Atmos. Chem. Phys. Discuss., 9, C9224–C9230, 2010
www.atmos-chem-phys-discuss.net/9/C9224/2010/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Parameterization of subgrid aircraft emission plumes for use in large-scale atmospheric simulations" *by* A. D. Naiman et al.

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Received and published: 4 January 2010

The discussion paper Naiman et al. (2009) describes a plume model to represent contrails in a large-scale atmospheric model. Their plume is assumed to have an ellipsoidal cross-section, which may get deformed by shear and which may widen by diffusion.

This is a simple and basically feasible approach. In fact, I follow a similar approach using a multiple Gaussian plume model concept (Schumann, 2009). The idea of using a multiple Gaussian plume model was first presented by Schumann and Konopka (1994) and later used in several papers from this institute. Konopka (1995) provided

the theoretical framework for the Gaussian plume expansion under shear and diffusion. Schumann et al. (1995) and Schlager et al. (1997) applied the Gaussian plume model to explain and to interpret measured plume concentration fields and to determine effective diffusivities. Dürbeck and Gerz (1996) showed that the effective diffusivities can be supported by comparisons to LES simulations for homogeneous turbulence. Gierens (1998) applied the concept to analyze the principle of contrail cirrus formation. Later the plume concept was used by several further authors from other institutes partially in cooperation with us (Meijer et al., 1997; Petry et al., 1998; Kraabol et al., 2000; 2002; Vohralik et al., 2008). Naiman et al. cite a few of these studies.

Conceptionally, the ellipsoidal model assumes constant concentrations inside the ellipse and zero outside. This is the main difference to a Gaussian plume model where the concentrations are steady functions decreasing exponentially with the square distance from the plume center line.

The problem with this model is that diffusion can only be represented qualitatively. The relations used for this, eqs. 3, 8 and 9, are justified only by scale analysis to order of magnitude. This is a consequence of the assumed plume concentration field which leaves the concentration gradient at the edge of the plume undefined. Consequently, gradient driven diffusion cannot be computed accurately with their model. But diffusion is important: Horizontal diffusion is important at short times; at large times, shear and vertical diffusion control plume dispersion (Schumann et al., 1995).

A further problem with eq (3) is that it assumes that diffusion is oriented in the direction of the variable ξ_i. In reality, diffusion may change the position of a piece of a plume cross-section either in positive or negative direction randomly.

As a consequence of the qualitative nature of eqs. (8, 9) also the solution given in eq. (21, 22) is correct only qualitatively. In the Gaussian plume model the horizontal plume variance scales with linear, quadratic and cubic parts of the diffusivity depending on the amount of shear. I am not sure whether the same behavior is represented by the present model.

However, at the end, this may impact the results only to a minor degree, because both the ellipsoidal and the Gaussian plume model are crude approximations to the real concentration field in a contrail and the diffusivities are not well known anyway.

The main purpose of this note, however, is to point out some formal errors in the interpretation of the results of the ellipsoidal model in terms of variances σ and the related equations (10 - 14) of the paper by Naiman et al. (2009).

The correction may explain the odd behavior shown in figure 3 (lower right panel) which shows σ_v^2 first increasing and then decreasing. I would expect a steady increase of this vertical variance with time, as shown by the Gaussian plume model. (Only the variance in the direction of the principal axis of the ellipse may decrease after some time).

The correct variances of an ellipsoidal domain with mayor radii a and b follow from

$$\sigma = \int\!\!\int (x \otimes x)\, c(x)\, dA \tag{1}$$

with the dyadic product $\otimes$ involving the position vector x relative to the plume center (see Konopka, 1995, eq. 35).

The concentration field $c(x)$ is normalized so that

$$\int\!\!\int \; c(x)\, dA = 1, \tag{2}$$

Hence, $c(x) = A^{-1}$ inside the ellipse with cross-section A, and zero outside; dA is a cross-section element of the x-plane. In general, the integrals go over the full space of x. However, since $c(x)$ is zero outside the ellipse, the integrals effectively integrate over the interior of the ellipse only.

For an ellipse with mayor radii a and b the cross-section is $A = \pi ab$.

With reference to Fig. 2 of Naiman et al., (2009), let $x = (z, s)$ be the spatial coordinates, and θ the angle of the major axis of the ellipse relative to the z-axis.

Then

$$\sigma_{zz} = (\pi ab)^{-1} \int\!\!\int \; z^2\, dA, \tag{3}$$

$$\sigma_{ss} = (\pi ab)^{-1} \int\!\!\int \; s^2\, dA, \tag{4}$$

$$\sigma_{zs} = \sigma_{sz} = (\pi ab)^{-1} \int\!\!\int \; z\, s\, dA, \tag{5}$$

Now we introduce transformed coordinates $z' = zC + sS$, $s' = -zS + sC$ and their inverse $z = z'C - s'S$, $s = z'S + s'C$, where $S = \sin(\theta)$, $C = \cos(\theta)$. This allows to reduce the integrals to those over an ellipse in its normal form (without inclination), for which the variances are

$$\sigma'_{zz} = a^2/4, \tag{6}$$

$$\sigma'_{ss} = b^2/4. \tag{7}$$

This follows from integration over a circle which results form the ellipse after linear scaling of the two axis with b^{-1} and a^{-1}, e.g.,

$$\sigma'_{ss} = \pi^{-1}\, 4\, b^2 \int_0^1 \; s^2\, (1 - s^2)^{1/2} ds = b^2/4. \tag{8}$$

Here the factor 4 arises because the integral covers a quarter of a circle.

Then the elements of the covariance matrix for the skewed ellipse are

$$\sigma_{zz} = \sigma'_{zz} C^2 + \sigma'_{ss} S^2, \tag{9}$$

$$\sigma_{ss} = \sigma'_{zz} S^2 + \sigma'_{ss} C^2, \tag{10}$$

$$\sigma_{zs} = (\sigma'_{zz} - \sigma'_{ss}) C\, S. \tag{11}$$

Hence, the variances should be computed from $\sigma_h^2 = \sigma_{ss}$, $\sigma_v^2 = \sigma_{zz}$, and $\sigma_s^2 = \sigma_{zs}$, instead of eqs. (10-14) of Naimann et al. (2009). In the Gaussian model, the corresponding variances are $\sigma'_{zz} = a^2/2, \sigma'_{ss} = b^2/2,$ i.e. they are a factor of two larger because of the smoother concentration profile.

It should be noted that the notation σ_s^2 for the off-diagonal elements is misleading, since this off-diagonal component of the variance matrix, which we denote as σ_{zs}, can be both positive and negative (this was also wrong in Dürbeck and Gerz, 1996). Moreover, we note that a factor of 2 was missing in eq. (9) of Dürbeck and Gerz (1996) which may have effected the analysis of the cross-section area A shown in Fig. 5 (right) of Naiman et al. (2009): The correct expression is $A = 2[det(\sigma)]^{1/2}$.

I expect that the results of the ellipsoidal model and the Gaussian model might agree better when the correct variance definitions are used for comparison.

At the end, however, comparisons with measurements in the atmosphere should be used to assess the validity of the approach. In particular, I would be interested to see the dilution of any passive tracer in the plume with plume age in comparison to measurements (Schumann et al., 1998).

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