

# Hybrid Formulation of Radiation Transport in Optically Thick Divertor Plasmas\*

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Kinetic Monte Carlo simulations of coupled atom-radiation transport in optically thick divertor plasmas can be computationally very demanding, in particular in ITER relevant conditions or even larger devices, e.g. for power plant divertor studies. At high ( $\sim 10^{15} \text{ cm}^{-3}$ ) atomic densities, it can be shown that sufficiently large divertors behave in certain areas like a black body near the first resonance line of hydrogen (Lyman  $\alpha$ ). This suggests that, at least in part, the use of continuum model (radiation hydrodynamics) can be sufficiently accurate, while being less time consuming. In this work, we report on the development of a hybrid model devoted to switch automatically between a kinetic and a continuum description according to the plasma conditions. Calculations of the photo-excitation rate in a homogeneous slab are performed as an illustration. The outlined hybrid concept might be also applicable to neutral atom transport, due to mathematical analogy of transport equations for neutrals and radiation.

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## 1 Introduction

The preparation of large-scale fusion reactor devices (ITER, DEMO) requires accurate transport models for the plasma edge able to account for neutral and charged particles in a self-consistent fashion. For certain, in particular ITER relevant, large and dense divertor configurations the run time in edge codes is currently reported to be so large (relative to accuracy criteria employed during the ITER divertor design phase) that it rules out any practical analysis of analogue results when extrapolating beyond ITER, e.g. towards conventional detached DEMO divertor scenarios [1]. Significant efforts are presently ongoing in order to either speed up the existing codes or to develop more modern computational tools [2]. A specific point that needs to be addressed concerns radiation transport in atomic lines. A few years ago, it was shown using B2-EIRENE that the trapping of Lyman photons may result in an alteration of the ionization-recombination balance [3]. An accurate description of the machine operation requires this process be properly accounted for. In its current version, the radiation transport model used in B2-EIRENE involves a kinetic transport equation for photons of the Boltzmann type (referred to as “equation of transfer” in the astrophysics literature) and this equation is solved using a Monte Carlo method, in the same way as the Boltzmann equation for neutrals is solved. In the most optically thick conditions (e.g. with an atomic density approaching locally values of  $10^{15} \text{ cm}^{-3}$  [3]), it can be shown that the divertor of ITER behaves in certain areas like a black body radiator near the first resonance line of hydrogen (Lyman  $\alpha$ ). This suggests that the use of a continuum model can be as accurate as a kinetic approach, while being less time consuming. In the same spirit as [4,5], we report on the development of a hybrid formulation of radiation transport, designed in such a way to switch automatically between a kinetic and a continuum description, according to the plasma conditions. First (Sec. 2), the theoretical framework of kinetic radiative transfer modeling is presented and specified to Lyman  $\alpha$  photons propagating in an optically thick plasma. In Sec. 3, we address the radiative transfer problem within the

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Monte Carlo terminology used in the EIRENE kinetic Monte Carlo Code ([www.eirene.de](http://www.eirene.de); see also [6]), which involves stochastic (random walk) processes and estimators. We examine an estimator based on the count of collisions, suitable for highly scattering media, and propose a modification based on the diffusion approximation and designed to reduce the CPU time. First prototypical applications to strongly reduced models are performed in Sec. 4 to demonstrate the feasibility of this hybrid approach. The issue of interfacing between kinetic and macroscopic (diffusion) zones is also discussed.

## 2 Kinetic modeling of radiation transport

The fundamental quantity of interest in radiative transfer is the spectral energy flux  $I(\omega, \vec{n}, \vec{r}, t)$  [ $\text{J m}^{-2} \text{s}^{-1} \text{sr}^{-1} (\text{rad/s})^{-1}$ ], referred to as “specific intensity” (e.g. [7]; note, we adopt here the angular frequency convention to make the notation consistent with previous works [8, 9]). A transport equation for this quantity is obtained from phase space balance considerations. In its usual form, this equation reads

$$\left( \frac{1}{c} \frac{\partial}{\partial t} + \vec{n} \cdot \vec{\nabla} \right) I = \eta - \chi I, \quad (1)$$

where  $\eta$  and  $\chi$  are source and loss terms, respectively, and express the interaction between the radiation field and the constituents of the matter present in the medium under consideration, for example atoms, molecules, or ions. For spectral line radiation with an atomic transition  $u \rightarrow d$ , these terms are given by

$$\eta = \frac{\hbar\omega_0}{4\pi} N_u A_{ud} \psi, \quad (2)$$

$$\chi = \frac{\hbar\omega_0}{4\pi} (N_d B_{du} \phi - N_u B_{ud} \psi), \quad (3)$$

where  $A_{ud}$ ,  $B_{du}$ , and  $B_{ud}$  are the Einstein coefficients for spontaneous emission, absorption, and stimulated emission, respectively;  $N_u$ ,  $N_d$  are the densities of atoms in the upper and lower states; and  $\psi$ ,  $\phi$  are the emission and absorption line shapes normalized such that  $\int d\omega d\Omega \phi = 4\pi = \int d\omega d\Omega \psi$ . They denote the conditional probability density function of emitting or absorbing a photon at the frequency  $\omega$ , given that the event of emission or absorption is already known to occur at a certain position. The fact that the stimulated emission is treated as a negative part in the absorption is only a matter of convention, which allows one to write the radiative transfer equation in the compact form given in Eq. (1). The Einstein A and B coefficients are related by  $g_u B_{ud} = g_d B_{du} = g_u A_{ud} 4\pi^3 c^2 / \hbar \omega_0^3$ , where  $g_u$  and  $g_d$  denote the statistical weights of the upper and lower level, respectively, and  $\omega_0$  is the Bohr frequency of the transition under consideration. The  $\eta$  coefficient (sometimes referred to as “emissivity”) describes the spontaneous emission from atoms excited due to both collisions and photon absorption; the latter contribution is usually interpreted as a scattering process and can be described in terms of the joint probability density function (“redistribution function”) for absorbing and reemitting a photon from one mode  $(\omega, \vec{n})$  to another one. In the case where only the two atomic levels  $u$ ,  $d$  are involved, and  $N_u$  is in collisional-radiative quasi steady state with  $N_d$ , the following relation holds

$$\begin{aligned} \eta(\omega, \vec{n}) &= \frac{\hbar\omega_0}{4\pi} A_{ud} \left[ \frac{C_{du} N_d \phi(\omega, \vec{n})}{A_{ud} + C_{ud}} + \frac{B_{du} N_d}{A_{ud} + C_{ud}} \int d\omega' \int \frac{d\Omega'}{4\pi} R(\omega, \vec{n}, \omega', \vec{n}') I(\omega', \vec{n}') \right] \\ &= \frac{\hbar\omega_0}{4\pi} N_u^* A_{ud} \phi(\omega, \vec{n}) + p_{sc} \int d\omega' \int \frac{d\Omega'}{4\pi} P(\omega, \vec{n} | \omega', \vec{n}') \chi(\omega', \vec{n}') I(\omega', \vec{n}'), \end{aligned} \quad (4)$$

where  $R$  is the redistribution function and the  $C_s$  are electronic collisional rates ( $\text{s}^{-1}$ ) and are related by the detailed balance  $g_u C_{ud} = g_d C_{du} \exp(\hbar\omega_0/k_B T_e)$ . Other notations are shortcut:  $N_u^* = C_{du} N_d / (A_{ud} + C_{ud})$  is the density of atoms excited by collisions,  $p_{sc} = A_{ud} / (A_{ud} + C_{ud})$  is the probability of reemitting a photon given that a photon has been absorbed, and  $P(\omega, \vec{n} | \omega', \vec{n}') = R(\omega, \vec{n}, \omega', \vec{n}') / \phi(\omega', \vec{n}')$  is the conditional probability density of emitting a photon  $(\omega, \vec{n})$  given that a photon  $(\omega', \vec{n}')$  has been absorbed. A decomposition similar to Eq. (4) holds for the stimulated emission, and it yields terms nonlinear in the specific intensity (stimulated scattering [10]). These processes will not be retained in the following.

### 3 Monte Carlo formulation

The structure of the transport equation (1) makes it suitable for kinetic Monte-Carlo simulations involving random walks. The specific intensity is proportional to the one-photon “Wigner” phase space distribution and can be used to calculate an observable quantity, using an appropriate detector function, in the same way as in classical kinetic theory for neutrons or other neutral particles. Features intrinsic to the wave nature of light (such as coherence [11, 12]) are not considered hereafter; what we refer to as a “photon” is a wave packet with a well defined position and with a size negligible with respect to other length scales of interest. We follow the terminology used in the EIRENE code and reported in the literature on neutron transport [13]. We define the photon collision density per spontaneous emission  $\Psi = \chi I / (\hbar \omega_0 A_{\text{ud}} \mathcal{N}_u^*)$  [with  $\mathcal{N}_u^* \equiv \int d^3 r N_u^*(\vec{r})$ ] and we write an integral equation for it, from integration of Eq. (1) along the characteristics:

$$\Psi(X) = S(X) + \int dX' K(X, X') \Psi(X'). \quad (5)$$

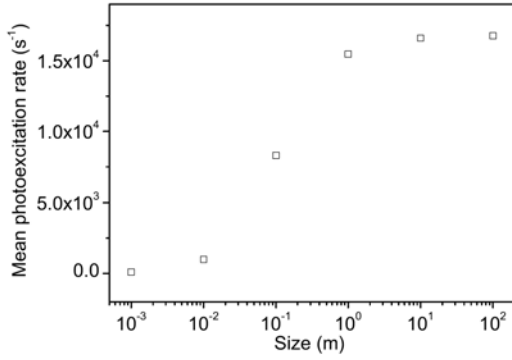
Here, the stationary regime has been assumed and  $X$  is a shortcut notation for  $(\omega, \vec{n}, \vec{r})$ . The source and the kernel correspond to the thermal- and scattering-emission, respectively. These terms are given by

$$S(X) = \int d^3 r' T(\vec{r}|\omega, \vec{n}, \vec{r}') \frac{\phi(\omega, \vec{n}, \vec{r}') N_u^*(\vec{r}')}{4\pi \mathcal{N}_u^*}, \quad (6)$$

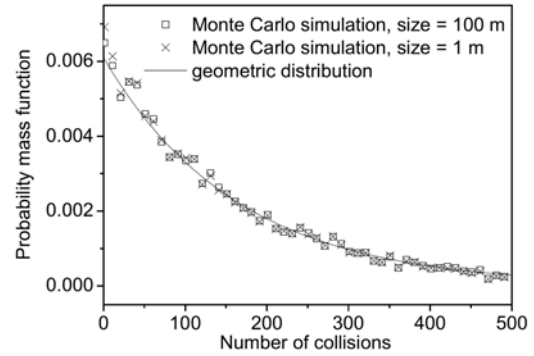
$$K(X, X') = T(\vec{r}|\omega, \vec{n}, \vec{r}') \frac{P(\omega, \vec{n}|\omega', \vec{n}', \vec{r}')}{4\pi} p_{\text{sc}}(\vec{r}'), \quad (7)$$

where  $T(\vec{r}|\omega, \vec{n}, \vec{r}') = H(\vec{n} \cdot (\vec{r} - \vec{r}')) \chi(\omega, \vec{n}, \vec{r}') \exp\left(-\int_0^{\vec{n} \cdot (\vec{r} - \vec{r}')} ds \chi(\omega, \vec{n}, \vec{r}' + \vec{n}s)\right) \delta(\vec{r}_\perp - \vec{r}'_\perp)$  is the conditional probability of a photon being absorbed at  $\vec{r}'$  ( $H$  is the Heaviside function and  $\perp$  refers to the plane perpendicular to  $\vec{n}$ ). The quantities  $S(X)$ ,  $K(X, X')$ , and  $p_{\text{abs}} = 1 - \int dX' K(X', X)$  are directly interpretable as probabilities associated with a continuous random walk process  $(X_1 \dots X_k)$ . This allows one to evaluate physical observables by generating a set of random sequences and using an appropriate estimator. In the following, we use the collision estimator [13], i.e., for any detector function  $g(X)$ , we evaluate the integral  $\int dX g(X) \Psi(X)$  from the expectation value of the random variable  $\nu = \sum_{m=1}^k g(X_m)$ . The collision estimator is suitable in particular for opaque regions where the photon mean free path  $\chi^{-1}$  is small. Variants (such as the track length estimator, the default estimator in EIRENE) can be used alternatively, e.g. in optically thin media where collisions are rare, but these latter do not translate immediately to proper estimators for diffusion equations, which will arise in the hybrid formulation.

As an example of application, consider the mean photoexcitation rate ( $\text{s}^{-1}$ ) in a homogeneous volume  $V$ : it is defined by  $W_{\text{du}} = B_{\text{du}} \int_V (d^3 r / V) \int d\omega \int (d\Omega / 4\pi) \phi(\omega, \vec{n}, \vec{r}) I(\omega, \vec{n}, \vec{r})$  and it can be evaluated using the collision estimator as  $A_{\text{ud}} N_u^* \langle k \rangle_V / N_d$  where  $\langle k \rangle_V$  is the mean number of collisions in  $V$ . An accurate description of this quantity is critical for the design of large scale (ITER- and DEMO-like) devices because the photoexcitation process plays a significant role in the ionization-recombination balance [3]. Figure 1 shows the dependence of the mean Lyman  $\alpha$  ( $n = 1 \rightarrow 2$ ) photoexcitation rate  $W_{12}$  on the medium size. A Monte Carlo simulation of radiation transport has been performed in a 1D slab with perfectly absorbing walls, using a three-level ( $n = 1, 2, \infty$ ) stationary collisional-radiative model and assuming a homogeneous plasma background with  $N_e = N_{\text{at}} = 10^{14} \text{ cm}^{-3}$  and  $T_e = T_{\text{at}} = 1 \text{ eV}$ . For the sake of simplicity complete redistribution has been assumed [i.e.,  $P(\omega, \vec{n}|\omega', \vec{n}') \equiv \phi(\omega, \vec{n})$ ] and only Maxwellian Doppler broadening has been retained in the line shape function. At these conditions, the photon mean free path at the line center ( $\omega = \omega_0$ ) is of the order of 1 mm. As can be seen, the photoexcitation rate increases and saturates when the size becomes much larger than the photon mean free path. At saturation, the number of collisions is distributed according to a geometric distribution of parameter  $p_{\text{sc}}$  (Fig. 2) and the mean number of collisions is given by  $1/(1 - p_{\text{sc}})$ . Note, if the atomic populations satisfy the Saha-Boltzmann relation, the value attained at the saturation corresponds to the value that would be obtained assuming a Planck radiation distribution (or Wien distribution if stimulated emission is neglected).



**Fig. 1** Plot of the Lyman  $\alpha$  photoexcitation rate calculated using the collision estimator. A homogeneous slab with  $N_e = N_{at} = 10^{14} \text{ cm}^{-3}$  and  $T_e = T_{at} = 1 \text{ eV}$  has been assumed. The photoexcitation rate increases and saturates when the size becomes much larger than the photon mean free path.



**Fig. 2** If the medium size is much larger than the photon mean free path, the number of collisions in a homogeneous medium is distributed according to a geometric distribution. Here, the probability mass function obtained from the Monte Carlo simulation is plotted together with the geometric distribution  $p(k) = (1 - p_{sc})p_{sc}^{k-1}$ . The same plasma conditions as in Fig. 1 and a size of 100 m and 1 m are assumed.

#### 4 Transition to a Monte Carlo continuum description

The plasma conditions assumed in the simulation presented above are such that the probability of scattering is larger than 99%. Even though the Monte Carlo calculation yields a correct estimation of the photoexcitation rate (as well as other moments of the specific intensity  $I$ ), it requires the counting of a large number of collisions, which can be CPU intensive in a realistic geometry where the photons are generated and tracked along many cells. A modification of the estimator that provides an analytical estimation of  $\langle k \rangle_V$  in highly scattering regions would be very beneficial. The geometric distribution corresponds to setting formally  $\chi \rightarrow \infty$  in the definition of the transport kernel (the mean free path tends to zero and the transport kernel tends to a delta function in space). An extension that accounts for finite mean free path can be devised by performing an expansion in powers of  $\chi^{-1}$ . We present hereafter a model adapted to the homogeneous slab discussed above. Like in other previous works [4, 5], we assume a rectangular line shape function (“grey” approximation) for the sake of simplicity; all frequency-dependent quantities are evaluated at the Bohr frequency  $\omega_0$  and the spectral band is set equal to the Doppler width  $\Delta\omega_D = \omega_0 v_0/c$  (with  $v_0 = \sqrt{2k_B T/m_{at}}$  being the thermal velocity). Let  $L$  be the slab size and  $z \in [0, L]$  the corresponding coordinate. The following relation holds for any function  $f$  (we set  $\mu \equiv \vec{n} \cdot \vec{e}_z$ ):

$$\int d^3r' T(\vec{r}|\omega, \vec{n}, \vec{r}') f(z') \quad \equiv \quad \int_0^\infty ds \chi e^{-\chi s} f(z - \mu s)$$

$$\underset{\chi \rightarrow \infty}{\sim} f(z) - \frac{\mu}{\chi} f'(z) + \frac{\mu^2}{\chi^2} f''(z). \quad (8)$$

It provides a simplification of the Monte Carlo equations (5), (6), and (7), because the spatial integral over the  $\vec{r}'$  variable has already been carried out. A discretization of the derivatives yields a balance relation which can be used in a Monte Carlo simulation. For example, consider a uniform grid with cell size  $\Delta z$  and take a centered difference scheme for the derivatives; Eq. (8) becomes

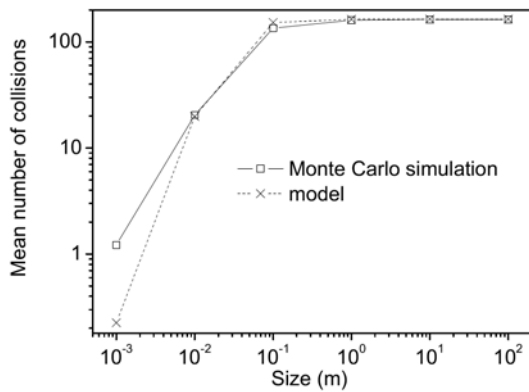
$$\int d^3r' T(\vec{r}|\omega, \vec{n}, \vec{r}') f(z') \simeq (1 - \alpha) f(z) + \left(\frac{\alpha}{2} - \beta\right) f(z + \Delta z) + \left(\frac{\alpha}{2} + \beta\right) f(z - \Delta z) \quad (9)$$

and it has a straightforward interpretation in random walks terms, namely, the number of photons leaving the cell centered at  $z$  is balanced with the number of photons coming from the two neighboring cells according to the probabilities  $\alpha/2 \pm \beta$ . The  $\alpha$  and  $\beta$  coefficients denote diffusion and advection contributions and are defined by  $\alpha = 2\mu^2/(\chi^2 \Delta z^2)$  and  $\beta = \mu/(2\chi \Delta z)$ . The collision estimator utilizes an angular average of these probabilities, so that there is no effective contribution of the advection term and  $\mu^2$  can be replaced by

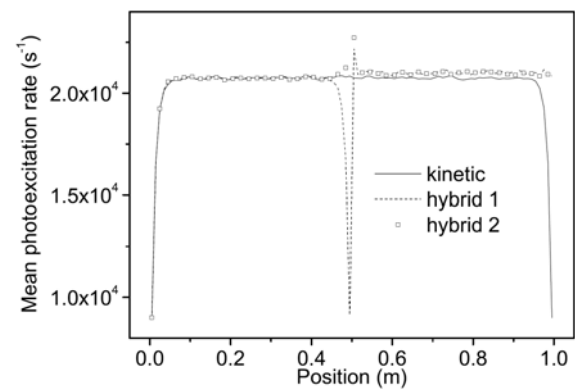
1/3 (because the line shape function assumed here is isotropic). This result is similar to that obtained from the radiative transfer equation within the so-called diffusion approximation [7, 14]. The applicability of Eq. (9) to generating trajectories and the counting of collisions can be illustrated through an application to the slab, setting formally  $\Delta z = L/2$  (one cell only) and assuming  $f(z \pm \Delta z) = 0$  for all functions present in the spatial integrals in Eqs. (5), (6), and (7) (perfectly absorbing walls). Algebraic manipulations yield the following expression

$$\langle k \rangle_V \simeq \frac{1}{1 - p_{sc} + 2p_{sc}/(3\chi^2\Delta z^2)}. \quad (10)$$

This expression coincides with the result of the geometric distribution at the  $\chi \rightarrow \infty$  limit and it provides an extension applicable to highly scattering media. Figure 3 shows a plot of the mean number of collisions estimated using the Monte Carlo simulation and compared to the result of Eq. (10), assuming different values of the size  $L$ . The model yields a result close to the Monte Carlo simulation (typically with a deviation smaller than 10%) if  $\langle k \rangle_V$  is large. The strong deviation that occurs at  $L = 10^{-3}$  m is due to the fact that the photon mean free path is of the same order as the slab size and the approximation (9) is not applicable.



**Fig. 3** Plot of the mean number of collisions calculated using the collision estimator (Monte Carlo simulation) and the model Eq. (10). The model is in a good agreement with the simulation in highly scattering media, i.e. if the mean number of collisions is large.



**Fig. 4** A hybrid Monte Carlo simulation that combines the kinetic equation and a fluid equation can be devised, provided a suitable interfacing between the regions is done. In the second hybrid simulation, the amount of photons escaping from the diffusive region (right) to the kinetic region (left) has been estimated using an ad hoc model.

A “hybrid” Monte Carlo simulation that involves random walks generated according to the kinetic equation (5) or its diffusive limit, according to the region under consideration, should involve a proper interfacing between the regions and a proper description of the boundary conditions. We present here the result of a simulation performed in the same plasma slab as above, assuming a uniform grid with 100 cells and a size  $L = 1$  m. The kinetic simulation is performed on the left half ( $z \in [0, L/2]$ ) and the diffusive limit process is applied to the right half ( $z \in [L/2, L]$ ). In the latter case, a random walk between neighboring cells is simulated, the probability that a photon leaves a cell is  $2/(3\chi^2\Delta z^2)$ , and the mean number of collisions is estimated as  $1/(1 - p_{sc})$ . If a photon initially present in the left half penetrates in the right half, the number of collisions  $k_l$  that have occurred in the left half is accounted for through the substitution  $p_{sc} \rightarrow p_{sc}^{k_l+1}$ . If a photon is initially present in the first cell of the diffusive region (here cell #51), it is allowed to escape in the kinetic region by advection if its velocity has a negative component on the  $z$  axis. Figure 4 shows a plot of the spatial dependence of the photoexcitation rate obtained from the hybrid simulation (referred to as “hybrid 2”) and compared to that obtained from the kinetic simulation. Also shown in the figure is the result of the hybrid simulation (referred to as “hybrid 1”) with no use of the procedure for photons reentering in the kinetic (left side) region. As can be seen, the model is in a good agreement with the fully kinetic simulation inside the diffusive region and the procedure for inserting photons from the diffusive to the kinetic region provides a fairly good estimate of the photoexcitation rate at the interface, with a deviation no larger than 30%. The overestimate near the right boundary is a feature of an incorrect description of boundary conditions. This issue is intrinsic to the use of a fluid model [4, 5, 14]; a

refinement of this work should involve the use of a model more elaborate than the approximation (9) and should be addressed in a future investigation.

## 5 Conclusion

Kinetic Monte Carlo simulations of coupled atom-radiation transport in optically thick divertor plasmas can be prohibitive, in particular in ITER (or beyond) relevant dense and cold divertor conditions. In this work, a hybrid formulation of radiation transport, designed in such a way to switch automatically between a kinetic and a fluid model according to the plasma conditions, has been developed and applied to idealized cases. The model involves a modification of the collision estimator used in standard kinetic Monte Carlo schemes and of the random walk process in highly collisional sub-domains. According to the region under consideration, the estimator counts the number of photon scatterings occurring in a given cell of the spatial grid or it automatically associates a mean number evaluated according to an analytical formula. A simplified random walk scheme based on a discretized diffusion approximation guides test particles across such diffusive sub-domains and provides entrance conditions to the remaining kinetic regions. By this a coupling scheme between kinetic and CFD codes and associated complexities (interfaces) can be avoided. A criterion that allows one to discriminate between the kinetic and fluid models is provided by the ratio between the photon mean free path and the cell's characteristic size. The issue of properly interfacing between the kinetic and fluid zones is still pending. An ad hoc procedure to account for photons initially present in the diffusion region and entering in the kinetic region has been proposed. The results obtained in our study have the correct order of magnitude but are dependent on the geometry under consideration. Further work should address the hybrid formulation in an arbitrary geometry. But we note that the concept outlined and verified in the present work remains equally valid in a regime in which not diffusive photons are interacting with (a bath of) atoms, but also if the atomic component of the gas is interacting (e.g. via resonant charge exchange as collision process then) with the background medium of charged plasma constituents.

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