Direct and Adjoint Monte Carlo Algorithms for the Footprint Problem

O. Kurbanmuradov[*], U. Rannik[†], K. Sabelfeld[‡]
and T. Vesala[†]

[*]Sci.Tech. Center *Climate*, Azadi 81, 744000 Ashkhabad, Turkmenistan

[†]Department of Physics, P.O. Box 9, FIN-00014, Helsinki University, Finland

[‡]Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstrasse 39, D – 10117 Berlin, Germany, E-mail: sabelfel@wias-berlin.de

This work is supported by Grant INTAS-RFBR N 95-IN-RU-726 and Nato Linkage Grant N 971664.

Abstract — Lagrangian stochastic models and algorithms are constructed and justified for solving the footprint problem, namely, the problem of calculation of the mean concentration and the flux of particles at a fixed point released from a source arbitrarily situated in the space. The direct and adjoint Monte Carlo algorithms are suggested, and rigorous justifications are given. Two different backward trajectory algorithms are considered: Thomson's method and a method based on probabilistic representations of the relevant initial value problem. The cost of the latter algorithm may increase with time, but it allows to treat the general situation when a set of reacting species is scattered by the flow. Thomson's approach is extended to general stochastic differental equations which is especially usefull when it is desired to find a solution at a fixed point, and for large time instances.

1 Introduction

The footprint problem as formulated in the literature (e.g., see [18], [3], [4], [5]) essentially deals with the calculation of the contribution to the mean concentration and its flux at a fixed point from an arbitrary given source of particles. There are mainly two different approaches: (1) conventional deterministic methods based on the semiempirical turbulent diffusion equation and closure assumptions (e.g., see [18]) and (2), stochastic approach which utilizes trajectory simulations (e.g., see [13], [9], [10], [14]-[21]).

The deterministic approach directly deals with the equation governing the mean concentration, but it is restricted by the use of the Boussinesq hypothesis whose applicability should be additionally studied (e.g., see [1]). For instance, this hypothesis can not be true if the concentration is calculated close to the sources [1], [11]. More generally, the high order closure methods are developed, but different closure hypotheses also should be made [11] .

Stochastic models do not require any closure hypotheses, and the main difficulty is to construct adequate Lagrangian trajectories with the desired statistical characteristics.

There are two main approaches in constructing stochastic methods. The first one is based on Monte Carlo simulation of the Eulerian random velocity fields (e.g., see [8], [13], [20]). Second approach treats the stochastic Lagrangian trajectories as solutions to the stochastic generalized Langevin equation (e.g., see [19], [16], [14]) .

The first approach is more rigorous, but generally it requires a lot of computer time. In addition, it needs a detailed information about statistical characteristics of the whole velocity field. In contrast, the second approach needs only one-pont probability density function (pdf) of the Eulerian velocity field, and is much more efficient in numerical calculations. It should be noted however, that this approach is rigorously justified only in the case of stationary isotropic turbulent flow. Even in the case of homogeneous but nonisotropic turbulence the justification problem remains unsolved; in particular there are several different stochastic models which satisfy the well-mixed condition [19], [15].

In this paper, we suggest direct and backward Monte Carlo algorithms for solving the footprint problem by simulation of Lagrangian trajectories as solutions to generalized Langevin equations. We derive random estimators for the mean concentration and its flux both for direct and backward schemes. Two different methods are compared: the adjoint scheme which is based on probabilistic representations of the relevant PDE [6] and the backward Thomson's scheme [19]. The last approach is extended to general stochastic differential equations.

2 Formulation of the problem

Let us consider a passive scalar dispersed by the turbulent velocity field in the surface layer of the atmosphere. The passive scalar is assumed to follow the streamlines of the flow. We assume that the source of particles is quite arbitrary, for instance, it might be situated on the surface or in the space, or even at given points. Let us denote by $q(\mathbf{x},t)$ the spatial-temporal density distribution function of the source, i.e, the number of emitted particles per unit volume in a unit time interval at the phase point $(\mathbf{x},t)$. Initially, the spatial density of particles is given by $q_0(\mathbf{x})$. The particles are transported by the 3D turbulent velocity field $\mathbf{u}(\mathbf{x},t)$ in the surface layer $D=\{\mathbf{x}=(x_1,x_2,x_3):\ x_3\geq 0\}$. Let us denote by $\mathbf{X}(t;\mathbf{x}_0,t_0)$ and $\mathbf{V}(t;\mathbf{x}_0,t_0)$ the Lagrangian spatial coordinates and the velocity, respectively.

The mean concentration at $(\mathbf{x},t)$ is defined by [11]:

$$\langle c(\mathbf{x},t)\rangle=\bar{c}(\mathbf{x},t)=\int\limits_0^t dt_0\int\limits_D d\mathbf{x}_0\, q(\mathbf{x}_0,t_0)p_L(\mathbf{x},t;\mathbf{x}_0,t_0)+\int\limits_D d\mathbf{x}_0\, q_0(\mathbf{x}_0)p_L(\mathbf{x},t;\mathbf{x}_0,0), \quad (2.1)$$

where

$$p_L(\mathbf{x},t;\mathbf{x}_0,t_0)=\langle\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,t_0))\rangle$$

is the probability density function (pdf) of the particle's coordinate at the time t which was started in the point $\mathbf{x}_0$ at the time t_0, $\delta(\cdot)$ is the Dyrac delta-function. Here and throughout the paper we use the notation $\langle\cdot\rangle$ for the averaging over the samples of the turbulent velocity field. We define also the concentration fluxes by

$$F_i(\mathbf{x},t)=\langle u_i(\mathbf{x},t)c(\mathbf{x},t)\rangle,\quad i=1,2,3,$$

where $c(\mathbf{x},t)$ is the instant concentration. As in the case (2.1), the fluxes can be represented in the integral form (see Appendix A):

$$\begin{aligned}F_i(\mathbf{x},t)=&\int\limits_{\mathbf{R}^3} d\mathbf{u}\int\limits_0^t dt_0\int\limits_D d\mathbf{x}_0\, u_i q(\mathbf{x}_0,t_0)p_L(\mathbf{x},\mathbf{u},t;\mathbf{x}_0,t_0)\\&+\int\limits_{\mathbb{R}^3} d\mathbf{u}\int\limits_D d\mathbf{x}_0\, u_i q_0(\mathbf{x}_0)p_L(\mathbf{x},\mathbf{u},t;\mathbf{x}_0,0).\end{aligned} \quad (2.2)$$

Here

$$p_L(\mathbf{x},\mathbf{u},t;\mathbf{x}_0,t_0)=\langle\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,t_0))\delta(\mathbf{u}-\mathbf{V}(t;\mathbf{x}_0,t_0))\rangle \quad (2.3)$$

is the pdf of the spatial-velocity phase point.

In the analysis, it is convenient to deal with a general quantity, the spatial-velocity distribution of an ensemble of particles:

$$\begin{aligned}p(\mathbf{x},\mathbf{u},t)=&\int\limits_0^t dt_0\int\limits_D d\mathbf{x}_0\, q(\mathbf{x}_0,t_0)p_L(\mathbf{x},\mathbf{u},t;\mathbf{x}_0,t_0)\\&+\int\limits_D d\mathbf{x}_0\, q_0(\mathbf{x}_0)p_L(\mathbf{x},\mathbf{u},t;\mathbf{x}_0,0).\end{aligned} \quad (2.4)$$

From (2.1), (2.2) and (2.4) we find

$$\bar{c}(\mathbf{x},t) = \int\limits_{\mathbb{R}^3} p(\mathbf{x},\mathbf{u},t)d\mathbf{u}\ , \quad F_i(\mathbf{x},t) = \int\limits_{\mathbb{R}^3} u_i\, p(\mathbf{x},\mathbf{u},t)d\mathbf{u}, \quad i=1,2,3.$$

It is of practical interest to calculate the mean concentration and relevant fluxes for arbitrarily situated surface sources. In the literature, this problem is called a footprint problem (e.g., see [18], [3], [5]). Note that in this problem, the mean concentration and fluxes are evaluated at a fixed point. We consider a more general function:

$$(p,h) = \int\limits_{\mathbb{R}^3} d\mathbf{u} \int\limits_0^T dt \int\limits_D d\mathbf{x}\ p(\mathbf{x},\mathbf{u},t)h(\mathbf{x},\mathbf{u},t),$$

where $h(\mathbf{x},\mathbf{u},t)$ is an arbitrary function which can be chosen relevant to the quantity of interest. For instance, in the case $h(\mathbf{y},\mathbf{u},s) = \delta(\mathbf{y}-\mathbf{x})\delta(s-t)$ we have $(p,h) = \bar{c}(\mathbf{x},t)$. If $h(\mathbf{y},\mathbf{u},s) = u_i\delta(\mathbf{y}-\mathbf{x})\delta(s-t)$, then $(p,h) = F_i(\mathbf{x},t)$. Thus we concentrate on the problem of calculation of the function (p,h).

3 Stochastic Lagrangian algorithm

To construct algorithms based on the representations given above, we need samples of the Lagrangian trajectories $\mathbf{X}(t) = \mathbf{X}(t;\mathbf{x}_0,t_0)$, $t \geq t_0$. Ideally, if we had samples of the velocity $\mathbf{u}(\mathbf{x},t)$, the trajectories could be simulated by solving the problem

$$\frac{d\mathbf{X}(t)}{dt} = \mathbf{u}(\mathbf{X}(t),t), \quad t > t_0 \quad \mathbf{X}(t_0) = \mathbf{x}_0\ .$$

In practice one uses approximate models of the velocity field. For instance, randomized models of the Gaussian velocity fields are used (e.g., see [13]). This approach is well developed and justified only in the case of homogeneous turbulence while inhomogeneous case requires further development. In general nonhomogeneous case one uses another approach based on stochastic differential equation of Langevin type governing directly the Lagrangian trajectory. This equation has the form (see, for instance, [19], [16], [15]):

$$\begin{aligned} d\mathbf{X}(t) &= \mathbf{V}(t)dt, \\ d\mathbf{V}(t) &= \mathbf{a}(t,\mathbf{X}(t),\mathbf{V}(t))dt + \sqrt{C_0\bar{\varepsilon}(\mathbf{X}(t),t)}\, d\mathbf{W}(t), \end{aligned} \tag{3.1}$$

where the function $\mathbf{a}$ is to be defined in each specific situation, C_0 is the universal Kolmogorov constant ($C_0 \approx 4 \div 6$), and $\bar{\varepsilon}(\mathbf{x},t)$ is the mean dissipation rate of the kinetic energy of turbulence, and $\mathbf{W}(t)$ is the standard 3D Wiener process. In this section, we deal with the general scheme.

Remark 3.1. Note that to complete the description of the Lagrangian stochastic model, we need to define the behaviour of $(\mathbf{X}(t),\mathbf{V}(t))$ in the neighbourhood of the boundary $\Gamma = \{\mathbf{x} = (x_1,x_2,x_3) : x_3 = 0\}$. We assume that the boundary is impenetrable, i.e., that $u_3(\mathbf{x})|_{\mathbf{x}\in\Gamma} = 0$. This implies that the Lagrangian trajectories satisfying (3.1) do never reach Γ. Therefore it is reasonable to require that the same property holds for $\mathbf{X}(t)$, the solutions to (3.1). This can be realized by special choice of the function $\bar{\varepsilon}(\mathbf{x},t)$ (see for details Sec. 4).

3.1 Direct Monte Carlo algorithm

Let $\mathbf{X}(t;\mathbf{x}_0,t_0)$, $\mathbf{V}(t;\mathbf{x}_0,t_0)$, $t \geq t_0$ be solutions to (3.1) satisfying the initial condition $\mathbf{X}(t_0) = \mathbf{x}_0$ with $\mathbf{V}(t_0) = \mathbf{u}_0$, where $\mathbf{u}_0$ is a random velocity whose pdf coincides with $p_E(\mathbf{u}_0;\mathbf{x}_0,t_0)$, the pdf of the Eulerian velocity $\mathbf{u}(\mathbf{x}_0,t_0)$.

It is convenient to use the representation $(p,h) = I + I_0$, where

$$I = \int\limits_{\mathbb{R}^3} d\mathbf{u} \int\limits_0^T dt \int\limits_D d\mathbf{x} h(\mathbf{x},\mathbf{u},t) \int\limits_0^t dt_0 \int\limits_D d\mathbf{x}_0\, q(\mathbf{x}_0,t_0) p_L(\mathbf{x},\mathbf{u},t;\mathbf{x}_0,t_0)$$
$$= \int\limits_0^T dt_0 \int\limits_D d\mathbf{x}_0 q(\mathbf{x}_0,t_0) \int\limits_{\mathbb{R}^3} d\mathbf{u} \int\limits_{t_0}^T dt \int\limits_D d\mathbf{x}\, h(\mathbf{x},\mathbf{u},t) p_L(\mathbf{x},\mathbf{u},t;\mathbf{x}_0,t_0),$$

and

$$I_0 = \int\limits_D d\mathbf{x}_0 q_0(\mathbf{x}_0) \int\limits_{\mathbb{R}^3} d\mathbf{u} \int\limits_0^T dt \int\limits_D d\mathbf{x} h(\mathbf{x},\mathbf{u},t)\, p_L(\mathbf{x},\mathbf{u},t;\mathbf{x}_0,0).$$

From this representations we can write down the Monte Carlo estimators for I and I_0. Let

$$Q = \int\limits_D d\mathbf{x} \int\limits_0^T dt\, q(\mathbf{x},t), \qquad Q_0 = \int\limits_D q_0(\mathbf{x}) d\mathbf{x},$$

and let $(\tilde{\mathbf{x}},\tilde{t})$ be a random point distributed in $D\times[0,T]$ with the pdf $q(\mathbf{x},t)/Q$, and $\tilde{\mathbf{x}}_0$ is a random point distributed in D with $q_0(\mathbf{x})/Q_0$. Standard arguments of the Monte Carlo theory [13] yield

$$I = Q\mathbb{E}_{(\tilde{\mathbf{x}},\tilde{t})}\mathbb{E}_{W(\cdot)} \int_{\tilde{t}}^T h(\mathbf{X}(t;\tilde{\mathbf{x}},\tilde{t}),\mathbf{V}(t;\tilde{\mathbf{x}},\tilde{t}),t)dt, \tag{3.2}$$

$$I_0 = Q_0\mathbf{E}_{\tilde{\mathbf{x}}_0}\mathbb{E}_{W(\cdot)} \int\limits_0^T h(\mathbf{X}(t;\tilde{\mathbf{x}}_0,0),\mathbf{V}(t;\tilde{\mathbf{x}}_0,0),t)\, dt. \tag{3.3}$$

Here $\mathbb{E}_{(\tilde{\mathbf{x}},\tilde{t})}\mathbf{E}_{W(\cdot)}$ means averaging, first, over all starting points $(\tilde{\mathbf{x}},\tilde{t})$ and, second, over all solutions of (3.1); these two averagings are taken independently. Similar notation is used in (3.3).

From the probabilistic representations (3.2),(3.3) we can construct the direct Monte Carlo algorithm. For this we need a numerical scheme for solving the stochastic differential equation (3.1). For simplicity, we choose the Euler scheme.

The algorithm can be described as follows. The mathematcal expectation in (3.2) is usually calculated as

$$I \simeq \frac{1}{N}\sum_{i=1}^N \xi_i,$$

where N is the number of samples and ξ_i, $i = 1,\ldots,N$, are independent samples of the random estimator

$$\xi = Q \int\limits_{\tilde{t}}^T h(\mathbf{X}(t;\tilde{\mathbf{x}},\tilde{t}),\mathbf{V}(t;\tilde{\mathbf{x}},\tilde{t}),t)dt.$$

First we choose the time step of integration as $\Delta t = T/N_t$, N_t is the total number of steps. Then the calculation of ξ_i is as follows.

Step 0.

$S := 0$, and sample the random point $(\tilde{\mathbf{x}}, \tilde{t})$ in $D \times [0, T]$
from the density $q(\mathbf{x}, t)/Q$; sample $\tilde{\mathbf{u}}_0$ in $\mathbf{R}^3$ from the density $p_E(\mathbf{u}_0; \tilde{\mathbf{x}}, \tilde{t})$;
put $t := \tilde{t}$, $\mathbf{X} := \tilde{\mathbf{x}}$, $\mathbf{V} := \tilde{\mathbf{u}}$;

Step 1.

$S := S + Q\Delta t h(\mathbf{X}, \mathbf{V}, t)$;
Sample a 3D standard gaussian random vector η;
put $\mathbf{X} := \mathbf{X} + \mathbf{V}\Delta t$, $\mathbf{V} := \mathbf{V} + \mathbf{a}(t, \mathbf{X}, \mathbf{V})\Delta t + \sqrt{C_0 \bar{\varepsilon}(\mathbf{X}, t)\Delta t}\eta$; $t := t + \Delta t$;
if $t > T$, then go to step 2. Otherwise go back to start the step 1.

Step 2.

put $\xi_i := S$;

3.2 Adjoint algorithm

Clearly, the direct algorithm is not practically applicable in general situation if the function $h(\mathbf{x}, \mathbf{u}, t)$ is concentrated on small domains. In this case, an adjoint scheme is preferable. For this purpose we need the probabilistic representation for $p(\mathbf{x}, \mathbf{u}, t)$. In what follows, we use the summation convention. The function $p_L(\mathbf{x}, \mathbf{u}, t; \mathbf{x}_0, t_0)$ defined in (2.3) satisfies the Kolmogorov-Fokker-Planck equation for the stochastic differential equation (3.1):

$$\frac{\partial p_L}{\partial t} + \frac{\partial (u_i p_L)}{\partial x_i} + \frac{\partial (a_i p_L)}{\partial u_i} = \frac{1}{2} C_0 \bar{\varepsilon}(\mathbf{x}, t) \frac{\partial^2}{\partial u_i \partial u_i} p_L(\mathbf{x}, \mathbf{u}, t; \mathbf{x}_0, t_0),$$

with the initial conditions

$$p_L(\mathbf{x}, \mathbf{u}, t; \mathbf{x}_0, t_0)|_{t=t_0} = \delta(\mathbf{x} - \mathbf{x}_0) p_E(\mathbf{u}; \mathbf{x}_0, t_0).$$

From this, using (2.4) we find

$$\frac{\partial p}{\partial t} + \frac{\partial (u_i p)}{\partial x_i} + \frac{\partial (a_i p)}{\partial u_i} = \frac{1}{2} C_0 \bar{\varepsilon}(\mathbf{x}, t) \frac{\partial^2 p(\mathbf{x}, \mathbf{u}, t)}{\partial u_i \partial u_i} + q(\mathbf{x}, t) p_E(\mathbf{u}; \mathbf{x}, t)$$

and

$$p(\mathbf{x}, \mathbf{u}, t)|_{t=0} = q_0(\mathbf{x}) p_E(\mathbf{u}; \mathbf{x}, 0).$$

Using the probabilistic representation given in Appendix B we get

$$\begin{aligned} p(\mathbf{x}, \mathbf{u}, t) = \mathbb{E}_{(\mathbf{x}, \mathbf{u}, t)} \Bigg\{ & \int_0^t q(\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}, \hat{\mathbf{V}}_{t_0}^{\mathbf{x},\mathbf{u},t}, t_0)\, p_E(\hat{\mathbf{V}}_{t_0}^{\mathbf{x},\mathbf{u},t}; \hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}, t_0) \\ & \times \exp\left(- \int_{t_0}^t \rho(\hat{\mathbf{X}}_{t_0'}^{\mathbf{x},\mathbf{u},t}, \hat{\mathbf{V}}_{t_0'}^{\mathbf{x},\mathbf{u},t}, t_0') dt_0' \right) dt_0 \qquad (3.4) \\ & + q_0(\hat{\mathbf{X}}_0^{\mathbf{x},\mathbf{u},t}) p_E(\hat{\mathbf{V}}_0^{\mathbf{x},\mathbf{u},t}; \hat{\mathbf{X}}_0^{\mathbf{x},\mathbf{u},t}, 0) \exp\left(- \int_0^t \rho(\hat{\mathbf{X}}_{t_0'}^{\mathbf{x},\mathbf{u},t}, \hat{\mathbf{V}}_{t_0'}^{\mathbf{x},\mathbf{u},t}, t_0') dt_0' \right) \Bigg\}. \end{aligned}$$

where $\rho(\mathbf{x},\mathbf{u},t) = \frac{\partial a_i(\mathbf{x},\mathbf{u},t)}{\partial u_i}$, and $\hat{\mathbf{X}}(t_0) \equiv \hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}$, $\hat{\mathbf{V}}(t_0) \equiv \hat{\mathbf{V}}_{t_0}^{\mathbf{x},\mathbf{u},t}$, $\quad t_0 \le t$ is the adjoint trajectory determined as the solution to the equation:

$$
\begin{aligned}
d\hat{\mathbf{X}}(t_0) &= \hat{\mathbf{V}}(t_0)dt_0, \\
d\hat{\mathbf{V}}(t_0) &= \mathbf{a}(t_0,\hat{\mathbf{X}}(t_0),\hat{\mathbf{V}}(t_0))dt_0 + \sqrt{C_0\bar{\varepsilon}(\hat{\mathbf{X}}(t_0),t_0)}\, d\hat{\mathbf{W}}(t_0),
\end{aligned}
$$

with the terminal conditions

$$
\hat{\mathbf{X}}(t_0)\Big|_{t_0=t} = \mathbf{x}, \quad \hat{\mathbf{V}}(t_0)\Big|_{t_0=t} = \mathbf{u}\ .
$$

Note that here $\mathbf{a}(\cdot)$ is the same function as in (3.1), and $\hat{\mathbf{W}}(t_0)$ is a standard 3D Wiener process.

From the probabilistic representation (3.4) we get

$$
\begin{aligned}
(p,h) = &\int\limits_{\mathbf{R}^3} d\mathbf{u} \int\limits_0^T dt \int\limits_D d\mathbf{x}\, h(\mathbf{x},\mathbf{u},t) \\
&\times \mathbb{E}_{(\mathbf{x},\mathbf{u},t)} \left\{ \int\limits_0^t q(\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}, \hat{\mathbf{V}}_{t_0}^{\mathbf{x},\mathbf{u},t}, t_0) p_E(\hat{\mathbf{V}}_{t_0}^{\mathbf{x},\mathbf{u},t}; \hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}, t_0) e_\rho^{t_0}(\mathbf{x},\mathbf{u},t)\, dt_0 \right. \\
&\qquad \left. + q_0(\hat{\mathbf{X}}_0^{\mathbf{x},\mathbf{u},t})\, p_E(\hat{\mathbf{V}}_0^{\mathbf{x},\mathbf{u},t}; \hat{\mathbf{X}}_0^{\mathbf{x},\mathbf{u},t}, 0)\, e_\rho^0(\mathbf{x},\mathbf{u},t) \right\}
\end{aligned}
$$

where

$$
e_\rho^\tau(\mathbf{x},\mathbf{u},t) = \exp\left(- \int\limits_\tau^t \rho(\hat{\mathbf{X}}_{t_0'}^{\mathbf{x},\mathbf{u},t}, \hat{\mathbf{V}}_{t_0'}^{\mathbf{x},\mathbf{u},t}, t_0') dt_0' \right).
$$

Now we are in position to write down the Monte Carlo estimator for $\hat{I}$ and $\hat{I}_0$.

Let $\pi(\mathbf{x},\mathbf{u},t)$ be an arbitrary probability density function in $D \times \mathbb{R}^3 \times [0,T]$ which satisfies the condition

$$
\pi(\mathbf{x},\mathbf{u},t) \neq 0 \quad \text{if } \ h(\mathbf{x},\mathbf{u},t) \neq 0.
$$

Let $(\hat{\mathbf{x}},\hat{\mathbf{u}},\hat{t})$ be a random point distributed in $D \times \mathbb{R}^3 \times [0,T]$ with density π. Then

$$
(p,h) = \mathbb{E}_{(\hat{\mathbf{x}},\hat{\mathbf{u}},\hat{t})} \mathbf{E}_{\hat{\mathbf{W}}(\cdot)} \hat{\xi},
$$

where

$$
\begin{aligned}
\hat{\xi} = \frac{h(\hat{\mathbf{x}},\hat{\mathbf{u}},\hat{t})}{\pi(\hat{\mathbf{x}},\hat{\mathbf{u}},\hat{t})} \Bigg[&\int\limits_0^{\hat{t}} \left\{ q(\hat{\mathbf{X}}_{t_0},t_0) p_E(\hat{\mathbf{V}}_{t_0}; \hat{\mathbf{X}}_{t_0}, t_0) e_\rho^{t_0}(\hat{\mathbf{x}},\hat{\mathbf{u}},\hat{t}) \right\} dt_0 \\
&+ q_0(\hat{\mathbf{X}}_0) p_E(\hat{\mathbf{V}}_0; \hat{\mathbf{X}}_0, 0) e_\rho^0(\hat{\mathbf{x}},\hat{\mathbf{u}},\hat{t}) \Bigg] .
\end{aligned}
$$

Here we used a brief notation,

$$
\hat{\mathbf{X}}_{t_0} \equiv \hat{\mathbf{X}}_{t_0}^{\hat{\mathbf{x}},\hat{\mathbf{u}},\hat{t}}, \quad \hat{\mathbf{V}}_{t_0} \equiv \hat{\mathbf{V}}_{t_0}^{\hat{\mathbf{x}},\hat{\mathbf{u}},\hat{t}}\ .
$$

The calculations are carried out according to

$$(p,h) \simeq \frac{1}{N}\sum_{i=1}^{N} \hat{\xi}_i,$$

where N is the number of samples, $\hat{\xi}_i$, $i = 1,\dots,N$, are independent samples of the random estimator $\hat{\xi}$.

The algorithm of calculation of the sample $\hat{\xi}_i$:

Step 0.

$S := 0$; sample the random point $(\hat{\mathbf{x}}, \hat{\mathbf{u}}, \hat{t})$ in $D \times \mathbf{R}^3 \times [0,T]$ from the density $\pi(\mathbf{x},\mathbf{u},t)$;
$Q := \frac{h(\hat{\mathbf{x}},\hat{\mathbf{u}},\hat{t})}{\pi(\hat{\mathbf{x}},\hat{\mathbf{u}},\hat{t})}$; put $t := \hat{t}$, $\mathbf{X} := \hat{\mathbf{x}}$, $\mathbf{V} := \hat{\mathbf{u}}$; $\mu := 1$.

Step 1.

$S := S + \Delta t q(\mathbf{X},t) p_E(\mathbf{V};\mathbf{X},t)\mu$;
Sample a 3D standard gaussian random vector η;
put $\mathbf{X} := \mathbf{X} - \mathbf{V}\Delta t$, $\mathbf{V} =: \mathbf{V} - \mathbf{a}(t,\mathbf{X},\mathbf{V})\Delta t + \sqrt{C_0 \bar{\varepsilon}(\mathbf{X},t)\Delta t}\,\eta$;
$\mu := \mu \exp(-\rho(\mathbf{X},\mathbf{V},t)\Delta t)$; $t := t - \Delta t$;
if $t < 0$, then go to step 2. Otherwise go back to start the step 1.

Step 2.

put $\hat{\xi}_i := Q[S + q_0(\mathbf{X}) p_E(\mathbf{V};\mathbf{X},0)\mu]$.

4 Impenetrable Boundary

Note that to complete the description of the Lagrangian stochastic model, we need to define the behaviour of $\mathbf{X}(t), \mathbf{V}(t)$, the solution to (3.1) in the neighbourhood of the boundary $\Gamma = \{\mathbf{x} : z = x_3 = 0\}$. We assume that the boundary is impenetrable, i.e., that $w = u_3 = 0$ at the boundary of Γ. This implies that the true Lagrangian trajectories do never reach Γ. Therefore it is reasonable to require that the same property holds for $\mathbf{X}(t)$, the solutions to (3.1). This can be done by special choice of the function $\bar{\varepsilon}(z,t)$. Indeed, in the neighbourhood of Γ, it is reasonable to consider the flow as neutrally stratified. Therefore, $p_E(w)$ is gaussian, with constant σ_w, and the vertical profile of $\bar{\varepsilon}(z)$ is given by [11]

$$\bar{\varepsilon}(z) = \frac{u_*^3}{\kappa z}, \quad \kappa \simeq 0.4, \quad z > z_0. \tag{4.1}$$

Here κ is the Karman constant, and z_0 is the roughness height.

The equation of vertical motion $Z(t) = X_3(t)$, $W(t) = V_3(t)$ then is

$$dZ = W\,dt, \quad dW(t) = -\frac{a}{Z}W(t)dt + \frac{b}{\sqrt{Z}}\,dB(t), \tag{4.2}$$

where

$$a = \frac{C_0 u_*^3}{2\kappa\sigma_w^2}, \quad b = \Big(\frac{C_0 u_*^3}{\kappa}\Big)^{\frac{1}{2}}.$$

If we assume that the formula (4.1) is true for all $z > 0$, then all the solutions to (4.2) do not reach the boundary Γ. Indeed, let τ be a random time (wich depends on the trajectory $Z(t)$) defined by

$$\tau(t) = \int_0^t \frac{ds}{Z(s)}.$$

Then, the vertical velocity $W(\tau)$ in new time variable τ satisfies the equation

$$dW(\tau) = -aW(\tau)d\tau + b\,dB(\tau).$$

Therefore, from

$$\frac{dZ}{d\tau} = \frac{dZ}{dt}\frac{dt}{d\tau} = W(\tau)Z(\tau)$$

we have

$$Z(\tau) = Z(0)\exp\{S(\tau)\}, \quad S(\tau) = \int_0^\tau W(\tau')\,d\tau'.$$

The function $W(\tau)$ is an Uhlenbeck-Ornstein process with continuous samples. Therefore, $|S(\tau)| < \infty$ with probability one for arbitrary $\tau > 0$. This implies that $Z(\tau) > 0$ provided that $Z(0) > 0$. Thus the function $Z(\tau)$ never reaches the boundary Γ. The same is true for $Z(t)$. To show this, it is sufficient to note that $t(\tau) \to \infty$ as $\tau \to \infty$. Let us show this property. We have

$$t(\tau) = \int_0^\tau \frac{dt}{d\tau'}\,d\tau' = \int_0^\tau Z(\tau')\,d\tau' = Z(0)\int_0^\tau \exp\{S(\tau')\}\,d\tau'.$$

In [9] it is shown that with probablity one,

$$\int_0^\infty \exp\{S(\tau)\}\,d\tau = \infty.$$

This implies that with probability one $t(\tau) \to \infty$ as $\tau \to \infty$.

In numerical implementation, it is convenient to simulate the trajectory in the neighbourhood of Γ by numerical solution to

$$\begin{aligned} \frac{d\ln Z(\tau)}{d\tau} &= W(\tau), \\ dW(\tau) &= -aW(\tau) + b\,dB(\tau) \\ \frac{dt(\tau)}{d\tau} &= Z(\tau). \end{aligned}$$

The Euler scheme reads

$$\begin{aligned} Z(\tau+\Delta\tau) &= Z(\tau)\exp\{W(\tau)\Delta\tau\}, \\ W(\tau+\Delta\tau) &= W(\tau) - aW(\tau)\Delta\tau + b\sqrt{\Delta\tau}\,\eta, \\ t(\tau+\Delta\tau) &= t(\tau) + Z(\tau)\Delta\tau, \end{aligned}$$

where $\Delta\tau$ is the discretization step, and η is a standard normal random number.

Note that by construction, this scheme ensures that the boundary is impenetrable, i.e., $Z(\tau) > 0$ for all τ.

5 Reacting Species

In this section we show that the backward trajectory technique can be extended to the case when a set of reacting species is in play. Assume that in the domain D with a boundary Γ which is impenetrable there are K reacting species governed in Lagrangian formulation by the system

$$\begin{aligned} d\mathbf{X}(t) &= \mathbf{V}(t)dt, \\ d\mathbf{V}(t) &= \mathbf{a}(t, \mathbf{X}(t), \mathbf{V}(t))dt + \sqrt{C_0\bar{\varepsilon}(\mathbf{X}(t), t)}\, d\mathbf{W}(t), \\ \frac{dN_k}{dt} &= f_k(t, \mathbf{X}, \mathbf{N}), \quad k = 1, 2. \ldots, K \end{aligned} \tag{5.1}$$

with the initial conditions:

$$\mathbf{X}(0; \mathbf{x}_0) = \mathbf{x}_0, \quad \mathbf{V}(0; \mathbf{x}_0) = \mathbf{v}_0, \quad N_k(0; \mathbf{x}_0) = q_k(\mathbf{x}_0),\ k = 1, \ldots, K,$$

where $\mathbf{v}_0$ is the initial random velocity whose pdf is $p_E(\mathbf{v}; \mathbf{x}_0)$, and $q_k(\mathbf{x}_0)$ is the initial spatial distribution of the species, $\mathbf{N} = (N_1, \ldots, N_K)$. The Eulerian concentration of k-th specie is given by

$$n_k(\mathbf{x}, t) = \int\limits_D d\mathbf{x}_0 q_k(\mathbf{x}_0)\delta(\mathbf{x} - \mathbf{X}(t; \mathbf{x}_0)), \quad k = 1, \ldots, K.$$

Then the mean is

$$\langle n_k(\mathbf{x}, t)\rangle = \int\limits_{\mathbf{R}^3} d\mathbf{v} \int d\mathbf{n} \int\limits_D d\,\mathbf{x}_0 n_k p_L(\mathbf{x}, \mathbf{v}, \mathbf{n}, t; \mathbf{x}_0), \quad k = 1, \ldots, K,$$

where

$$p_L(\mathbf{x}, \mathbf{v}, \mathbf{n}, t; \mathbf{x}_0) = \langle \delta(\mathbf{x} - X(t; \mathbf{x}_0))\delta(\mathbf{v} - \mathbf{V}(t; \mathbf{x}_0))\delta(\mathbf{n} - \mathbf{N}(t; \mathbf{x}_0))\rangle.$$

This pdf satisfies the Kolmogorov-Fokker-Planck equation

$$\frac{\partial p_L}{\partial t} + \frac{\partial}{\partial x_i}(v_i p_L) + \frac{\partial}{\partial v_i}(a_i p_L) + \frac{\partial}{\partial n_k}(f_k p_L) = \frac{C_0\bar{\varepsilon}}{2}\frac{\partial^2 p_L}{\partial v_i \partial v_j}$$

with the initial condition:

$$p_L(\mathbf{x}, \mathbf{v}, \mathbf{n}, 0; \mathbf{x}_0) = \delta(\mathbf{x} - \mathbf{x}_0)\, p_E(\mathbf{v}; \mathbf{x}_0)\delta(\mathbf{n} - \mathbf{q}(\mathbf{x}_0)).$$

Here $\mathbf{q}(\mathbf{x}_0) = (q_1(\mathbf{x}_0), \ldots, q_K(\mathbf{x}_0))$. The flux of k-th specie in i-th direction is given by $(k = 1, \ldots, K)$:

$$\langle v_i(\mathbf{x}, t)n_k(\mathbf{x}, t)\rangle = \int\limits_{\mathbb{R}^3} d\mathbf{v} \int d\mathbf{n} \int\limits_D d\,\mathbf{x}_0 v_i n_k\, p_L(\mathbf{x}, \mathbf{v}, \mathbf{n}, t; \mathbf{x}_0).$$

Generally, the integral

$$I_h(\mathbf{x}, t) = \int\limits_{\mathbb{R}^3} d\mathbf{v} \int d\mathbf{n} \int\limits_D d\,\mathbf{x}_0\, h(\mathbf{x}, \mathbf{v}, \mathbf{n}, t)\, p_L(\mathbf{x}, \mathbf{v}, \mathbf{n}, t; \mathbf{x}_0) \tag{5.2}$$

is to be evaluated for a given function h. Let

$$\theta(\mathbf{x},\mathbf{v},\mathbf{n},t)=\int\limits_D d\,\mathbf{x}_0\,p_L(\mathbf{x},\mathbf{v},\mathbf{n},t;\mathbf{x}_0).$$

Then this function satisfies

$$\frac{\partial\theta}{\partial t}+\frac{\partial}{\partial x_i}(v_i\theta)+\frac{\partial}{\partial v_i}(a_i\theta)+\frac{\partial}{\partial n_k}(f_k\theta)=\frac{C_0\bar{\varepsilon}}{2}\frac{\partial^2\theta}{\partial v_i\partial v_j}$$

and the initial condition

$$\theta(\mathbf{x},\mathbf{v},\mathbf{n},0)=p_E(\mathbf{v};\mathbf{x})\delta(\mathbf{n}-\mathbf{q}(\mathbf{x})).$$

The probabilistic representation given in Appendix B in this case yields:

$$\begin{aligned}\theta(\mathbf{x},\mathbf{v},\mathbf{n},t)=\mathbf{E}\,p_E(\mathbf{V}_0^{\mathbf{x},\mathbf{v},t};\mathbf{X}_0^{\mathbf{x},\mathbf{v},t})\exp\left\{-\int\limits_0^t\frac{\partial a_i}{\partial v_i}(s,\mathbf{X}_s^{\mathbf{x},\mathbf{v},t},\mathbf{V}_s^{\mathbf{x},\mathbf{v},t})ds\right\}\\ \times\exp\left\{-\int\limits_0^t\frac{\partial f_k}{\partial n_k}(s,\mathbf{X}_s^{\mathbf{x},\mathbf{v},t},\mathbf{N}_s^{\mathbf{x},\mathbf{v},\mathbf{n},t})ds\right\}\delta(\mathbf{N}_0^{\mathbf{x},\mathbf{v},\mathbf{n},t}-\mathbf{q}(\mathbf{X}_0^{\mathbf{x},\mathbf{v},t})),\end{aligned}\tag{5.3}$$

where $\mathbf{X}(s)=\mathbf{X}_s^{\mathbf{x},\mathbf{v},t}$, $\mathbf{V}(s)=\mathbf{V}_s^{\mathbf{x},\mathbf{v},t}$ and $\mathbf{N}(s)=\mathbf{N}_s^{\mathbf{x},\mathbf{v},\mathbf{n},t}$, $0\le s\le t$ are the adjoint Lagrangian processes defined as the solutions to

$$\begin{aligned}d\mathbf{X}(s)&=\mathbf{V}(s)ds,\\ d\mathbf{V}(s)&=\mathbf{a}(s,\mathbf{X}(s),\mathbf{V}(s))ds+\sqrt{C_0\bar{\varepsilon}(\mathbf{X}(s),s)}\,d\mathbf{W}(s),\\ \frac{dN_k}{ds}&=f_k(s,\mathbf{X},\mathbf{N}),\quad k=1,2\ldots,K\end{aligned}$$

with the terminal conditions

$$\mathbf{X}(t)=\mathbf{x},\quad \mathbf{V}(t)=\mathbf{v},\quad N_k(t)=n_k,\ k=1,\ldots,K.$$

The expectation $\mathbb{E}$ is taken over all backward Lagrangian trajectories. From (5.2) and (5.3) we find

$$\begin{aligned}I_h(\mathbf{x},t)=\int\limits_{\mathbf{R}^3}d\mathbf{v}\int d\mathbf{n}\,h(\mathbf{x},\mathbf{v},\mathbf{n},t)\\ \times\mathbb{E}p_E(\mathbf{V}_0^{\mathbf{x},\mathbf{v},t};\mathbf{X}_0^{\mathbf{x},\mathbf{v},t})Q_a(\mathbf{x},\mathbf{v},t)Q_f(\mathbf{x},\mathbf{v},\mathbf{n},t)\delta(\mathbf{N}_0^{\mathbf{x},\mathbf{v},\mathbf{n},t}-\mathbf{q}(\mathbf{X}_0^{\mathbf{x},\mathbf{v},t})),\end{aligned}$$

where

$$Q_a(\mathbf{x},\mathbf{v},t)=\exp\left\{-\int\limits_0^t\frac{\partial a_i}{\partial v_i}(s,\mathbf{X}_s^{\mathbf{x},\mathbf{v},t},\mathbf{V}_s^{\mathbf{x},\mathbf{v},t})ds\right\},$$

$$Q_f(\mathbf{x},\mathbf{v},\mathbf{n},t)=\exp\left\{-\int\limits_0^t\frac{\partial f_k}{\partial n_k}(s,\mathbf{X}_s^{\mathbf{x},\mathbf{v},t},\mathbf{N}_s^{\mathbf{x},\mathbf{v},\mathbf{n},t})ds\right\}.$$

Hence,

$$I_h(\mathbf{x},t) = \mathbf{E}\int\limits_{\mathbf{R}^3} d\mathbf{v} p_E(\mathbf{V}_0^{\mathbf{x},\mathbf{v},t};\mathbf{X}_0^{\mathbf{x},\mathbf{v},t}) Q_a(\mathbf{x},\mathbf{v},t) \\ \times \int d\mathbf{n}\, Q_f(\mathbf{x},\mathbf{v},\mathbf{n},t) h(\mathbf{x},\mathbf{v},\mathbf{n},t)\delta(\mathbf{N}_0^{\mathbf{x},\mathbf{v},\mathbf{n},t} - \mathbf{q}(\mathbf{X}_0^{\mathbf{x},\mathbf{v},t})). \tag{5.4}$$

To evaluate the last integral in (5.4) we use the following known formula. Let F be a function of $\mathbf{x} = (x_1,\ldots,x_m)$, and g be a vector-function $g(\mathbf{x}) = (g_1(\mathbf{x}),\ldots,g_m(\mathbf{x}))$, whose inverse g^{-1} exists, and let $\mathbf{b} = (b_1,\ldots,b_m)$ be a fixed vector. Then

$$\int F(\mathbf{x})\delta(g(\mathbf{x}) - \mathbf{b})\, d\mathbf{x} = \frac{F(\mathbf{x}_b)}{J(\mathbf{x}_b)}, \tag{5.5}$$

where $\mathbf{x}_b = g^{-1}(\mathbf{b})$, and

$$J(\mathbf{x}) = Det \left|\left| \frac{\partial g_i(\mathbf{x})}{\partial x_j} \right|\right|$$

is the Jacobian of the transformation $\mathbf{x} \to g(\mathbf{x})$. Applying (5.5), we can evaluate the last integral in (5.4). Indeed, the transformation $g : \mathbf{N} \to \mathbf{N}_0^{\mathbf{x},\mathbf{v},\mathbf{n},t}$ has the Jacobian $Q_f(\mathbf{x},\mathbf{v},\mathbf{n},t)$. Choosing $\mathbf{b} = \mathbf{q}(\mathbf{X}_0^{\mathbf{x},\mathbf{v},t})$ we find that $g^{-1}(\mathbf{b}) = \mathbf{N}(t;\mathbf{b})$ where $\mathbf{N}(s;\mathbf{b})$ is the solution to

$$\frac{d\mathbf{N}}{ds} = f(\mathbf{N}, \mathbf{X}_s^{\mathbf{x},\mathbf{v},t}, s), \quad \mathbf{N}(0;\mathbf{b}) = \mathbf{b}.$$

Thus we have

$$I_h(\mathbf{x},t) = \mathbf{E}\int\limits_{\mathbb{R}^3} d\mathbf{v} p_E(\mathbf{V}_0^{\mathbf{x},\mathbf{v},t};\mathbf{X}_0^{\mathbf{x},\mathbf{v},t}) Q_a(\mathbf{x},\mathbf{v},t) h(\mathbf{x},\mathbf{v},\mathbf{n}(t;\mathbf{q}(\mathbf{X}_0^{\mathbf{x},\mathbf{v},t})),t).$$

Now we can formulate the backward algorithm for solving the problem (5.1). Introduce a probability density function $r(\mathbf{V}) > 0$ in $\mathbb{R}^3$, and use the notation $\tilde{\mathbf{V}}$ for a sample from this density. We write for simplicity $\tilde{\mathbf{X}}_{t_0} = \mathbf{X}_{t_0}^{\mathbf{x},\tilde{\mathbf{V}},t}$ and $\tilde{\mathbf{V}}_{t_0} = \mathbf{V}_{t_0}^{\mathbf{x},\tilde{\mathbf{V}},t}$. We denote by $\tilde{\mathbf{N}}(s)$ the solution to

$$\frac{d\tilde{\mathbf{N}}}{ds} = f(\tilde{\mathbf{N}}, \tilde{\mathbf{X}}_s, s), \quad \tilde{\mathbf{N}}(0) = \mathbf{q}(\tilde{\mathbf{X}}_0).$$

The random estimator has the form:

$$\xi(\mathbf{x},\tilde{\mathbf{V}},t) = \frac{1}{r(\tilde{\mathbf{V}})} p_E(\tilde{\mathbf{V}}_0;\tilde{\mathbf{X}}_0)\, Q_a(\mathbf{x},\tilde{\mathbf{V}},t) h(\mathbf{x},\tilde{\mathbf{V}},\tilde{\mathbf{N}}(t),t),$$

hence,

$$I_h(\mathbf{x},t) = \mathbb{E}_{\tilde{\mathbf{V}}}\mathbb{E}\,\xi(\mathbf{x},\tilde{\mathbf{V}},t).$$

Here $\mathbb{E}_{\tilde{\mathbf{V}}}$ means averaging over the samples $\tilde{\mathbf{V}}$, and $\mathbf{E}$ is the averaging over the trajectories $\tilde{\mathbf{X}}_s, \tilde{\mathbf{V}}_s$, $0 \le s \le t$.

6 Numerical simulations

Numerical simulations are carried out for the following problem. A horizontally homogeneous, stationary, neutrally stratified surface layer is considered. The source starts to generate particles at the time $t = 0$. It is uniformly distributed over the plane at the height $z = z_s$. In this section we use the SI metric system of units. We calculate the mean concentartion and its vertical flux at a fixed point at the height $z = z_d$ by three methods: the direct Monte Carlo described in Sect.3.1, and two backward in time Monte Carlo algorithms presented in Sect.3.2 and in Appendix C: the adjoint algorithm based on the probabilistic representation, and the backward method due to Thomson [19]. Comparison of the cost of these three methods is given.

Since our problem is described by horizontally homogeneous parameters, it is governed by one-dimensional stochastic model (4.1), (4.2).

First, let us present the details of random estimators for the direct estimator of the type (3.2). In our case it takes the form:

$$\bar{c}(z_d, t) = Q\, \mathbf{E} \sum_{j=1}^{\nu_t(z_d)} \frac{1}{|W(\tau_j)|} \tag{6.1}$$

for the mean concentration, and

$$F(z_d, t) = Q\, \mathbf{E} \sum_{j=1}^{\nu_t(z_d)} \frac{W(\tau_j)}{|W(\tau_j)|} \tag{6.2}$$

for the vertical concentration flux. Here $(Z(\tau), W(\tau))$ is the solution to (4.2) with the initial condition $Z(0) = z_s$, $W(0) = w_0$ where w_0 is a random velocity distributed with the Eulerian gaussian pdf $p_E(w) = \exp\{-w^2/2\sigma_w^2\}/\sqrt{2\pi\sigma_w^2}$. The values τ_j are random times at which the process $Z(s)$ intersects the level $z = z_d$, and $\nu_t(z_d)$ is the total number of such events in the interval $0 \le s \le t$. The constant Q is the strength of the surface-area source.

The derivation of the estimator (6.1) can be obtained as folllows.

Note that

$$\begin{aligned}
\bar{c}(z_d, t) &= \int_{-\infty}^{\infty} dw \int_0^t dt_0 \int_0^{\infty} dz_0 \delta(z_0 - z_s) \int_{-\infty}^{\infty} dw_0 p_E(w_0) p_L(z_d, w, t; z_0, w_0, t_0) \\
&= \int_{-\infty}^{\infty} dw \int_0^t dt_0 \int_0^{\infty} dz_0 \delta(z_0 - z_s) \int_{-\infty}^{\infty} dw_0 p_E(w_0) \\
&\times \int_0^{\infty} dz \delta(z - z_d) p_L(z, w, \tau; z_0, w_0, t_0) = \mathbf{E} \int_0^t \delta(Z_\tau^{z_s, \tilde{w}_0} - z_d)\, d\tau.
\end{aligned}$$

Here $\tilde{w}_0$ is a random number distributed with $p_E(w_0)$, $Z_t^{z,w}$ is the solution to the system (4.2) with the initial deterministic condition $Z_0^{z,w} = z$, $W_0^{z,w} = w$. It remains to note that for arbitrary continuously differentiable function $Z(\tau)$

$$\int_0^t \delta(Z(\tau) - z)\, d\tau = \sum_{j=1}^{\nu_t(z)} \frac{1}{\left|\frac{dZ(\tau_j)}{d\tau}\right|},$$

where $\nu_t(z)$ is the number of intersections of the level z by the trajectory $Z(\tau)$ in the interval $0 \le \tau \le t$, and τ_j are the intersection times.

The random estimator of Thomson's backward algorithm used in [5] is constructed on the solutions to backward-time stochastic differential equation:

$$d\hat{Z}(t_0) = \hat{W}(t_0)dt_0, \quad d\hat{W}(t_0) = \frac{a}{\hat{Z}}\hat{W}(t_0)dt_0 + \frac{b}{\sqrt{\hat{Z}}}\,dB(t_0),$$

with terminal condition $\hat{Z}(t) = z_d$, $\hat{W}(t) = \hat{w}$ where $\hat{w}$ is a random number distributed with gaussian $p_E(w)$ given above. Here

$$a = \frac{C_0 u_*^3}{2\kappa\sigma_w^2}, \quad b = \Big(\frac{C_0 u_*^3}{\kappa}\Big)^{\frac{1}{2}}.$$

The random estimators read

$$\bar{c}(z_d, t) = Q\,\mathbb{E}\sum_{j=1}^{\nu_t(z_s)} \frac{1}{|\hat{W}(\tau_j)|}\ , \tag{6.3}$$

for the mean concentration, and

$$F(z_d, t) = Q\,\mathbb{E}\sum_{j=1}^{\nu_t(z_s)} \frac{\hat{W}(t)}{|\hat{W}(\tau_j)|}\ , \tag{6.4}$$

for the vertical concentration flux.

Here the values τ_j are random times at which the process $\hat{Z}(t_0)$ $(0 \le t_0 \le t)$ intersects the level $z = z_s$, and $\nu_t(z_s)$ is the total number of such events in the interval $0 \le t_0 \le t$.

Finally, let us consider the adjoint estimator based on probabilistic representation. The probabilistic representation (3.4) in our case (1D) reads

$$p(z, w, t) = \mathbb{E}_{z,w}\int_0^t \delta(\tilde{Z}(t_0) - z_s)p_E(\tilde{W}(t_0))\exp\left\{\int_{t_0}^t \frac{b\,ds}{\tilde{Z}(s)}\right\}dt_0, \tag{6.5}$$

where $\tilde{Z}(t_0) = Z_{t_0}^{z,w}, \tilde{W}(t_0)) = W_{t_0}^{z,w}$, $0 \le t_0 \le t$ is the adjoint trajectory defined by

$$d\tilde{Z}(t_0) = \tilde{W}(t_0)\,dt, \quad d\tilde{W}(t_0) = -\frac{a}{\tilde{Z}}\tilde{W}(t_0)dt_0 + \frac{b}{\sqrt{\tilde{Z}}}\,dB(t_0),$$

with terminal condition $\tilde{Z}(t) = z$, $\tilde{W}(t) = w$.

Now, substitute (6.5) in

$$\bar{c}(z_d, t) = \int_{-\infty}^{+\infty} p(z_d, w, t)\,dw\ .$$

This yields

$$\bar{c}(z_d, t) = \int_{-\infty}^{+\infty} dw\mathbb{E}_{z_d,w}\sum_{j=1}^{\tilde{\nu}_t(z_s)} \frac{p_E(\tilde{W}(\tau_j))}{|\tilde{W}(\tau_j)|}\exp\left\{\int_{\tau_j}^t \frac{b\,ds}{\tilde{Z}(s)}\right\}. \tag{6.6}$$

Here we used the relation

$$\int_0^t \delta(\tilde{Z}(t_0)-z_s)p_E(\tilde{W}(t_0))\exp\left\{\int_{t_0}^t \frac{b\,ds}{\tilde{Z}(s)}\right\}dt_0 = \sum_{j=1}^{\tilde{\nu}_t(z_s)} \frac{p_E(\tilde{W}(\tau_j))}{|\tilde{W}(\tau_j)|}\exp\left\{\int_{\tau_j}^t \frac{b\,ds}{\tilde{Z}(s)}\right\}\ , \quad (6.7)$$

where $\tilde{\nu}_{t(z_s)}$ is the number of intersections of the level $z=z_s$ by the trajectory $Z_{t_0}^{z_d,w}$, $0\le t_o\le t$, and $\tau_1,\dots,\tau_j,\dots$ are the intersection times.

The resulting estimator is

$$\bar{c}(z_d,t) = \mathbb{E}\left\{\frac{1}{r(\tilde{w})}\sum_{j=1}^{\tilde{\nu}_t(z_s)} \frac{p_E(W_{\tau_j}^{z_d,\tilde{w}})}{|W_{\tau_j}^{z_d,\tilde{w}}|}\exp\left\{\int_{\tau_j}^t \frac{b\,ds}{Z_\tau^{z_d,\tilde{w}}}\right\}\right\}, \quad (6.8)$$

where $r(w)$ is a pdf which is positive in $(-\infty,+\infty)$, and $\tilde{w}$ is a random number distributed with $r(w)$.

Analogous arguments lead to the random estimator for the vertical concentration flux:

$$F(z_d,t) = \mathbf{E}\left\{\frac{\tilde{w}}{r(\tilde{w})}\sum_{j=1}^{\tilde{\nu}_t(z_s)} \frac{p_E(W_{\tau_j}^{z_d,\tilde{w}})}{|W_{\tau_j}^{z_d,\tilde{w}}|}\exp\left\{\int_{\tau_j}^t \frac{b\,ds}{Z_\tau^{z_d,\tilde{w}}}\right\}\right\}. \quad (6.9)$$

In numerical calculations, one takes a cut-off in the integral over w in (6.6), and integrates from, say, $-A$ to A, A being sufficiently large; in our case we have chosen $A=5\sigma_w$. Further parameters in calculations are: $\sigma_w = 1.25\,u_*$, $u_*=0.4$, the function $\bar{\varepsilon}$ is defined in (4.1).

As to the penetrable boundary conditions, in calculations it cannot be satisfied strictly. In the numerical scheme it is convenient to follow the trajectories till some reflection height $z=z_r<z_0$ and then reflect them according to some reflection law. In calculations we found that beginning from $z_r<z_0/5$, the results are stable with respect to further decreasing of the reflection height z_r. The perfect reflection (symmetric to the plane $z=z_r$) was used.

It should be noted that usually (e.g., see [3]) one reflects the trajectories at the height $z=z_0$ which does not affect the calculations at large (compared to z_0) heights, but at height of several z_0 the error may be about 10-30 %.

In Table 1 we present the mean concentration and its vertical flux obtained by the direct (6.1), (6.2), the adjoint (6.8), (6.9), and the backward method (6.3), (6.4). The calculations are made for four time instances $t=T_L(z_s)$, $2T_L(z_s)$, $4T_L(z_s)$ and $8T_L(z_s)$, for $z_d=1$, $z_s=0.5$. The unit source strength uniformly distributed over the plane $z=z_s$ was taken. The Lagrangian time scale $T_L=T_L(z_s)$ is given by [16] $T_L(z_s) = 2\sigma_w^2/C_0\bar{\varepsilon}(z_s) = z_s/a = 0.39$. The error shown in the table is the statistical error measured as $3\times$ standard deviation$/\sqrt{\text{number of samples}}$, the *cost* means the computer time of a 233 MHz PC computer.

The results presented in the table show that in this special case of horizontally homogeneous problem the direct and backward methods have approximately equal cost and are both much more efficient than the adjoint method. It should be emphasized however that this is because our model problem is actually one-dimensional and the source is stationary. In general case of 3D problems with a source generating particles during a short period of time the backward algorithm is much more efficient.

Table 1. Comparison of different methods.

method		$t = T_L$	$t = 2T_L$	$t = 4T_L$	$t = 8T_L$
Direct	$\bar{c}$	$2.08e-3 \pm 1.95e-4$	$8.94e-2 \pm 3.90e-3$	0.467 ± 0.031	1.26 ± 0.11
	F	$2.71e-3 \pm 2.47e-4$	$6.48e-2 \pm 1.60e-3$	0.213 ± 0.006	0.4 ± 0.015
	cost	200 [sec]	200 [sec]	85 [sec]	60 [sec]
Adjoint	$\bar{c}$	$1.95e-3 \pm 1.40e-4$	$8.42e-2 \pm 3.70e-3$	0.471 ± 0.032	1.19 ± 0.15
	F	$2.51e-3 \pm 2.00e-4$	$6.10e-2 \pm 3.30e-3$	0.216 ± 0.022	0.34 ± 0.075
	cost	400 [sec]	1800 [sec]	2000 [sec]	2200 [sec]
Backward	$\bar{c}$	$1.95e-3 \pm 1.77e-4$	$9.03e-2 \pm 3.69e-3$	0.468 ± 0.017	1.21 ± 0.11
	F	$2.50e-3 \pm 2.37e-4$	$6.58e-2 \pm 3.35e-3$	0.205 ± 0.010	0.37 ± 0.06
	cost	180 [sec]	300 [sec]	300 [sec]	40 [sec]

As to the adjoint method, although our calculations show that it requires a lot of computer time, it has the following important advantages. The method allows to solve problems of transport of reacting species as described in Sect.5. Another advantage of the adjoint method is in treating the problems with boundary conditions. It should be noted that it is not evident how to extend the backward method described in Appendic C to the case of boundary value problems.

7 Conclusion

A generalized footprint problem is treated as a calculation of an integral over space, velocity and time of the space-velocity distribution of ensemble of particles in a turbulent flow. The Lagrangian stochastic description is used to solve this problem. As important particular cases, the mean concentration and its flux are analysed in details.

Three different algorithms are presented: (1) direct Monte Carlo, (2) adjoint Monte Carlo, and (3) backward Monte Carlo algorithms. The direct Monte Carlo algorithm is quite general but it is not efficient in estimation of local functions like, e.g, the concentration and its flux at a fixed point.

The adjoint method is also general and is especially convenient for evaluation of local functionals. The method is based on the well developed probabilistic representations for the boundary value problems. Therefore, it allows to solve problems with quite general boundary conditions. Unfortunately, the method requires a lot of computer time because the variance increases with time very fast.

The backward algorithm originally presented by Thomson is extended to more general case when the transport in the phase space is described by a general stochastic differential equation. This extension allows to treat problems with absorption of particles, which is of our current interest.

Appendix A. Flux representation

Here we derive the representation (2.2). By the definition, the instant concentration is

$$c(\mathbf{x},t)=\int\limits_0^t dt_0\int\limits_D d\mathbf{x}_0\,q(\mathbf{x}_0,t_0)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,t_0))+\int\limits_D d\mathbf{x}_0\,q_0(\mathbf{x}_0)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,0)).$$

From this,

$$F_i(\mathbf{x},t)=\langle u_i(\mathbf{x},t)c(\mathbf{x},t)\rangle=\int\limits_0^t dt_0\int\limits_D d\mathbf{x}_0\,q(\mathbf{x}_0,t_0)\langle u_i(\mathbf{x},t)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,t_0))\rangle$$

$$+\int\limits_D d\mathbf{x}_0\,q_0(\mathbf{x}_0)\langle u_i(\mathbf{x},t)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,0))\rangle. \qquad (A1)$$

Since

$$\begin{aligned}u_i(\mathbf{x},t)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,t_0)) &= u_i(\mathbf{X}(t;\mathbf{x}_0,t_0),t)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,t_0))\\ &= V_i(t;\mathbf{x}_0,t_0)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,t_0)),\end{aligned}$$

then

$$\langle u_i(\mathbf{x},t)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,t_0))\rangle=\langle V_i(t;\mathbf{x}_0,t_0)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,t_0))\rangle$$
$$=\int\limits_{\mathbf{R}^3}d\mathbf{V}\int\limits_D d\mathbf{X}\,V_i\delta(\mathbf{x}-\mathbf{X})p_L(\mathbf{X},\mathbf{V},t;\mathbf{x}_0,t_0)=\int\limits_{\mathbf{R}^3}V_ip_L(\mathbf{x},\mathbf{V},t;\mathbf{x}_0,t_0)\,d\mathbf{V}.$$

From this we get in view of (A1) the desired representation (2.2).

Appendix B. Probabilistic representation

Let us write down the probabilistic representation of the function $\theta(\mathbf{y},t)=\theta(y_1,\ldots,y_n,t)$, the solution to the following general parabolic equation

$$\frac{\partial\theta}{\partial t}+A_i(\mathbf{y},t)\frac{\partial\theta}{\partial y_i}+\frac{1}{2}B_{ij}(\mathbf{y},t)\frac{\partial^2\theta}{\partial y_i\partial y_j}+\beta(\mathbf{y},t)\theta+f(\mathbf{y},t)=0,\qquad t\in[0,T),$$

with the terminal condition

$$\theta(\mathbf{y},t)|_{t=T}=f_0(\mathbf{y}).$$

The probabilistic representation to this problem has the form [6]:

$$\theta(\mathbf{y},t)=\mathbf{E}_{(\mathbf{y},t)}\left\{\int\limits_t^T f(\mathbf{Y}_s^{\mathbf{y},t},s)\exp\Big(\int\limits_t^s\beta(\mathbf{Y}_\tau^{\mathbf{y},t},\tau)d\tau\Big)ds+f_0(\mathbf{Y}_T^{\mathbf{y},t})\exp\Big(\int\limits_t^T\beta(\mathbf{Y}_\tau^{\mathbf{y},t},\tau)d\tau\Big)\right\}, \qquad (B1)$$

where $\mathbf{Y}_s^{\mathbf{y},t} \equiv \mathbf{Y}(s)$, $s \geq t$ solves the problem

$$dY_i(s) = A_i(\mathbf{Y}(s), s)ds + \sigma_{ij}(\mathbf{Y}(s), s)dW_j(s),\ s > t,\ \ \mathbf{Y}(s)|_{s=t} = \mathbf{y}. \qquad (B2)$$

Here $\sigma_{ik}\sigma_{jk} = B_{ij}$. In (B1), $\mathbb{E}_{(\mathbf{y},t)}$ stands for the expectation taken over all trajectories (solutions to (B2)) starting from $\mathbf{y}$ at time t.

Note that the solution to the equation

$$\frac{\partial\theta}{\partial t} + A_i(\mathbf{y},t)\frac{\partial\theta}{\partial y_i} + \beta(\mathbf{y},t)\theta = \frac{1}{2}B_{ij}(\mathbf{y},t)\frac{\partial^2\theta}{\partial y_i \partial y_j} + f(\mathbf{y},t), \qquad t \in [0,T),$$

satisfying $\theta(y,0) = f_0(y)$, has the probabilistic representation:

$$\begin{aligned}\theta(\mathbf{y},t) \;=\; & \mathbf{E}_{(\mathbf{y},t)}\left\{\int_0^t f(\mathbf{X}_{t_0}^{\mathbf{y},t}, t_0)\exp\Big(-\int_{t_0}^t \beta(\mathbf{X}_{t_0'}^{\mathbf{y},t}, t_0')dt_0'\Big)dt_0\right. \\ & \left. +\ f_0(\mathbf{X}_0^{\mathbf{y},t})\exp\Big(-\int_0^t \beta(\mathbf{X}_{t_0}^{\mathbf{y},t}, t_0)dt_0\Big)\right\},\end{aligned}$$

where $\mathbf{X}_{t_0}^{\mathbf{y},t} \equiv \mathbf{X}(t_0)$, $0 \leq t_0 \leq t$ solves the problem

$$\begin{aligned} dX_i(t_0) \;&=\; A_i(\mathbf{X}(t_0), t_0)dt_0 + \sigma_{ij}(\mathbf{X}(t_0), t_0)dW_j(t_0), \quad 0 \leq t_0 \leq t, \\ \mathbf{X}(t_0)|_{t_0=t} \;&=\; \mathbf{y}.\end{aligned}$$

Appendix C. Forward and Backward trajectory estimators

In this Appendix we treat the evaluation of the integral:

$$I_{h,q} = \int_D d\mathbf{y}\int_0^T dt\int_D d\mathbf{y}_0\int_0^t dt_0\, h(\mathbf{y},t)q(\mathbf{y}_0,t_0)p^f(\mathbf{y},t;\mathbf{y}_0,t_0), \qquad (C1)$$

where D is a domain in $\mathbb{R}^n$, $T > 0$, h and q are functions defined in $D \times [0,T]$, and $p^f(\mathbf{y},t;\mathbf{y}_0,t_0) = \langle\delta(\mathbf{y} - \mathbf{Y}_t^{\mathbf{y}_0,t_0})\rangle$ is the transition density of the n-dimensional diffusion process $\mathbf{Y}_t^{\mathbf{y}_0,t_0}$, the solution to

$$dY_i(t) = A_i(\mathbf{Y}(t),t)dt + \sigma_{ij}(\mathbf{Y}(t),t)dW_j(t),\ t > t_0,\ \ \mathbf{Y}(t)|_{t=t_0} = \mathbf{y}_0. \qquad (C2)$$

We assume that the boundary of D is impenetrable, i.e., the trajectories determined by (C2) do not reach the boundary. The Direct Monte Carlo estimator for evaluating the integral (C1) is straightforward:

$$\begin{aligned} I_{h,q} \;&=\; \int_D d\mathbf{y}_0\int_0^T dt_0\int_D d\mathbf{y}\int_{t_0}^T dt\, h(\mathbf{y},t)q(\mathbf{y}_0,t_0)p^f(\mathbf{y},t;\mathbf{y}_0,t_0) \\ &=\; \mathbb{E}\Big\{\frac{q(\tilde{\mathbf{y}}_0,\tilde{t}_0)}{p_0(\tilde{\mathbf{y}}_0,\tilde{t}_0)}\int_{\tilde{t}_0}^T h(\mathbf{Y}_t^{\tilde{\mathbf{y}}_0,\tilde{t}_0},t)\,dt\Big\}.\end{aligned}$$

Here $p_0(\mathbf{y}_0, t_0)$ is an arbitrary pdf in $D \times [0,T]$ consistent with the function $q(\mathbf{y}_0, t_0)$ in the sense that $p_0(\mathbf{y}_0, t_0) > 0$ if $q_0(\mathbf{y}_0, t_0) \neq 0$, and the expectation is taken over all sample points $(\tilde{\mathbf{y}}_0, \tilde{t}_0)$ and sample trajectories $\mathbf{Y}_t^{\tilde{\mathbf{y}}_0, \tilde{t}_0}$, $\tilde{t}_0 \leq t \leq T$; the random points $\tilde{\mathbf{y}}_0, \tilde{t}_0$ are distributed with $p_0(\mathbf{y}_0, t_0)$.

A backward estimator can be obtained by a generalization of Thomson's approach [19]. Assume that we have a positive function $\rho(\mathbf{y}, t)$ defined on $D \times [0,T]$ as a solution to the equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial y_i}(A_i \rho) = \frac{1}{2} \frac{\partial^2 (B_{ij} \rho)}{\partial y_i \partial y_j}, \tag{C3}$$

where $\sigma_{ik}\sigma_{jk} = B_{ij}$. Let $p^b(\mathbf{y}_0, t_0; \mathbf{y}, t) = \langle \delta(\mathbf{y}_0 - \mathbf{Z}_{t_0}^{\mathbf{y},t}) \rangle$ be the transition density of the diffusion process $Z_{t_0}^{\mathbf{y},t}$, $0 \leq t_0 \leq t$ which is defined by

$$dZ_i = A_i^*(\mathbf{Z}, t_0)\, dt_0 + B_{ij}(\mathbf{Z}, t_0), t_0)\, dW_j(t_0), \quad t_0 < t, \quad \mathbf{Z}(t) = \mathbf{y}. \tag{C4}$$

Here

$$A_i^*(\mathbf{y}, t) = A_i(\mathbf{y}, t) - \frac{1}{\rho(\mathbf{y}, t)} \frac{\partial}{\partial y_j}(B_{ij}(\mathbf{y}, t)\rho(\mathbf{y}, t)).$$

We assume again, that the solutions to (C4) do never reach the boundary of D. Then the following relation is true:

$$\rho(\mathbf{y}_0, t_0) p^f(\mathbf{y}, t; \mathbf{y}_0, t_0) = \rho(\mathbf{y}, t) p^b(\mathbf{y}_0, t_0; \mathbf{y}, t). \tag{C5}$$

To prove it, we first remark that the function p^b and

$$F(\mathbf{y}_0, t_0; \mathbf{y}, t) = \frac{\rho(\mathbf{y}_0, t_0)}{\rho(\mathbf{y}, t)} p^f(\mathbf{y}, t; \mathbf{y}_0, t_0)$$

satisfy the equations

$$\mathcal{L}_{\mathbf{y}_0, t_0} F = 0, \quad \mathcal{L}_{\mathbf{y}_0, t_0} p^b = 0$$

where the operator $\mathcal{L}_{\mathbf{y}_0, t_0}$ acts on a function $g(\mathbf{y}_0, t_0)$ as follows:

$$\mathcal{L}_{\mathbf{y}_0, t_0} g = \frac{\partial g}{\partial t} + \frac{\partial}{\partial y_{0i}}(A_i^* g) + \frac{1}{2} \frac{\partial^2 (B_{ij} g)}{\partial y_{0i} \partial y_{0j}}.$$

Since the values of the functions F and p^b at $t_0 = t$ coincide:

$$p^b(\mathbf{y}_0, t; \mathbf{y}, t) = F(\mathbf{y}_0, t; \mathbf{y}, t) = \langle \delta(\mathbf{y} - \mathbf{y}_0) \rangle, \tag{C6}$$

we conclude that $F \equiv p^b$, provided that the equation $\mathcal{L}_{\mathbf{y}_0, t_0} g = 0$ with initial condition $g(t, \mathbf{y}_0) = \delta(\mathbf{y}_0 - \mathbf{y})$ has a unique solution. This implies that (C5) is true. Now we note that $\mathcal{L}_{\mathbf{y}_0, t_0} p^b = 0$ is true indeed, since it is the first Kolmogorov equation for p^b. The equality $\mathcal{L}_{\mathbf{y}_0, t_0} F = 0$ then follows from (C3), the inverse Kolmogorov's equation

$$\frac{\partial p^f(\mathbf{y}, t; \mathbf{y}_0, t_0)}{\partial t_0} + A_i(\mathbf{y}_0, t_0) \frac{\partial p^f}{\partial y_{0i}} + \frac{1}{2} B_{ij}(\mathbf{y}_0, t_0) \frac{\partial^2 p^f}{\partial y_{0i} \partial y_{0j}} = 0\ ,$$

and the expression for $A_i^*(\mathbf{y}_0, t_0)$ through A_i and B_{ij} given above.

Now, we present the backward Monte Carlo algorithm based on the property (C5). We proceed as follows: substitute the expression for p^f from (C5) into (C1), then

$$I_{h,q} = \int\limits_D d\mathbf{y} \int\limits_0^T dt \int\limits_D d\mathbf{y}_0 \int\limits_0^t dt_0 h(\mathbf{y},t) q(\mathbf{y}_0,t_0) \frac{\rho(\mathbf{y},t)}{\rho(\mathbf{y}_0,t_0)} p^b(\mathbf{y}_0,t_0;\mathbf{y},t). \qquad (C7)$$

Let $r(\mathbf{y},t)$ be a probability density in $D\times[0,T]$ consistent with $h\rho$, i.e., $r>0$ if $h\rho\neq 0$. Then from (C7) we get

$$I_{h,q} = \mathbb{E}\left\{ \frac{h(\tilde{\mathbf{y}},\tilde{t})\rho(\tilde{\mathbf{y}},\tilde{t})}{r(\tilde{\mathbf{y}},\tilde{t})} \int\limits_0^{\tilde{t}} \frac{q(\mathbf{Z}_{t_0}^{\tilde{\mathbf{y}},\tilde{t}},t_0)}{\rho(\mathbf{Z}_{t_0}^{\tilde{\mathbf{y}},\tilde{t}},t_0)}\, dt_0 \right\}. \qquad (C8)$$

Here the expectation is taken over the random points $(\tilde{\mathbf{y}},\tilde{t})$ distributed in $D\times[0,T]$ with density $r(\mathbf{y},t)$, and backward trajectories $Z_{t_0}^{\tilde{\mathbf{y}},\tilde{t}}$, $0\le t_0\le\tilde{t}$.

Another backward trajectory estimator which generalizes the estimator presented in Sect.3.2 can be obtained as follows. Let

$$\theta(\mathbf{y},t) = \int\limits_D d\mathbf{y}_0 \int\limits_0^t dt_0 q(\mathbf{y}_0,t_0) p^f(\mathbf{y},t;\mathbf{y}_0,t_0).$$

This function solves the problem

$$\frac{\partial\theta}{\partial t} + \frac{\partial(A_i\theta)}{\partial y_i} = \frac{1}{2}\frac{\partial^2(B_{ij}\theta)}{\partial y_i \partial y_j} + q(\mathbf{y},t), \quad \theta(\mathbf{y},0)=0. \qquad (C9)$$

From the probabilistic representation given in Appendix B we get

$$\theta(\mathbf{y},t) = \mathbb{E}\left\{ \int\limits_0^t q(\mathbf{X}_{t_0}^{\mathbf{y},t},t_0) \exp\Big\{ -\int\limits_{t_0}^t R(\mathbf{X}_s^{\mathbf{y},t},s)\, ds\Big\} dt_0 \right\},$$

where the expectation is taken over the backward trajectories $\mathbf{X}_{t_0}^{\mathbf{y},t}$, $0\le t_0\le t$ determined from

$$dX_i(t_0) = \hat{A}_i(\mathbf{X}(t_0),t_0)\, dt_0 + B_{ij}(\mathbf{X}(t_0),t_0)\, dW_j(t_0), \quad t_0\le t, \quad \mathbf{X}(t)=\mathbf{y}.$$

Here

$$\hat{A}_i(\mathbf{x},t) = A_i(\mathbf{x},t) + 2\frac{\partial B_{ik}(\mathbf{x},t)}{\partial x_k},$$

and

$$R(\mathbf{x},t) = \frac{\partial A_i(\mathbf{x},t)}{\partial x_i} + \frac{\partial^2 B_{ij}(\mathbf{x},t)}{\partial x_i \partial x_j}.$$

Thus we have

$$\begin{aligned} I_{h,q} &= \int\limits_D d\mathbf{y} \int\limits_0^T dt\; h(\mathbf{y},t)\theta(\mathbf{y},t) \\ &= \int\limits_D d\mathbf{y} \int\limits_0^T dt\; h(\mathbf{y},t) \mathbb{E}_{\mathbf{X}} \left\{ \int\limits_0^t q(\mathbf{X}_{t_0}^{\mathbf{y},t},t_0) \exp\Big\{ -\int\limits_{t_0}^t R(\mathbf{X}_s^{\mathbf{y},t},s)\, ds\Big\} dt_0 \right\}. \end{aligned}$$

Here $\mathbf{E}_{\mathbf{X}}$ stands for averaging over trajectories $\mathbf{X}_{t_0}^{\mathbf{y},t}$, $0 \le t_0 \le t$. From this we find:

$$I_{h,q} = \mathbf{E}\left(\frac{h(\tilde{\mathbf{y}},\tilde{t})}{r(\tilde{\mathbf{y}},\tilde{t})}\left\{\int_0^{\tilde{t}} q(\mathbf{X}_{t_0}^{\tilde{\mathbf{y}},\tilde{t}},t_0)\exp\Big\{-\int_{t_0}^{\tilde{t}} R(\mathbf{X}_s^{\tilde{\mathbf{y}},\tilde{t}},s)\,ds\Big\}dt_0\right\}\right), \qquad (C10)$$

where $\tilde{\mathbf{y}},\tilde{t}$ is a random point distributed in $D\times[0,T]$ with density $r(\mathbf{y},t)$ consistent with $h(\mathbf{y},t)$. The notation $\mathbf{E}$ means the expectation over the random points $\tilde{\mathbf{y}},\tilde{t}$ and trajectories $\mathbf{X}_{t_0}^{\tilde{\mathbf{y}},\tilde{t}}$, $0\le t_0\le\tilde{t}$.

Remark. In this appendix, we assumed that the boundary is impenetrable. However in practice one treats also situations where a part of boundary (say, the upper bound of a layer) can be reached by the Lagrangian trajectories. In this case boundary conditions should be given. For instance, an absorption, reflection or other behaviour at the boundary can be considered. For the direct algorithm this can be taken into account by simulating the relevant behaviour of the trajectories of (C2) at the boundary (e.g., the trajectories are absorbing at the absorbing boundary, reflecting at the reflection boundary, etc.). In the backward algorihm based on (C5) the situation is more complicated. Indeed, it is not clear how to arrange the behaviour of trajectories, the solutions to (C4), to guarantee that (C5) is fulfilled. Note that in the approach based on (C10) there is a need in the generalization of probabilistic representation of the solution to (C9) with the relevant boundary conditions. This can be done on the basis of the well known probabilistic representations [6].

References

[1] N.L. Bysova, E.K. Garger and V.N. Ivanov. Experimental studies of atmospheric diffusion and calculation of pollutant dispersion. Gidrometeoizdat., L., 1991. (in Russian).

[2] I.T. Drummond, S. Duane S. and R.R. Horgan. Scalar diffusion in simulated helical turbulence with molecular diffusivity. *J. Fluid Mech.*, **138**, 75-91 (1984).

[3] T.K. Flesch. The footprint for flux measurements, from backward Lagrangian stochastic models. *Boundary-Layer Meteorology*, **78**, 399-404 (1996).

[4] T.K. Flesch and J.D. Wilson. A two-dimensional trajectory-simulation model for non-gaussian, inhomogeneous turbulence within plant canopies. *Boundary-Layer Meteorology*, **61**, 349-374 (1992).

[5] T.K. Flesch and J.D. Wilson. Backward-time Lagrangian stochastic dispersion models and their application to estimate gaseous emissions. *Journal of Applied Meteorology*, **34**, 1320-1332 (1995).

[6] M.I. Freidlin and A.D. Wentzell. *Random Perturbations of Dynamical Systems.* Springer-Verlag, New York - Berlin, 1983.

[7] J.C.H. Fung, J.C.R. Hunt, N.A. Malik and R.J. Perkins. Cinematic simulation of homogeneous turbulence by unsteady random Fourier modes. *J. Fluid Mech.*, **236**, 281-318 (1992).

[8] R.H. Kraichnan. Diffusion by a random velocity field. *Phys. Fluids*, **9**, 1728-1752 (1970).

[9] O.A. Kurbanmuradov. A new Lagrangian model of two-particle relative turbulent dispersion. *Monte Carlo Methods and Applications*, **1** (1995), N2, 83–100.

[10] A.K. Luhar, R.E. Britter. A random walk model for dispersion in inhomogeneous turbulence in a convective boundary layer. *Atmospheric Environment*, **21** (1989), N9, 1911-1924.

[11] A.S. Monin and A.M. Yaglom. *Statistical Fluid Mechanics.* Vol. **2** M.I.T. Press, Cambridge, Massachusets, 1975.

[12] E.A. Novikov. A relation between the Lagrangian and Eulerian description of turbulence. *Appl. Math. Mech.*, **33**, No.5, 887–888 (1969), (in Russian).

[13] K.K. Sabelfeld. *Monte Carlo Methods in Boundary Value Problems.* Springer-Verlag, Heidelberg – New York – Berlin, 1991.

[14] K.K. Sabelfeld and O.A. Kurbanmuradov. Numerical statistical model of classical incompressible isotropic turbulence. *Sov. Journal on Numer. Analysis and Math. Modelling*, **5**, No.3, 251-263 (1990).

[15] K.K. Sabelfeld and O.A. Kurbanmuradov. One-particle stochastic Lagrangian model for turbulent dispersion in horizontally homogeneous turbulence. *Monte Carlo Methods and Applications*, **4** (1998), N2, 127–140.

[16] B.L. Sawford. Lagrangian statistical simulation of concentration mean and fluctuation fields *J. Clim. Appl. Met.*, **24**, 1152-1166 (1985).

[17] B.L. Sawford and F.M. Guest. Uniqueness and universality of Lagrangian stochastic models of turbulent dispersion. *Proceed. AMS 8th Symp. on Turbulence and Diffusion.* San Diego, pp.96-99 (1988).

[18] H.P. Schmid. Source areas for scalar and scalar fluxes. *Boundary-Layer Meteorology*, **67**, 293-318 (1994).

[19] D.J. Thomson. Criteria for the selection of stochastic models of particle trajectories in turbulent flows. *J. Fluid. Mech.*, **180**, 529–556 (1987).

[20] C. Turfus and J.C.R. Hunt. A stochastic analysis of the displacements of fluid elements in inhomogeneous turbulence using Kraichnan's method of random modes. In *Advances in Turbulence* (ed. G. Comte-Bellot and J. Mathieu), Springer-Verlag, Berlin, 191-203 (1987).

[21] J.D. Wilson and B.L. Sawford. Revew of Lagrangian stochastic models for trajectories in the turbulent atmosphere. *Boundary Layer Met.*, **78**, 191-210 (1996).