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Eulerian backtracking of atmospheric tracers: I Adjoint derivation and parametrisation of subgrid-scale transport

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SUMMARY

The problem of identification of sources of atmospheric tracers is most classically addressed through either Lagrangian backtracking or adjoint integration. On the basis of physical considerations, the retro-transport equation, which is at the basis of Lagrangian backtracking, can be derived in a Eulerian framework as well. Because of a fundamental time symmetry of fluid transport, Lagrangian or Eulerian backtracking can be used for inverting measurements of the concentration of an atmospheric tracer. The retro-transport equation turns out to be the adjoint of the direct transport equation, with respect to the scalar product defined by integration with respect to air mass (Hourdin et Issartel, 2000, Geophys. Res. Lett. 27:2245–2248). In the present paper, the exact equivalence between the physically-derived retro-transport and adjoint equations is proved. The transformation from the direct to the retro-transport equation requires only simple transformations. The sign of terms describing explicit advection is changed. Terms describing linear sources or sinks of tracers are kept unchanged. Terms representing diffusion by unresolved time symmetric motions of the transporting air are also unchanged. This is rigorously shown for turbulent eddy-diffusion or mixing length theory. The case of subgrid-scale vertical transport by non time-symmetric motions of air is studied on the example of the Tiedtke mass-flux scheme for cumulus convection. The retro-transport equation is then obtained by simply inverting the roles of updraughts and downdraughts, as well as of entrainment and detrainment. Conservation of mass of the transporting air is critical for all those properties to hold.

1. INTRODUCTION

The identification of sources of atmospheric tracers (i. e., the spatial and temporal localisation of the sources, as well as the quantification of the amount of emitted tracers) is a fundamental question in many aspects of environmental science. A typical example is the identification of natural or anthropic emissions of CO_2 (Kaminski et al., 1999b; Rayner et al., 1999; Bousquet and Peylin, 2000; Gurney et al., 2002), in the perspective of control of those emissions. Inventories of emissions of pollutants are also necessary for the study and reduction of urban pollution (see e. g. Menut et al., 2000). Another example is identification of the source of unexpected emissions of tracers, as can occur for instance on the occasion of an accident in a nuclear plant. A particular example, which was actually at the origin of the work presented here, is the identification, as part of the verification of the Comprehensive Test Ban Treaty (CTBT), of possible nuclear tests (Pudykiewicz, 1998; Hourdin and Issartel, 2000).

The expression *inverse transport* will denote hereafter any technique used for identifying the source of a tracer from measurements of concentration of that tracer. Inverse transport can be in itself a powerful tool for analysing the dynamics and chemistry of the atmosphere. A first approach to inverse transport, often referred to as *Lagrangian backtracking*, consists in inverting the trajectories of individual air parcels. In the case of a unique detector, this technique gives access rather efficiently to a qualitative description of the origin of air masses (Merrill, 1994; Veron et al., 2000; Hess et al., 1996; Ramonet et al., 1996; Chiapello et al.,

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1997). In this *receptor-oriented* approach, turbulent mixing can be accounted for on the basis of assumed random motion of air particles (Flesch et al., 1995; Vautard et al., 2001; Siebert and Frank, 2003). However, the computation of back-trajectories is most often restricted to scales of motion that are explicitly resolved by the transport model.

As noticed by Hourdin et al. (1999), there is in fact no reason to favour Lagrangian rather than Eulerian formalism for backtracking. This remark is at the basis of *Eulerian backtracking*, which is described in detail in the present paper.

Direct transport of a perfect tracer describes the temporal evolution of a scalar field conserved along air trajectories. In a symmetric way, one can define the *retro-transport* of a perfect retro-tracer which describes the reversed temporal evolution of a scalar field conserved along the same air trajectories. Even though retro-transport is a purely virtual process, all the methods used for the representation of direct transport (Lagrangian and Eulerian formulations, Reynolds decomposition between explicitly resolved and unresolved scales, more or less sophisticated positive or monotonic advection schemes, parametrisation of subgrid-scale transport) can also be used for the representation of retro-transport.

Retro-transport can be used for inverting measurements of atmospheric composition by taking advantage of an intrinsic *time symmetry of atmospheric transport*. In the absence of other sources or sinks, the concentration at a detector, at detection time t_D, following the release of a given tracer amount at a point source at time $t_S < t_D$, can be computed as well as the concentration in the source at time t_S of a *retro-tracer* emitted in the same amount in the detector at time t_D. The distribution of this retro-tracer is, up to a scaling factor, the distribution of that particular air which will be sampled for the measurement. Note that this does not violate irreversibility of atmospheric transport. A stronger dispersion in the direct world is associated with a broader initial distribution of the air that will eventually reach a given detector, and corresponds to a stronger dispersion in the retro-transport computation as well. The irreversibility or loss of information is the same for direct and retro-transport.

Another approach to identify sources of tracers is to use a full numerical transport model, containing a description of all physical processes considered as relevant, and to implement on that model the classical techniques of assimilation of observations, such as variants of optimal interpolation or three-dimensional variational assimilation (Pétron et al., 2002), Kalman filter and Kalman smoother (Haas-Laursen et al., 1996, Zhang et al., 1999). We will particularly concentrate here on methods based on the adjoint technique. The adjoint technique, which originated in the works of Lions and Marchuk (see, e. g., Lions, 1971, or Marchuk, 1974, 1982), is a systematic and powerful method for determining numerical sensitivities. It is usually described on the basis of purely mathematical arguments, without reference to a possible physical significance.

Given a model for direct transport (either a mathematical model, or a discretised numerical model), backward integration of the adjoint of the model provides the sensitivity of any observable (such as the concentration of a tracer at a measurement station) with respect to any input parameter of the model (such as surface emission or initial tracer distribution). The adjoint technique is widely used for many meteorological or oceanographical applications, in particular for variational assimilation of observations (Penenko and Obraztsov, 1976; Le Dimet and Talagrand, 1986; Talagrand and Courtier, 1987; Courtier and Talagrand, 1987). It has also been used by a number of authors in order to invert observed atmospheric concentrations of tracers (Uliasz and Pielke, 1991; Pudykiewicz, 1998; Kaminski et al., 1999a,b; Vukićević and Hess, 2000; Robertson and Persson, 1992; Houweling et al., 1999). If the observable under consideration is the concentration of an atmospheric tracer at a given time at a given station, the adjoint transport equation or model is in effect a receptor-oriented model of the atmospheric transport, restricted to those processes that will influence the observed concentration. The adjoint computation determines the sensitivity, or *influence function*, which, combined with the tracer source or initial concentration, will produce the observed concentration.

Hourdin and Issartel (2000) observe that the equation they obtain for backtracking from the time symmetry of atmospheric transport is also the adjoint of the direct transport equation for the particular *air-mass-weighted scalar product*

$$\langle \phi, \psi \rangle = \int \rho \phi \psi \ \mathbf{dx} dt \tag{1}$$

where ϕ and ψ are tracer concentrations per unit mass of transporting air (ρ being the density of transporting air, and $\mathbf{dx}$ and dt volume and time elements respectively). In this particular case, the adjoint of an equation can be derived on purely physical considerations (and not, as usually done, through mathematical manipulations involving, among others, repeated integrations by parts). In addition, the adjoint equation for scalar product (1) is obtained by only changing the sign of a number of terms in the direct equation.

With a more straightforward scalar product of the form $[\phi, \psi] = \int \phi\psi \mathbf{dx} dt$ the symmetry is broken and the direct and adjoint transport equations take a different form (see e. g. Pudykiewicz, 1998; Vukićević and Hess, 2000). Uliasz and Pielke (1991) arrived at symmetric equations for the direct and adjoint transports, despite the fact they used a non-weighted scalar product. The reason is that they considered a Boussinesq fluid for which air density is absent from the continuity equation, making all those scalar products equivalent. Uliasz and Pielke (1991) also already recognised the essential result that "the influence function can be calculated from backward trajectories of particles if a Lagrangian dispersion model is used. Eulerian models governed by partial differential equations are formulated in a variational framework and then the influence function is obtained as a solution of adjoint equations backward in time with the receptor R as a source term". We would rather rephrase this in a more symmetric way. The influence function can be derived either from backtracking of the air sampled at the receptor or as a solution of the adjoint transport equation, and that independently of the particular framework (Eulerian or Lagrangian) retained for the representation of atmospheric transport.

The purpose of the present paper is to give a further and more detailed discussion of inverse transport, as studied from the different views of physical analysis of retro-transport and formal mathematical adjoint sensitivity. The paper contains in particular a mathematical proof of the conclusions previously obtained on the basis of physical considerations. The next section starts with a brief summary of previous work and presents the mathematical derivation of the adjoint of the linear transport equation associated with a linear source or sink of tracer. The adjoint formalism, and the discussion of its connection with the underlying physics, is extended to turbulent eddy-diffusion, surface emission

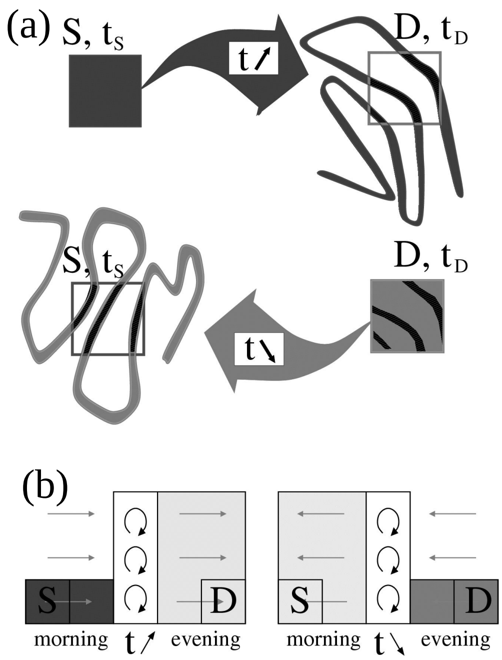

Figure 1. Illustration of the time symmetry of atmospheric transport. **a**: The domain S originally occupied by the tracer at time t_S is transformed by the motion into a filamented structure at time t_D (dark grey). The air in D at t_D consists of air coming from S (intersection with the filamented structure, black) and tracer-free air. When tracking single particles back in time from D at t_D, the particles in the black area come back in S whereas the other particles spread outside S (light grey filament). **b**: Schematic view of the dilution of a tracer injected near the surface under the effect of a strong convective mixing in the planetary boundary layer during the day. The evening concentration in D can be obtained through direct transport and convective mixing from the source S. It can be obtained as well as morning concentration in S through retro-transport from D subject to the same mixing as in the direct computation.

and parametrisation of convective processes (Section 3). Concluding remarks are given in Section 4. Numerical aspects are discussed in a companion paper.

2. Time symmetry of atmospheric transport and adjoint transport

(*a*) *Time symmetry of atmospheric transport*

Following Hourdin et al. (1999) and Hourdin and Issartel (2000), we will first introduce the symmetry of atmospheric transport considering the case of a perfect tracer uniformly distributed with respect to air mass in a volume S at initial time t_S. The mean mass concentration of this tracer is measured later on in volume D at detection time t_D. For a total initial amount Q of tracer (in kg, atoms, ...), the mean mass concentration $\mathcal{M}$ in D at t_D can be expressed as

$$\mathcal{M} = Q \, \frac{m^{ex}(S, t_S, D, t_D)}{m(S, t_S) m(D, t_D)} \tag{2}$$

where $m(\mathcal{V}, t)$ is the mass of air contained in volume $\mathcal{V}$ at time t and $m^{ex}(S, t_S, D, t_D)$ is the mass of the air exchanged between the two volumes. Expression (2) is clearly symmetric and can be evaluated either as the mean concentration in (D, t_D) following the injection of an amount Q of tracer in (S, t_S) or as the mean concentration in (S, t_S) resulting from the injection of the same amount of tracer in (D, t_D), following the air trajectories backward in time. This time symmetry is essentially a kinematical fact and is illustrated in Fig. 1.

Defined in that way, the time symmetry can be extended to a number of non conservative processes. Considering the case of a radioactive tracer, if the same decay rate λ is applied to the direct and retro-tracer, the same concentration

$$\mathcal{M} = Q\ exp\left[-\lambda\left(t_D - t_S\right)\right] \frac{m^{ex}(S, t_S, D, t_D)}{m(S, t_S)m(D, t_D)} \tag{3}$$

can be obtained by injecting the radio-element at (S, t_S) and measuring it at (D, t_D), or by injecting it at (D, t_D) and measuring it at (S, t_S) after a backward integration. This extends in fact to any linear sink (or source) of tracer with decay rate $\lambda\left(\mathbf{x}, t\right)$ (chemical reaction with a dominant species not affected by the reaction, simple parametrisations of scavenging, ...). In this case, the mean concentration $\mathcal{M}$ can be expressed as

$$\mathcal{M} = \frac{Q}{m(S, t_S)m(D, t_D)} \int_{\gamma \text{ in } \Gamma_{S,D}} \exp\left[-\int_{t_S}^{t_D} \lambda\left(\gamma, t\right) dt\right] \rho(\mathbf{x}, t_S) d\Omega_S \tag{4}$$

where $\Gamma_{S,D}$ is the ensemble of trajectories originating in S at time t_S and ending in D at time t_D, $d\Omega_S$ is an elementary volume in S at the origin of the trajectory γ and $\lambda\left(\gamma, t\right)$ is the value of λ at time t along γ. Since the integral bears on trajectories connecting (S, t_S) and (D, t_D), the expression above is unmodified if the mass element $\rho(\mathbf{x}, t_S)d\Omega_S$ in the source is changed into a mass element $\rho(\mathbf{x}, t_D)d\Omega_D$ in the detector. For $\lambda = 0$, the integral reduces to $m^{ex}(S, t_S, D, t_D)$.

The quantity $\mathcal{M}$ in Eq. (4) can be computed by a forward integration of the equation

$$\frac{\partial c}{\partial t} + \mathbf{v}.\mathbf{grad}\ c + \lambda c = \sigma \tag{5}$$

where $c\left(\mathbf{x}, t\right)$ is the tracer concentration per unit mass of air and $\sigma\left(\mathbf{x}, t\right)$ is the source distribution, equal to $Q\ \delta(t - t_S)/m(S, t_S)$ inside S, and 0 outside, with the additional conditions that $c\left(\mathbf{x}, t\right) = 0$ at some time $t_i < t_S$, and that there is no inflow of tracer along the lateral boundaries of the domain Ω under consideration.

Alternatively, $\mathcal{M}$ can be computed by a backward integration of the equation

$$-\frac{\partial c^*}{\partial t} - \mathbf{v}.\mathbf{grad}\ c^* + \lambda c^* = \mu \tag{6}$$

where $c^*\left(\mathbf{x}, t\right)$ is the retro-tracer concentration per unit mass of air and $\mu(\mathbf{x}, t)$, the distribution of the measurement, is equal to $\delta(t - t_D)/m(D, t_D)$ inside D, and 0 outside, with the additional conditions that $c^*\left(\mathbf{x}, t\right) = 0$ at a time $t_f > t_D$, and that there is no lateral inflow again for backward transport.

The time symmetry of atmospheric transport then reads

$$\mathcal{M} = \int_{\Omega\times\tau} \rho\mu c \mathbf{dx} dt = \int_{\Omega\times\tau} \rho\sigma c^* \mathbf{dx} dt \tag{7}$$

where $\tau = [t_i, t_f]$ is the time domain. Note that with the notations above, $(\sigma/Q, c/Q)$ and (μ, c^*) play a symmetric role with units (kg^{-1} s^{-1}, kg^{-1}). As also mentioned by Hourdin and Issartel (2000), because of the linearity of the transport equation, this approach easily extends to non local sources and measurements σ and μ.

In the absence of any other source of tracer, the solution of Eq. (5) is a uniquely defined linear function $c \equiv \mathcal{L}(\sigma)$ of the source σ. Similarly, the solution of Eq. (6) is a uniquely defined linear function $c^* \equiv \mathcal{L}^*(\mu)$ of the measurement distribution μ. With those notations, the time symmetry (Eq. (7)) is expressed as

$$\langle \mathcal{L}(\sigma), \mu \rangle = \langle \sigma, \mathcal{L}^*(\mu) \rangle \tag{8}$$

where $\langle , \rangle$ is the air-mass-weighted scalar product

$$\langle \phi, \psi \rangle = \int_{\Omega \times \mathcal{T}} \rho \phi \psi \mathbf{dx} dt \tag{9}$$

already defined in Eq. (1). Eq. (8) expresses that the operators $\mathcal{L}$ and $\mathcal{L}^*$ are adjoint of each other with respect to the scalar product $\langle , \rangle$. This result has been here obtained on the basis of kinematical considerations only.

(*b*) *Adjoint derivation*

We are now going to use the formal adjoint approach to establish Eq. (7). This will be done in a broader context than before. We consider a measurement of concentration

$$\mathcal{M} \equiv \int_{\Omega \times \mathcal{T}} \rho \mu c \ \mathbf{dx} dt \tag{10}$$

where $\mu(\mathbf{x}, t)$ is the fraction of tracer observed at point $\mathbf{x}$ and time t, per unit mass of transporting air and per unit time. We consider the dependence of $\mathcal{M}$ with respect to the emission $\sigma(\mathbf{x}, t)$, which can now be any space time distribution, and also with respect to the initial distribution of the tracer $c(\mathbf{x}, t_i)$ and to a possible lateral inflow of tracer. Such a lateral inflow can occur only along the *inflow boundary* $\partial\Omega_i$ of Ω, i. e. along the part of the boundary $\partial\Omega$ where the velocity $\mathbf{v}$ is directed towards the interior of Ω ($\mathbf{v}.\mathbf{n} < 0$ where $\mathbf{n}$ is the unit outward normal vector).

The adjoint method defines a general approach to explicitly determine the link between any observable quantity (here $\mathcal{M}$) and any of the input parameters (which are here the source, initial concentration and lateral inflow of tracer). Equation (5) is introduced in Eq. (10) as

$$\begin{aligned} \mathcal{M} &= \int_{\Omega \times \mathcal{T}} \rho \mu c \ \mathbf{dx} dt \\ &- \int_{\Omega \times \mathcal{T}} \rho c^* \left[\frac{\partial c}{\partial t} + \mathbf{v}.\mathbf{grad} c + \lambda c - \sigma \right] \ \mathbf{dx} dt \end{aligned} \tag{11}$$

where the function c^* $(\mathbf{x}, t)$ (which is basically a Lagrange multiplier) is to be defined. Let us transform through integration by parts the advective part in Eq. (11):

$$I \equiv \int_{\Omega \times \mathcal{T}} \rho c^* \left[\frac{\partial c}{\partial t} + \mathbf{v}.\mathbf{grad} c \right] \mathbf{dx} dt \tag{12}$$

$$\begin{aligned} &= \int_{\Omega} [\rho c^* c]_{t_i}^{t_f} \ \mathbf{dx} + \int_{\partial\Omega \times \mathcal{T}} \rho c^* c \ \mathbf{v}.\mathbf{n}_{|\partial\Omega} \ ds dt \\ &- \int_{\Omega \times \mathcal{T}} c \left[\frac{\partial \rho c^*}{\partial t} + \text{div} \ (\rho \mathbf{v} c^*) \right] \mathbf{dx} dt \end{aligned} \tag{13}$$

One recognises in the last integral the conservative flux form of the continuity equation for c^*, which can be transformed into its advective form by using the continuity equation

$$\frac{\partial \rho}{\partial t} + \text{div}\,(\rho \mathbf{v}) = 0 \tag{14}$$

so that, after rearrangement of terms,

$$\begin{aligned}\mathcal{M} \;=\; & \int_{\Omega\times\mathcal{T}} \rho c^* \sigma \;\mathbf{dx}dt \\ - & \int_{\Omega} [\rho c^* c]_{t_i}^{t_f} \;\mathbf{dx} - \int_{\partial\Omega\times\mathcal{T}} \rho c^* c \;\mathbf{v}.\mathbf{n}_{|\partial\Omega}\; dsdt \\ + & \int_{\Omega\times\mathcal{T}} \rho c \left[\frac{\partial c^*}{\partial t} + \mathbf{v}.\mathbf{grad} c^* - \lambda c^* + \mu\right] \;\mathbf{dx}dt\end{aligned} \tag{15}$$

By taking for c^* the solution of Eq. (6) defined by the condition that $c^* = 0$ at time t_f and along the outflow boundary $\partial\Omega_o$ $(\mathbf{v}.\mathbf{n} > 0)$, we finally obtain

$$\mathcal{M} = \int_{\Omega} \rho c^* c_{|_{t_i}} \mathbf{dx} - \int_{\partial\Omega_i\times\mathcal{T}} \rho c^* c \;\mathbf{v}.\mathbf{n}_{|\partial\Omega_i}\; dsdt + \int_{\Omega\times\mathcal{T}} \rho c^* \sigma \;\mathbf{dx}dt \tag{16}$$

which explicitly expresses $\mathcal{M}$ as a function of the initial concentration c at t_i, of the tracer inflow $\rho c\ \mathbf{v}.\mathbf{n}_{|\partial\Omega_i}$ and of the tracer emission σ. The corresponding multiplicative factors depend linearly on the adjoint variable c^*, which turns out to be identical with the retro-tracer concentration introduced in the previous section.

In the absence of tracer at time t_i and of lateral inflow, expression (16) reduces to its last term. This completes the mathematical proof for the time symmetry of atmospheric transport (Eq. (7)) introduced previously on kinematic arguments.

Note that with the same algebra, it can be shown that for times at which no emission nor measurement occurs, and in the absence of lateral inflow of tracer,

$$\frac{d}{dt} \int_{\Omega} \rho c c^* \mathbf{dx} = 0 \tag{17}$$

At any time between the end of the emission and the beginning of the measurement process, the integral $\int_\Omega \rho c c^* \mathbf{dx}$ is equal to the measurement $\mathcal{M}$ which is thus expressed as a combination of the distribution of the tracer coming from the source and of the retro-tracer coming from the detector.

(c) *Time symmetry and conservation*

In the case of pure advection ($\lambda = 0$), the homogeneous part of the advection equation (5), which reduces to

$$\frac{\partial c}{\partial t} + \mathbf{v}.\mathbf{grad}\; c = 0 \tag{18}$$

is identical with the homogeneous part of its adjoint (6) with respect to the air-mass-weighted scalar product (9). This self-adjointness of the transport equation is linked to the conservation of the mass of air and tracer. It was mentioned by Talagrand and Courtier (1987) that, if a linear evolution equation

$$\frac{dc}{dt} = Lc \tag{19}$$

conserves a scalar product $\{,\}$ in time, meaning that for any solution c of Eq. (19), the quantity $\{c, c\}$ is constant in time, then that equation is identical with its adjoint with respect to the conserved scalar product. The latter reads

$$-\frac{dc^*}{dt} = L^* c^* \tag{20}$$

where L^* is the adjoint of L with respect to $\{,\}$.

A proof is obtained from the following transformations of the time derivative of the conserved quantity $\{c, c\}$

$$\frac{d}{dt}\{c, c\} = \left\{\frac{dc}{dt}, c\right\} + \left\{c, \frac{dc}{dt}\right\} = \{Lc, c\} + \{c, Lc\} = \{(L + L^*)\, c, c\} \tag{21}$$

(note that the first transformation requires some degree of smoothness, not discussed here, in the case of an infinite dimension functional space). Thus, $\{(L + L^*)\, c, c\} = 0$ for any c. This implies $L + L^* = 0$ and shows that Eq. (19) and Eq. (20) are identical. Conversely, the condition $L + L^* = 0$ implies conservation of $\{c, c\}$.

In the case of pure advection, the tracer mass concentration c is conserved for any air mass element $dm = \rho \mathbf{dx}$. This means that the quantity $\int \rho c^2 \mathbf{dx}$, where the integral is taken over a given mass of air, is conserved in time. The proof that has just been given underlines the link between conservation of this integral and self-adjointness of the transport equation with respect to the air-mass-weighted scalar product (9).

In the adjoint derivation above, it is the presence of the density ρ in the second integral in Eq. (11) which allows to take advantage of the conservation of mass (14) and to obtain the exact symmetry between Eq. (6) and Eq. (5).

3. Parameterisation of subgrid-scale motions and surface emissions

(*a*) *Separation between resolved and unresolved scales*

An observation system cannot resolve all scales of motions, nor can a numerical model. A distinction must be made between explicitly resolved scales and unresolved or turbulent scales. The interaction between the resolved and unresolved scales must be treated through an appropriate statistical closure procedure.

The classical introduction of turbulent closures relies on the notion of an ensemble average. The ensemble average $\overline{q}$ is defined as the average of a quantity q taken over a set of independent random realizations of turbulent motions. For compressible flows, it is convenient to introduce an air-mass-weighted average $\tilde{q} = \overline{\rho q}/\overline{\rho}$ and a perturbation $q' = q - \tilde{q}$, so that $\overline{\rho q'} = 0$.

Taking the ensemble average of the flux form of the transport equation

$$\frac{\partial \rho c}{\partial t} + \mathrm{div}\,(\rho \mathbf{v} c) = \rho \sigma, \tag{22}$$

and noting that

$$\overline{\rho \mathbf{v} c} = \overline{\rho} \tilde{\mathbf{v}} \tilde{c} + \overline{\rho \mathbf{v}' c'}, \tag{23}$$

lead to

$$\frac{\partial \overline{\rho} \tilde{c}}{\partial t} + \mathrm{div}\,(\overline{\rho} \tilde{\mathbf{v}} \tilde{c}) + \mathrm{div}\left(\overline{\rho \mathbf{v}' c'}\right) = \overline{\rho} \tilde{\sigma} \tag{24}$$

The large scale variables $\overline{\rho}$, $\tilde{\mathbf{v}}$, $\tilde{c}$, $\tilde{\sigma}$ and $\tilde{\mu}$ will be denoted ρ, $\mathbf{v}$, c, σ and μ hereafter. Coming back to the advective form, we obtain the following advection-diffusion equation

$$\frac{\partial c}{\partial t} + \mathbf{v}.\mathbf{grad}c + \frac{1}{\rho}\text{div}\left(\overline{\rho \mathbf{v}' c'}\right) = \sigma \tag{25}$$

Exactly the same treatment can be applied to the backward transport equation leading to

$$-\frac{\partial c^*}{\partial t} - \mathbf{v}.\mathbf{grad}c^* - \frac{1}{\rho}\text{div}\left(\overline{\rho \mathbf{v}' c^{*\prime}}\right) = \mu \tag{26}$$

The turbulent term in Eq. (25) is often defined in meteorological or climate models as the sum of two terms. The first one accounts for the turbulent transport in the planetary boundary layer and is most classically treated with a turbulent eddy-diffusion approach. The second one accounts for vertical transport by cumulus convection. Both cases are considered below.

(b) *Turbulent eddy-diffusion and surface emissions*

(i) *Physical derivation*

Eddy-diffusion parametrisations of turbulence are based upon the idea that unresolved turbulence consists of statistically symmetric upward and downward motions (we restrict here the presentation to the transport by the turbulent fluctuations of the vertical wind, w', which generally dominate, but the derivation below extends easily to horizontal turbulent transport). Those motions produce a diffusion of atmospheric tracers just as random walk of molecules produces molecular diffusion. When inverting the direction of time and motions, unresolved motions still consist of upward and downward motions which have the same statistical effect as in the forward march in time. For Lagrangian models, which account for turbulent diffusion through random perturbations of the air-trajectories, the same random perturbations must be applied to retro-trajectories (see e. g., Flesch et al., 1995; Vautard et al., 2001). In the Eulerian framework, eddy-diffusion can be introduced through the mixing length theory (Prandtl and Tietjens, 1934). In this approach, the concentration for a given realization $c + c'$, in, say, a subsiding motion, is considered as representative of the air at a typical distance l (the mixing length) above. Thus, $c' = c(z + l) - c(z)$ for downward motions ($w' < 0$) and $c' = c(z - l) - c(z)$ for upward motions, resulting for both cases in $w'c' \simeq -|w'| l \partial c/\partial z$. This leads to the turbulent eddy-diffusion formulation

$$\overline{\rho w' c'} = -\rho K_z \frac{\partial c}{\partial z} \tag{27}$$

where $K_z = \widetilde{|w'|l}$ is the eddy-diffusivity. The transport equation thus finally reads

$$\frac{\partial c}{\partial t} + \mathbf{v}.\mathbf{grad}\ c - \frac{1}{\rho}\frac{\partial}{\partial z}\left(\rho K_z \frac{\partial c}{\partial z}\right) = \sigma \tag{28}$$

Note that the closure consisting in expressing K_z as a function of the large scale meteorological variables can be quite complex (including for instance formulations based on a prognostic equation for the turbulent kinetic energy, as in Yamada, 1983).

The vertical turbulent flux of the retro-tracer can be treated with the same mixing length approach except that, since the tracer is advected back in time along air trajectories, positive values of w' are associated with retro-tracer concentrations representative of the air situated above, so that

$$\overline{\rho w' c^{*\prime}} = \rho K_z \frac{\partial c^*}{\partial z} \tag{29}$$

and

$$-\frac{\partial c^*}{\partial t} - \mathbf{v}.\mathbf{grad}\ c^* - \frac{1}{\rho}\frac{\partial}{\partial z}\left(\rho K_z \frac{\partial c^*}{\partial z}\right) = \mu \tag{30}$$

Note that the tracer flux is $\overline{\rho w' c'}$ for direct transport and $-\overline{\rho w' c^{*\prime}}$ for retro-transport so that both fluxes are down-gradient with respect to the tracer or retro-tracer concentrations respectively.

In a number of applications, one is led to consider tracers that are emitted or absorbed at the surface. In this case, sources and sinks are generally treated as a boundary condition for vertical diffusion

$$\frac{\partial c}{\partial t} + \mathbf{v}.\mathbf{grad}\ c - \frac{1}{\rho}\frac{\partial}{\partial z}\left(\rho K_z \frac{\partial c}{\partial z}\right) = 0 \tag{31}$$

$$-K_z \rho \frac{\partial c}{\partial z}_{|\text{surf}} = \Sigma \tag{32}$$

$$-K_z \rho \frac{\partial c}{\partial z}_{|\infty} = 0 \tag{33}$$

(here we assume that the vertical domain extends from the surface upwards to infinity where the density of the atmosphere and the turbulent fluxes vanish).

When interpreting a particular measurement, and tracking back in time the distribution of air, no source must be added at the surface (air mass conservation) so we can hypothesize that the boundary condition for the retro-diffusion will be a zero flux at the surface. Since a source Σ will at first increase the tracer concentration at the surface, it is also possible to argue that c^* at the surface will give the sensitivity to surface emissions as well. This is confirmed by the adjoint analysis which follows.

(ii) *Adjoint derivation*

We consider the effect of advection and diffusion only and, similarly to what was done on Eq. (11), write the measurement as

$$\mathcal{M} = \int_{\Omega\times\mathcal{T}} \rho\mu c\ \mathbf{dx}dt \tag{34}$$

$$- \int_{\Omega\times\mathcal{T}} \rho c^* \left[\frac{\partial c}{\partial t} + \mathbf{v}.\mathbf{grad}c - \frac{1}{\rho}\frac{\partial}{\partial z}\left(\rho K_z \frac{\partial c}{\partial z}\right)\right] \mathbf{dx}dt \tag{35}$$

The vertical diffusion term is transformed through a double integration by parts

$$\int_{\text{surf}}^{\infty} c^* \frac{\partial}{\partial z}\left(\rho K_z \frac{\partial c}{\partial z}\right) dz = \left[c^* \rho K_z \frac{\partial c}{\partial z}\right]_{\text{surf}}^{\infty} - \left[c\rho K_z \frac{\partial c^*}{\partial z}\right]_{\text{surf}}^{\infty} + \int_{\text{surf}}^{\infty} c \frac{\partial}{\partial z}\left(\rho K_z \frac{\partial c^*}{\partial z}\right) dz \tag{36}$$

Taking for the adjoint or retro-tracer, the solution of

$$-\frac{\partial c^*}{\partial t} - \mathbf{v}.\mathbf{grad}\ c^* - \frac{1}{\rho}\frac{\partial}{\partial z}\left(\rho K_z \frac{\partial c^*}{\partial z}\right) = \mu \tag{37}$$

$$K_z \rho \frac{\partial c^*}{\partial z}_{|\text{surf}} = 0 \tag{38}$$

$$K_z \rho \frac{\partial c^*}{\partial z}_{|\infty} = 0 \tag{39}$$

with $c^* = 0$ at time t_f, assuming that there is no resolved boundary advective flow and using Eq. (32) and Eq. (33), the measurement simply reads

$$\mathcal{M} = \int_\Omega \rho c^* c_{|t_i} \mathbf{dx} + \int_{\mathcal{S}\times\mathcal{T}} \Sigma c^* dxdydt \tag{40}$$

($\mathcal{S}$ is the domain of the horizontal integration) as the sum of the contributions of initial concentration and of surface emissions.

This derivation confirms the results obtained from physical considerations on the symmetry of turbulent eddy-diffusion. It also shows that the air origin distribution c^* gives the sensitivity to both initial conditions and surface emissions.

(*c*) *Non local parametrisation of convective transport*

(i) *Mass flux parametrisations*

State-of-the-art parametrisations of cumulus convection are based on so-called mass-flux parametrisations (Arakawa and Schubert, 1974; Tiedtke, 1989; Emanuel, 1991). Mass flux parametrisations have also been applied more recently to the dry convective boundary layer (Hourdin et al., 2002). Some of those parametrisations consider a full spectrum of ascending plumes or columns. We consider below the case where each atmospheric column is divided into two or three sub-columns: one for concentrated updraughts, one (optional) for strong (often precipitating) downdraughts, and one for compensatory slower motion (generally subsidence) in the environment. The derivation below applies directly to the Tiedtke (1989) convection scheme and the Hourdin et al. (2002) thermal plume model and can easily be extended to other convection schemes.

The updraught is characterised by a mass flux $\hat{f}(z)$ (expressed in kg m^{-2} s^{-1}). The lateral exchange of air between updraught and environment is prescribed through an entrainment rate $\hat{e}(z)$ and a detrainment $\hat{d}(z)$ (in kg m^{-3} s^{-1}). For the downdraught, we define similarly a mass flux $\check{f}(z)$, entrainment $\check{e}(z)$ and detrainment $\check{d}(z)$. The convective column is assumed to be stationary over one time step of the full model so that the continuity equation for the air reads

$$\frac{\partial \hat{f}}{\partial z} = \hat{e} - \hat{d} \tag{41}$$

and

$$-\frac{\partial \check{f}}{\partial z} = \check{e} - \check{d} \tag{42}$$

(with the convention that $\hat{f}$, $\check{f}$, $\hat{e}$, $\check{e}$, $\hat{d}$ and $\check{d}$ are positive variables, equal to zero at the upper and lower boundaries). The mass flux in the up- and downdraughts

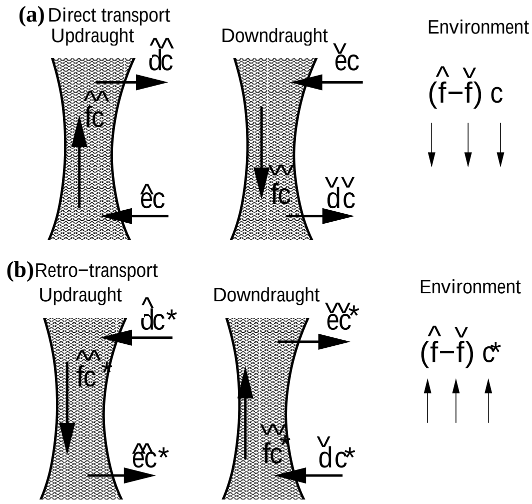

Figure 2. Notation for direct (a) and retro (b) mass-flux schemes. See text for details.

are compensated by a flux, which is generally slower and directed downward, in the environment, $f_e = \hat{f} - \check{f}$.

For inclusion of the tracer component, the following classical approximations are made. The tracer is in a steady state regime, both in the updraught and downdraught. The fractional area covered by rapid motions is negligible so that the tracer concentration c in the environment is equal to the mean concentration in the mesh. This leads to the following expression for the subgrid-scale vertical flux

$$\overline{\rho w' c'} = \hat{f}\hat{c} - \check{f}\check{c} - (\hat{f} - \check{f})c \tag{43}$$

where the tracer concentrations per unit mass of transporting air in the updraught ($\hat{c}$) and downdraught ($\check{c}$) verify the equations

$$\frac{\partial \hat{f}\hat{c}}{\partial z} = \hat{e}c - \hat{d}\hat{c} \tag{44}$$

$$-\frac{\partial \check{f}\check{c}}{\partial z} = \check{e}c - \check{d}\check{c} \tag{45}$$

as illustrated in Fig. 2(a). Eq. (44) must be integrated from the physically necessary condition $\hat{c} = c$ at the bottom level of the updraught ($\check{c} = c$ at the top of the downdraught for Eq. (45)).

As explained by Hourdin and Issartel (2000), mass-flux parametrisations can also be used for backtracking by just reversing the flow direction in the various sub-columns (reversing the direction of all the arrows as illustrated in Fig. 2(b)). For backtracking, the air is for instance carried down rapidly in the updraught, entrainment at the base of the column playing now the role of detrainment. This gives the following expression, similar to Eq. (43), for the subgrid-scale vertical flux

$$-\overline{\rho w' c^{*\prime}} = -\hat{f}\hat{c}^* + \check{f}\check{c}^* - (-\hat{f} + \check{f})c^* \tag{46}$$

where, similarly to Eq. (44) and Eq. (45), the concentrations of the retro-tracer in the updraught ($\hat{c}^*$) and in the downdraught ($\check{c}^*$) are solutions of

$$-\frac{\partial \hat{f}\hat{c}^*}{\partial z} = \hat{d}c^* - \hat{e}\hat{c}^* \tag{47}$$

$$\frac{\partial \check{f}\check{c}^*}{\partial z} = \check{d}c^* - \check{e}\check{c}^* \tag{48}$$

with $\hat{c}^* = c^*$ and $\check{c}^* = c^*$ at the top of the updraught and bottom of the downdraught respectively.

One sees that the retro-transport mass flux scheme (respectively Eqs. 46 to 48) is derived from the direct scheme (Eqs. 43 to 45) by changing (c, $\hat{c}$, $\hat{f}$, $\hat{e}$, $\hat{d}$, $\check{c}$, $\check{f}$, $\check{e}$, $\check{d}$) into (c^*, $\check{c}^*$, $\check{f}$, $\check{d}$, $\check{e}$, $\hat{c}^*$, $\hat{f}$, $\hat{d}$, $\hat{e}$). In practice, the only change to be performed when switching to backward mode in a numerical model is to replace ($\hat{e}$, $\hat{d}$, $\check{e}$, $\check{d}$) by ($\check{d}$, $\check{e}$, $\hat{d}$, $\hat{e}$), $\hat{f}$ and $\check{f}$ being recomputed from Eqs. (41) and (42), and $\hat{c}$ and $\check{c}$ (or $\hat{c}^*$ and $\check{c}^*$ for retro-transport) being dummy internal variables of the parametrisation.

This model of convective retro-transport was introduced in the LMDZ general circulation model on the basis of the above kinematical considerations (Hourdin and Issartel, 2000) much before obtaining the mathematical proof which we are going to present now. Note that Siebert and Frank (2003) reached similar conclusions for the inversion of the parametrisation of convection in a Lagrangian framework.

(ii) *Adjoint derivation*

For the mathematical derivation, and to avoid useless duplications, we restrict the direct model to updraught plus environment ($\check{f} = \check{e} = \check{d} = 0$).

The direct transport model for a conserved tracer is then

$$\frac{\partial c}{\partial t} + \mathbf{v}.\mathbf{grad}\ c + \frac{1}{\rho}\frac{\partial \hat{f}\ (\hat{c} - c)}{\partial z} = \sigma \tag{49}$$

$\hat{c}$ being taken as solution of Eq. (44).

We first rewrite the measurement $\mathcal{M}$ as

$$\mathcal{M} = \int_{\Omega\times\mathcal{T}} \rho\mu c\ \mathbf{dx}dt \tag{50}$$

$$- \int_{\Omega\times\mathcal{T}} \rho c^* \left[\frac{\partial c}{\partial t} + \mathbf{v}.\mathbf{grad}c + \frac{1}{\rho}\frac{\partial \hat{f}\ (\hat{c} - c)}{\partial z} - \sigma\right] \mathbf{dx}dt \tag{51}$$

$$- \int_{\Omega\times\mathcal{T}} \hat{c}^* \left[\frac{\partial \hat{f}\hat{c}}{\partial z} - \hat{e}c + \hat{d}\hat{c}\right] \mathbf{dx}dt \tag{52}$$

The convective terms are transformed by using successively Eqs. (44) and (41):

$$I \equiv \int_{\text{surf}}^{\infty} \left[c^*\frac{\partial \hat{f}\ (\hat{c} - c)}{\partial z} + \hat{c}^*\left(\frac{\partial \hat{f}\hat{c}}{\partial z} - \hat{e}c + \hat{d}\hat{c}\right)\right] dz \tag{53}$$

$$= \int_{\text{surf}}^{\infty} \left[c^*\left(\hat{e}c - \hat{d}\hat{c} - \frac{\partial \hat{f}c}{\partial z}\right) + \hat{c}^*\left(\frac{\partial \hat{f}\hat{c}}{\partial z} - \hat{e}c + \hat{d}\hat{c}\right)\right] dz \tag{54}$$

$$= \int_{\text{surf}}^{\infty} \left[c^*\left(\hat{d}(c - \hat{c}) - \hat{f}\frac{\partial c}{\partial z}\right) + \hat{c}^*\left(\hat{f}\frac{\partial \hat{c}}{\partial z} + \hat{e}(\hat{c} - c)\right)\right] dz \tag{55}$$

Finally, after integrating by parts (considering that $\hat{f}=0$ at the top and bottom) and reordering terms,

$$I=\int_{\text{surf}}^{\infty}\left[c\left(\hat{d}c^*+\frac{\partial \hat{f}c^*}{\partial z}-\hat{e}\hat{c}^*\right)+\hat{c}\left(-\hat{d}c^*-\frac{\partial \hat{f}\hat{c}^*}{\partial z}+\hat{e}\hat{c}^*\right)\right]\,dz \qquad (56)$$

Taking for $\hat{c}^*$ the solution of

$$-\frac{\partial \hat{f}\hat{c}^*}{\partial z}=\hat{d}c^*-\hat{e}\hat{c}^* \qquad (57)$$

the measurement finally reads

$$\begin{aligned}\mathcal{M} &= \int_{\Omega\times\mathcal{T}}\rho c^*\sigma\mathbf{dx}dt\\ &- \int_{\Omega}[\rho c^* c]_{t_i}^{t_f}\,\mathbf{dx}-\int_{\partial\Omega\times\mathcal{T}}\rho c^* c\ \mathbf{v}.\mathbf{n}_{|\partial\Omega}\ dsdt\\ &+ \int_{\Omega\times\mathcal{T}}\rho c\left[\frac{\partial c^*}{\partial t}+\mathbf{v}.\mathbf{grad}c^*+\frac{1}{\rho}\frac{\partial\hat{f}\,(\hat{c}^*-c^*)}{\partial z}+\mu\right]\ \mathbf{dx}dt \qquad (58)\end{aligned}$$

(59)

Taking c^* as the solution of

$$-\frac{\partial c^*}{\partial t}-\mathbf{v}.\mathbf{grad}c^*-\frac{1}{\rho}\frac{\partial\hat{f}\,(\hat{c}^*-c^*)}{\partial z}=\mu \qquad (60)$$

expresses $\mathcal{M}$ as a function of initial and boundary conditions (as well as surface emission if included in the direct model).

Without physical intuition, it would have been easy also to formally derive the adjoints of the direct equations (44) and (49). But one could have missed the intrinsic symmetry of transport and ended up with an apparently different set of equations. It is this symmetry which allows one to use the same algorithms in the two modes of integration.

(*d*) *Exchange matrices*

Some parametrisations make direct use of an exchange matrix on the vertical. It is the case for instance for the transilient matrices approach proposed by Stull (1984) for the parametrisation of the convective boundary layer. The transilient or exchange matrix consists of explicit exchange coefficients between origin and target layers. Turbulent eddy-diffusion is typically associated with a tridiagonal matrix in that formalism whereas non local transport will add terms farther away from the diagonal. Ebert et al. (1989) used transilient matrices to summarise the vertical transport from results of a Large Eddy Simulations of the dry convective boundary layer. Pleim and Chang (1992) proposed an asymmetric model, also based on transilient matrices, retaining only a rapid transport from the lowest layer to all the other ones, compensated by a gradual subsidence. Note also that the Emanuel (1991) scheme for deep convection makes use of a combination of mass fluxes as explained above and of an exchange matrix.

For transilient or exchange matrices, reversing transport simply consists in inverting the role of the origin and target for the exchange coefficients.

4. Conclusion

We have established, for linear tracers, the exact equivalence between retro- and adjoint transport for the air-mass-weighted scalar product. This equivalence relies on the time symmetry of atmospheric transport. The direct and retro-transport are in a sense symmetric by construction since they consist of exploring the same trajectories forward and backward. The time symmetry used for tracer inversion requires however in addition that the transformation of space defined by following air trajectories conserves a certain measure, here the mass of transporting air. Mathematically, air mass conservation allows to invert the roles of target and origin in integral (4); the continuity equation for the large scale flow (14) and for the convective mass-flux (41) are also necessary for the transformations from (11) to (15) and from (54) to (55) respectively; the position of ρ in the expression for turbulent diffusion (28) is intimately related to air mass and tracer conservation and is also essential to obtain a symmetric form after the double integration by parts (36). For the case of pure advection, the additional conservation of $\int \rho c^2 \mathbf{dx}$ implies self-adjointness of the transport equation for the air-mass-weighted scalar product. The equations are not self-adjoint anymore with diffusion of form $1/\rho \times \text{div}\,(\rho K \mathbf{grad}\ c)$ for which both $\int \rho c^2 \mathbf{dx}$ and $\int \rho c^{*2} \mathbf{dx}$ decrease with the same rate $-\int \rho K (\mathbf{grad}\ c)^2 \mathbf{dx}$ for forward and backward time integration respectively.

Though mathematically equivalent, the retro-transport and adjoint approaches are conceptually quite different. The adjoint approach is a systematic mathematical technique providing the sensitivity of any objective function with respect to all control parameters (here initial or boundary conditions as well as 4D sources or surface emission). On the other hand, in the retro-transport approach, which is entirely based on physical considerations, a tracer following air trajectories backward in time is treated with the physical tools usually applied to forward atmospheric transport, including Eulerian description or parametrisation of subgrid-scale motions. The retro-transport algorithms are generally obtained through simple formal transformations, which is of course of practical advantage.

Application of backtracking in a Eulerian rather than Lagrangian framework allows to benefit from the great effort developed in terms of parametrisation of subgrid-scale processes, both for meteorological and climatological applications. When applying those parametrisations to backtracking, the direction of wind must be inverted for the subgrid-scale motions that are at the basis of the parametrisations. The classical turbulent eddy-diffusion is unchanged in the reverse world because it is based on the assumption of symmetric upward and downward motions. Non local transport by convective plumes must be inverted carefully. Concentrated updraughts will be replaced by concentrated downdraughts. Note however that,in both cases, convective motions will generally increase dispersion in both the direct and reverse worlds.

If mathematically equivalent to retro-transport, the adjoint derivation may lead to a set of equations which is apparently different from that obtained from the symmetry of atmospheric transport. The adjoint and retro-transport approaches may also lead to different numerical implementations. Because of the peculiarities of the numerical discretisation, the retro-transport model obtained by the simple transformations mentioned above may actually differ from the exact adjoint of the direct numerical model with implications for practical use in inversion algorithms. Those aspects are discussed in details in the companion paper.

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