad W = -\Omega'(0), \quad D = \tfrac{1}{2}\Omega''(0) \tag{21}$$

and that the TOF experiment determines all these quantities, at least in principle.

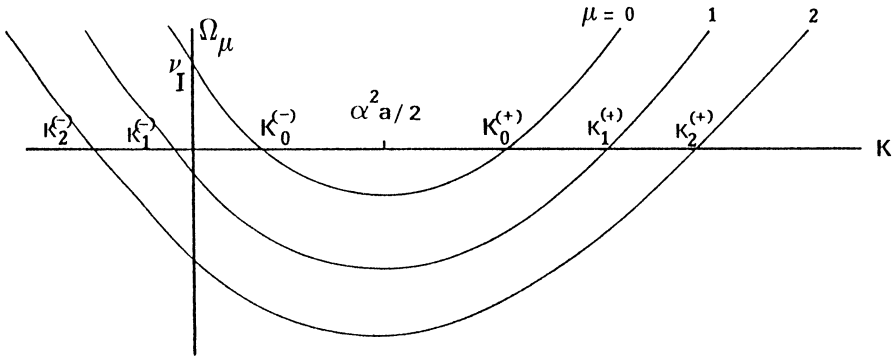

Fig. 2. Dispersion relations $\Omega_\mu(K)$ for the Fokker–Planck collision model operator (Standish 1987), where the intercepts on the K-axis are given by equation (26).

3. Boltzmann Equation Solution

We consider firstly an instantaneous source of electrons activated at time $t = t_0$. The electron phase space distribution function $f(z, \mathbf{c}, t)$ is governed by the

Boltzmann equation, from the solution of which we obtain the number density (Robson 1991):

$$\begin{aligned} n(z,t) &= \int \mathrm{d}\mathbf{c}\, f(z,\mathbf{c},t) \\ &= \Theta(t-t_0)\frac{2\sigma}{\ell}\sum_{\mu}\sum_{j=1}^{\infty} A_\mu(K_j)\exp[\Omega_\mu(K_j)(t-t_0) \\ &\quad + \Lambda(z-z_0)]\sin k_j z_0 \sin k_j z\,, \end{aligned} \tag{22}$$

where

$$k_j = j\pi/\ell, \qquad K_j = \Lambda + \mathrm{i}k_j \quad (j=1,2,\ldots)\,, \tag{23}$$

$$\Lambda = a\alpha^2/2, \qquad \alpha^2 = m/kT_0\,, \tag{24}$$

T_0 is the gas temperature and $-\Omega_\mu(K)$ are eigenvalues of $\hat{M}+Kc_z$, and where $\hat{M} = J+a\partial c_z$, i.e.

$$(\hat{M} + Kc_z + \Omega_\mu)\psi_\mu(\boldsymbol{c}|K) = 0\,. \tag{25}$$

The index μ orders these eigenvalues, with $\Omega_0 > \Omega_1 \geq \Omega_2 \geq \ldots$. The amplitudes $A_\mu(K)$ are given by certain velocity integrals over the eigenfunctions $\psi_\mu(\mathbf{c}|K)$. A typical family of 'dispersion' curves $\Omega_\mu(K)$, generated by solving (25) with a model collision operator J, is shown in Fig. 2. Note the intersections on the Ω and K axes, for these have particular physical significance. The intercepts on the K-axis for this model are given by

$$K_\mu^{(\pm)} = \tfrac{1}{2}\alpha^2 a \pm [(\tfrac{1}{2}\alpha^2 a)^2 + \alpha^2\nu_{\mathrm{m}}(\mu\nu_{\mathrm{m}} - \nu_{\mathrm{I}})]^{\frac{1}{2}}\,, \tag{26}$$

where ν_m is the momentum transfer collision frequency. It is emphasised that the following discussion is, however, independent of the details of J, and the results are therefore quite general.

If the source in Fig. 1 operates in a *continuous* mode, the corresponding solution may be found by integrating over all t_0. In the asymptotic time regime $t \to \infty$, a steady state density profile $n_\infty(z)$ is attained in which *both* zeros $K_\mu^{(\pm)}$ of Ω_μ appear in exponential growth terms, $\exp[K_\mu^{(\pm)}(z-z_0)]$. In the limit when $\ell \to \infty$, however, only the lower zero $K_\mu^{(-)}$ plays a role *downstream* from the source $z > z_0$, i.e. the expression for $n_\infty(z)$ consists of a sum of exponentials

$$n_\infty(z) = \sum_\mu B_\mu^{(-)} \exp[K_\mu^{(-)}(z-z_0)] \qquad (z > z_0)\,, \tag{27}$$

where $B_\mu^{(-)}$ are constants. The fundamental velocity mode $\mu = 0$ dominates the sum for large downstream distances $z-z_0$, since $K_0^{(-)} > K_1^{(-)} > K_2^{(-)} \ldots$. Thus we have asymptotically at large $z-z_0$, $n_\infty(z) \sim \mathrm{e}^{\alpha_T(z-z_0)}$, where $\alpha_{\mathrm{T}} = K_0^{(-)}$ is again identified as the Townsend primary ionisation coefficient.

On the other hand, *upstream* from the source (which is assumed far removed from the boundary at $z = 0$), we find that only the *larger* zeros $K_\mu^{(+)}$ contribute:

$$n_\infty(z) = \sum_\mu B_\mu^{(+)} \exp[-K_\mu^{(+)}\,|z-z_0|]\,, \tag{28}$$

the $B_\mu^{(+)}$ being constant amplitudes. The fundamental mode $\mu = 0$ again dominates asymptotically. Note that an important result of the eigenvalue analysis is that (Robson 1991)

$$K_\mu^{(+)} = 2\Lambda - K_\mu^{(-)}, \tag{29}$$

where Λ is defined by (24). When $T_0 \to 0$, then $\Lambda \to \infty$ and the larger zeros $K_\mu^{(+)}$ become infinite. This is in contrast to the corresponding result for the diffusion equation, obtained directly from (14),

$$K_+ = 2\lambda - K_-, \tag{30}$$

where λ is given by (9) and remains *finite* as $T_0 \to 0$. The situation is depicted schematically in Fig. 3.

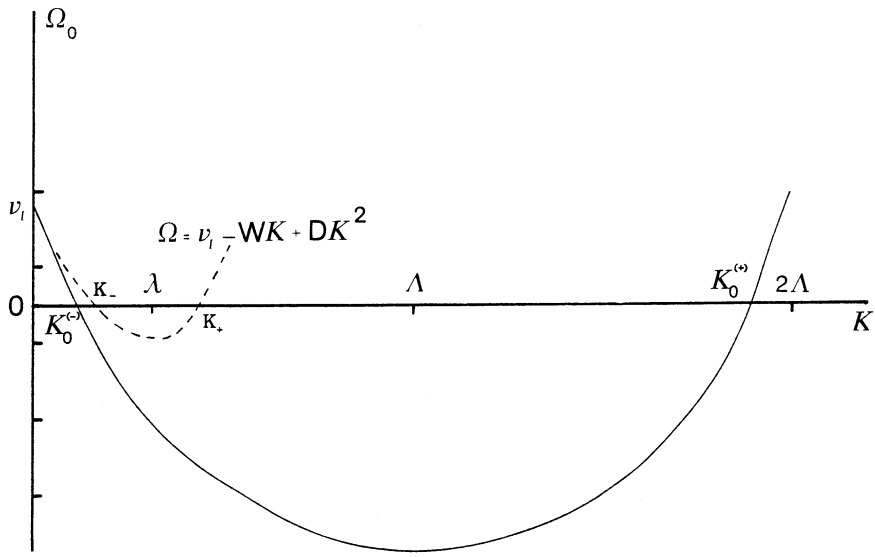

Fig. 3. Schematic representation of 'dispersion curves' for the diffusion equation (3) and the fundamental mode of the Boltzmann eigenvalue problem (25). The lower intercepts on the K-axis are close, i.e. $K_- \approx K_0^{(-)}$, but $K_0^{(+)} \gg K_+$.

While the lower roots are nearly the same for both Boltzmann and diffusion equation solutions, as might be expected since the coefficients of the diffusion equation are effectively chosen to produce an accurate, small-K representation of $\Omega_0(K)$, i.e.

$$K_- \approx K_0^{(-)} \equiv \alpha_T, \tag{31}$$

the upper root is not even closely represented by the diffusion equation value, with

$$K_+ \ll K_0^{(+)} \tag{32}$$

at lower gas temperatures. Calculations for a specific case are reported below. We shall discuss this startling difference and its ramifications from another angle in the next section.

For practical purpose, the SST experiment can therefore be dealt with by solving the eigenvalue problem (25) with Ω_μ set equal to zero, i.e.

$$(\hat{M} + Kc_z)\psi = 0\,. \tag{33}$$

Now K can be considered to play the role of an eigenvalue. In solving (33), we expect to find two spectral sets $\{K_\mu^{(-)}\}$ and $\{K_\mu^{(+)}\}$, of which only the first plays any role if downstream regions are being considered and boundaries negelected. In fact, if the $K_\mu^{(-)}$ are known, then $K_\mu^{(+)}$ can be found from (29), if upstream/finite geometry situations are under examination. Of these, only the fundamental model $\mu = 0$ need be considered in asymptotic regions.

Table 1. Estimates of eigenvalues $K_\pm$ and $K_0^{(\pm)}$ from the diffusion equation (14) and the Boltzmann eigenvalue problem (33), respectively, for an electron swarm in water vapour at $T_0 = 293$ K, using the cross-section data set of Ness and Robson (1988). The reasonably good agreement between K_- and $K_0^{(-)}$ is in stark contrast with the enormous disparity between K_+ and $K_0^{(+)}$

E/n_0 (Td)	K_-/n_0	$K_0^{(-)}/n_0$ (10^{-21} m^2)	K_+/n_0	$K_0^{(+)}/n_0$ (10^{-20} m^2)
200	0·93	0·94	6·54	$7{\cdot}92\times10^2$
300	3·10	3·10	6·40	$1{\cdot}19\times10^3$
400	5·70	5·58	5·43	$1{\cdot}58\times10^3$
500	8·41	8·14	4·55	$1{\cdot}98\times10^3$
600	11·2	10·3	3·89	$2{\cdot}38\times10^3$

The general Boltzmann eigenvalue problem (25) and the reduced problem (33) specific to the SST experiment have been solved for electrons in water vapour (Robson and Ness 1990), using the cross-section set of Ness and Robson (1988). Estimates of eigenvalues found from the diffusion equation result (14) and from (33) are shown in Table 1 for E/n_0 over a range where ionisation is appreciable. (Note 1 Td $\equiv 10^{-17}$ V cm^2.)

The fairly good agreement between K_- and $K_0^{(-)}$ shown in the first two columns supports the approximation (31), at least in this case. However, K_+ is several orders of magnitude less than $K_0^{(+)}$. Thus, while the diffusion equation offers a reasonable way of modelling downstream density, it is not even qualitatively correct upstream.

To conclude this section, we observe that the eigenvalue equations shown here have appeared many times before in the literature, although the true nature of the problem has not always been recognised (Robson 1991). It would seem that the role played by equation (25) in the kinetic theory of swarms was first recognised by Kumar (1984). Standish (1989) adapted Kumar's theory to SST. Our results are essentially in accord with his observations, although the remarkable difference *in general* between the upper roots K_+ and $K_0^{(+)}$ of the diffusion equation and Boltzmann equation dispersion relations, $\Omega(K)$ and $\Omega_0(K)$ respectively, is lost for the particular collision model chosen by Standish: For the Fokker–Planck model,

$\Omega_0(K)$ is a quadratic in K, identical to $\Omega(K)$ and hence $\lambda = \Lambda$ and $K_+ \equiv K_0^{(+)}$ in that case.

4. Discussion

Although we have focussed on the SST experiment, it is worth a reminder that other experiments can also be analysed in terms of these dispersion curves appearing above (Robson 1991). Thus while SST effectively determines the intersections on the K-axis, the TOF experiment measures the intersection on the Ω-axis and the slope and curvature at small K (see equations 20 and 21). Apart from the upstream behaviour in SST, it is the small $-K$ properties of $\Omega_0(K)$ which are generally sampled in experiment. The significance of this is that the diffusion equation could then be expected to be useful in analysing these experiments, since it is essentially a weak-gradient (small-K) model of reality. Put another way, $\Omega(K) \approx \Omega_0(K)$ for small K (cf. Fig. 3). The large gradient/large-K situation is, however, quite different and the total inadequacy of the diffusion equation in the region upstream of the source in the SST experiment is an example of this.

A brief digression from the mathematics to consider a physical picture will serve to further highlight the qualitative inadequacy of the diffusion equation. Firstly, note that the diffusion equation (3) contains only an integrated source strength: There is no information as to *how* the particles actually enter the gas upon creation. No matter whether they are created at rest, or with an isotropic or anisotropic distribution of speeds, only the total strength σ appears. This detailed information must, of course, be specified when solving Boltzmann's equation, but at the level of the diffusion equation only the value integrated over all velocities enters the calculations. Thus, the diffusion equation cannot discriminate between the details of various types of sources and, consequently, neither do the expressions for density resulting from it, e.g. equations (18) and (19) for the upstream profile. The gas temperature T_0 plays a very important role in this upstream distribution, as we illustrate in the following example, but does not enter into the diffusion equation or its results except implicitly through the transport coefficients. On the other hand, T_0 appears explicitly in the Boltzmann equation formalism, through equation (24).

To understand how T_0 plays such an important role, consider a situation where the particles are created at rest and assume a cold gas, $T_0 \to 0$. This means that the particles drift and diffuse downstream only and can never gain energy and momentum through collisions with neutral molecules to diffuse upstream against the field. That is, the density $n(z)$ must be identically zero upstream and (18) and (19) are simply wrong in this case. On the other hand, if K_+ in (19) is replaced with the Boltzmann $K_0^{(+)}$ given by (29), then as $T_0 \to 0$, we see that $K_0^{(+)} \to \infty$ and the density vanishes everywhere upstream, as required by the above physical considerations.

Tagashira *et al.* (1994) have recognised the shortcomings in the diffusion equation upstream of the source in the SST experiment, but have attempted to come to terms with this problem by effectively introducing a different diffusion equation for the upstream region with different coefficients W', D' and ν_I', resulting in different zeros $K_\pm'$. Such an *ad hoc* recipe is, however, at odds with the functional premise that the coefficients in (3) are constants, determined solely

by the field, gas properties (density, temperature) and fundamental collision cross sections. That the real diffusion equation may fail hopelessly upstream is not grounds for replacing it with an artificial one. In fact, if an artificial transport equation is to be introduced, there is no good reason that it should be a parabolic, second order differential equation like the diffusion equation: *Any* equation of *arbitrary* order would do, as long as it produced the same *upper* exponent $K_0^{(+)}$! Of course, the only correct transport equation, producing true values of both exponents $K_0^{(+-)}$, is the Boltzmann equation. For these reasons we feel that the only tenable alternative is to solve the full Boltzmann equation, along the lines reported in Robson (1991) or by other means (Sugawara *et al.* 1994).

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