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Evaluation of Mean Concentration and Fluxes in Turbulent Flows by Lagrangian Stochastic Models

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Abstract

Forward and backward stochastic Lagrangian trajectory simulation methods for calculation of the mean concentration of scalars and their fluxes for sources arbitrarily distributed in space and time are constructed and justified. Generally, absorption of scalars by medium is taken into account. A special case of the source structure, when the scalar is generated by a plane source, say, located close to the ground, is treated. This practically interesting particular case is known in the literature as the *footprint problem.*

1 Introduction

The turbulent dispersion of particles in the framework of statistical fluid mechanics is described as particles' transport in random velocity field (e.g., [17]). In particular, the concentration of scalars and their fluxes are random fields. There are mainly two different approaches for calculation of the mean values of these fields: conventional deterministic methods based on the semiempirical turbulent diffusion equation and closure assumptions (e.g., see [6], [18], [26]), and stochastic approach which utilizes trajectory simulations (e.g., see [5], [8], [11], [21] [28], [29], [32]).

The deterministic approach directly deals with the equation governing the mean concentration, and relies on the Bousinesque hypothesis whose applicability is restricted (e.g., see [1], [19]). For instance, this hypothesis cannot be true if the concentration is calculated close to the sources [1], [17]. More generally, the high order closure methods are developed, but different closure hypothesis also should be made (see, e.g. [7], [17]).

Stochastic approach based on modelling of stochastic Lagrangian trajectories in principle does not require any closure hypotheses. Two main issues in this approach are (i) development of adequate Lagrangian stochastic models governed by generalized Langevin-type equations, and (ii) construction of Monte Carlo random estimators for evaluation of desired statistical characteristics (for instance, the mean concentration, the mean height of a cloud of particles, etc.).

It should be noted that in the Monte Carlo methods, when using the random estimators, the results are obtained with statistical errors. Remind that a random variable ξ is said to be a Monte Carlo estimator for a quantity a if the mathematical expectation of ξ is equal to a: $\mathbf{E}\xi = a$. If $\xi_1, \xi_2, ...\xi_N$ are N independent samples of the random variable ξ then the average $S_N = \frac{1}{N}\sum_{i=1}^{N}\xi_i$ tends to a almost sure (i.e., with probability one) as N tends to infinity, and the error in using S_N to approximate $a = \mathbf{E}\xi$ (for sufficiently large N) is proportional to the standard deviation of ξ. As N increases, this statistical error decreases as $N^{-1/2}$. The well known "law of three sigmas" gives the rate of convergence: $\mathbf{P}(|S_N - a| < 3\sigma_\xi/\sqrt{N}) \approx 0.997$. Here $\sigma_\xi = (\mathbf{E}\xi^2 - \mathbf{E}^2\xi)^{1/2}$ is the standard deviation of ξ.

The larger N, the closer the distribution of S_N to the Gaussian one, and the better this approximation.

The issue (i) attracts attention in many recent publications (e.g., see [12], [20], [23], [31], [32]). In this paper we concentrate on the issue (ii). It should be noted that this field is not well developed, and we can give only few references [4], [13], [24], [28].

In this paper we treat simulation methods based on the forward and backward Lagrangian trajectories. The general principle is quite clear: one uses the backward trajectories originating at the detector, if it is a point detector in space (or the detector occupies a small volume); the forward trajectories are used if the detector is quite extended in space.

The paper is organized as follows. In Section 2 one relates the calculation of the mean concentration and its flux with the averages over Lagrangian trajectories governed by generalized Langevin-type equations. The forward and backward estimators are presented in Section 3. Applications of these estimators to the footprint problem are given in Section 4. Some technical details are included in Appendices A-C.

2 Formulation of the problem

Let us assume that a passive but generally non-conservative scalar is dispersed by a turbulent velocity field $\mathbf{u}(\mathbf{x},t)$ in the half-space $D = \{\mathbf{x} = (x_1, x_2, x_3) : \; x_3 \geq 0\}$, for example in the surface layer of the atmosphere. Throughout this paper the following notation of spatial and velocity co-ordinates is used: $\mathbf{x} = (x_1, x_2, x_3) = (x, y, z)$ and $\mathbf{u} = (u_1, u_2, u_3) = (u, v, w)$; and analogously $\mathbf{X} = (X_1, X_2, X_3) = (X, Y, Z)$ and $\mathbf{V} = (V_1, V_2, V_3) = (U, V, W)$ for the Lagrangian co-ordinates.

The passive scalar is assumed to be uninertial, i.e., it follows the streamlines of the flow.

The evolution of scalar concentration field from a source of intensity $q(\mathbf{x},t)$ (the amount of emitted scalar per unit volume in a unit time interval at the phase point $(\mathbf{x},t)$) is controlled by the turbulent transport and absorption by a medium:

$$\frac{\partial c(\mathbf{x},t)}{\partial t} + u_i(\mathbf{x},t)\frac{\partial c}{\partial x_i} + \gamma(\mathbf{x},t)c(\mathbf{x},t) = q(\mathbf{x},t)\ , t>0; \quad c(\mathbf{x},0) = q_0(\mathbf{x})\ ,$$

where $\gamma(\mathbf{x},t)$ ($\gamma \geq 0$) denotes the coefficient of absorption, the initial spatial distribution of concentration is given by $q_0(\mathbf{x})$, and the molecular diffusion is neglected. Here and in what follows the summation convention is assumed over repeated indices.

The turbulent velocity field $\mathbf{u}(\mathbf{x},t)$ is considered to be incompressible three-dimensional (3D) random field. Accordingly, the concentration $c(\mathbf{x},t)$ is also a scalar random field. We consider the simplest statistical characteristics of this field, the mean concentration $\langle c(\mathbf{x},t)\rangle$, the mean flux of scalar concentration $\langle u_i(\mathbf{x},t)c(\mathbf{x},t)\rangle$ and spatial-temporal average of these statistical characteristics. Here and below the angle brackets denote the average over samples of turbulent velocity fluctuations.

The above-mentioned means are calculated by simulation of Lagrangian trajectories $\mathbf{X}(t) = \mathbf{X}(t;\mathbf{x}_0,t_0)$, $t \geq t_0$, determined by

$$\frac{dX_i(t)}{dt} = u_i(\mathbf{X}(t),t) = V_i(t), \quad \mathbf{X}(t_0) = \mathbf{x}_0\ ,$$

where $\mathbf{V}(t) = \mathbf{V}(t; \mathbf{x}_0, t_0)$ is the Lagrangian velocity.

The instantaneous concentration can be expressed as (see Appendix A)

$$\begin{aligned} c(\mathbf{x}, t) = & \int_0^t dt_0 \int_D d\mathbf{x}_0\, \mu(t; \mathbf{x}_0, t_0) q(\mathbf{x}_0, t_0) \delta(\mathbf{x} - \mathbf{X}(t; \mathbf{x}_0, t_0)) \\ & + \int_D d\mathbf{x}_0\, \mu(t; \mathbf{x}_0, 0) q_0(\mathbf{x}_0) \delta(\mathbf{x} - \mathbf{X}(t; \mathbf{x}_0, 0)), \end{aligned} \qquad (1)$$

where $\delta(\cdot)$ is the Dirac delta function, and $\mu(t) = \mu(t; \mathbf{x}_0, t_0)$ is defined by

$$\frac{d\mu(t)}{dt} + \gamma(\mathbf{X}(t; \mathbf{x}_0, t_0), t)\mu(t) = 0\,, \quad \mu(t_0) = 1\,. \qquad (2)$$

The expression for instantaneous concentration can be rewritten as

$$\begin{aligned} c(\mathbf{x}, t) = & \int_{\mathbb{R}^3} d\mathbf{u} \int_0^\infty d\mu \int_0^t dt_0 \int_D d\mathbf{x}_0\, \mu\, Q(\mathbf{x}_0, t_0) \\ & \times \delta(\mathbf{x} - \mathbf{X}(t; \mathbf{x}_0, t_0)) \delta(\mathbf{u} - \mathbf{V}(t; \mathbf{x}_0, t_0)) \delta(\mu - \mu(t; \mathbf{x}_0, t_0))\,, \end{aligned}$$

where $Q(\mathbf{x}_0, t_0) = q(\mathbf{x}_0, t_0) + q_0(\mathbf{x}_0)\delta(t_0)$. Averaging the last equation yields the mean concentration

$$\langle c(\mathbf{x}, t) \rangle = \int_{\mathbb{R}^3} d\mathbf{u} \int_0^\infty d\mu \int_0^t dt_0 \int_D d\mathbf{x}_0\, \mu\, Q(\mathbf{x}_0, t_0) p_L(\mathbf{x}, \mathbf{u}, \mu, t; \mathbf{x}_0, t_0)\,, \qquad (3)$$

where

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

is the joint probability density function (pdf) of Lagrangian characteristics $\mathbf{X}(t; \mathbf{x}_0, t_0)$, $\mathbf{V}(t; \mathbf{x}_0, t_0)$, and $\mu(t; \mathbf{x}_0, t_0)$.

Analogously, the mean flux of concentration can be represented as

$$\langle u_i(\mathbf{x}, t) c(\mathbf{x}, t) \rangle = \int_{\mathbb{R}^3} d\mathbf{u} \int_0^\infty d\mu \int_0^t dt_0 \int_D d\mathbf{x}_0\, u_i \mu Q(\mathbf{x}_0, t_0) p_L(\mathbf{x}, \mathbf{u}, \mu, t; \mathbf{x}_0, t_0)\,, i = 1, 2, 3. \quad (4)$$

For convenience, the mean characteristics (3) and (4) will be written in the general form

$$< g(\mathbf{u}(\mathbf{x}, t)) c(\mathbf{x}, t) >= \int_{\mathbb{R}^3} d\mathbf{u} \int_0^\infty d\mu \int_0^t dt_0 \int_D d\mathbf{x}_0\, g(\mathbf{u}) \mu\, Q(\mathbf{x}_0, t_0) p_L(\mathbf{x}, \mathbf{u}, \mu, t; \mathbf{x}_0, t_0)\,, \quad (5)$$

where $g(\mathbf{u})$ equals 1 and u_i for the mean concentration and fluxes, respectively.

Our problem now can be formulated as follows: it is necessary to represent the integral (5) as an expectation of a random estimator defined on Lagrangian trajectories. But since the exact form of $p_L(\mathbf{x}, \mathbf{u}, \mu, t; \mathbf{x}_0, t_0)$ is not known, we have to use some approximation, usually taken as a pdf of the solution to the following generalized Langevin-type equation (e.g., see [28]):

$$\begin{aligned} d\mathbf{X}(t) &= \mathbf{V}(t)dt, \\ d\mathbf{V}(t) &= \mathbf{a}(t,\mathbf{X}(t),\mathbf{V}(t))dt + \sqrt{C_0\bar{\varepsilon}(\mathbf{X}(t),t)}\, d\mathbf{W}(t), \end{aligned} \tag{6}$$

where C_0 is the universal Kolmogorov constant ($C_0 \approx 4 \div 6$), $\bar{\varepsilon}(\mathbf{x},t)$ is the mean dissipation rate of the kinetic energy of turbulence, and $\mathbf{W}(t) = (W_1(t), W_2(t), W_3(t))$ is the standard 3D Wiener process. The function $\mathbf{a}$ is to be specified in each specific situation (e.g., [3], [15], [28], [32]). We mention only that in all these models Thomson's well-mixed condition should be satisfied [28].

We will deal in this paper with two different types of random estimators, namely, with forward estimators, which are defined on forward Lagrangian trajectories which emanate from the source and move toward the detector, and with backward estimators which are defined on backward trajectories starting at the detector and moving toward the source.

More exactly, the solution to (6) with the initial conditions

$$\mathbf{X}(t_0) = \mathbf{x}_0, \quad \mathbf{V}(t_0) = \mathbf{u}_0$$

is called *forward Lagrangian trajectory*. We denote it by $\mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$ and $\mathbf{V}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$. Then the true Lagrangian trajectory $\mathbf{X}(t;\mathbf{x}_0,t_0)$, $\mathbf{V}(t;\mathbf{x}_0,t_0)$ can be approximated by the model trajectory $\mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$ and $\mathbf{V}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$ with the random initial velocity $\mathbf{u}_0$ chosen according to the Eulerian pdf p_E which is defined by $p_E(\mathbf{u};\mathbf{x}_0,t_0) = \langle \delta(\mathbf{u} - \mathbf{u}(\mathbf{x}_0,t_0))\rangle$.

Let $p_L(\mathbf{x},\mathbf{u},\mu,t;\mathbf{x}_0,\mathbf{u}_0,t_0)$ be the conditional pdf under the condition that $\mathbf{V}(t;\mathbf{x}_0,t_0) = u_0$:

$$\begin{aligned} &p_L(\mathbf{x},\mathbf{u},\mu,t;\mathbf{x}_0,\mathbf{u}_0,t_0) \\ &\quad = \langle \delta(\mathbf{x} - \mathbf{X}(t;\mathbf{x}_0,t_0))\delta(\mathbf{u} - \mathbf{V}(t;\mathbf{x}_0,t_0))\delta(\mu - \mu(t;\mathbf{x}_0,t_0)) |\, \mathbf{V}(t;\mathbf{x}_0,t_0) = u_0\rangle. \end{aligned}$$

By the theorem on conditional probability we get

$$p_L(\mathbf{x},\mathbf{u},\mu,t;\mathbf{x}_0,t_0) = \int\limits_{\mathbb{R}^3} d\mathbf{u}_0\, p_E(\mathbf{u}_0;\mathbf{x}_0,t_0) p_L(\mathbf{x},\mathbf{u},\mu,t;\mathbf{x}_0,\mathbf{u}_0,t_0)\,.$$

Let us introduce the model conditional pdf:

$$p_L^f(\mathbf{x},\mathbf{u},\mu,t;\mathbf{x}_0,\mathbf{u}_0,t_0) = \mathbb{E}_{\mathbf{x}_0,\mathbf{u}_0,t_0}\left\{\delta(\mathbf{x} - \mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0})\delta(\mathbf{u} - \mathbf{V}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0})\delta(\mu - \mu_t^{\mathbf{x}_0,\mathbf{u}_0,t_0})\right\}\,, \tag{7}$$

where $\mu(t) = \mu_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$ is defined by

$$\frac{d\mu(t)}{dt} + \gamma(\mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}, t)\mu(t) = 0\,, \quad \mu(t_0) = 1\,.$$

Here $\mathbb{E}_{\mathbf{x}_0,\mathbf{u}_0,t_0}$ means the expectation over samples of stochastic processes $\mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$, $\mathbf{V}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$, and $\mu_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$, starting at time $t = t_0$ from the point $\mathbf{x}_0, \mathbf{u}_0, 1$. Taking the model transition density $p_L^f(\mathbf{x},\mathbf{u},\mu,t;\mathbf{x}_0,\mathbf{u}_0,t_0)$ as an approximation to $p_L(\mathbf{x},\mathbf{u},\mu,t;\mathbf{x}_0,\mathbf{u}_0,t_0)$, the true Lagrangian pdf $p_L(\mathbf{x},\mathbf{u},\mu,t;\mathbf{x}_0,t_0)$ is approximated

$$p_L(\mathbf{x},\mathbf{u},\mu,t;\mathbf{x}_0,t_0) \approx \int\limits_{\mathbb{R}^3} d\mathbf{u}_0\, p_E(\mathbf{u}_0;\mathbf{x}_0,t_0) p_L^f(\mathbf{x},\mathbf{u},\mu,t;\mathbf{x}_0,\mathbf{u}_0,t_0). \tag{8}$$

Substituting the approximation (8) into the integral (5), we come to the approximate equality

$$\langle g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t)\rangle = \int\limits_{\mathbb{R}^3} d\mathbf{u} \int\limits_0^\infty d\mu \int\limits_0^t dt_0 \int\limits_D d\mathbf{x}_0\, g(\mathbf{u})\mu\, Q(\mathbf{x}_0,t_0) \times \int\limits_{\mathbb{R}^3} d\mathbf{u}_0\, p_E(\mathbf{u}_0;\mathbf{x}_0,t_0) p_L^f(\mathbf{x},\mathbf{u},\mu,t;\mathbf{x}_0,\mathbf{u}_0,t_0)\,. \tag{9}$$

The *backward Lagrangian trajectory*, denoted in what follows by $\hat{\mathbf{X}}(t_0) = \hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}$, $\hat{\mathbf{V}}(t_0) = \hat{\mathbf{V}}_{t_0}^{\mathbf{x},\mathbf{u},t}$, $t_0 \le t$, is defined as the solution to (e.g, [4], [28])

$$\begin{aligned} d\hat{\mathbf{X}}(t_0) &= \hat{\mathbf{V}}(t_0)dt_0, \\ d\hat{\mathbf{V}}(t_0) &= \hat{\mathbf{a}}(t_0,\hat{\mathbf{X}}(t_0),\hat{\mathbf{V}}(t_0))dt_0 + \sqrt{C_0\bar{\varepsilon}(\hat{\mathbf{X}}(t_0),t_0)}\; \overleftarrow{d}\, \mathbf{W}(t_0), \end{aligned} \tag{10}$$

with the terminal condition

$$\hat{\mathbf{X}}(t) = \mathbf{x}, \quad \hat{\mathbf{V}}(t) = \mathbf{u}\,,$$

where the drift term $\hat{\mathbf{a}} = (\hat{a}_1, \hat{a}_2, \hat{a}_3)$ of the backward model (10) is related to the drift term $\mathbf{a} = (a_1, a_2, a_3)$ of the forward model (6) via

$$\hat{a}_i(t,\mathbf{x},\mathbf{u}) = a_i(t,\mathbf{x},\mathbf{u}) - C_0\bar{\varepsilon}(\mathbf{x},t)\frac{\partial}{\partial u_i}\ln p_E(\mathbf{u};\mathbf{x},t)\,. \tag{11}$$

This form of the drift term is the consequence of Thomson's well-mixed condition (see [28]). It ensures the relation between the forward and backward pdf's used in the construction of backward algorithms in Section 3.3. Note that in Appenix B such a relation is given for a more general case.

Remark. *In (10), the differential* $\overleftarrow{d}\, W$ *means that here the backward Ito integral is taken*[1]*. From this, the finite-difference form of the backward Ito equation (10) reads:*

$$\begin{aligned} &\hat{\mathbf{X}}(t_0) - \hat{\mathbf{X}}(t_0 - \Delta t_0) = \hat{\mathbf{V}}(t_0)\Delta t_0, \\ &\hat{\mathbf{V}}(t_0) - \hat{\mathbf{V}}(t_0 - \Delta t_0) = \hat{\mathbf{a}}(t_0,\hat{\mathbf{X}}(t_0),\hat{\mathbf{V}}(t_0))\Delta t_0 + \sqrt{C_0\bar{\varepsilon}(\hat{\mathbf{X}}(t_0),t_0)}\,\Big[W(t_0) - W(t_0 - \Delta t_0)\Big], \end{aligned}$$

where the integration step Δt_0 *is positive.*

Thus we will deal in this paper with the construction of Monte Carlo estimators for the integral (9) based on simulation of forward and backward Lagrangian trajectories.

[1] The backward Ito integral is defined by

$$\int\limits_s^t \xi(\tau)\, \overleftarrow{d}\, W(\tau) := \int\limits_{T-t}^{T-s} \xi(T-\tau)\, dW_T(\tau),$$

$s \le t \le T$, $W_T(\tau) := W(T) - W(T-\tau)$ is a standard Wiener process. This integral does not depend on the choice of T. For details see, e.g., [9].

3 Monte Carlo estimators for the mean concentration and fluxes

In this section we construct Monte Carlo estimators for the mean concentration and fluxes at a fixed point and for integrals over space and time of these mean fields. In Sect.3.1 we deal with forward estimators for the general case of nonstationary, possibly horizontally inhomogeneous turbulence. In Sect.3.2 we modify these estimators to the horizontally homogeneous turbulence. Backward estimators are suggested in Sect.3.3.

3.1 Forward estimator

Calculation of the mean concentration and fluxes at a fixed point by forward simulation is generally not possible (e.g., [4]).

However if it is desired to calculate an integral of $< g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t) >$ over space and time,

$$I_H = \int\limits_D d\mathbf{x} \int\limits_0^T dt \; < g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t) > H(\mathbf{x},t)\,, \tag{12}$$

where $T > 0$ and $H(\mathbf{x},t)$ is a weight function defined on $D \times [0,T]$, then the forward estimator can be successfully used. As one example, we mention the problem of evaluation of the centre and size of a cloud.

Let us give now a forward Monte Carlo estimator for the integral (12) with arbitrary function $H(\mathbf{x},t)$. Substituting (9) into the right-hand side of (12), we get

$$\int\limits_D d\mathbf{x} \int\limits_0^T dt \, \langle g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t)\rangle \, H(\mathbf{x},t) = \int\limits_0^T dt_0 \int\limits_D d\mathbf{x}_0 \, g(\mathbf{u})\mu \, Q(\mathbf{x}_0,t_0) \int\limits_{\mathbb{R}^3} d\mathbf{u}_0 p_E(\mathbf{u}_0;\mathbf{x}_0,t_0)$$

$$\times \int\limits_D d\mathbf{x} \int\limits_{t_0}^T dt \int\limits_{\mathbb{R}^3} d\mathbf{u} \int\limits_0^\infty d\mu \, H(\mathbf{x},t) p_L^f(\mathbf{x},\mathbf{u},\mu,t;\mathbf{x}_0,\mathbf{u}_0,t_0) =$$

$$\int\limits_0^T dt_0 \int\limits_D d\mathbf{x}_0 \, Q(\mathbf{x}_0,t_0) \int\limits_{\mathbb{R}^3} d\mathbf{u}_0 \, p_E(\mathbf{u}_0;\mathbf{x}_0,t_0) \mathbb{E}_{\mathbf{x}_0,\mathbf{u}_0,t_0} \int\limits_{t_0}^T dt \, \mu_t^{\mathbf{x}_0,\mathbf{u}_0,t_0} g(\mathbf{V}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}) H(\mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0},t)$$

where $\mathbb{E}_{\mathbf{x}_0,\mathbf{u}_0,t_0}$ is the expectation over samples of stochastic processes $\mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$, $\mathbf{V}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$, $\mu_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$ (for fixed $\mathbf{x}_0$, $\mathbf{u}_0$, t_0). The forward estimator can be obtained by applying the randomisation procedure (see e.g. [14], and [21]) to the integrals (over t_0, $\mathbf{x}_0$ and $\mathbf{u}_0$) in the second line of the last equality. Randomisation can be done by choosing an arbitrary pdf $r(\mathbf{x},t)$ defined in $D \times [0,T]$ which is consistent with $Q(\mathbf{x},t)$ in the sense that $r(\mathbf{x},t) \neq 0$ if $Q(\mathbf{x},t) \neq 0$. If $(\mathbf{x}_0,t_0)$ is a random point in $D \times [0,T]$ with the pdf $r(\mathbf{x},t)$, and $\mathbf{u}_0$ is a 3D random variable with the pdf $p_E(\mathbf{u};\mathbf{x}_0,t_0)$, then

$$\int\limits_D d\mathbf{x} \int\limits_0^T dt \; < g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t) > H(\mathbf{x},t) = \mathbb{E}\xi_H,$$

where

$$\xi_H = \frac{Q(\mathbf{x}_0,t_0)}{r(\mathbf{x}_0,t_0)} \int\limits_{t_0}^{T} dt \mu_t^{\mathbf{x}_0,\mathbf{u}_0,t_0} g(\mathbf{V}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}) H(\mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0},t) , \quad (13)$$

and $\mathbf{E}$ stands for the expectation over ensemble of trajectories $\mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$, $\mathbf{V}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$, $\mu_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$ with random initial points $\mathbf{x}_0, \mathbf{u}_0, t_0$.

It is reasonable to choose $r(\mathbf{x},t)$ proportional to $Q(\mathbf{x},t)$. In this case the factor Q/r in (13) is a constant, and this might result in a variance reduction.

3.2 Modified forward estimators in case of horizontally homogeneous turbulence

3.2.1 Time averaged mean characteristics

In this subsection the turbulence is assumed to be horizontally homogeneous, generally non-stationary, and the coefficient of absorption does not depend on the horizontal coordinates: $\gamma(\mathbf{x},t) = \gamma(z,t)$.

We use the horizontal homogeneity to calculate the time averaged mean $\int_0^T dt\, \langle g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t)\rangle h(t)$ at a fixed point $\mathbf{x} = (x,y,z)$. Here $h(t)$ is a weight function defined on $[0,T]$.

From the horizontal homogeneity it follows that

$$p_L^f(x,y,z,\mathbf{u},\mu,t;x_0,y_0,z_0,\mathbf{u}_0,t_0) = p_L^f(x-x_0,y-y_0,z,\mathbf{u},\mu,t;0,0,z_0,\mathbf{u}_0,t_0) .$$

Taking into account that $p_E(\mathbf{u}_0;\mathbf{x}_0,t_0) = p_E(\mathbf{u}_0;z_0,t_0)$ we get

$$\int_0^T dt\, \langle g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t)\rangle\, h(t) = \int\limits_0^T dt_0 \int\limits_0^\infty dz_0 \int\limits_{\mathbb{R}^3} d\mathbf{u}_0\, p_E(\mathbf{u}_0;z_0,t_0)$$

$$\times \int\limits_{t_0}^T dt\, h(t) \int\limits_D d\mathbf{x}' \int\limits_{\mathbb{R}^3} d\mathbf{u} \int\limits_0^\infty d\mu \delta(z-z') g(\mathbf{u})\, \mu\, Q(x-x',y-y',z_0,t_0)$$

$$\times p_L^f(\mathbf{x}',\mathbf{u},\mu,t;0,0,z_0,\mathbf{u}_0,t_0) = \int\limits_0^T dt_0 \int\limits_0^\infty dz_0 \int\limits_{\mathbb{R}^3} d\mathbf{u}_0\, p_E(\mathbf{u}_0;z_0,t_0) \mathbf{E}_{z_0,\mathbf{u}_0,t_0}$$

$$\times \int\limits_{t_0}^T dt\, h(t) \delta(z - Z_t^{z_0,\mathbf{u}_0,t_0}) g(\mathbf{V}_t^{z_0,\mathbf{u}_0,t_0}) \mu_t^{z_0,\mathbf{u}_0,t_0} Q(x - X_t^{z_0,\mathbf{u}_0,t_0}, y - Y_t^{z_0,\mathbf{u}_0,t_0}, z_0, t_0), \quad (14)$$

where $\mathbf{E}_{z_0,\mathbf{u}_0,t_0}$ is the expectation over ensemble of trajectories $\mathbf{X}_t^{z_0,\mathbf{u}_0,t_0}$, $\mathbf{V}_t^{z_0,\mathbf{u}_0,t_0}$, $\mu_t^{z_0,\mathbf{u}_0,t_0}$, $t \geq t_0$, which are defined as $\mathbf{X}_t^{z_0,\mathbf{u}_0,t_0} = (X_t^{z_0,\mathbf{u}_0,t_0}, Y_t^{z_0,\mathbf{u}_0,t_0}, Z_t^{z_0,\mathbf{u}_0,t_0}) = \mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$, $\mathbf{V}_t^{z_0,\mathbf{u}_0,t_0} = (U_t^{z_0,\mathbf{u}_0,t_0}, V_t^{z_0,\mathbf{u}_0,t_0}, W_t^{z_0,\mathbf{u}_0,t_0}) = \mathbf{V}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$, $\mu_t^{z_0,\mathbf{u}_0,t_0} = \mu(t;\mathbf{x}_0,t_0)$, with $\mathbf{x}_0 = (0,0,z_0)$.

Now we will use the following property of the Dirac delta function (e.g., see [30], p.36, formula (9.3)): for arbitrary continuous function $f(\tau)$ and continuously differentiable function $Z(\tau)$

$$\int_0^t f(\tau)\delta(Z(\tau)-z)\,d\tau = \sum_{j=1}^{\nu_t(z)} \frac{f(\tau_j)}{\left|\frac{dZ(\tau_j)}{d\tau}\right|}\,, \tag{15}$$

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.

Thus, from (14), taking into account (15), we find

$$\int_0^T dt\,\langle g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t)\rangle\,h(t) = \int_0^T dt_0 \int_0^\infty dz_0 \int_{\mathbb{R}^3} d\mathbf{u}_0\,p_E(\mathbf{u}_0;z_0,t_0)$$

$$\times \mathbb{E}_{z_0,\mathbf{u}_0,t_0}\cdot \sum_{j=1}^{\nu_{t_0,T}(z)} h(\tau_j)\frac{g(\mathbf{V}_{\tau_j}^{z_0,\mathbf{u}_0,t_0})}{|W_{\tau_j}^{z_0,\mathbf{u}_0,t_0}|}\mu_{\tau_j}^{z_0,\mathbf{u}_0,t_0} Q(x-X_{\tau_j}^{z_0,\mathbf{u}_0,t_0}, y-Y_{\tau_j}^{z_0,\mathbf{u}_0,t_0}, z_0,t_0)\,,$$

where $\nu_{t_0,T}(z)$ is the number of intersections of the level z by the trajectory $Z_t^{z_0,\mathbf{u}_0,t_0}$ in the interval $t_0 \le t \le T$, and τ_j are the intersection times. Now the randomisation of integrals over t_0, z_0 and $\mathbf{u}_0$ in the right-hand side of the last equality enables to obtain the final estimator. For this, consider a pdf $r(z_0,t_0)$ on $[0,\infty)\times[0,T]$ which is consistent with the source $Q(x,y,z,t)$ in the sense that $r(z_0,t_0)\neq 0$ if there exist x, y such that $Q(x,y,z_0,t_0)\neq 0$. Then,

$$\int_0^T dt\,\langle g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t)\rangle h(t) = \mathbb{E}\xi_1(\mathbf{x}),$$

where

$$\xi_1(\mathbf{x}) = \frac{1}{r(z_0,t_0)} \sum_{j=1}^{\nu_{t_0,T}(z)} h(\tau_j)\frac{g(\mathbf{V}_{\tau_j}^{z_0,\mathbf{u}_0,t_0})}{|W_{\tau_j}^{z_0,\mathbf{u}_0,t_0}|}\mu_{\tau_j}^{z_0,\mathbf{u}_0,t_0} Q(x-X_{\tau_j}^{z_0,\mathbf{u}_0,t_0}, y-Y_{\tau_j}^{z_0,\mathbf{u}_0,t_0}, z_0,t_0)\,.$$

Here z_0,t_0 is a 2D random variable chosen from $[0,\infty)\times[0,T]$ with the pdf $r(z_0,t_0)$, and $\mathbf{u}_0$ is a $3D$ random variable with the pdf $p_E(\mathbf{u}_0;z_0,t_0)$.

3.2.2 Crosswind and time averaged mean characteristics

In this subsection the turbulence is assumed to be horizontally homogeneous (generally nonstationary), and the coefficient of absorption does not depend on the horizontal coordinates : $\gamma(\mathbf{x},t) = \gamma(z,t)$. Let us estimate the crosswind and time averaged mean characteristic $I_h = \int_0^T dt \int_{-\infty}^\infty dy\,\langle g(\mathbf{u}(x,y,z,t))c(x,y,z,t)\rangle\,h(y,t)$ at a fixed point (x,z). Here $h(y,t)$ is a weight function defined on $(-\infty,\infty)\times[0,T]$. Using the same arguments as in the previous subsection we get

$$I_h = \int_0^T dt \int_{-\infty}^\infty dy\,\langle g(\mathbf{u}(x,y,z,t))c(x,y,z,t)\rangle\,h(y,t)$$

$$= \int_0^T dt_0 \int_{-\infty}^\infty dy_0 \int_0^\infty dz_0 \int_{\mathbb{R}^3} d\mathbf{u}_0\,p_E(\mathbf{u}_0;z_0,t_0)\mathbb{E}_{y_0,z_0,\mathbf{u}_0,t_0}\int_{t_0}^T dt\,h(Y_t^{y_0,z_0,\mathbf{u}_0,t_0},t)$$

$$\times\,\delta(z-Z_t^{y_0,z_0,\mathbf{u}_0,t_0})g(\mathbf{V}_t^{y_0,z_0,\mathbf{u}_0,t_0})\mu_t^{y_0,z_0,\mathbf{u}_0,t_0}Q(x-X_t^{y_0,z_0,\mathbf{u}_0,t_0},y_0,z_0,t_0)\,, \tag{16}$$

where $\mathbf{E}_{y_0,z_0,\mathbf{u}_0,t_0}$ is the expectation over the ensemble of trajectories $\mathbf{X}_t^{y_0,z_0,\mathbf{u}_0,t_0}$, $\mathbf{V}_t^{y_0,z_0,\mathbf{u}_0,t_0}$, $\mu_t^{y_0,z_0,\mathbf{u}_0,t_0}$, $t \geq t_0$, which are defined as

$$\begin{aligned}\mathbf{X}_t^{y_0,z_0,\mathbf{u}_0,t_0} &= (X_t^{y_0,z_0,\mathbf{u}_0,t_0}, Y_t^{y_0,z_0,\mathbf{u}_0,t_0}, Z_t^{y_0,z_0,\mathbf{u}_0,t_0}) = \mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}\,, \\ \mathbf{V}_t^{y_0,z_0,\mathbf{u}_0,t_0} &= (U_t^{y_0,z_0,\mathbf{u}_0,t_0}, V_t^{y_0,z_0,\mathbf{u}_0,t_0}, W_t^{y_0,z_0,\mathbf{u}_0,t_0}) = \mathbf{V}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}\,, \mu_t^{y_0,z_0,\mathbf{u}_0,t_0} = \mu(t;\mathbf{x}_0,t_0)\,,\end{aligned}$$

with $\mathbf{x}_0 = (0, y_0, z_0)$.

From (16) we get by the property (15) that

$$I_h = \int_0^T dt_0 \int_{-\infty}^{\infty} dy_0 \int_0^{\infty} dz_0 \int_{\mathbb{R}^3} d\mathbf{u}_0\, p_E(\mathbf{u}_0, z_0, t_0)\, \mathbf{E}_{y_0,z_0,\mathbf{u}_0,t_0} \sum_{j=1}^{\nu_{t_0,T}(z)} h(Y_{\tau_j}^{y_0,z_0,\mathbf{u}_0,t_0}, \tau_j)$$
$$\times \frac{g(\mathbf{V}_{\tau_j}^{y_0,z_0,\mathbf{u}_0,t_0})}{|W_{\tau_j}^{y_0,z_0,\mathbf{u}_0,t_0}|} \mu_{\tau_j}^{y_0,z_0,\mathbf{u}_0,t_0} Q(x - X_{\tau_j}^{y_0,z_0,\mathbf{u}_0,t_0}, y_0, z_0, t_0)\,, \tag{17}$$

where $\nu_{t_0,T}(z)$ is the number of intersections of the level z by the trajectory $Z_t^{y_0,z_0,\mathbf{u}_0,t_0}$ during the interval $t_0 \leq t \leq T$, and τ_j are the intersection times.

Now, it is not difficult to construct a random estimator for I_h by applying a standard Monte Carlo randomisation procedure for evaluation of integrals. In our case we apply it to the multiple integral in (17) over t_0, y_0, z_0 and $\mathbf{u}_0$. To this end, we consider a probability density $r(y_0, z_0, t_0)$ on $(-\infty, \infty) \times [0, \infty) \times [0, T]$ which is consistent with the source $Q(x, y, z, t)$ in the sense that $r(y_0, z_0, t_0) \neq 0$ if there exists x such that $Q(x, y_0, z_0, t_0) \neq 0$. Then,

$$\mathbf{E}\xi_2(x, z) = \int_0^T dt \int_{-\infty}^{\infty} dy\, \langle g(\mathbf{u}(x, y, z, t)) c(x, y, z, t)\rangle\, h(y, t)$$

where

$$\begin{aligned}\xi_2(x, z) = \quad & \frac{1}{r(y_0, z_0, t_0)} \sum_{j=1}^{\nu_{t_0,T}(z)} h(Y_{\tau_j}^{y_0,z_0,\mathbf{u}_0,t_0}, \tau_j) \frac{g(\mathbf{V}_{\tau_j}^{y_0,z_0,\mathbf{u}_0,t_0})}{|W_{\tau_j}^{y_0,z_0,\mathbf{u}_0,t_0}|} \mu_{\tau_j}^{y_0,z_0,\mathbf{u}_0,t_0} \\ & \times Q(x - X_{\tau_j}^{y_0,z_0,\mathbf{u}_0,t_0}, y_0, z_0, t_0)\,.\end{aligned}$$

Here y_0, z_0, t_0 is a random variable chosen in $(-\infty, \infty) \times [0, \infty) \times [0, T]$ with the density $r(y_0, z_0, t_0)$, and $\mathbf{u}_0$ is a $3D$ random variable with the pdf $p_E(\mathbf{u}_0; z_0, t_0)$.

3.2.3 Stationary turbulence

In this subsection the turbulence is assumed to be horizontally homogeneous and stationary, and the coefficient of absorption depends only on heigth: $\gamma(\mathbf{x}, t) = \gamma(z)$. In addition, the initial concentration is assumed to be zero: $q_0(\mathbf{x}) = 0$. These assumptions allow to estimate $< g(\mathbf{u}(\mathbf{x}, t))c(\mathbf{x}, t) >$ directly at a fixed point $(\mathbf{x}, t)$. Indeed, under conditions assumed

$$p_L^f(x, y, z, \mathbf{u}, \mu, t; x_0, y_0, z_0, \mathbf{u}_0, t_0) = p_L^f(x - x_0, y - y_0, z, \mathbf{u}, \mu, t - t_0; 0, 0, z_0, \mathbf{u}_0, 0)\,.$$

Therefore, by $p_E(\mathbf{u}_0; \mathbf{x}_0, t_0) = p_E(\mathbf{u}_0; z_0)$ we get

$$< g(\mathbf{u}(\mathbf{x}, t))c(\mathbf{x}, t) >= \int_0^{\infty} dz_0 \int_{\mathbb{R}^3} d\mathbf{u}_0\, p_E(\mathbf{u}_0; z_0) \int_0^t d\tau \int_D d\mathbf{x}' \int_{\mathbb{R}^3} d\mathbf{u} \int_0^{\infty} d\mu \delta(z - z')$$

$$\times g(\mathbf{u})\,\mu\, q(x-x', y-y', z_0, t-\tau) p_L^f(\mathbf{x}', \mathbf{u}, \mu, \tau; 0, 0, z_0, \mathbf{u}_0, 0) = \int\limits_0^\infty dz_0 \int\limits_{\mathbb{R}^3} d\mathbf{u}_0\, p_E(\mathbf{u}_0; z_0)$$

$$\times \mathbb{E}_{z_0,\mathbf{u}_0} \int\limits_0^t d\tau \delta(z - Z_\tau^{z_0,\mathbf{u}_0}) g(\mathbf{V}_\tau^{z_0,\mathbf{u}_0}) \mu_\tau^{z_0,\mathbf{u}_0} q(x - X_\tau^{z_0,\mathbf{u}_0}, y - Y_\tau^{z_0,\mathbf{u}_0}, z_0, t-\tau)\,, \qquad (18)$$

where $\mathbb{E}_{z_0,\mathbf{u}_0}$ is the expectation over the ensemble of trajectories $\mathbf{X}_\tau^{z_0,\mathbf{u}_0}$, $\mathbf{V}_\tau^{z_0,\mathbf{u}_0}$, $\mu_\tau^{z_0,\mathbf{u}_0}$, $\tau \geq 0$, which are defined as

$\mathbf{X}_\tau^{z_0,\mathbf{u}_0} = (X_\tau^{z_0,\mathbf{u}_0}, Y_\tau^{z_0,\mathbf{u}_0}, Z_\tau^{z_0,\mathbf{u}_0}) = \mathbf{X}_\tau^{\mathbf{x}_0,\mathbf{u}_0,0}$, $\mathbf{V}_\tau^{z_0,\mathbf{u}_0} = (U_\tau^{z_0,\mathbf{u}_0}, V_\tau^{z_0,\mathbf{u}_0}, W_\tau^{z_0,\mathbf{u}_0}) = \mathbf{V}_\tau^{\mathbf{x}_0,\mathbf{u}_0,0}$, $\mu_\tau^{z_0,\mathbf{u}_0} = \mu(\tau; \mathbf{x}_0, 0)$, with $\mathbf{x}_0 = (0, 0, z_0)$.

Now, from (18) we get by (15)

$$< g(\mathbf{u}(\mathbf{x},t)) c(\mathbf{x},t) >= \int\limits_0^\infty dz_0 \int\limits_{\mathbb{R}^3} d\mathbf{u}_0\, p_E(\mathbf{u}_0, z_0) \mathbb{E}_{z_0,\mathbf{u}_0} \sum_{j=1}^{\nu_t(z)} \frac{g(\mathbf{V}_{\tau_j}^{z_0,\mathbf{u}_0})}{|W_{\tau_j}^{z_0,\mathbf{u}_0}|} \mu_{\tau_j}^{z_0,\mathbf{u}_0} \times q(x - X_{\tau_j}^{z_0,\mathbf{u}_0}, y - Y_{\tau_j}^{z_0,\mathbf{u}_0}, z_0, t - \tau_j)\,,$$

where $\nu_t(z)$ is the number of intersections of the level z by the trajectory $Z_\tau^{z_0,\mathbf{u}_0}$ during the interval $0 \leq \tau \leq t$, and τ_j are the intersection times.

We apply here the standard Monte Carlo randomisation procedure to evaluate the integrals over z_0 and $\mathbf{u}_0$. To this end, we consider a probability density $r(z_0)$ on $[0, \infty)$ which is consistent with the source $q(x, y, z, t)$ in the sense that $r(z_0) \neq 0$ if there exist x, y, t such that $q(x, y, z_0, t) \neq 0$. Then,

$$\langle g(\mathbf{u}(\mathbf{x}, t)) c(\mathbf{x}, t)\rangle = \mathbb{E}\xi_3(\mathbf{x}, t)$$

where

$$\xi_3(\mathbf{x}, t) = \frac{1}{r(z_0)} \sum_{j=1}^{\nu_t(z)} \frac{g(\mathbf{V}_{\tau_j}^{z_0,\mathbf{u}_0})}{|W_{\tau_j}^{z_0,\mathbf{u}_0}|} \mu_{\tau_j}^{z_0,\mathbf{u}_0} q(x - X_{\tau_j}^{z_0,\mathbf{u}_0}, y - Y_{\tau_j}^{z_0,\mathbf{u}_0}, z_0, t - \tau_j)\,. \qquad (19)$$

Here z_0 is a random variable chosen in $[0, \infty)$ with the density $r(z_0)$, and $\mathbf{u}_0$ is a $3D$ random variable with the pdf $p_E(\mathbf{u}_0; z_0)$.

Analogously the crosswind averaged mean can be evaluated at a fixed point (x, z, t): $\int_{-\infty}^{\infty} dy \langle g(\mathbf{u}(x, y, z, t)) c(x, y, z, t)\rangle\, h(y)$. Here $h(y)$ is a weight function defined on $(-\infty, \infty)$. Let $r(y_0, z_0)$ be a probability density defined on $(-\infty, \infty) \times [0, \infty)$ which is consistent with the source $q(x, y, z, t)$ in the sense that $r(y_0, z_0) \neq 0$ if there exist x, t such that $q(x, y_0, z_0, t) \neq 0$. Then,

$$\int_{-\infty}^{\infty} dy\ < g(\mathbf{u}(x, y, z, t)) c(x, y, z, t) >\ h(y) = \mathbb{E}\xi_4(x, z, t),$$

where

$$\xi_4(x, z, t) = \frac{1}{r(y_0, z_0)} \sum_{j=1}^{\nu_t(z)} h(Y_{\tau_j}^{y_0,z_0,\mathbf{u}_0}) \frac{g(\mathbf{V}_{\tau_j}^{y_0,z_0,\mathbf{u}_0})}{|W_{\tau_j}^{y_0,z_0,\mathbf{u}_0}|} \mu_{\tau_j}^{y_0,z_0,\mathbf{u}_0} q(x - X_{\tau_j}^{y_0,z_0,\mathbf{u}_0}, y_0, z_0, t - \tau_j)\,.$$

Here (y_0, z_0) is a random variable chosen in $(-\infty, \infty) \times [0, \infty)$ with the density $r(y_0, z_0)$, $\mathbf{u}_0$ is a $3D$ random variable with the pdf $p_E(\mathbf{u}_0; z_0)$ and $\mathbf{X}_\tau^{y_0,z_0,\mathbf{u}_0}$, $\mathbf{W}_\tau^{y_0,z_0,\mathbf{u}_0}$, $\mu_\tau^{y_0,z_0,\mathbf{u}_0}$ $(\tau \geq 0)$ are stochastic processes defined as $\mathbf{X}_\tau^{y_0,z_0,\mathbf{u}_0} = (X_\tau^{y_0,z_0,\mathbf{u}_0}, Y_\tau^{y_0,z_0,\mathbf{u}_0}, Z_\tau^{y_0,z_0,\mathbf{u}_0}) = \mathbf{X}_\tau^{\mathbf{x}_0,\mathbf{u}_0,0}$, $\mathbf{V}_\tau^{y_0,z_0,\mathbf{u}_0} = (U_\tau^{y_0,z_0,\mathbf{u}_0}, V_\tau^{y_0,z_0,\mathbf{u}_0}, W_\tau^{y_0,z_0,\mathbf{u}_0}) = \mathbf{V}_\tau^{\mathbf{x}_0,\mathbf{u}_0,0}$, $\mu_\tau^{y_0,z_0,\mathbf{u}_0} = \mu(\tau; \mathbf{x}_0, 0)$, with $\mathbf{x}_0 = (0, y_0, z_0)$.

3.3 Backward estimator

Unlike to forward algorithm, the backward technique enables to estimate the mean concentration and fluxes at a fixed point in space and time, even in general case of non-stationary turbulence. Therefore, the estimation can be done directly for $\langle g(\mathbf{u})c\rangle$. Note that taking $g(\mathbf{u})$ equal to 1 or to u_i, we get $\langle\, g(\mathbf{u})c\rangle\ = \langle c\rangle$ or $\langle\, g(\mathbf{u})c\rangle\ = \langle u_i c\rangle$, respectively.

Analogously to forward Lagrangian pdf (7), the backward Lagrangian pdf can be defined as

$$p_L^b(\mathbf{x}_0, \mathbf{u}_0, \mu_0, t_0; \mathbf{x}, \mathbf{u}, t) = \mathbb{E}_{\mathbf{x},\mathbf{u},t}\left\{\delta(\mathbf{x}_0 - \hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t})\delta(\mathbf{u}_0 - \hat{\mathbf{V}}_{t_0}^{\mathbf{x},\mathbf{u},t})\delta(\mu_0 - \hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t})\right\} ,$$

where $\hat{\mu}(t_0) = \hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t}$ is defined by

$$\frac{d\hat{\mu}(t_0)}{dt_0} = \gamma(\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}, t_0)\hat{\mu}(t_0) , \quad \hat{\mu}(t) = 1 ,$$

and $\mathbb{E}_{\mathbf{x},\mathbf{u},t}$ means the expectation over samples of stochastic processes $\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}$, $\hat{\mathbf{V}}_{t_0}^{\mathbf{x},\mathbf{u},t}$, and $\hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t}$, $t_0 \le t$, starting at final time $t_0 = t$ at point $\mathbf{x}, \mathbf{u}, 1$. In appendix C it is shown that

$$p_E(\mathbf{u}_0; \mathbf{x}_0, t_0)p_L^f(\mathbf{x}, \mathbf{u}, \mu, t; \mathbf{x}_0, \mathbf{u}_0, t_0) = p_E(\mathbf{u}; \mathbf{x}, t)p_L^b(\mathbf{x}_0, \mathbf{u}_0, \mu, t_0; \mathbf{x}, \mathbf{u}, t) . \qquad (20)$$

Substituting the right-hand side of this equality to the right-hand side of (9), we get

$$< g(\mathbf{u}(\mathbf{x}, t))c(\mathbf{x}, t) >= \int_{\mathbb{R}^3} d\mathbf{u} \int_0^\infty d\mu \int_0^t dt_0 \int_D d\mathbf{x}_0\, g(\mathbf{u})\mu\, Q(\mathbf{x}_0, t_0) \int_{\mathbb{R}^3} d\mathbf{u}_0\, p_E(\mathbf{u}; \mathbf{x}, t)$$
$$\times\ p_L^b(\mathbf{x}_0, \mathbf{u}_0, \mu, t_0; \mathbf{x}, \mathbf{u}, t) = \int_{\mathbb{R}^3} d\mathbf{u}\, p_E(\mathbf{u}; \mathbf{x}, t)g(\mathbf{u})\mathbb{E}_{\mathbf{x},\mathbf{u},t} \int_0^t dt_0\, \hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t} Q(\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}, t_0) .$$

From the last expression, using the standard Monte Carlo arguments, one gets

$$\langle g(\mathbf{u}(\mathbf{x}, t))c(\mathbf{x}, t)\rangle = \mathbb{E}\hat{\xi}(\mathbf{x}, t) , \qquad (21)$$

where

$$\begin{aligned}\hat{\xi}(\mathbf{x}, t) &= g(\mathbf{u}) \int_0^t dt_0\, \hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t} Q(\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}, t_0) \\ &= g(\mathbf{u}) \left(\hat{\mu}_0^{\mathbf{x},\mathbf{u},t} q_0(\hat{\mathbf{X}}_0^{\mathbf{x},\mathbf{u},t}) + \int_0^t dt_0\, \hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t} q(\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}, t_0)\right) . \qquad (22)\end{aligned}$$

Here $\mathbf{u}$ is $3D$ random variable with the pdf $p_E(\mathbf{u}; \mathbf{x}, t)$.

Now we are in a position to construct a Monte Carlo estimator for the integral (12) from $\langle g(\mathbf{u})c\rangle$ over space and time with an averaging function $H(\mathbf{x}, t)$. For this, we consider an arbitrary pdf $p(\mathbf{x}, t)$ defined in $D \times [0, T]$ which is consistent with $H(\mathbf{x}, t)$ in the sense that $p(\mathbf{x}, t) \neq 0$ if $H(\mathbf{x}, t) \neq 0$. Let $(\mathbf{x}, t)$ be a random point in $D \times [0, T]$ with the pdf

$p(\mathbf{x},t)$, and $\mathbf{u}$ be a $3D$ random variable with the pdf $p_E(\mathbf{u};\mathbf{x},t)$. Then from (21)-(22) and the standard Monte Carlo arguments it follows that the random variable

$$\begin{aligned}\hat{\xi}_H &= \frac{H(\mathbf{x},t)}{p(\mathbf{x},t)} g(\mathbf{u}) \int_0^t dt_0\, \hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t} Q(\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}, t_0) \\ &= \frac{H(\mathbf{x},t)}{p(\mathbf{x},t)}\, g(\mathbf{u}) \left(\hat{\mu}_0^{\mathbf{x},\mathbf{u},t} q_0(\hat{\mathbf{X}}_0^{\mathbf{x},\mathbf{u},t}) + \int_0^t dt_0\, \hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t} q(\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}, t_0) \right)\end{aligned}$$

is a Monte Carlo estimator for the integral (12):

$$\int_D d\mathbf{x} \int_0^T dt\, \langle g(\mathbf{u}(\mathbf{x},t)) c(\mathbf{x},t) \rangle H(\mathbf{x},t) = \mathbb{E}\hat{\xi}_H\ .$$

4 Application to the footprint problem

The footprint problem as formulated in the literature (e.g., see [2], [27]) essentially deals with the calculation of the contribution to the mean concentration and its flux at a fixed point from a surface source of a scalar.

Let us consider a surface sourse at a height z_s and let $F(x,y,t)$ be an amount of emitted scalar per unite time and area (at time t near the surface point (x,y)). Then the distribution function $q(\mathbf{x},t)$ has the form:

$$q(\mathbf{x},t) = q(x,y,z,t) = F(x,y,t)\ \delta(z-z_s). \tag{23}$$

We assume that the turbulence is horizontally homogeneous and stationary. The coefficient of absorption is assumed to depend only on height: $\gamma(\mathbf{x},t) = \gamma(z)$. The initial concentration distribution is assumed to be zero: $q_0(\mathbf{x}) = 0$. The Lagrangian trajectories are perfectly reflected at roughness height z_*. Therefore we will naturally assume that $z_s \geq z_*$.

First, let us construct a Monte Carlo estimator for $\langle g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t)\rangle$ based on *the forward Lagrangian trajectory* $\mathbf{X}_\tau^{z_s,\mathbf{u}_0}$, $\mathbf{V}_\tau^{z_s,\mathbf{u}_0}$, $\mu_\tau^{z_s,\mathbf{u}_0}$, $\tau \geq 0$ (see Sect. 3.2.3). Indeed, choosing in (19) $r(z_0) = \delta(z_0 - z_s)$ and taking into account (23), we have

$$\langle g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t)\rangle = \mathbb{E}_{z_s,\mathbf{u}_0} \left(\sum_{j=1}^{\nu_t(z)} \frac{g(\mathbf{V}_{\tau_j}^{z_s,\mathbf{u}_0})}{|W_{\tau_j}^{z_s,\mathbf{u}_0}|} \mu_{\tau_j}^{z_s,\mathbf{u}_0} F(x - X_{\tau_j}^{z_s,\mathbf{u}_0}, y - Y_{\tau_j}^{z_s,\mathbf{u}_0}, t - \tau_j) \right), \tag{24}$$

where $\mathbf{u}_0$ is a $3D$ random variable with the pdf $p_E(\mathbf{u}_0; z_s)$ and $\mathbb{E}_{z_s,\mathbf{u}_0}$ means an expectation over samples of the stochastic processes $\mathbf{X}_\tau^{z_s,\mathbf{u}_0}$, $\mathbf{V}_\tau^{z_s,\mathbf{u}_0}$, $\mu_\tau^{z_s,\mathbf{u}_0}$, $\tau \geq 0$.

In practical implementation the mathematical expectation in the right-hand side of (24) is approximately calculated as

$$\begin{aligned}\mathbb{E}_{z_s,\mathbf{u}_0} &\left(\sum_{j=1}^{\nu_t(z)} \frac{g(\mathbf{V}_{\tau_j}^{z_s,\mathbf{u}_0})}{|W_{\tau_j}^{z_s,\mathbf{u}_0}|} \mu_{\tau_j}^{z_s,\mathbf{u}_0} F(x - X_{\tau_j}^{z_s,\mathbf{u}_0}, y - Y_{\tau_j}^{z_s,\mathbf{u}_0}, t - \tau_j) \right) \\ &\simeq \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{\nu_i} \frac{g(\mathbf{V}_{\tau_{ij}}^i)}{|W_{\tau_{ij}}^i|} \mu_{\tau_{ij}}^i F(x - X_{\tau_{ij}}^i, y - Y_{\tau_{ij}}^i, t - \tau_{ij})\ ,\end{aligned} \tag{25}$$

where i denotes the trajectory starting with the initial velocity $\mathbf{u}_{0i}$ (which is random with the pdf $p_E(\mathbf{u}_0; z_s)$ and independent for different i), N is the number of trajectories, ν_i is the number of intersections of the level z by i-th trajectory, and τ_{ij} are the intersection times.

Now, let us construct a Monte Carlo estimator for $\langle g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t)\rangle$ based on *the backward Lagrangian trajectory* $\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}$, $\hat{\mathbf{V}}_{t_0}^{\mathbf{x},\mathbf{u},t}$, and $\hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t}$, $t_0 \le t$ (see Sect.3.3). First we will assume that $z_s > z_*$. Taking into account (23) and using the property (15) of the Dirac delta function, from (21)-(22) we find

$$\begin{aligned}\langle g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t)\rangle &= \mathbb{E}_{\mathbf{x},\mathbf{u},t}\left(g(\mathbf{u})\int_0^t dt_0\, \hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t} q(\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}, t_0)\right)\\ &= \mathbb{E}_{\mathbf{x},\mathbf{u},t}\left(g(\mathbf{u})\sum_{j=1}^{\hat{\nu}_t(z_s)} \frac{\hat{\mu}_{\tau_j}^{\mathbf{x},\mathbf{u},t}}{|\hat{W}_{\tau_j}^{\mathbf{x},\mathbf{u},t}|} F(\hat{X}_{\tau_j}^{\mathbf{x},\mathbf{u},t}, \hat{Y}_{\tau_j}^{\mathbf{x},\mathbf{u},t}, \tau_j)\right) , \qquad (26)\end{aligned}$$

where $\hat{\nu}_t(z_s)$ is the number of intersections of the level z_s by the backward trajectory $\hat{Z}_{\tau}^{\mathbf{x},\mathbf{u},t}$ in the interval $0 \le \tau \le t$; τ_j are the intersection times; $\mathbf{u}$ is $3D$ random variable with the pdf $p_E(\mathbf{u}; \mathbf{x}, t)$, and $\mathbb{E}_{\mathbf{x},\mathbf{u},t}$ is the expectation taken over samples of the stochastic processes $\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}$, $\hat{\mathbf{V}}_{t_0}^{\mathbf{x},\mathbf{u},t}$, and $\hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t}$, $t_0 \le t$. The surface emission at the height where the trajectories are reflected, (the case $z_s = z_*$) can be handled by letting $z_s \to z_*$ $(z_s > z_*)$. Taking into account that for each time τ_j the trajectory $\hat{Z}_{\tau}^{\mathbf{x},\mathbf{u},t}$ will simultaneously pass twice (first in dawnward direction and, then, in upward one) the level z_s, it is easy to establish that:

$$\begin{aligned}\langle g(\mathbf{u}(\mathbf{x},t))c(\mathbf{x},t)\rangle &= \mathbb{E}\left(g(\mathbf{u})\int_0^t dt_0\, \hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t} q(\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}, t_0)\right)\\ &= 2\,\mathbb{E}\left(g(\mathbf{u})\sum_{j=1}^{\hat{\nu}_t(z_*)} \frac{\hat{\mu}_{\tau_j}^{\mathbf{x},\mathbf{u},t}}{|\hat{W}_{\tau_j}^{\mathbf{x},\mathbf{u},t}|} F(\hat{X}_{\tau_j}^{\mathbf{x},\mathbf{u},t}, \hat{Y}_{\tau_j}^{\mathbf{x},\mathbf{u},t}, \tau_j)\right) . \qquad (27)\end{aligned}$$

In practice, the approximate calculation of mathematical expectations in the right-hand sides of (26)-(27) is carried out by similiar technique as in (25). For example, in the case $z_s = z_*$ we have

$$\mathbb{E}_{\mathbf{x},\mathbf{u},t}\left(g(\mathbf{u})\sum_{j=1}^{\hat{\nu}_t(z_*)} \frac{\hat{\mu}_{\tau_j}^{\mathbf{x},\mathbf{u},t}}{|\hat{W}_{\tau_j}^{\mathbf{x},\mathbf{u},t}|} q(\hat{\mathbf{X}}_{\tau_j}^{\mathbf{x},\mathbf{u},t}, \tau_j)\right) \simeq 2\,\frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{\hat{\nu}_i} g(\mathbf{u})\frac{\hat{\mu}_{\tau_{ij}}^{i}}{|\hat{W}_{\tau_{ij}}^{i}|} F(\hat{X}_{\tau_{ij}}^{i}, \hat{X}_{\tau_{ij}}^{\mathbf{x},\mathbf{u},t}, \tau_{ij}). \quad (28)$$

Appendix A. Representation of concentration in Lagrangian description

Here we show that the equality (1) is true. The total instantaneous concentration $c(\mathbf{x},t)$ can be represented as the sum of $c_0(\mathbf{x},t)$ and $c_1(\mathbf{x},t)$, defined by

$$\frac{\partial c_0(\mathbf{x},t)}{\partial t} + u_i(\mathbf{x},t)\frac{\partial c_0}{\partial x_i} + \gamma(\mathbf{x},t)c_0(\mathbf{x},t) = 0\,, t > 0; \quad c_0(\mathbf{x},0) = q_0(\mathbf{x})\,, \qquad (A1)$$

and

$$\frac{\partial c_1(\mathbf{x},t)}{\partial t} + u_i(\mathbf{x},t)\frac{\partial c_1}{\partial x_i} + \gamma(\mathbf{x},t)c_1(\mathbf{x},t) = q(\mathbf{x},t)\ , t>0; \quad c_1(\mathbf{x},0)=0\ ,$$

respectively. First we show that

$$c_0(\mathbf{x},t) = \int\limits_D d\mathbf{x}_0\, \mu(t;\mathbf{x}_0,0)q_0(\mathbf{x}_0)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,0)). \tag{A2}$$

According to (A1) the function $C_0(t) = C_0(t;\mathbf{x}_0) = c_0(\mathbf{X}(t;\mathbf{x}_0,0),t)$ satisfies the equation

$$\frac{dC_0(t)}{dt} + \gamma(\mathbf{X}(t;\mathbf{x}_0,0),t)C_0(t) = 0\ , \quad C_0(0) = q_0(\mathbf{x}_0)\ .$$

Therefore from the definition of $\mu(t;\mathbf{x}_0,t_0)$ given by (2) it follows that $C_0(t;\mathbf{x}_0) = \mu(t;\mathbf{x}_0,0)q_0(\mathbf{x}_0)$, and

$$\begin{aligned}\int\limits_D d\mathbf{x}_0\, \mu(t;\mathbf{x}_0,0)q_0(\mathbf{x}_0)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,0)) &= \int\limits_D d\mathbf{x}_0\, c_0(\mathbf{X}(t;\mathbf{x}_0,0),t)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,0)) \\ &= \int\limits_D d\mathbf{y}_0 c_0(\mathbf{y}_0,t)\delta(\mathbf{x}-\mathbf{y}_0) = c_0(\mathbf{x},t)\ .\end{aligned}$$

Here in the last integral the substitution of variables $\mathbf{x}_0 \to \mathbf{y}_0 = \mathbf{X}(t;\mathbf{x}_0,0)$ was performed, and it was taken into account that the Jakobian of this transformation equals unity due to incompressibility of the velocity field $\mathbf{u}(\mathbf{x},t)$ ([16]). With this, (A2) is established.

Now the following equality will be shown:

$$c_1(\mathbf{x},t) = \int\limits_0^t dt_0 \int\limits_D d\mathbf{x}_0\, \mu(t;\mathbf{x}_0,t_0)q(\mathbf{x}_0,t_0)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,t_0))\ . \tag{A3}$$

Indeed, it can be easily shown (by taking suitable derivatives) that

$$c_1(\mathbf{x},t) = \int\limits_0^t dt_0\, g_{t_0}(\mathbf{x},t)\ , \tag{A4}$$

where $g_{t_0}(\mathbf{x},t)$, $(t_0>0)$ is defined by

$$\frac{\partial g_{t_0}(\mathbf{x},t)}{\partial t} + u_i(\mathbf{x},t)\frac{\partial g_{t_0}}{\partial x_i} + \gamma(\mathbf{x},t)g_{t_0}(\mathbf{x},t) = 0\ , t>t_0; \quad g_{t_0}(\mathbf{x},t_0) = q(\mathbf{x},t_0)\ . \tag{A5}$$

From (A5) and by the definition of the function $\mu(t;\mathbf{x}_0,t_0)$ given by (2), it follows that

$$g_{t_0}(\mathbf{X}(t;\mathbf{x}_0,t_0),t) = \mu(t;\mathbf{x}_0,t_0)q(\mathbf{x}_0,t_0)\ .$$

From this equality and since the Jakobian of the transformation $\mathbf{x}_0 \to \mathbf{y}_0 = \mathbf{X}(t;\mathbf{x}_0,t_0)$ is equal to unity, we obtain

$$\begin{aligned}\int\limits_D d\mathbf{x}_0\, \mu(t;\mathbf{x}_0,t_0)q(\mathbf{x}_0,t_0)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,t_0)) &= \int\limits_D d\mathbf{x}_0\, g_{t_0}(\mathbf{X}(t;\mathbf{x}_0,t_0),t)\delta(\mathbf{x}-\mathbf{X}(t;\mathbf{x}_0,t_0)) \\ &= \int\limits_D d\mathbf{y}_0 g_{t_0}(\mathbf{y}_0,t)\delta(\mathbf{x}-\mathbf{y}_0) = g_{t_0}(\mathbf{x},t)\ .\end{aligned}$$

The last equality and (A4) yields (A3). Since $c(\mathbf{x},t) = c_0(\mathbf{x},t) + c_1(\mathbf{x},t)$, from (A2) and (A3) it follows that the representation (1) holds.

Appendix B. Relation between forward and backward transition density functions

Here we present the relation between the forward and backward pdf's used further in Appendix C. Let $p^f(\mathbf{y},t;\mathbf{y}_0,t_0) = \langle \delta(\mathbf{y} - \mathbf{Y}_t^{\mathbf{y}_0,t_0}) \rangle$ be the transition density function of the n-dimensional diffusion process $\mathbf{Y}_t^{\mathbf{y}_0,t_0}$, the solution to

$$dY_i(t) = A_i(\mathbf{Y}(t),t)dt + \sigma_{ij}(\mathbf{Y}(t),t)dW_j(t),\ t > t_0,\ i = 1,\dots,n,\ \mathbf{Y}(t)|_{t=t_0} = \mathbf{y}_0, \quad (B1)$$

where $A_i(\mathbf{y},t)$ and $\sigma_{ij}(\mathbf{y},t)$ are functions defined in $D \times [0,T]$; $W_1(t),\dots,W_n(t)$ are independent standard Wiener processes; D is a domain in $\mathbb{R}^n$, $T > 0$.

We assume that the boundary of D is impenetrable, i.e., the trajectories determined by (B1) do not reach the boundary. Assume that we have a positive function $\rho(\mathbf{y},t)$ defined on $D \times [0,T]$ as a solution to the equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial y_i}(A_i \rho) = \frac{1}{2}\frac{\partial^2 (B_{ij}\rho)}{\partial y_i \partial y_j}, \quad (B2)$$

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 $Z_{t_0}^{\mathbf{y},t}$, $0 \le t_0 \le t$ which is defined by

$$dZ_i = A_i^*(\mathbf{Z},t_0)\,dt_0 + \sigma_{ij}(\mathbf{Z},t_0),t_0)\ \overleftarrow{d}\ W_j(t_0), \quad t_0 < t, \quad \mathbf{Z}(t) = \mathbf{y}. \quad (B3)$$

Here $\overleftarrow{d}\ W_j(t_0)$ is defined as in the footnote to (10) in Sect.2, and

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

We assume again, that the solutions to (B3) do never reach the boundary of D. Then the following relation is true (see [13], Appendix C):

$$\rho(\mathbf{y}_0,t_0)p^f(\mathbf{y},t;\mathbf{y}_0,t_0) = \rho(\mathbf{y},t)p^b(\mathbf{y}_0,t_0;\mathbf{y},t). \quad (B4)$$

Appendix C. Derivation of the relation (20)

Here the derivation of the relation between forward and backward Lagrangian transition pdf's, equation (20), is presented. It is assumed that the boundary $z = 0$ is impenetrable, i.e., the trajectory, the solution to (6), will never reach this boundary.

Let us define $C(t) = C_t^{\mathbf{x}_0,\mathbf{u}_0,c_0,t_0}$ as the solution to

$$\frac{dC(t)}{dt} + \gamma(\mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0},t)C(t) = 0\ , \quad t > t_0; \quad C(t_0) = c_0\ ,$$

and the extended forward Lagrangian transition pdf

$$P_L^f(\mathbf{x},\mathbf{u},c,t;\mathbf{x}_0,\mathbf{u}_0,c_0,t_0) = \mathbb{E}_{\mathbf{x}_0,\mathbf{u}_0,c_0,t_0}\left\{\delta(\mathbf{x}-\mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0})\delta(\mathbf{u}-\mathbf{V}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0})\delta(c-C_t^{\mathbf{x}_0,\mathbf{u}_0,c_0,t_0})\right\},$$

where the forward Lagrangian trajectory $\mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$, $\mathbf{V}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$ is defined in Sect.2 and $\mathbb{E}_{\mathbf{x}_0,\mathbf{u}_0,c_0,t_0}$ means an expectation over samples of stochastic processes $\mathbf{X}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$, $\mathbf{V}_t^{\mathbf{x}_0,\mathbf{u}_0,t_0}$, and $C_t^{\mathbf{x}_0,\mathbf{u}_0,c_0,t_0}$ starting at time $t=t_0$ from the point $\mathbf{x}_0,\mathbf{u}_0,c_0$. Analogously, we define $\hat{C}(t_0)=\hat{C}_{t_0}^{\mathbf{x},\mathbf{u},c,t}$ as the solution to

$$\frac{d\hat{C}(t_0)}{dt_0}+\gamma(\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t},t_0)\hat{C}(t_0)=0\,,\quad t_0<t;\quad \hat{C}(t)=c\,,$$

and the extended backward Lagrangian transition pdf

$$P_L^b(\mathbf{x}_0,\mathbf{u}_0,c_0,t_0;\mathbf{x},\mathbf{u},c,t) = \mathbb{E}_{\mathbf{x},\mathbf{u},c,t}\left\{\delta(\mathbf{x}-\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t})\delta(\mathbf{u}-\hat{\mathbf{V}}_{t_0}^{\mathbf{x},\mathbf{u},t})\delta(c-\hat{C}_{t_0}^{\mathbf{x},\mathbf{u},c,t})\right\}\ ,$$

where $\mathbb{E}_{\mathbf{x},\mathbf{u},c,t}$ means the expectation over samples of stochastic processes $\hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t}$, $\hat{\mathbf{V}}_{t_0}^{\mathbf{x},\mathbf{u},t}$, $\hat{C}_{t_0}^{\mathbf{x},\mathbf{u},c,t}$, $t_0\le t$, starting at final time $t_0=t$ at point $\mathbf{x},\mathbf{u},c$.

To derive the relation (20), first we establish the following equality:

$$\frac{p_E(\mathbf{u}_0;\mathbf{x}_0,t_0)}{c_0}P_L^f(\mathbf{x},\mathbf{u},c,t;\mathbf{x}_0,\mathbf{u}_0,c_0,t_0) = \frac{p_E(\mathbf{u};\mathbf{x},t)}{c}P_L^b(\mathbf{x}_0,\mathbf{u}_0,c_0,t_0;\mathbf{x},\mathbf{u},c,t)\,. \qquad (C1)$$

To this end, we use the well-mixed condition [28]:

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

Denote

$$\rho(\mathbf{x},\mathbf{u},c,t)=\frac{p_E(\mathbf{u};\mathbf{x},t)}{c}\,.$$

From the well-mixed condition we get

$$\frac{\partial\rho}{\partial t}+\frac{\partial(u_i\rho)}{\partial x_i}+\frac{\partial(a_i\rho)}{\partial u_i}+\frac{\partial(-\gamma(\mathbf{x},t)\;c\;\rho)}{\partial c}=\frac{1}{2}C_0\bar{\varepsilon}(\mathbf{x},t)\frac{\partial^2\rho}{\partial u_i\partial u_i}\,. \qquad (C2)$$

Now (C1) follows from (C2) and from the result obtained in Appendix B.

Using

$$p_L^f(\mathbf{x},\mathbf{u},c,t;\mathbf{x}_0,\mathbf{u}_0,t_0)=P_L^f(\mathbf{x},\mathbf{u},c,t;\mathbf{x}_0,\mathbf{u}_0,1,t_0)$$

and assuming in (C1) that $c_0=1$ and $c=\mu$, we get

$$p_E(\mathbf{u}_0;\mathbf{x}_0,t_0)p_L^f(\mathbf{x},\mathbf{u},\mu,t;\mathbf{x}_0,\mathbf{u}_0,t_0)=\frac{p_E(\mathbf{u};\mathbf{x},t)}{\mu}P_L^b(\mathbf{x}_0,\mathbf{u}_0,1,t_0;\mathbf{x},\mathbf{u},\mu,t)\,. \qquad (C3)$$

Further taking into account that

$$\hat{C}_{t_0}^{\mathbf{x},\mathbf{u},\mu,t}=\frac{\mu}{\hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t}}\,,$$

and using the following property of the Dirac delta function

$$\delta(a\mu - b) = \frac{1}{a}\delta(\mu - \frac{b}{a}) , \quad \mu, a, b \in (-\infty, \infty) ,$$

with $b = 1$ and $a = 1/\hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t}$, we get

$$\delta(1 - \hat{C}_{t_0}^{\mathbf{x},\mathbf{u},\mu,t}) = \delta(\frac{\mu}{\hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t}} - 1) = \hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t}\delta(\mu - \hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t}) = \mu\delta(\mu - \hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t}) .$$

From this and the definition of the function P_L^b it follows that

$$P_L^b(\mathbf{x}_0, \mathbf{u}_0, 1, t_0; \mathbf{x}, \mathbf{u}, \mu, t)$$
$$= \mu\mathbf{E}_{\mathbf{x},\mathbf{u},t}\left\{\delta(\mathbf{x}_0 - \hat{\mathbf{X}}_{t_0}^{\mathbf{x},\mathbf{u},t})\delta(\mathbf{u}_0 - \hat{\mathbf{V}}_{t_0}^{\mathbf{x},\mathbf{u},t})\delta(\mu_0 - \hat{\mu}_{t_0}^{\mathbf{x},\mathbf{u},t})\right\} = \mu p_L^b(\mathbf{x}_0, \mathbf{u}_0, \mu_0, t_0; \mathbf{x}, \mathbf{u}, t) .$$

Substitution of the right-hand side of the last equality into (C3) completes the proof of the relation (20).

5 Conclusion

Direct and backward Lagrangian stochastic algorithms for the numerical evaluation of the mean concentration of scalars and its fluxes are suggested and justified. The random estimators are constructed in the form of expectations over stochastic Lagrangian trajectories governed by Langevin type equations derived from Thomson's well-mixed condition. The transported scalar may be absorbed. Detailed expressions for random estimators for the mean characteristics (concentration, fluxes, time and space averages of concentration and fluxes) for quite general cases of sources are given. A practically important case of a plane source (related to the so-called "footprint problem") is treated in details. Advantages of the methods developed are that they are flexible to the structure of the source and the measured statistical characteristics.

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