

On the slowing down of charged particles in a binary stochastic mixture

JEAN-FRANÇOIS CLOUET

CEA/Bruyères, Bruyères-le-Chatel, 91297 Arpajon Cedex, F.

FRANÇOIS GOLSE

Centre de Mathématiques, Ecole Polytechnique, 91128 Palaiseau Cedex, F.

MARJOLAINE PUEL

Laboratoire MIP, Université paul Sabatier, 31062 Toulouse, F.

RÉMI SENTIS ¹

CEA/Bruyères, Bruyères-le-Chatel, 91297 Arpajon Cedex, F.

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Abstract. A kinetic equation is addressed for the straight line slowing-down of charged particles, the geometrical domain consists of randomly distributed spherical grains of dense material imbedded in a light material. The dense material is assumed to be a Boolean medium (the sphere centers are sampled according to a Poisson random field). We focus on the fraction of particles P which stop in the light medium. After setting some properties of the Boolean medium, we perform an asymptotic analysis in two extreme cases corresponding to grain radius very small and very large with respect to the stopping distance of the dense material. A fitted analytic formula is proposed for the quantity P and results of numerical simulations are presented in order to validate the proposed formula.

Running head: Slowing down in a binary stochastic mixture

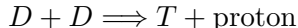
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¹communicating author, remi.sentis@cea.fr

1 Introduction

The motivation of this study is the following. In the framework of Inertial Confinement Fusion experiments with Deuterium (D) targets, the thermonuclear reaction



creates Tritium (T) ions with a very high velocity - so they are called suprathermal. These tritium ions travel in the plasma and after slowing down they stop and may undergo new thermonuclear reactions with the Deuterium ions creating neutrons (the corresponding cross section is much larger than the one of $D + D$ reactions). So it is of primal interest to know where the Tritium ions stop. Here we are concerned with this problem in the case of a heterogeneous plasma. This plasma consists of a mixture of two materials: the Deuterium which is called the "light" material and a dense one whose presence is due to the hydrodynamic instabilities during the implosion (see Lindl [11] for physical background). Therefore, one has to estimate the fraction of suprathermal ions which stop in each material in order to estimate accurately the number of $D + T$ reactions.

For the modeling of this problem, one has to describe the motion of particles in the plasma and to know the mixture characteristic. Slowing down of suprathermal particles is classically described by a linear Vlasov equation (see eq. (1) below); the slowing down is assumed to be on straight line, that is to say the scattering phenomena are neglected. But, the structure of heterogeneous medium is not well known because it arises from complex hydrodynamic flow and we have to adopt a statistical description. This problem has been addressed in numerous articles [17], [18], [8], [10]; but in these papers, the heterogeneous medium is always assumed to be Markovian with the same law in all directions. Although it enables to compute explicitly the fraction of particles lost in the dense material and leads to simple formulas, this model should be questioned because it seems not to be realistic (it is not clear that such a medium may be built easily in the three-dimensional case, see the end of §5 for this point).

In this paper, we use a different approach. The heterogeneous medium is assumed to consist of randomly distributed spherical grains of dense material embedded in the light material. With classical tools of stochastic geometry (see [16], [21]), the dense material is built as a Boolean medium \mathcal{G} which is statistically homogeneous and isotropic. The problem may be studied by an asymptotic analysis in two extreme cases corresponding to grain radius which are very small and very large with respect to the stopping distance in the dense material \mathcal{G} . So, for these two extreme cases, we may evaluate the fraction P of particles which stop in the light material \mathcal{G}^c , by an analytical way. In the sequel this fraction P is expressed as a function of the relevant parameters of the model and mainly the volume fraction of \mathcal{G} , so we often write $P = P(f)$. For the general cases, we have to fit a formula which interpolate the ones obtained by asymptotic analysis; it is done by performing a set of numerical simulations corresponding to different physical coefficients and to various sampling of the Boolean medium \mathcal{G} .

The paper is organized as follows. In section 2, we describe the physical model and we build the stochastic Boolean medium \mathcal{G} . The relevant parameters of the model are exhibited and

some properties of the Boolean medium are also given, especially the estimation of the mean chord lengths, using the so-called capacity functional [21]. Section 3 is devoted to the asymptotic analysis of the problem in the cases where the grain radius is very small or very large (compared to the grain stopping distance) and we write the corresponding analytic formulas for the fraction of particles $P(f)$ which stop in the light material. We state also a fitted formula for $P(f)$ which may be applied to general cases. In section 4, we present the results of the numerical simulations in various situations for the validation of the previous formula. Our results are also compared with those of [8].

2 The physical model and the geometry

In this paper, we assume that the slowing down of the suprathreshold particles occurs only on straight lines (the scattering phenomena are neglected; for a more realistic model, see [3]). Let us denote $\mathbf{v} = \Omega w$ the particle velocity of the particles, with $w \in \mathbf{R}^+$ and $\Omega \in \mathbf{S}^2$, the unit sphere. To model the behavior of the density of the charged particles $u = u(t, \mathbf{x}, w, \Omega)$ at time t , position $\mathbf{x} \in \mathbf{R}^3$ and velocity Ωw , we consider the transport equation

$$\frac{\partial u}{\partial t} + w\Omega \cdot \frac{\partial u}{\partial \mathbf{x}} = k(\mathbf{x}) \frac{\partial}{\partial w} (S(w)u). \quad (1)$$

Here the slowing down function is assumed to be factorized by a product of an universal function $S(w) = s_0(w^2/\beta^3 + 1/w)$ with a slowing coefficient $k(x)$ depending only on the space variable. One assumes that the heterogeneous medium consists of two materials : the sub-domain \mathcal{G} is the union of spherical granules of a "dense" plasma (the pollutant) and in the other one \mathcal{G}^c there is the reacting matter, called "light". So one states $k(\mathbf{x}) = k_g$ in \mathcal{G} and $k(\mathbf{x}) = k_l$ in \mathcal{G}^c . In the function S , the w^2 term models the interactions with the electrons while the $1/w$ term models the interactions with ions (the coefficient β depends mainly on the ionization level, the atomic number of the ion and the electron temperature of the plasma and is assumed to be constant in this paper).

The particles are assumed to be created with an uniform angular direction and a fixed energy, corresponding to the velocity w_{\max} , that is to say the initial velocity distribution is

$$d\Omega \delta_{w_{\max}}(dw) \quad (\delta_{w_{\max}}, \text{ the Dirac mass in } w_{\max}).$$

We assume also that all the particles are created uniformly in the sub-domain \mathcal{G}^c , then the initial value of u may read as

$$u(0, \mathbf{x}, w, \Omega) dw d\Omega = u^0(\mathbf{x}, w, \Omega) dw d\Omega \equiv \mathbf{1}_{\mathcal{G}^c}(\mathbf{x}) \delta_{w_{\max}}(dw) d\Omega.$$

It is easy to show that for t large enough, $u(t, x, w, \Omega) dw$ converges to a Dirac mass at $w = 0$ (the particle stops after a finite time). We want to determine the probability that the particles stop in the light medium \mathcal{G}^c , that is to say we wish to get an evaluation of the following quantity

$$P = \lim_{t \rightarrow \infty} \frac{\int \int \int \mathbf{1}_{\mathcal{G}^c}(\mathbf{x}) u(t, x, \Omega, w) \frac{d\Omega}{4\pi} d\mathbf{x} dw}{\int \mathbf{1}_{\mathcal{G}^c}(\mathbf{x}) d\mathbf{x}} \quad (2)$$

As a matter of fact the above limit is reached for t large enough (see the remark below).

2.1 Stopping distances

We address first the case where the slowing down coefficient k is constant. For a fixed value of the variable Ω , the solution u of equation (1) may be replaced by $u = u(t, y, w)$ (where $y \in \mathbf{R}^+$ corresponds to an abscissa along a trajectory) which is solution to

$$\frac{\partial u}{\partial t} + w \frac{\partial u}{\partial y} = k \frac{\partial}{\partial w} (S(w)u).$$

The characteristic curves $(Y(t), W(t))$ for this equation are given by

$$dY(t) = W(t)dt, \quad dW(t) = -kS(W(t))dt$$

thus we get

$$\frac{W(t)}{S(W(t))} dW(t) = -k dY(t).$$

Defining the function H by $H(W) = \int_0^W \frac{v}{S(v)} dv = \frac{\beta^3}{3s_0} \log(1 + \frac{W^3}{\beta^3})$, for $W > 0$, we have for all t^1, t^2 (with $t^2 > t^1$)

$$k(Y(t^2) - Y(t^1)) = H(W(t^1)) - H(W(t^2)).$$

Recall that the initial velocity is $W(0) = w_{\max}$, then the velocity becomes zero after a finite distance which is equal to $k^{-1}H(w_{\max})$. This distance is called the stopping distance. The coefficient s_0 is chosen such that $H(w_{\max}) = 1$ (that is $s_0 = \frac{\beta^3}{3} \log(1 + w_{\max}^3/\beta^3)$). Then the stopping distance is equal to k^{-1} .

In our model, two stopping distances are to be considered: k_l^{-1} in the light medium \mathcal{G}^c and k_g^{-1} in \mathcal{G} . We always have $k_l^{-1} > k_g^{-1}$.

Remark. Since $k(Y)dt = -S(W(t))^{-1}dW(t)$, the stopping time is bounded from above by t_{\max} which satisfies

$$k_l t_{\max} = \int_0^{w_{\max}} \frac{1}{S(v)} dv \leq \frac{\beta^2}{2s_0} \int_0^\infty \frac{dz}{1+z^{3/2}} \leq \frac{3\beta^2}{2s_0} = \frac{9}{2\beta \log(1 + w_{\max}^3/\beta^3)}$$

Thus by setting $t_{\max} = (k_l \frac{2}{9} \beta \log(1 + w_{\max}^3/\beta^3))^{-1}$, formula (2) may be simplified and reads as

$$P = \frac{\int \int \int \mathbf{1}_{\mathcal{G}^c}(\mathbf{x}) u(t_{\max}, \mathbf{x}, \Omega, w) \frac{d\Omega}{4\pi} d\mathbf{x} dw}{\int \mathbf{1}_{\mathcal{G}^c}(\mathbf{x}) d\mathbf{x}}$$

2.2 Stochastic geometry

In the sequel, for any compact set A , one denotes by $|A|$ its volume, by $A_{(\mathbf{z})}$ the compact set translated by a vector \mathbf{z} and by $S_{\mathbf{o}}$ the sphere of radius r (which is a deterministic value) whose center is located at a fixed point \mathbf{o} . Moreover let us set $A \oplus A' = \{\mathbf{x} + \mathbf{x}'/\mathbf{x} \in A, \mathbf{x}' \in A'\}$ and by $\#\{\cdot\}$ the cardinal on a discrete set.

Let us now define the random closed set \mathcal{G} . For the sake of simplicity, it is done in the whole space \mathbf{R}^3 , but from the numerical point of view, we shall consider the problem on a bounded set, more precisely on a torus of \mathbf{R}^3 (the numerical simulations based on the equation (1) will be performed on such a torus). We assume that

$$\mathcal{G} = \cup_{\mathbf{q}} S_{\mathbf{q}}$$

where $S_{\mathbf{q}}$ is the sphere of radius r whose centers is the random point \mathbf{q} and the set of points $\{\mathbf{q}\}$ is a stationary Poisson point process whose intensity is equal to a constant λ times the Lebesgue measure. Such a medium is called in the literature a *Poisson germ-grain random closed set* or shortly a *Boolean medium* (see for instance [21]). Recall that the Poisson point process satisfies

$$\mathbb{P}(\#\{\text{points } \mathbf{q} \text{ in } A\} = n) = \frac{(\lambda|A|)^n}{n!} \exp(-\lambda|A|), \quad \text{for all compact set } A$$

and for two disjoint compact sets A and A' , the random variables $\#\{\text{points } \mathbf{q} \text{ in } A\}$ and $\#\{\text{points } \mathbf{q} \text{ in } A'\}$ are independent; moreover $\lambda|A|$ is the mean number of points \mathbf{q} in A . Of course, we allow overlapping of the spheres $S_{\mathbf{q}}$. Notice that the construction of a random closed set without overlapping of spheres is more delicate, see [1] for instance.

Remark. The hypothesis that the granules are spherical may be weakened from a theoretical point of view (the sphere may be replaced by a very smooth convex body) but in this paper we wish to perform numerical calculus so it is better to deal with spheres in order to have fast computations. To assume that the radius of the sphere is equal to a fixed deterministic value is clearly not realistic; but in practice it may be assumed that in a small region (at macroscopic level), the typical diameter of the heterogeneities is a random variable whose standard deviation is small. On the other hand, we will see that the final formulas for P are smooth functions of the parameter r , so if the probability distribution function is centered around a mean value \bar{r} , we may think that the expected value of P for a random distribution of r may be roughly approximated by the value of P evaluated with the mean value \bar{r} . ■

The Boolean medium \mathcal{G} is statistically homogeneous and isotropic. According to the stationarity of \mathcal{G} , we have $\mathbb{P}(A \cap \mathcal{G} \neq \emptyset) = \mathbb{P}(A_{(\mathbf{z})} \cap \mathcal{G} \neq \emptyset)$ for all compact set A . Moreover, $\mathbb{P}(\mathbf{x} \in \mathcal{G})$ does not depend on the deterministic point \mathbf{x} ; this justifies to set

$$f = \mathbb{P}(\mathbf{x} \in \mathcal{G}) \quad \text{for all fixed point } \mathbf{x}$$

This quantity is called the mean volume fraction f of the Boolean medium \mathcal{G} ; it corresponds to the intuitive definition of the volume fraction, according to the simple but fundamental result.

Lemma 1. For any deterministic compact set A , we get

$$f = \frac{1}{|A|} \mathbb{E} \left(|A \cap \mathcal{G}| \right)$$

Moreover, it satisfies

$$f = 1 - \exp(-\lambda |S_{\mathbf{o}}|) \quad (3)$$

For any deterministic compact set B , we get

$$\mathbb{P}(B \cap \mathcal{G} \neq \emptyset) = 1 - \exp(-\lambda |S_{\mathbf{o}} \oplus B|). \quad (4)$$

Proof. According to the definition of f , we get

$$f = \frac{1}{|A|} \int_A \mathbb{P}(\mathbf{x} \in \mathcal{G}) d\mathbf{x} = \frac{1}{|A|} \mathbb{E} \left(\int_A 1_{\mathcal{G}}(\mathbf{x}) d\mathbf{x} \right) = \frac{1}{|A|} \mathbb{E} \left(|A \cap \mathcal{G}| \right)$$

We now prove (4) [notice that (3) follows from that relation with $B = \{\mathbf{o}\}$]. Notice that $1 - \mathbb{P}(B \cap \mathcal{G} \neq \emptyset) = \mathbb{P}(\mathbf{x} \notin (\cup_{\mathbf{q}} S_{\mathbf{q}}), \forall \mathbf{x} \in B)$. But $\mathbf{x} \notin S_{\mathbf{q}}$ means that $\mathbf{q} \notin (S_{\mathbf{o}})_{(\mathbf{x})}$, thus

$$\mathbb{P}(\mathbf{x} \notin \cup_{\mathbf{q}} S_{\mathbf{q}}, \forall \mathbf{x} \in B) = \mathbb{P}[\text{no point } \mathbf{q}, \text{ s.t. } \mathbf{q} \in S_{\mathbf{o}} \oplus \{\mathbf{x}\}, \forall \mathbf{x} \in B] = \exp(-\lambda |S_{\mathbf{o}} \oplus B|),$$

according to the Poisson law. ■

Remark. As it is claimed in [21], it may be checked that the Boolean medium \mathcal{G} is mixing, that is to say if $\mathbf{z} \rightarrow \infty$, we get for all compact sets A, B

$$\mathbb{P}(A \cap \mathcal{G} \neq \emptyset, B_{(\mathbf{z})} \cap \mathcal{G} \neq \emptyset) \rightarrow \mathbb{P}(A \cap \mathcal{G} \neq \emptyset) \mathbb{P}(B \cap \mathcal{G} \neq \emptyset)$$

(indeed A and $B_{(\mathbf{z})}$ are disjoint for \mathbf{z} large enough). Therefore \mathcal{G} is ergodic. As a consequence, according to the ergodic property, one has $\lim_{\alpha \rightarrow \infty} \frac{|\mathcal{G} \cap (\alpha B)|}{\alpha |B|} = f$, almost surely (αB denotes the set $\{\alpha \mathbf{x} / \mathbf{x} \in B\}$).

The functional defined for all compact set A by $\mathbb{P}(A \cap \mathcal{G} \neq \emptyset)$ is called the Choquet's capacity functional related to the Boolean medium \mathcal{G} . ■

As it is explained above, we shall have to consider the problem on a torus for numerical purpose. So, we introduce a characteristic length \mathcal{L} which is somehow the observation length of the phenomena (this length is larger than k_l^{-1}) and one considers a Poisson point process $\{\mathbf{q}\}$ and a Boolean medium \mathcal{G} which are defined on the torus $[0, \mathcal{L}]^3$. Since $\lambda \mathcal{L}^3$ is the mean number of points \mathbf{q} in the torus, we may state

$$\lambda = N \mathcal{L}^{-3}$$

where N is the mean number of sphere centers. Notice that if the volume fraction is small, there is few overlapping and f is close to $\frac{N}{\mathcal{L}^3} |S_{\mathbf{o}}|$.

Lastly, it may be also interesting to address two-dimensional problems; then of course \mathcal{L}^3 has to be replaced by \mathcal{L}^2 in the previous formulas.

2.3 Trajectories and chord lengths.

The trajectory of a given particle belongs to a half line D (corresponding to an angular direction Ω); besides its initial position Y^0 (in \mathcal{G}^c) it is characterized by the intersections of D with the Boolean medium \mathcal{G} . So denote by Y^i the i -th entrance intersection of D with \mathcal{G} and by $Y^{i,s}$ the corresponding exit intersection; Y^e is the final point of the particle trajectory, that is to say the point where its velocity vanishes.

Let $l_g^i = |Y^{i,s} - Y^i|$ and $l_l^i = |Y^i - Y^{i-1,s}|$ (for $i \geq 2$) be the length of the i -th section of the trajectory respectively in \mathcal{G} and in the light medium \mathcal{G}^c .

According to the calculus made above, there are two formulas satisfied by Y^e according to the medium in which the particle stops: either there exists i such that

$$1 = k_l |Y^1 - Y^0| + k_g l_g^1 + k_l l_l^2 \dots + k_l l_l^i + k_g l_g^i + k_l |Y^e - Y^{i,s}| \quad (5)$$

then it stops in the light medium, or

$$1 = k_l |Y^1 - Y^0| + k_g l_g^1 + k_l l_l^2 \dots + k_l l_l^i + k_g |Y^e - Y^i| \quad (6)$$

then it stops in a grain (by convention in these formulas, if $i = 1$, then $k_g l_g^1 + \dots + k_l l_l^i$ is withdrawn).

Thus the probability P to stop outside the Boolean medium \mathcal{G} is given by

$$P = \mathbb{P}(k_l |Y^1 - Y^0| > 1) + \sum_{i \geq 1} \mathbb{P}(k_l |Y^1 - Y^0| + k_g l_g^1 + \dots + k_g l_g^i \leq 1 \text{ and } k_l |Y^1 - Y^0| + k_g l_g^1 + \dots + k_g l_g^i + k_l l_l^{i+1} > 1).$$

Mean chord lengths.

Since the Boolean medium is statistically homogeneous and isotropic, the chords l_g^i are independent and equidistributed and the chords l_l^i are independent and equidistributed. The following result related to the chord length in a Boolean medium is useful for the sequel.

Proposition 1. Underwood's theorem [19]. *Let $S(\mathcal{G})$ the expected value of the interface area $\partial\mathcal{G}$ divided by \mathcal{L}^3 , then we get*

$$\begin{aligned} \mathbb{E}(l_g) &= 4f/S(\mathcal{G}), \\ \mathbb{E}(l_l) &= 4(1-f)/S(\mathcal{G}). \end{aligned}$$

It is proved in appendix where the expression of $S(\mathcal{G})$ is also given. In 2D the coefficient 4 has to be replaced by π .

Therefore, we get

$$\frac{\mathbb{E}(l_l)}{\mathbb{E}(l_g)} = \frac{1-f}{f} \quad (7)$$

The problem of finding the chord-length distribution of a binary stochastic mixture is an important one, which has been dealt in numerous studies since Debye et al. [4], see [20], [14], [15], [12], [16].

3 An analytic formula for the probability $P(f)$

There are four characteristic lengths

$$r, \quad k_g^{-1}, \quad k_l^{-1}, \quad \mathcal{L},$$

and one parameter f which is called the mean volume fraction of the granules. We always have

$$k_g^{-1} \leq k_l^{-1} \leq \mathcal{L} \quad \text{and} \quad r \leq \mathcal{L}$$

$$\text{Moreover} \quad k_l^{-1} \sim \mathcal{L}$$

We present in the two first paragraphs some mathematical arguments to compute the probability $P = P(f)$ to stop in the light medium when the sphere radius r is respectively much smaller or much larger than to the stopping distance k_g^{-1} corresponding to the medium \mathcal{G} . In the third paragraph, we propose an analytic formula to model this probability $P(f)$.

3.1 Case of homogenization.

We address the case where

- the stopping distances $k_g^{-1} \sim k_l^{-1}$ are of order \mathcal{L} ,
- the radius of the sphere is small, i.e. $r = \varepsilon \ll \mathcal{L}$.

Notice that, since f is fixed, the mean number of granules N in the torus $[0, \mathcal{L}]^3$ is of order of ε^{-3} . We now introduce a different scaling in the space variable and we denote

$$L_g^k = l_g^k / \varepsilon, \quad L_l^k = l_l^k / \varepsilon, \quad \tilde{L}_l^1 = |Y^1 - Y^0| / \varepsilon, \quad \tilde{Y}^e = Y^e / \varepsilon.$$

So we get

$$\varepsilon^{-1} = k_l \tilde{L}_l^1 + k_g L_g^1 + \dots + k_g L_g^{i-1} + k_l |\tilde{Y}^e - \tilde{Y}^{i-1,s}|, \quad (8)$$

if the particle stops in the light medium and

$$\varepsilon^{-1} = k_l \tilde{L}_l^1 + k_g L_g^1 + \dots + k_l L_l^i + k_g |\tilde{Y}^e - \tilde{Y}^i|$$

if the particle stops in a granule.

We want to estimate the following quantity

$$\begin{aligned}
P_\varepsilon &= \mathbb{P}\left(k_l \tilde{L}_l^1 > \frac{1}{\varepsilon}\right) + \sum_{i \geq 1} \\
&\mathbb{P}\left(k_l \tilde{L}_l^1 + k_g L_g^1 + \dots + k_g L_g^i < \frac{1}{\varepsilon} \text{ and } k_l \tilde{L}_l^1 + k_g L_g^1 + \dots + k_g L_g^i + k_l L_l^{i+1} \geq \frac{1}{\varepsilon}\right).
\end{aligned} \tag{9}$$

Proposition 2. *Assume that the random variables (L_l^i) are identically distributed, the random variables (L_g^i) are identically distributed and that all the random variables (L_g^i) and (L_l^i) are independent. Then when ε goes to 0, we get*

$$P_\varepsilon \rightarrow \frac{k_l \mathbb{E}(L_l)}{k_g \mathbb{E}(L_g) + k_l \mathbb{E}(L_l)}$$

Proof. The probability distribution of \tilde{L}_l^1 is not the same as for the L_l^i , but since we are concerned with the formula (9) with small ε , one sees that P_ε has the same limit that P^ε which is obtained by replacing \tilde{L}_l^1 by a random variable L_l^1 which is distributed as the other L_l^i ; that is P^ε reads as

$$P^\varepsilon = \sum_{i=1}^{\infty} \mathbb{P}\left(\sum_{j=1}^i (k_l L_l^j + k_g L_g^j) < \frac{1}{\varepsilon} < \sum_{j=1}^i (k_l L_l^j + k_g L_g^j) + k_l L_l^{i+1}\right)$$

Then, using the independence between $k_l L_l^{i+1}$ and $\sum_{j=1}^i (k_l L_l^j + k_g L_g^j)$, we get

$$\begin{aligned}
P^\varepsilon &= \sum_{i=1}^{\infty} \int_0^{1/\varepsilon} \mathbb{P}\left(\sum_{j=1}^i (k_l L_l^j + k_g L_g^j) \in [x, x + dx]\right) \mathbb{P}\left(\frac{1}{\varepsilon} < x + k_l L_l^{i+1}\right) \\
&= \int_0^\infty \sum_{i=1}^{\infty} \mathbb{P}\left(\sum_{j=1}^i (k_l L_l^j + k_g L_g^j) \in \left[\frac{1}{\varepsilon} - y, \frac{1}{\varepsilon} - y + dy\right]\right) \mathbb{P}(k_l L_l > y) \mathbf{1}_{y < 1/\varepsilon}
\end{aligned}$$

Since the random variables $k_l L_l^j + k_g L_g^j$ are identically distributed and independent, we can build the renewal process associated to these variables. Let us recall the renewal theorem (cf. [2], chap. 11). If Z^j denote independent identically distributed random variables and $U(x, dx) = \mathbb{P}\left(\cup_i (\sum_{j=1}^i Z^j \in [x, x + dx])\right)$ the renewal measure, then the theorem claims that $U(x, dx) \rightarrow dx/\mathbb{E}(Z^1)$ when $x \rightarrow \infty$. Notice that $U(x, dx)$ is the expected number of points of the renewal process $\sum_{j=1}^i Z^j$ in the interval $[x, x + dx]$.

We now apply this theorem to the random variables $Z^j = k_l L_l^j + k_g L_g^j$. So, when $x \rightarrow \infty$, we have

$$\sum_{i=1}^{\infty} \mathbb{P}\left(\sum_{j=1}^i (k_l L_l^j + k_g L_g^j) \in [x, x + dx]\right) \rightarrow \frac{dx}{\mathbb{E}(k_g L_g + k_l L_l)} \tag{10}$$

Let now $\varepsilon \rightarrow 0$. Since the function $y \rightarrow P(k_l L_l > y) \mathbf{1}_{y < 1/\varepsilon}$ is bounded by $P(k_l L_l > y)$ which is integrable, according to Lebesgue theorem, the property (10) implies that

$$P^\varepsilon = \int_0^\infty U \left(\frac{1}{\varepsilon} - y, dy \right) \mathbb{P}(k_l L_l > y) \mathbf{1}_{y < \frac{1}{\varepsilon}} \rightarrow \frac{1}{\mathbb{E}(k_g L_g + k_l L_l)} \int_0^\infty \mathbb{P}(k_l L_l > y) dy.$$

Since $\int_0^\infty \mathbb{P}(L_l > y/k_l) dy = \int_0^\infty k_l z \mathbb{P}(L_l \in [z, z + dz]) = k_l \mathbb{E}(L_l)$, we get the result. \blacksquare According to this proposition and relation (7), we may state that, when $k_g r \ll 1$, one have

$$P_\varepsilon \simeq P_{\text{hom}}(f) \equiv \frac{k_l(1-f)}{k_l(1-f) + k_g f} \quad (11)$$

Remark. Since $f k_g + (1-f) k_l$ is the averaged value \bar{k} of k , the coefficient $k = k_\varepsilon$ whose values in \mathcal{G} and \mathcal{G}^c are k_g and k_l , converges towards \bar{k} in L^2 weakly. Then the justification of (11) can be reinforced by the result obtained in [6] which claims that the solution u_ε of the initial problem $\frac{\partial}{\partial t} u_\varepsilon + w \Omega \cdot \frac{\partial}{\partial \mathbf{x}} u_\varepsilon = k_\varepsilon \frac{\partial}{\partial w} (S(w) u_\varepsilon)$ may be approximated (with some technical assumptions on the random heterogeneous medium) by the solution U to the homogenized problem

$$\frac{\partial U}{\partial t} + w \Omega \cdot \frac{\partial}{\partial \mathbf{x}} U = \bar{k} \frac{\partial}{\partial w} (S(w) U),$$

The technical arguments of the proof are analogous to the ones used in [5].

3.2 Case of small stopping distances

We address now the case where

- the radius r of the spheres is of order \mathcal{L} .
- the stopping distance k_g^{-1} is very small with respect to k_l^{-1} and r , that is

$$k_g^{-1} \ll k_l^{-1} \quad \text{and} \quad k_g^{-1} \ll r$$

In this asymptotic, we want to express the fact that if a particle crosses a sphere, it stops in this sphere since the slowing power is very large compared to the radius of the spheres.

Then, if one assumes that a particle is initially located at point \mathbf{y} chosen uniformly in \mathcal{G}^c and that its direction is equal to a fixed vector Ω , its probability $P(f)$ to stop in \mathcal{G}^c is nearly equal to the probability $P_{ssd}(f)$ that the travel distance of this particle up to the set \mathcal{G} is smaller than k_l^{-1} . So, introducing this travel distance $d(\mathbf{y}) = \inf(s/\mathbf{y} + s\Omega \in \mathcal{G})$, we have to evaluate the quantity $\mathbb{P}(d(\mathbf{y}) < k_l^{-1})$.

Proposition 3. *For any point \mathbf{y} in \mathcal{G}^c , we get*

$$P_{ssd} = \mathbb{P}(d(\mathbf{y}) < k_l^{-1}) = \exp\left(\frac{3}{4k_l r} \log(1-f)\right) = (1-f)^{3/4k_l r}$$

Proof. Consider a random point \mathbf{y} uniformly distributed in $[0, \mathcal{L}]^3$ independently from the points \mathbf{q} . According to the definition of f , we have

$$\begin{aligned} 1 - P_{ssd} &= \mathbb{P}(d(\mathbf{y}) > k_l^{-1} / \mathbf{y} \in \mathcal{G}^c) \\ &= \mathbb{P}([d(\mathbf{y}) > k_l^{-1}] \cap [\mathbf{y} \in \mathcal{G}^c]) / \mathbb{P}(\mathbf{y} \in \mathcal{G}^c) \\ &= \mathbb{P}([d(\mathbf{y}) > k_l^{-1}] \cap [\mathbf{y} \in \mathcal{G}^c]) / (1 - f) \end{aligned}$$

Denote by Γ the cylinder whose base is the half sphere $S_{\mathbf{o}}$ and whose length is equal to k_l^{-1} , we get

$$\mathbb{P}([d(\mathbf{y}) > k_l^{-1}] \cap [\mathbf{y} \in \mathcal{G}^c]) = \mathbb{P}(\mathbf{y} \notin \mathcal{G} \oplus \Gamma) = \mathbb{P}(\mathbf{o} \notin \mathcal{G} \oplus \Gamma)$$

indeed these quantities do not depend on the point \mathbf{y} . But $\mathbf{o} \in \mathcal{G} \oplus \Gamma$ means that $\mathbf{o} - \mathbf{z} \in \mathcal{G}$ for one point $\mathbf{z} \in \Gamma$. Then $\mathbb{P}(\mathbf{o} \in \mathcal{G} \oplus \Gamma) = \mathbb{P}((-\Gamma) \cap \mathcal{G} \neq \emptyset)$. According to lemma 1, we see that

$$\mathbb{P}(\mathbf{o} \notin \mathcal{G} \oplus \Gamma) = 1 - \mathbb{P}(\Gamma \cap \mathcal{G} \neq \emptyset) = \exp(-\lambda|S_{\mathbf{o}} \oplus \Gamma|) = \exp(-\lambda|S_{\mathbf{o}}|) \exp(-\lambda|\Gamma|).$$

Since $|\Gamma| = \pi r^2 k_l^{-1} = \frac{3}{4k_l r} |S_{\mathbf{o}}|$, the result comes from relation (3). ■

In two-dimension case, the volume of the cylinder is equal to $2rk_l^{-1}$, then the same argument leads to $P_{ssd}(f) = \exp(\frac{2}{\pi k_l r} \log(1 - f))$. So one can state, for whatever dimension

$$P_{ssd}(f) = \exp\left(\frac{\alpha}{k_l r} \log(1 - f)\right),$$

with $\alpha = 2/\pi$ in the two-dimension case and $\alpha = 3/4$ in the three-dimension case.

3.3 Fitting by an analytic formula

We wish to find a fitting formula which would be valid when the parameters range over a wide domain, for instance

$$k_l r \in [10^{-1}, 10], \quad k_g r \in [10^{-1}, 10^2], \quad k_g/k_l \in [1, 10].$$

For the volume fraction f , it suffices for a practical point of view to assume $f \in [0, 0.6]$. For

this purpose, to approximate $P(f)$ we propose a combination of the two formulas $P_{ssd}(f)$ and $P_{hom}(f)$ found above

$$P_{hom} = \frac{k_l(1 - f)}{k_l(1 - f) + k_g f}, \quad P_{ssd}(f) = \exp\left(\frac{\alpha}{k_l r} \log(1 - f)\right)$$

In other words, we look for a fitting function Z such that :

$$P(f) = P_{\text{ssd}}(f)Z + P_{\text{hom}}(f)(1 - Z), \quad \text{with } 0 \leq Z \leq 1.$$

When r becomes very small compared to k_l^{-1} and k_g^{-1} , one must have $Z \simeq 0$, and when $k_l r$ and $k_g r$ becomes large one must have $Z \simeq 1$. It is natural to search a fitting function Z depending only on the quantity $k_g r$ that is to say the ratio between the granule radius and the slowing distance in the granules. The simplest choice is $Z = \exp(-bk_g r)$ with b constant. With the help of the numerical results presented below, we may adjust the constant b and it turns out that a good choice is $b = 1$.

Finally, we propose the following analytic formula

$$P_{\text{fit}}(f) = \exp\left(\frac{\alpha}{k_l r} \log(1 - f)\right) (1 - e^{-k_g r}) + e^{-k_g r} \frac{k_l(1 - f)}{k_l(1 - f) + k_g f} \quad (12)$$

4 Numerical results

In this section, numerical simulations are presented for estimating the probability $P(f)$ as a function of f . The numerical algorithm is based on the solution of the initial kinetic equation (1) by a Monte-Carlo method; its description of the is sketched in appendix 1.

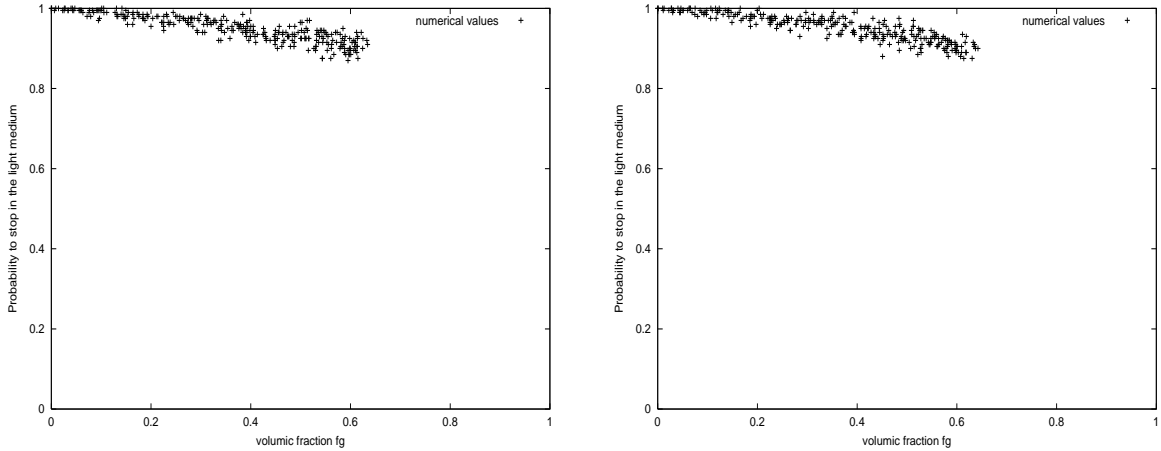


Figure 1: Case of large sphere radius: $r k_l = 6$. Left: $k_g = k_l$, Right: $k_g = 9k_l$, Two-dimension computations

We first consider the case where the radius of the spheres is very large with respect to the stopping distance in the light medium, here $r k_l = 6$. We check on Fig. 1 that the probability $P(f)$ depends weakly on the volume fraction f and we recover – what we mathematically expected – that $P(f)$ does not depend any more on the ratio between k_g and k_l since the particle will stop in the first sphere encountered whatever k_g is.

We now compare the numerical results with the analytic formula P_{fit} given by (12) for a representative panel of parameters. We observe that the analytic formula is a good

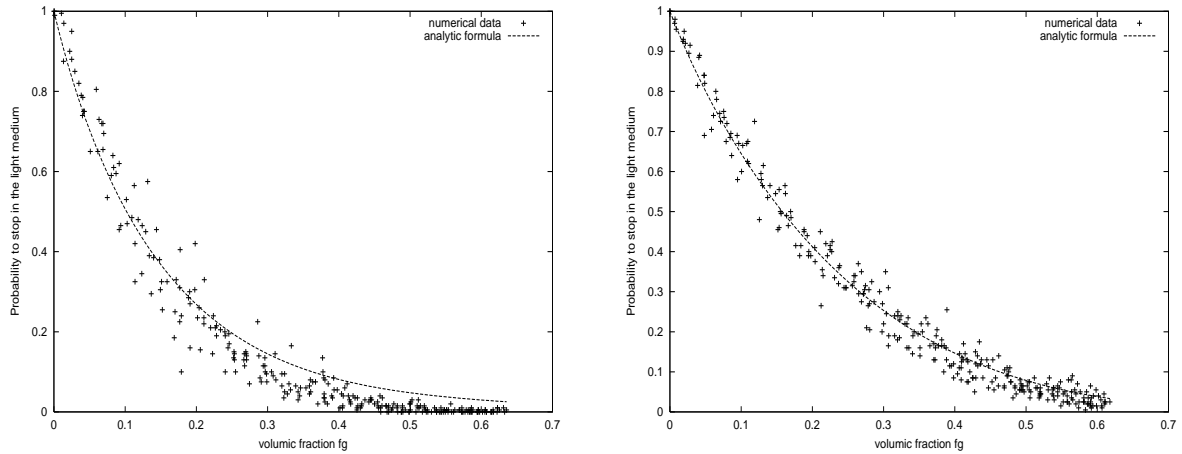


Figure 2: Case of small sphere radius: $rk_l = 0.1$ and $rk_g = 0.9$. Left: 2-dim.; Right: 3-dim. computations

approximation in the two extremal cases of characteristic length and for any ratio of the slowing distances.

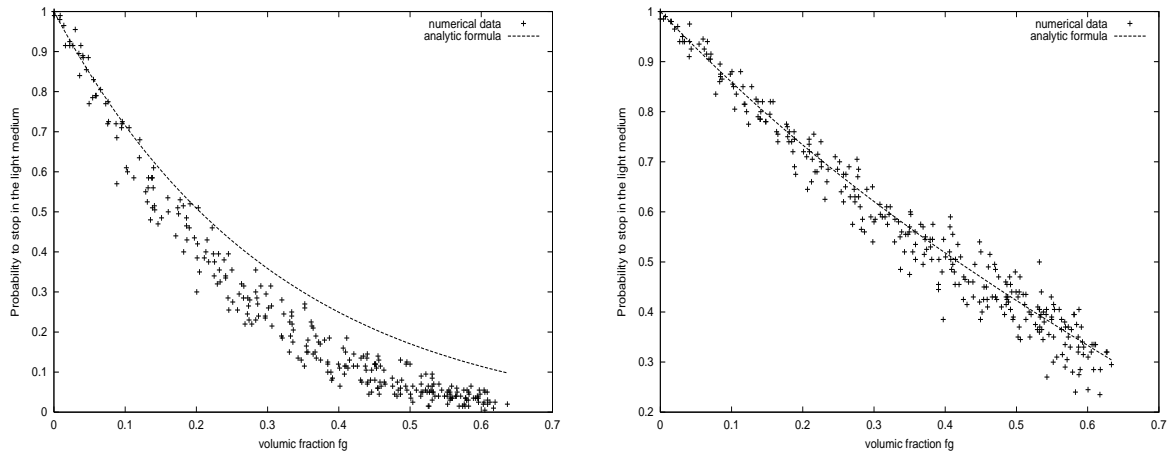


Figure 3: Case of small sphere radius: $rk_l = 0.1$. Left: $rk_g = 0.3$; Right: $rk_g = 0.1$ (3-dim. computations)

The first considered cases correspond to a sphere radius which is small compared with the stopping distance in \mathcal{G}^c : $rk_l = 0.1$. In these cases, the radius of the spheres is small enough so that the particles go through a large number of spheres before stopping.

On Fig. 2 computations performed in the two-dimension and the three-dimension framework are plotted in the case $rk_g = 0.9$. On Fig. 3, the computations are performed for other values of rk_g (the computation are made in three-dimension as in the sequel). We check on Fig. 2 and Fig. 3 that the numerical simulations are in agreement with the mathematical estimation of $P(f)$ which is here very close to $P_{\text{hom}}(f)$. On Fig. 4, we have plotted results

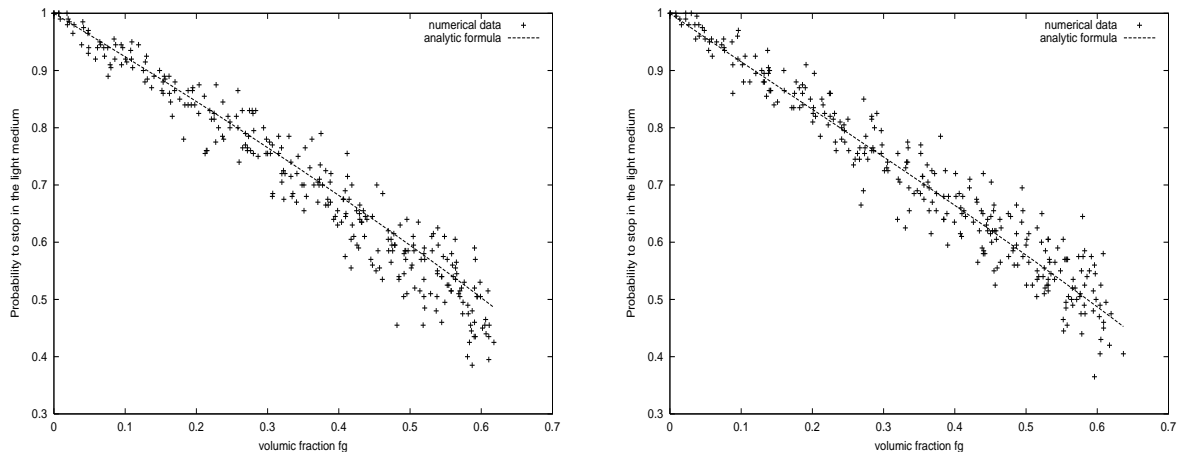


Figure 4: Case $rk_l = 1$. Left: $rk_g = 9$; Right: $rk_g = 3$,

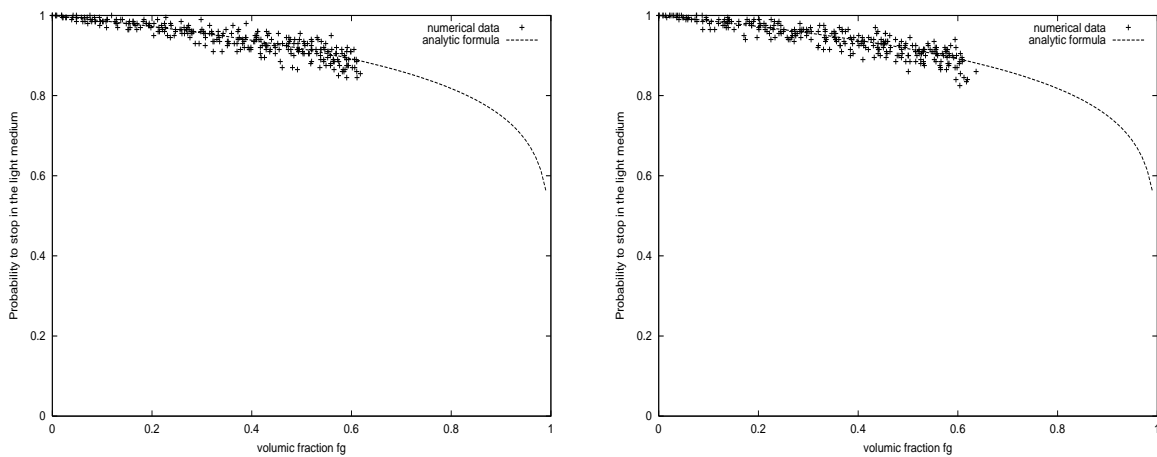


Figure 5: case of large sphere radius: $rk_l = 6$. Left: $rk_g = 54$; Right: $k_g = 18$,

obtained in cases where the characteristic lengths r and k_l^{-1} are such that $rk_l = 1$; they are performed for two different values of rk_g . On fig 5, we have plotted results obtained for a sphere radius which is large compared with the stopping distance in \mathcal{G}^c , here we choose $rk_l = 6$. They are also performed for two different values of rk_g . One can check that in all the cases there is a good agreement between the numerical results and our analytic formula P_{fit} .

5 Comparison with a Markovian medium

In this section, we would like to compare our results based on a representation of the heterogeneous binary mixture by a Boolean medium with the ones obtained in [8] by another representation of the mixture, see also [10] [17], [18]. In these paper, the main hypothesis is that the length of both media are distributed according Markovian laws (so the approach is specially one-dimensional). For this model, one has to introduce the characteristic stopping

distance of each material which are equal to k_l^{-1} and k_g^{-1} and some characteristic lengths of each medium λ_l, λ_g .

Then the proposed analytical approximation reads as follows

$$P(f) = P_{\text{ev}}(f) = \frac{k_l \lambda_l}{k_l \lambda_l + k_g \lambda_g} + \frac{k_g \lambda_g}{k_l \lambda_l + k_g \lambda_g} \exp\left(-\frac{1}{k_l \lambda_l} - \frac{1}{k_g \lambda_g}\right).$$

In order to make comparison, we have to define precisely the two quantities λ_l, λ_g in the framework of the Boolean medium ; it is natural to claim that these quantities are the mean chord length for \mathcal{G}^c and for \mathcal{G} . So, according to (7), we get

$$\lambda_l = \lambda_g(1 - f)/f$$

Underwood's theorem yields a value for λ_g which is not very handy in the general case; so we choose for λ_g the mean chord length of a isolated sphere, that is to say $\lambda_g = r/\alpha$, where α is a constant depending on the dimension ($\alpha = 2/\pi$ or $\alpha = 3/4$ as above). Therefore, denoting $f_l = 1 - f$, we get $\lambda_l = r f_l / (\alpha f)$ and the approximation proposed in [8] reads as

$$\begin{aligned} P_{\text{ev}}(f) &= \frac{k_l f_l}{k_l f_l + k_g f} + \frac{k_g f}{k_l f_l + k_g f} \exp\left(-\frac{\alpha}{r} \left(\frac{1}{k_g} + \frac{f}{f_l k_l}\right)\right), \\ &= \frac{k_l f_l}{k_l f_l + k_g f} \left(1 - \exp\left(-\frac{\alpha}{k_g r}\right) \exp\left(-\frac{\alpha f}{f_l k_l r}\right)\right) + \exp\left(-\frac{\alpha}{k_g r}\right) \exp\left(-\frac{\alpha f}{f_l k_l r}\right), \end{aligned}$$

We can now compare this formula with our formula

$$P_{\text{fit}}(f) = \exp\left(\frac{\alpha}{k_l r} \log(1 - f)\right) (1 - Z) + Z \frac{k_l f_l}{k_l f_l + k_g f}, \quad \text{with } Z = \exp(-k_g r).$$

Notice that in the case where $k_g r \ll 1$ that is to say $Z \simeq 1$, we have $P_{\text{fit}} = P_{\text{ev}} = P_{\text{hom}}$. Now in the case where $k_g r \gg 1$, and $k_g/k_l \gg 1$, that is to say $Z \simeq 0$, we have $P_{\text{fit}}(f) \simeq \exp(\frac{\alpha}{k_l r} \log(1 - f))$, but $P_{\text{ev}}(f) \simeq \exp\left(-\frac{\alpha}{k_l r} \frac{f}{1-f}\right)$. Therefore one checks that for very small values of f , the two quantities are very close, but at second order with respect to f , there is a difference between these two quantities ($\log(1 - f)$ is not equal to $-f/(1 - f)$ at second order with respect to f).

Let us now perform some numerics to compare the two approaches. On Fig. 6, the results given by the numerical simulations are compared with the two analytic formulas P_{ev} and P_{fit} in two cases: firstly when the sphere radius is small and the ratio between the two stopping distances is large; secondly when the sphere radius is of order 1 and the stopping distances are equal.

The comparison between the two analytic formula suggests that the two models do not differ a lot when the stopping distance are of the same order of magnitude but in the other case our formula P_{fit} is a better one.

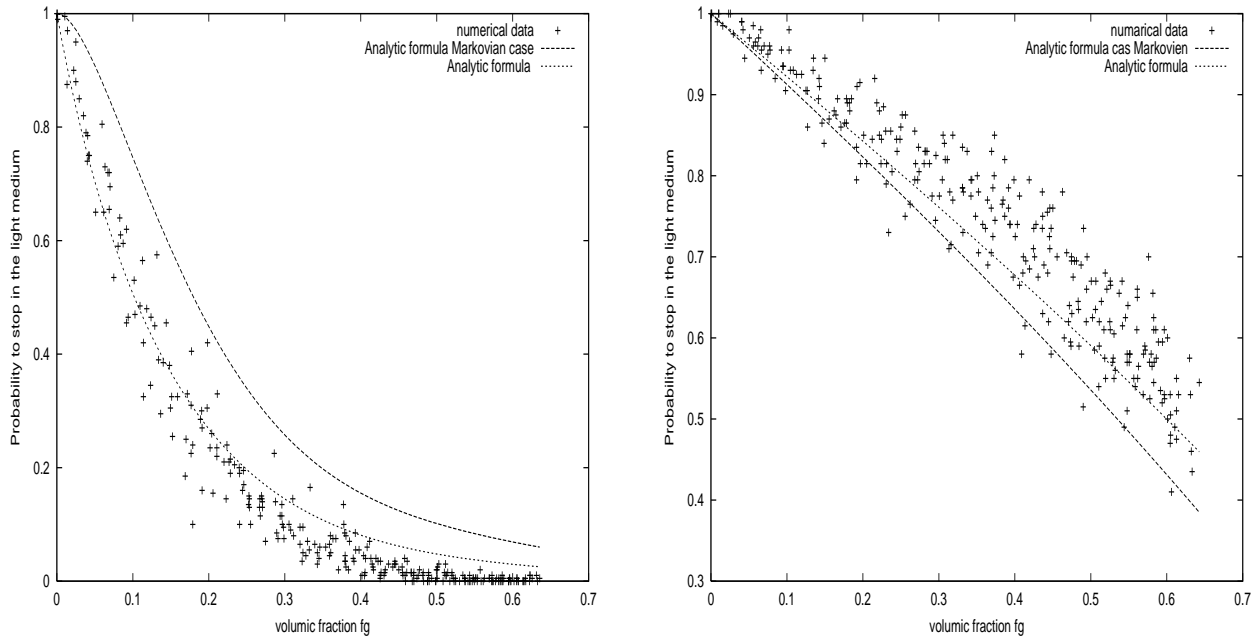


Figure 6: Comparison between numerical simulations and the formulas P_{fit} (dotted line) and P_{ev} (dashed line). Both figures correspond to $rk_g = 1$ and (on the left) to $rk_l = 0.1$ and (on the right) to $rk_l = 1$.

For understanding the difference between the two approaches, it must be noticed that the building of the random medium considered in [8], [9], [10] is basically a one dimensional construction and the way to extend their results to a fully three dimensional random medium is not clear. Particularly, it is easy to find examples where the chord distribution is exponential but depends on the direction (simply think to a stratified medium), but the assumption that the distribution of chords is markovian with the **same** law in each direction (which is the case if the medium is isotropic) is a very strong condition. In [13], it is claimed that for a binary random mixture with non-overlapping disks or spheres, the chord-length distribution in the background material is approximatively of exponential type (and thus Markovian) if the volume fraction f is not too large; but the chord-length distribution for the spheres is not of the same type. For the sake of completeness, let us mention [22] for an example in 2D of isotropic binary mixture where the distribution of chords is Markovian for both materials (but this building is quite complicated).

Nevertheless, although the mixture we consider in our paper does not fullfill the assumptions of a Markovian medium, the two approaches give results which are not dramatically different (provided that the mean chord lengths are properly defined).

6 Conclusion

In the framework of a stochastic binary mixture with spherical heterogeneities, we have proposed an analytical formula for the fraction $P(f)$ of suprathreshold particles stopped in the light material as a function of the size of heterogeneities, the stopping distances in

each material and the volume fraction f . We addressed the issue of the influence of the details of the distribution of heterogeneities : the main conclusion is that it is not of primal importance to know these details since we are only interested in results on the mean fraction of particles stopped in \mathcal{G}^c . For this purpose, the analytical formula is obtained on one hand by direct numerical simulations on a large number of realistic mixtures and on the other hand by interpolation between asymptotic results obtained in idealized situations.

Appendix 1: Description of the algorithm for the numerical simulations

In practice, we don't start from a given volume fraction to construct a heterogeneous medium. In fact, we first construct the heterogeneous medium and afterwards we evaluate the volume fraction and the probability to stop in the light medium for this given configuration. Thus to build the binary mixture, we fix a value for the sphere radius and we simply sample the location of the centers of the spheres according to the above Poisson law. Once, the geometry is given, a classical Monte-Carlo method is used to solve the transport equation (1) (see for example [7]). So, we have to perform two steps.

Step 1: Initialization. We sample the random variables

- the initial position of the particles
- the direction of the velocity of the particles.

The initial position must be in \mathcal{G}^c . So we sample it uniformly in the torus and if it is not in \mathcal{G}^c , we have to sample out another point until we find a point in the light medium \mathcal{G}^c . Notice that since we apply this to a large number of points, this step allows us to estimate numerically the volume fraction f of the heavy medium.

Step 2: Iterations to compute the stopping point.

Recall that we use formula (5) and (6) to compute the trajectory of the particle. The numerical computation can be reduced to compute the position of $(Y^i; Y^{i,s})$.

At each iteration i corresponding to $(Y^{i-1}; Y^{i,s})$, we compute the remaining potential H^i by subtracting to H^{i-1} the distance needed to reach $Y^{i,s}$ multiplied by the slowing coefficient corresponding to the medium where the particle moves. We iterate the computation as long as the remaining potential is strictly positive. When the potential becomes negative, it means that the particle stopped before reaching $Y^{i,s}$. Therefore, for any configuration of the binary mixture, we may estimate the probability P to stop in the light medium by using the formula (2).

Appendix 2: Proof of proposition 1

Step i). Let \mathbf{y} be an arbitrary fixed point and Ω an arbitrary unit vector. Since the Boolean medium \mathcal{G} is isotropic, one may define a function M on \mathbf{R}^+ by the following relation

$$M(z) = \mathbb{P}[\mathbf{y} \in \mathcal{G}, \mathbf{y} + z\Omega \in \mathcal{G}^c]$$

($-M(z)$ is the correlation function of the Boolean medium up to an additive constant). We have $(\mathbf{o} \in \mathcal{G}) \cap (\mathbf{o} + z\Omega \in \mathcal{G}^c) = [(\mathbf{o} \in \mathcal{G}) \cup (\mathbf{o} + z\Omega \in \mathcal{G})] - [\mathbf{o} + z\Omega \in \mathcal{G}]$. Then, according to lemma 1, we get

$$\begin{aligned} f + M(z) &= \mathbb{P}[(\mathbf{o} \in \mathcal{G}) \cup (\mathbf{o} + z\Omega \in \mathcal{G})] = \mathbb{P}[\mathcal{G} \cap \{\mathbf{o}, \mathbf{o} + z\Omega\} \neq \emptyset] \\ &= 1 - \exp(-\lambda |S_{\mathbf{o}} \oplus \{\mathbf{o}, \mathbf{o} + z\Omega\}|) \end{aligned}$$

But $|S_{\mathbf{o}} \oplus \{\mathbf{o}, \mathbf{o} + z\Omega\}| = 2|S_{\mathbf{o}}| - |S_{\mathbf{o}} \cap S_{\mathbf{o}+z\Omega}|$ and after some tedious calculus it may be found that $|S_{\mathbf{o}} \cap S_{\mathbf{o}+z\Omega}| = |S_{\mathbf{o}}| - \pi r^2(z - z^3 r^{-2}/12)$ (for z smaller than $2r$). Therefore, we get

$$f + M(z) = 1 - (1 - f) \exp\left(-\lambda \pi r^2 \left(z - \frac{z^3}{12r^2}\right)\right),$$

$$\frac{\partial M}{\partial z}(0) = (1 - f) \lambda \pi r^2. \quad (13)$$

Step ii). Following [16], introduce also the lineal-path function $L_c(z)$ which is the probability that a line segment $[\mathbf{y}, \mathbf{y} + z\Omega]$ lies in \mathcal{G} (it is independent from the initial point \mathbf{y}). For small values of z , we can easily see that $L_c(z) = \mathbb{P}[\mathbf{y} \in \mathcal{G}, \mathbf{y} + z\Omega \in \mathcal{G}] + o(z)$. Then we have

$$\mathbb{P}[\mathbf{y} \in \mathcal{G}] = f = M(z) + L_c(z) + o(z)$$

Therefore, by deriving this relation with respect to z , we get

$$\frac{\partial L_c}{\partial z}(0) + \frac{\partial M}{\partial z}(0) = 0. \quad (14)$$

Step iii). Let $p_c(z)$ the probability law density of the chord length l_g , then

$$\mathbb{E}(l_g) = \int z p_c(z) dz.$$

Let us now show that the probability that the point \mathbf{y} belongs to \mathcal{G} and that the line segment $[\mathbf{y}, \mathbf{y} + z\Omega]$ is included in a chord of \mathcal{G} is equal to

$$L_c(z) = f \frac{\int_z^\infty (x - z) p_c(x) dx}{\mathbb{E}(l_g)}. \quad (15)$$

see [16]. Indeed, on a arbitrary line, the probability that a fixed point \mathbf{y} on this line belongs to a chord l_g of length in $[x, x + dx]$ is equal to $x p_c(x) dx / \mathbb{E}(l_g)$. Moreover, the probability that a fixed line segment $[\mathbf{y}, \mathbf{y} + z\Omega]$ is included in a chord of length x , knowing that \mathbf{y} belongs to this chord is equal to $\frac{x-z}{x} \mathbf{1}_{z < x}$. Then, the probability that the line segment $[\mathbf{y}, \mathbf{y} + z\Omega]$ is included in a chord l_g knowing that \mathbf{y} belongs to this chord is $\int_z^\infty (x - z) p_c(x) dx / \mathbb{E}(l_g)$ and (15) follows.

Since we have $\frac{\partial L_*}{\partial z}(0) = -f/\mathbb{E}(l_g)$, according to (14) and (13) we get

$$\frac{f}{\mathbb{E}(l_g)} = (1-f)\lambda\pi r^2. \quad (16)$$

So, denoting $S(\mathcal{G}) = (1-f)\lambda 4\pi r^2$, the first part of the theorem follows. For proving the second part of the theorem, it suffices to reverse the part of \mathcal{G} and \mathcal{G}^c in steps ii) and iii) above. ■

Notice that this quantity $S(\mathcal{G})\mathcal{L}^3$ may be considered as the expected value of the interface area $\partial\mathcal{G}$. Moreover

$$\mathbb{E}(l_g) = f((1-f)\lambda|S_{\bullet}|)^{-1} \frac{4r}{3} = \frac{4r}{3} \frac{f}{(1-f)|\log(1-f)|} \simeq \frac{4r}{3}$$

for f small. Therefore we find the classical result that for a isolated sphere of radius r , the mean value of the chord length is equal to $r\frac{4}{3}$.

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