Atmos. Chem. Phys. Discuss., 2, S377–S386, 2002
www.atmos-chem-phys.org/acpd/2/S377/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "A condensed-mass advection based model for the simulation of liquid polar stratospheric clouds" *by* D. Lowe et al.

D. Lowe et al.

Received and published: 9 September 2002

Referee 1

Comment 1:

"Eq. (9) is split in two in order to solve it... Here, some additional remarks are necessary"

Reply:

To solve equation 9, we use the method of fractional steps. The following changes have beeen made to the paper to clarify this:

Page 695, line 2, change to first sentence:

"Equation 9 can be solved by splitting it into two parts, allowing the use of the method of fractional steps (Yanenko, 1971; Toro, 1999, Chapter 15)."

Page 695, line 8, addition of following paragraph:

"The fractional step method advances the solution of eq. 9 in one co-ordinante direction at a time. The advantage of this method is that it allows us to choose the most suitable schemes for solving each part of Eq. (9). However, it is limited by the need to use small time-steps, ensuring that the properties of the system do not appreciably change during the time-step."

Comment 2:

"It is not easy to understand the WAF-approach described at page 695. What is the definition of the mass flux f^{waf} if compared with eq. (11)? In addition, I would recommend to shift this part of the manuscript to the appendix."

Reply:

The following changes have been made to the paper:

Page 695, addition to the paragraph ending on line 15:

"This method calculates the flux of mass between adjacent size bins ($f_i^{waf} = p_i H$), which is used to solve Eq. 11."

Section 2.2, from line 16 on page 695 to line 10 on page 697, will be moved to the appendix.

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Comment 3:

"...the presentation in section 3 has to be improved."

a)

"Please adjust the notation used in this section to the notation in section 2.1."

Reply:

The notation used has been changed, and the text around Eqs. (23) and (24) has been reduced to reflect these changes:

"The analytical solution developed by Fernández Díaz et al. is based on Pilinis's work (Eq. 9). They solved Eq. (9) for both $H = 0$ and $H \neq 0$, and studied three growth laws: diffusion; surface reaction; and volume reaction. We shall use their solutions for $H \neq 0$ and the diffusional growth law."

b)

"Because only eq. (32) is important for the discussion, I would recommend to reduce (remove) the text between eqs. (24) and (31) or to shift this part of the manuscript to the appendix."

Reply:

The text between Eqs. (24) and (31) has been reduced to:

"The growth rate for a particle of size μ is:

$$\frac{d\mu}{dt} = \frac{1}{3} H \,. \tag{1}$$

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Interactive Comment

This equation defines a characteristic curve in the (μ, t) coordinate system. Equation (25) is integrated to obtain the equation of the characteristic curve:

$$\mu = f(\mu_0, t_0, t) \tag{2}$$

which may be inverted

$$\mu_0 = f_0(\mu, t_0, t) \tag{3}$$

where $J = J_0$ when $t = t_0$. This integration will be performed later for the diffusion case.

Using the method of characteristics, Fernández Díaz et al. solved Eq. (9) for $H \neq 0$,

$$p_i(\mu, t) = \frac{H(f_0(\mu, t_0, t))}{H(\mu)} \left(\left[\exp(3(\mu - f_0(\mu, t_0, t)) - 1 \right] \times A_i p(f_0(\mu, t_0, t), t_0) + p_i(f_0(\mu, t_0, t), t_0) \right). \tag{4}$$

where

$$A_i = \frac{H_i(J, t)}{H(J, t)}. \tag{5}$$

This analytical solution is valid while A_i is constant, and H_i is a function of separable variables ($H_i = H_i^{\mu}(\mu) H_i^{t}(t)$)."

Comment 4:

"In section 2.3, the model physics based on eq. (22) is introduced. The authors should explain at this place the connection of this model physics with the main eqs. (10) and (11). What is the definition of H in this context."

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Reply:

The following text replaces the start of the first paragraph on page 698:

"The growth rates for each component can be determined by substituting for dm_i/dt in Eq. (3). These are calculated assuming uncoupled mass fluxes between the gas and liquid phases for each component i of the multicomponent particle (e.g. Vesala, 1991):"

Comment 5:

"The questions of the required CPU time and of the tractability of MADVEC for coupling with a CTM are not discussed in the paper. Here, more details are desirable."

Reply:

This question is covered in the second referee's comments 2-4, which we answer below.

Referee 2

Comment 1:

"The authors mention that higher HNO3 concentration could lead to NAT formation. A recent paper by Knopf et al (ACP, 2002) shows that the homogeneous nucleation rate from the liquid phase is much too low to explain the number density of large NAT particles observed by Fahey et al (Science, 2000). Thus, this makes the desire of such a treatment much weaker."

Reply:

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It seems to us a little harsh to judge the usefulness of our work of several years, reported here, on the basis of a single very recent (and disputed) publication. However, that said, we agree that homogeneous nucleation of NAT is likely to occur at rates too low to make it a significant source of the observed large NAT particles.

In the Conclusions section of the paper we refer to work by Bogdan et al., which indicates that heterogeneous nucleation of NAT is very likely to be composition dependent, and could occur up to 8 degrees above the ice point. If this proves to be true, and a working parameterisation can be formulated, then the non-equilibrium modelling of STS particles will be important.

Comments 2+3:

"For the implementation of MADVEC into a 3D-model extra efforts (e.g. the proper parameterisation of the mountain wave activities) are required."

"However, how can the particles be transported in a 3D-model is not discussed here. This is a crucial problem... because the clouds could be very patchy and have strong number density gradient in space. How can one transport a PSC-cloud from one grid-box to another box with an affordable CPU time in 3D-models avoiding artificial numeric diffusion?"

Reply:

This paper is intended to present our box-model, not to solve all the problems involved with efficiently implementing such a model into a CTM. The following has been added to the Conclusions section (the matter of particle transport is addressed in our reply to comment 4):

"Due to the fixed size distribution, MADVEC is suitable for use within global and mesoscale CTMs. However full non-equilibrium modelling of PSC particles will require

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high resolution parameterisation of mountain waves and of the PSCs created by them. Mesoscale models can, at high resolution, capture the larger scale features of mountain waves (Leutbecher and Volkert, 2000). However these models still fail to capture the smaller scale fluctuations (with wavelengths of a few km), which have a large effect on the composition of STS particles (Voigt et al., 2000). Sedimentation of particles from PSCs, a proposed source of "NAT-rocks", also require higher vertical resolutions than those currently available (Fueglistaler et al., 2002). Further development of the parameterisation of these small-scale features is needed."

Comment 4:

"A summary of accuracy concerning numeric diffusion, composition, and CPU time expense of different schemes... would be useful..."

Reply:

At the moment we are just using the simple Eulerian forward integration (we are not happy with our implementation of SVODE, and have made relavent changes to the original paper, as indicated below), so we cannot make a comparision of the different schemes. However we have added the following summary to the conclusions:

"The four-hour test case used in this paper takes approximately 1000 CPU seconds on a Sparc IIi 248MHz processor. Reducing the resolution of the model (i.e. the number of size bins) can decrease the cost of the model by upto 30%. It is envisaged that particles will be transported between grid cells using an adaption of the scheme used to advect trace gases. This would result in [number of components * number of size bin] tracers, thus at the resolution of 50 size bins the transport of 150 tracers would be required, while a 20-bin model would require 60 tracers. This will be expensive, but is achievable for the mesoscale modelling of mountain waves for a few days at a time."

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Minor comments:

Fig.4:

“The same colour bars for panel a) and b) should be used”

Reply:

We have re-adjusted the colour bars.

Fig.5:

“The maximum of the HNO3 wt% from MADVEC is about 4% lower than the Lagrangian solution... This should be improved, or at least understood.”

Reply:

This figure has been changed due to changes in the ODE solver. The relevant discussion is included below.

General Amendments

Since submitting this paper we have discovered that our implementation of SVODE calculated HNO3 mass fractions, for the smallest particles, which were unrealistically high (up to 47% HNO3 at 190K). Because of this we are currently using only the Eulerian foward step as our ODE solver, which correctly calculates the expected decrease in the volatile mass fractions with particle size for the smallest particles due to the Kelvin effect. The paper has been altered to reflect this, including new figures (figures 4b, 5, and 6).

Because this change only affects the smallest particles, which contain very little mass, the aerosol distribution and mass fractions are not greatly changed from those originally

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presented in the paper. The HNO3 mass fractions at 190K are 1–2% lower than those calculated using SVODE, however the mass fraction maxima is of the same magnitude ($\approx 47\%$).

The comparison with the results of Meilinger et al. (1995) (Figure 5 in the original paper) is therefore changed. The HNO3 mass fractions determined by MADVEC are approximately 3% lower than those reached by Meilinger et al. A new discussion of the differences has been inserted in the text. Lines 14-15 on page 704 have been changed to:

"However at 190K, the HNO3 mass fractions determined by MADVEC are approximately 3% lower than those reached by Meilinger et al."

The following discussion is appended to line 19 on page 704:

"The difference in HNO3 mass fractions between our results and those of Meilinger et al. (1995) is not sensitive to the resolution of MADVEC (tested by doubling the resolution of MADVEC relative to that used to produce Figure 5). Neither is there any indication of significant numerical diffusion when MADVEC is tested against the analytical solution (Figures 1 and 2; but see also the discussion below). It is likely, therefore, that the difference between the models is due to small differences in physical parameters such as vapour pressure, density, surface tension, etc."

References

[1] Fueglistaler, S., Luo, B. P., Voigt, C., Carslaw, K. S., and Peter, Th: NAT-rock formation by mother clouds: a microphysical model study, Atmos. Chem. Phys., 2, 93–98, 2002.

[2] Leutbecher, M., and Volkert, H.: The propagation of mountain waves into the strato-

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sphere: quantitative evaluation of three-dimensional simulations, J. Atmos. Sci., 57, 3090–3108, 2000.

[3] Voigt, C., Tsias, A., Dörnbrack, A., Meilinger, S., Luo, B., Schreiner, J., Larsen, N., Mauersbergerk K., and Peter, T.: Non-equilibrium compositions of liquid polar stratospheric clouds in gravity waves, Geophys. Res. Lett., 27, 3873–3876, 2000.

[4] Yanenko, N. N.: The Method of Fractional Steps, Springer, Berlin, 1971.

Interactive comment on Atmos. Chem. Phys. Discuss., 2, 689, 2002.