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Collided-flux-expansion method for the transport of muonic deuterium in finite media

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Transport of muonic deuterium atoms in a slab of thickness d filled with a molecular deuterium gas is described by means of the multiple-collision expansion in the framework of a time-dependent theory. The relevant expressions for the emerging flux are derived. Numerically generated results are presented for several different cases, some of which are under experimental investigation. A justification of the approximations made in a previous work is given.

I. INTRODUCTION

In this work we investigate the efficiency of the multiple-collision expansion, Refs. [1] and [2], and references therein, as a tool for modeling the transport of muonic atoms in a molecular gas. The multiple-collision expansion is nothing other than a Neumann series solution of the integral form of the transport equation (Ref. [6], p. 48) and may thus be considered a perturbation series, analogous to the Dyson series of QED. This series converges rapidly when the optical thickness of the medium being studied is small. As discussed in Ref. [3], a diffusion approximation can be applied to optically thick media [(optical thickness)=(cross section)×(thickness)]. Our work is intended to extend the transport calculations presented in Sec. V of Ref. [3] to include certain anisotropy effects and energy-dependent cross sections [4,5].

In Ref. [2], multiple-collision theory has been used to describe neutron transport in infinite media. An essential feature in the successful application of this method to infinite geometry is the fact that the solution is factorizable into a function of t multiplied by a function of μ and of $y=x/vt$, where μ is the cosine of the angle variable. Although this property does not carry over to finite geometry, our physical intuition would suggest that the multiple-collision-expansion theory is perfectly applicable to problems involving finite media of moderate thickness, as pointed out by Case and Zweifel [6], since the streaming out of particles should leave inside only low-order collided particles and, therefore, only a few terms in the collision expansion should play a significant role.

In Ref. [3], Rusjan and Zweifel have calculated the emerging flux of muonic deuterium atoms from a slab of molecular deuterium, via multiple-collision expansion with a one-speed approximation. Our purpose is to develop the relevant equations and carry out the numerical analysis in order to remove certain simplifying assumptions imposed in the quoted reference. In particular, we want to remove the assumption that all atoms contributing to the once-collided particle flux travel with the same speed, the assumption that the once-collided particles are generated by an isotropic source, the assumption of isotropic scattering in the center-of-mass reference frame, and we want also to take the scattering cross sections to be continuously dependent on the energy. Our goal is to evaluate the effectiveness of the approximations made in Ref. [3], considering both the accuracy that can be reached in the calculation of the emerging flux and the computer resources needed by such work. This investigation is required because for many cases of practical interest high-order collision terms need to be evaluated, but there is no hope of performing the relevant numerical calculations without certain appropriate simplifying assumptions.

Here we address these questions for cases of particular interest to us; in particular, we study cases under experimental investigation, as pointed out to us by Siegel [7]. In Sec. II we develop the relevant mathematical framework, following the standard prescriptions of particle transport theory. We conclude, in Sec. III, that modern computers can successfully tackle such complicated problems, because the simplifying assumptions of Ref. [3], required to render the method practical, are verified.

II. APPLICATION TO THIN MEDIA

Let us concentrate first on optically thin media, from which most atoms escape without undergoing a single collision. Let us consider a slab of thickness d filled with molecular deuterium at a temperature T and at a pressure p, and assume there is a source of muonic deuterium atoms of the form $S(E,t)=S_0\delta(t)\delta(E-E_0)$. Assuming also that the muonic atoms are produced in such a way as to respect the statistical mixture of doublet (D) and quadruplet (Q) states, i.e., $S_0=S_{0D}+S_{0Q}$ and $S_{0D}=S_{0Q}/2$. This models the experimental setup for muon experiments, and is also of interest for the study of muon catalyzed fusion [8–15].

Expanding the angular flux ϕ_a for $a=D,Q$ as

$$\phi_a=\sum_{m=0}^{\infty}\phi_a^{(m)}\,, \tag{1}$$

where $\phi_a^{(m)}$ is the flux of particles of species a that have undergone m collisions, we have

$$\phi_a^{(m)}(t,x,\mu,E)=\int_0^t v\exp\left[-v\Sigma_a(E,x-\mu v(t-\tau))v(t-\tau)\right]S_a^{(m-1)}(\tau,x-\mu v(t-\tau),\mu,E)d\tau . \quad (2)$$

This can be viewed both as the solution to the transport equation

$$\frac{1}{v}\frac{\partial\phi_a^{(m)}}{\partial t}+\mu\frac{\partial\phi_a^{(m)}}{\partial x}+\Sigma_a\phi_a^{(m)}=S_a^{(m-1)} \quad (3)$$

via integration along the characteristics [6], or as a balance equation in the phase space of the system [16],[17]. In turn, $S_a^{(m)}$ is expressed as

$$S_a^{(m)}(t,x,\mu,E)=\int_0^\infty dE'\int_{-1}^1 d\mu'\Sigma_{aa}(E'\to E,\mu'\to\mu;x)\phi_a^{(m)}(t,x,\mu',E') + \int_0^\infty dE'\int_{-1}^1 d\mu'\Sigma_{ba}(E'\to E,\mu'\to\mu;x)\phi_b^{(m)}(t,x,\mu',E') , \quad (4)$$

where $\Sigma_a(E,x)$ is the total macroscopic cross section for atoms of species a and v is their speed. $S_a^{(m)}(t,x,\mu,E)$ represents the number of m-collided particles with energy E and direction μ that are produced by collisions suffered by the (m-1)-collided particles in the unit volume around x at time t. $\Sigma_{aa}(E'\to E,\mu'\to\mu;x)$ is the transfer function for collisions of particles a to remain particles a and to change energy from E' to E and direction from μ' to μ at the position x. $\Sigma_{ba}(E'\to E,\mu'\to\mu;x)$ has the same meaning but for inelastic collisions that change particles b into particles a.

Let us assume, now, that our slab is homogeneous and isotropic. Then we can perform the standard analysis of those functions via orthogonal polynomials (see Ref. [6], [18], and [19], for instance) and write

$$\Sigma(E'\to E,\mu'\to\mu;x)=H(d/2-|x|)\Sigma(E'\to E,\mu'\to\mu) \quad \text{(homogeneous medium)} , \quad (5)$$

$$\Sigma(E'\to E,\mu'\to\mu)=\sum_{l=0}^\infty\frac{2l+1}{2}P_l(\mu)P_l(\mu')\Sigma^l(E'\to E) \quad \text{(isotropic medium)} , \quad (6)$$

$$\Sigma^l(E'\to E)=\int_{-1}^{-1}\Sigma(E'\to E,\mu)P_l(\mu)d\mu , \quad (7)$$

$$\phi_{al}^{(m)}(t,x,E)=\int_{-1}^{-1}\phi_a^{(m)}(t,x,\mu,E)P_l(\mu)d\mu , \quad (8)$$

where H is the Heaviside function. Substituting into Eq. (4) we get

$$S_a^{(m)}(t,x,\mu,E)=\int_0^\infty dE'\int_{-1}^1 d\mu'\phi_a^{(m)}(t,x,\mu',E')\sum_{l=0}^\infty\frac{2l+1}{2}\Sigma_{aa}^l(E'\to E;x)P_l(\mu)P_l(\mu') + \int_0^\infty dE'\int_{-1}^1 d\mu'\phi_b^{(m)}(t,x,\mu',E')\sum_{l=0}^\infty\frac{2l+1}{2}\Sigma_{ba}^l(E'\to E;x)P_l(\mu)P_l(\mu') . \quad (9)$$

If we go one step beyond the assumption of isotropic scattering and stop our sums at $l=1$, then $S_a^{(m)}$ is the sum of four terms only, namely,

$$S_a^{(m)}=\int_0^\infty dE'\{\tfrac{1}{2}[\Sigma_{aa}^0\phi_{a0}^{(m)}+\Sigma_{ba}^0\phi_{b0}^{(m)}] + \tfrac{3}{2}\mu[\Sigma_{aa}^1\phi_{a1}^{(m)}+\Sigma_{ba}^1\phi_{b1}^{(m)}]\} . \quad (10)$$

We need to know the form of the transfer functions that appear in (9). Through a classical procedure [18,20], assuming stationary scattering centers and defining the function Λ as $\Lambda(E,E')=H(E-E^-(E'))-H(E-E^+(E'))$, we get

$$\Sigma_{aa}^0(E'\to E;x)=H(d/2-|x|)\frac{\Sigma_{aa}(E')}{(1-\alpha)E'}\times[H(E'-E)-H(E'-E/\alpha)] , \quad (11)$$

where

$$\alpha=\left[\frac{A-1}{A+1}\right]^2 ,$$

1 is the projectile mass and A is the target mass,

$$E^\pm=E'\left[\frac{A\beta(E')\pm 1}{A+1}\right]^2 ,$$

and

$$\beta(E')=\left[1+\frac{A+1}{A}\frac{U}{E'}\right]^{1/2} ,$$

in which U is the projectile potential-energy change in the inelastic collision, and

$$\Sigma_{QD}^0(E'\to E;x)=H(d/2-|x|)\frac{\Sigma_{QD}(E')}{(1-\alpha)E'\beta(E')}\Lambda(E,E') , \quad (12)$$

$$\Sigma_{DQ}^0(E'\to E;x)=H(d/2-|x|)\times\begin{cases}0 & \text{if } 0\le E'<-\frac{A+1}{A}U\\ \frac{\Sigma_{DQ}(E')}{(1-\alpha)E'\beta(E')}\Lambda(E,E') & \text{if } E'\ge\frac{A+1}{A}U ,\end{cases} \quad (13)$$

$$\Sigma^1_{ac}(E'\to E;x)=\tfrac{1}{2}\Sigma^0_{ac}(E'\to E;x)[(A+1)\sqrt{E/E'}-(A-1)\sqrt{E'/E}], \quad (14)$$

for $c=b$ and $c=a$. Note that in Ref. [3] the $U_{\rm eff}$ term given in Ref. [20] was used for the calculations relevant to the transport of muonic hydrogen, instead of U. The symbols used in [3] and [20] are Q and $Q_{\rm eff}$. Here we are not going to make that correction to the value of U because the change is negligible when muonic deuterium is considered.

In order to have an analytical expression for $S_a^{(m)}$ in (10), we need to know the form of $\phi^{(m)}_{D0},\phi^{(m)}_{Q0},\phi^{(m)}_{D1},\phi^{(m)}_{Q1}$, which are known if $S_a^{(m-1)}$ is known. Then we may start from $\phi_a^{(0)}(t,x,\mu,E)$ and its zeroth and first moments, and iteratively construct all the others. This can be done by first solving

$$\frac{1}{v_0}\frac{\partial\phi_a^{(0)}}{\partial t}+\mu\frac{\partial\phi_a^{(0)}}{\partial x}+\Sigma_a\phi_a^{(0)}=S_{0a}\delta(t)\delta(E-E_0)\ . \quad (15)$$

In Ref. [3] Eq. (15) was solved with $S_0=1/2d$ and $\phi^{(0)}_{a0}(t,x,E)$ and $\phi^{(0)}_{a1}(t,x,E)$ were given analytically. This allows us to compute the emerging uncollided flux $X_a^{(0)}(t,E_0)=2\phi^{(0)}_{a1}(t,d/2,E_0)$, which agrees with that in Ref. [3], and it yields an analytical expression for $S_a^{(0)}$:

$$S_a^{(0)}(t,x,\mu,E)=H(d/2-|x|)\Bigg[\frac{1}{2}[\Sigma^0_{aa}(E_0\to E)\phi^{(0)}_{a0}(t,x,E_0)+\Sigma^0_{ba}(E_0\to E)\phi^{(0)}_{b0}(t,x,E_0)]$$
$$+3[\Sigma^1_{aa}(E_0\to E)\phi^{(0)}_{a1}(t,x,E_0)+\Sigma^1_{ba}(E_0\to E)\phi^{(0)}_{b1}(t,x,E_0)]\frac{\mu}{2}\Bigg]\ . \quad (16)$$

Substituting (16) into (2) one may derive an analytical expression for $\phi_a^{(1)}(t,d/2,\mu,E)$, namely,

$$\phi_a^{(1)}(t,d/2,\mu,E)=\frac{ve^{v\Sigma_a(E)t}}{2}\Bigg[[\Sigma^0_{aa}(E_0\to E)I_0^{aa}(t,d/2,\mu,E)+\Sigma^0_{ba}(E_0\to E)I_0^{ba}(t,d/2,\mu,E)]$$
$$+\frac{3\mu v}{2}[\Sigma^1_{aa}(E_0\to E)I_1^{aa}(t,d/2,\mu,E)+\Sigma^1_{ba}(E_0\to E)I_1^{ba}(t,d/2,\mu,E)]\Bigg] \quad (17)$$

for $a\neq b$, where

$$I_0^{ca}(t,d/2,\mu,E)=\int_0^t H\left[\frac{d}{2}-\left|\frac{d}{2}-\mu v(t-\tau)\right|\right]\phi^{(0)}_{c0}\left[\tau,\frac{d}{2}-\mu v(t-\tau),E_0\right]e^{v\Sigma_a(E)\tau}d\tau$$
$$=S_0\Bigg[\frac{2v_0}{L_{ca}(E,E_0)}(e^{L_{ca}(E,E_0)t}-e^{L_{ca}(E,E_0)T_i'})-\frac{v_0+\mu v}{L_{ca}(E,E_0)}(e^{L_{ca}(E,E_0)T_{f1}}-e^{L_{ca}(E,E_0)T_{i1}})$$
$$+\frac{v_0-\mu v}{L_{ca}(E,E_0)}(e^{L_{ca}(E,E_0)T_{f1}}-e^{L_{ca}(E,E_0)T_{i1}})$$
$$+\mu vt\{E_1[-L_{ca}(E,E_0)T_{i1}]-E_1[-L_{ca}(E,E_0)T_{f1}]\}$$
$$-(d-\mu vt)\{E_1-[L_{ca}(E,E_0)T_{i2}]-E_1[-L_{ca}(E,E_0)T_{f2}]\}\Bigg]\ , \quad (18)$$

where $T_i'=0$ if $t\le d/(2\mu v)$ and $T_i'=\max[0,t-d/(\mu v)]$ if $t>d/(2\mu v)$, and

$$I_1^{ca}(t,d/2,\mu,E)=\int_0^t H\left[\frac{d}{2}-\left|\frac{d}{2}-\mu v(t-\tau)\right|\right]\phi^{(1)}_{c0}\left[\tau,\frac{d}{2}-\mu v(t-\tau),E_0\right]e^{v\Sigma_a(E)\tau}d\tau$$
$$=\frac{S_0}{v_0}\Bigg[\frac{v_0^2-\mu^2v^2}{2L_{ca}(E,E_0)}(e^{L_{ca}(E,E_0)T_{f1}}-e^{L_{ca}(E,E_0)T_{i1}}-e^{L_{ca}(E,E_0)T_{f2}}+e^{L_{ca}(E,E_0)T_{i2}})$$
$$+\mu^2v^2t\{E_1[-L_{ca}(E,E_0)T_{i1}]-E_1[-L_{ca}(E,E_0)T_{f1}]\}$$
$$+\mu v(d-\mu vt)\{E_1[-L_{ca}(E,E_0)T_{i2}]-E_1[-L_{ca}(E,E_0)T_{f2}]\}$$
$$-\frac{(\mu vt)^2}{2}\left[\frac{E_2[-L_{ca}(E,E_0)T_{i1}]}{T_{i1}}-\frac{E_2[-L_{ca}(E,E_0)T_{f1}}{T_{f1}}\right]$$
$$+\frac{(d-\mu vt)^2}{2}\left[\frac{E_2[-L_{ca}(E,E_0)T_{i2}]}{T_{i2}}-\frac{E_2[-L_{ca}(E,E_0)T_{f2}]}{T_{f2}}\right]\Bigg] \quad (19)$$

for $c=b$ and $c=a$. Here $L_{ca}(E,E_0)=v\Sigma_a(E)-v_0\Sigma_c(E_0)$,

$$E_n(x)=\int_1^\infty \frac{e^{-xt}}{t^n}dt \quad \text{for } n=1,2 \ , \tag{20}$$

and

$$T_{ij}=T_{ij}(t,\mu,v)=\max\left[t_{ij}(t,\mu,v),t-\frac{d}{\mu v}\right],\quad T_{fj}=T_{fj}(t,\mu,v)=\max\left[t_{fj}(t,\mu,v),t-\frac{d}{\mu v}\right] \quad \text{if } t-\frac{t}{2\mu v}\geq t_{fj}(t,\mu,v)\ , \tag{21}$$

$$T_{ij}=T_{ij}(t,\mu,v)=\max\left[t_{ij}(t,\mu,v),t-\frac{d}{\mu v}\right],\quad T_{fj}=T_{fj}(t,\mu,v)=t_{fj}(t,\mu,v) \quad \text{if } t_{ij}(t,\mu,v)<t-\frac{t}{2\mu v}<t_{fj}(t,\mu,v)\ , \tag{22}$$

$$T_{ij}=T_{ij}(t,\mu,v)=t_{ij}(t,\mu,v),\quad T_{fj}=T_{fj}(t,\mu,v)=t_{fj}(t,\mu,v) \quad \text{if } t-\frac{t}{2\mu v}\leq t_{ij}(t,\mu,v) \tag{23}$$

for $j=1,2$, where the following must be used:

$$t_{i1}(t,\mu,v)=\min\left[t,\frac{\mu v t}{v_0+\mu v}\right]\ ,\qquad t_{f1}(t,\mu,v)=t\ , \tag{24}$$

$$t_{i2}(t,\mu,v)=\begin{cases}\min\left[t,\max\left[0,\dfrac{d-\mu v t}{v_0-\mu v}\right]\right], & v_0>\mu v\\ \left.\begin{array}{l} t_{f2}(t,\mu,v)\ \text{ if } d-\mu v t>0\ ,\\ 0\ \text{ if } d-\mu v t\leq 0\ ,\end{array}\right\} & v_0=\mu v\\ 0, & v_0<\mu v\ ,\end{cases} \tag{25}$$

$$t_{f2}(t,\mu,v)=\begin{cases} t, & v_0\geq\mu v\\ \max\left[0,\min\left[t,\dfrac{d-\mu v t}{v_0-\mu v}\right]\right], & v_0<\mu v\ .\end{cases} \tag{26}$$

The last step is to compute, with the aid of a computer, the experimentally measurable quantity, that is,

$$X(t)=\sum_{m=0}^{\infty}X^{(m)}(t)=\sum_{m=0}^{\infty}[X_D^{(m)}(t)+X_Q^{(m)}(t)]\ , \tag{27}$$

where

$$X_a^{(m)}(t)=2\int_0^\infty dE\int_0^1 d\mu[\mu\phi_a^{(m)}(t,d/2,\mu,E)]\ . \tag{28}$$

In our case we determine the contribution of the zeroth- and first-order collided particles only, as done in Ref. [3], in order to assess the validity of

$$X(t)\simeq X^{(0)}(t)+X^{(1)}(t) \tag{29}$$

and to compare our results with those given in Ref. [3], Fig. 1.

III. NUMERICAL RESULTS

Numerically we have computed the quantities given in (28) and (29) and the integrated flux

$$F(t)=\int_0^t X(s)ds \tag{30}$$

starting from the knowledge of the analytical expression for $\phi_a^{(0)}$ and $\phi_a^{(1)}$. Three numerical integrations had to be performed: one over the angle variable, one over the en-

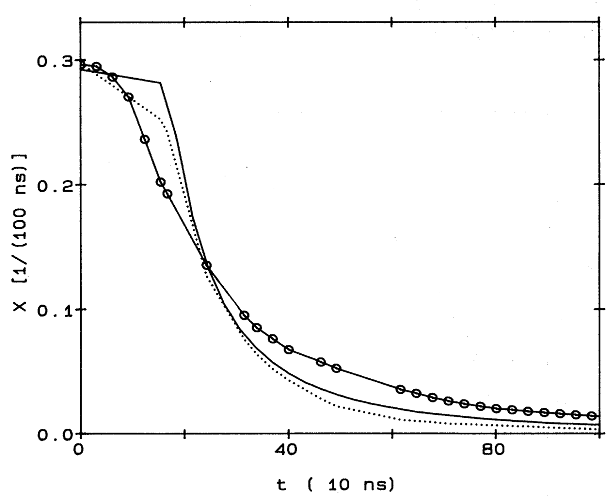

FIG. 1. Comparison between our calculation (the solid line) and Fig. 5 in Ref. [3] for the case where $E_0=2$ eV, $T=300$ K, $d=0.23$ cm, $p=0.188$ bar. Here, the solid line with circles gives the results of a Monte Carlo simulation, while the dotted line represents what can be obtained by the method presented in Ref. [3].

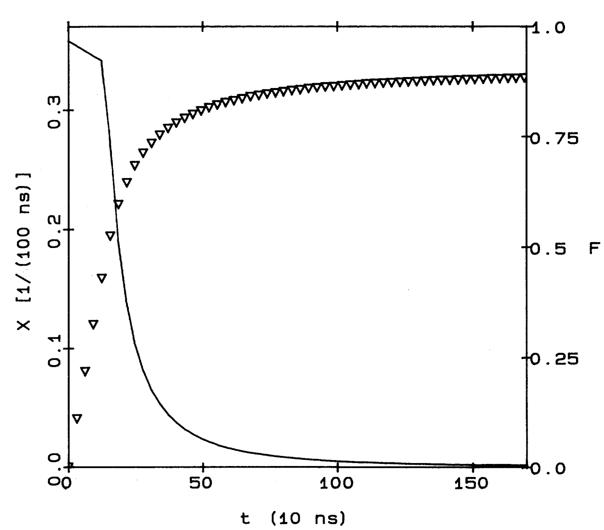

FIG. 2. $E_0=3$ eV, $T=500$ K, $d=0.23$ cm, $p=0.375$ bar. After 1.7 μs the flux has become negligible. The contribution of zeroth and first order will exceed 85%.

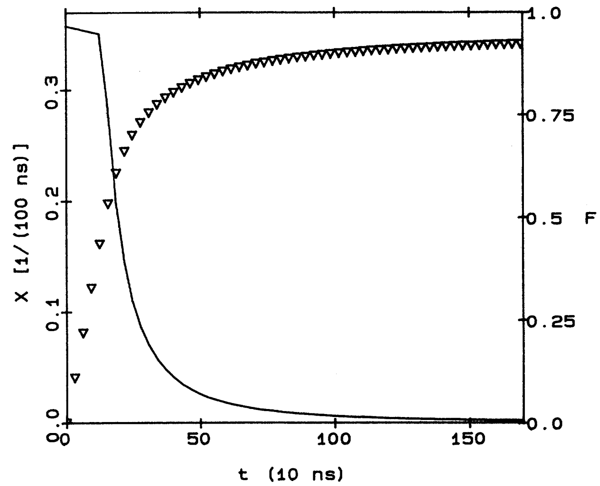

FIG. 3. $E_0=3$ eV, $T=1200$ K, $d=0.23$ cm, $p=0.375$ bar. The contribution of zeroth and first order exceeds 90%.

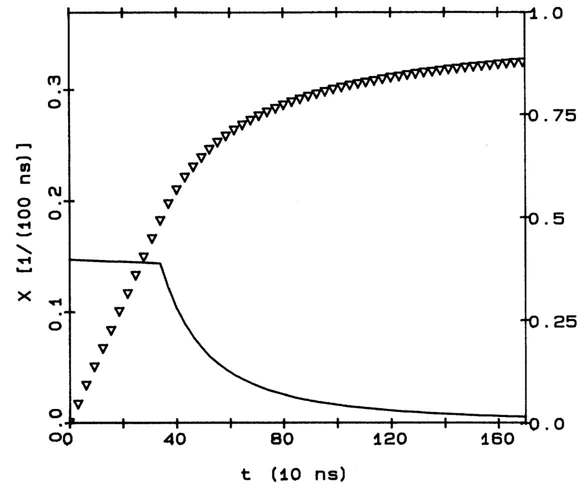

FIG. 5. $E_0=2$ eV, $T=1200$ K, $d=0.4572$ cm, $p=0.188$ bar. The contribution of zeroth and first order is more than 85%.

ergy variable, and one over the time variable, in the given order. For the first integration we performed accuracy tests on several different integration routines, as available to us, which convinced us to choose the routine QDAGS, of the vectorized IMSL-MATH/11 package available on the Pittsburgh Cray Y-MP computer, and the routine GAULEG, presented in Ref. [21]. Of these, QDAGS is to be preferred on the grounds of CPU-time performance, as our program runs about 20 times faster when QDAGS is used as compared to when the same program is run with GAULEG. The integration over energy was performed through a standard but fine (approximately 30 groups) multigroup approximation of the continuous distribution. Note that the integral over the energy only apparently goes from 0 to ∞, since there are no particles of zeroth and first collision order with energy higher than E_0+U. Finally, the integration over the time variable was performed through an integration routine devised by us and based on the trapezoid rule. We observe that the expressions (11)-(14) assume that the target molecules are at rest; thus they apply strictly only for $T=0$. For $T>0$, the thermal motion of the scattering centers must be taken into account, and two corrections must be introduced: (a) the Doppler broadening (or Wigner-Wilkins effect), and (b) the temperature-dependent effect of the chemical bond. We have introduced these two corrections by averaging over Maxwellian distribution and by multiplying the free microscopic cross sections by a temperature-dependent factor, following the same procedure discussed in Ref. [20]. The other obvious effect of the temperature is on the density of the scattering centers, which were assumed to be the constituents of a perfect gas. Some results, are given in Figs. 1–8. Note that in all the figures, with the exception of Fig. 1, the y axis on the left refers to

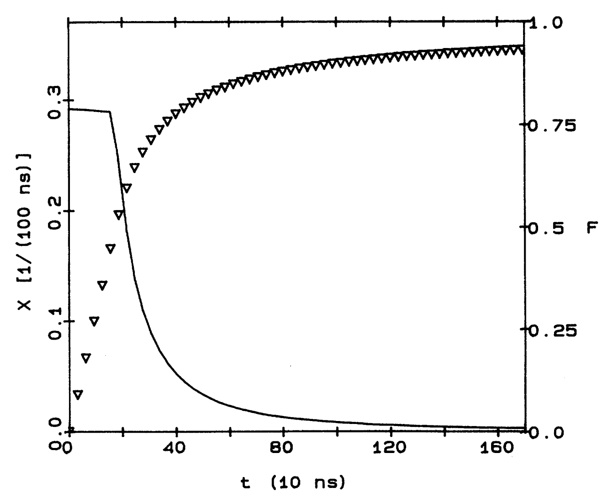

FIG. 4. $E_0=2$ eV, $T=1200$ K, $d=0.23$ cm, $p=0.188$ bar. The contribution of zeroth and first order exceeds 90%.

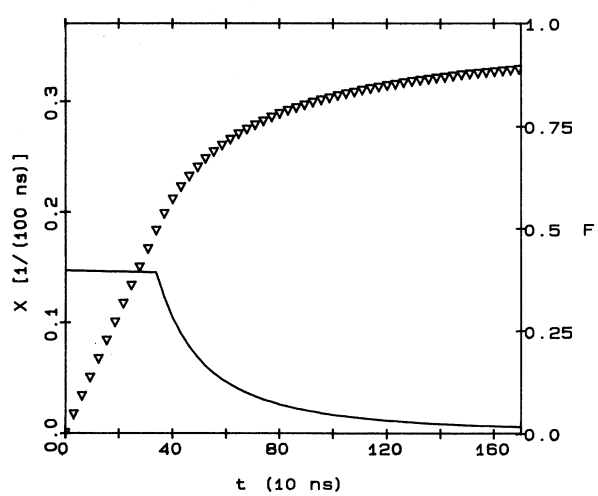

FIG. 6. $E_0=2$ eV, $T=1200$ K, $d=0.4572$ cm, $p=0.094$ bar. The contribution of zeroth and first order is about 90%.

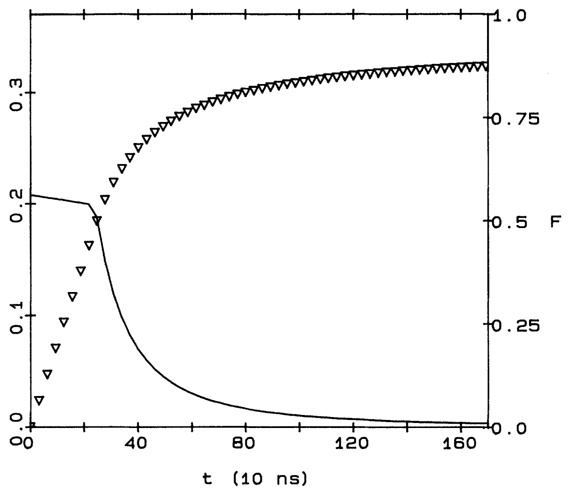

FIG. 7. $E_0=4$ eV, $T=300$ K, $d=0.4572$ cm, $p=0.094$ bar. The contribution of zeroth and first order is about 90%.

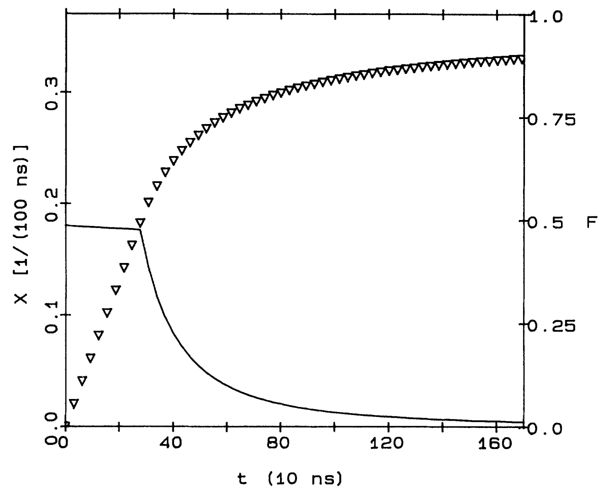

FIG. 8. $E_0=3$ eV, $T=1200$ K, $d=0.4572$ cm, $p=0.188$ bar. The contribution of zeroth and first order is about 90%.

the solid line, i.e., to the emerging flux $X(t)$, while the y axis on the right refers to the triangles, i.e., to $F(t)$, which represents the fraction of particles of zeroth and first order that escaped from the medium in the time interval $[0,t]$.

Our results show good agreement with the calculations previously published for the optically thin media considered in Ref. [3]. For such media, the difference between our calculation and that of Rusjan and Zweifel amounts to about 1% when the emerging flux X is considered, and about 5% for the integrated emerging flux; see Fig. 1. This may be taken, then, as a bound on the performance of the simpler scheme outlined by those authors.

For increased accuracy and to consider somewhat thicker slabs, it will be necessary to consider higher-order collided fluxes. Here, the inclusion of anisotropy and energy dependence complicates greatly the necessary analytical development and increases the computer-resource needs, and so the approach of Ref. [3] is likely to be necessary for practical considerations. Indeed, our analysis shows that the approximations of one energy group, isotropic scattering, and the isotropic source of once-collided particles can be made without causing serious errors, and with the advantage that calculations can be carried out within reasonable time limits, thus making feasible a higher-order collision-expansion analysis. The method presented in Ref. [3] is the only one, of which we are currently aware, capable of achieving such results.

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