Using Meteorological Analyses for Off-Line Chemical Transport Modelling

Martyn P. Chipperfield

Institute for Atmospheric Science, School of the Environment, University of Leeds, U.K.
martyn@env.leeds.ac.uk

ABSTRACT

Issues related to how off-line chemical transport models (CTMs) use meteorological analyses are discussed. The principles behind the off-line approach and mass conservations are described. The use of chemical data assimilation to overcome shortcomings in the forcing meteorology is outlined.

1 Introduction

In recent years 'off-line' chemical transport models (CTMs) have become increasingly common. In these models the meteorology (winds and temperatures) are prescribed while the model calculates the chemistry. The forcing winds can be taken from a general circulation model, but there are advantages in taking the winds and temperatures from meteorological analyses. In this case the chemical fields calculated by the CTM can be compared directly with observations at a given time/location. Thus, off-line CTMs are very powerful tools for diagnosing past changes in the atmosphere.

While the principle of using meteorological analyses to force an off-line CTM is straightforward, there are a number of issues and potential problems which need to be carefully addressed. The realism of the chemical fields calculated by the CTM will often be limited by how this is done. The effect of the meteorological analyses on the CTM simulations can be divided into two categories:

- How model uses the analyses.
- The quality of analyses themselves.

This paper discusses aspects of these issues with reference to the our experiences in developing and using the TOMCAT and SLIMCAT 3D CTMs.

2 TOMCAT and SLIMCAT CTMs

The TOMCAT and SLIMCAT off-line 3D CTMs are two related models which share much common code. The distinction between the two models is the vertical coordinate: TOMCAT uses a hybrid σ-pressure coordinate while SLIMCAT uses a hybrid σ-θ one. Because it uses isentropic (θ) levels in the stratosphere, SLIMCAT has the option (default) for calculating the vertical (diabatic) transport by using heating rates. The following table summarises the two models.

	TOMCAT	SLIMCAT
Vertical coordinate	σ-p	σ-θ
Horizontal coordinate	Longitude - regular Latitude - anything	*as TOMCAT* *as TOMCAT*
Horizontal Resolution Vertical Resolution	Variable Variable	*as TOMCAT* Variable
Winds	Spectral or Grid point (u,v,w)	*as TOMCAT*
Advection Scheme	Default: Prather [1986] Other: Semi-Lagrangian	*as TOMCAT*

For consistency, the dynamics of the CTM ought to reproduce that of the forcing meteorological model. However, other considerations mean that it is desirable (often necessary) for the CTM to be run at a different resolution or with different coordinates.

3 Issues

3.1 Vertical Coordinate

There are a number of possible vertical coordinates that can be used in an off-line CTM. This coordinate is, in general, completely independent of the forcing meteorological model, though care must be taken when averaging/interpolating fields between grids. Near the surface a terrain-following coordinate is useful and as the analyses contain surface pressure, a coordinate based on this is easy to employ. At higher altitudes (e.g. the stratosphere) a pressure coordinate is useful for keeping track of mass conservation. However, isentropic (θ) coordinates are the 'natural' system which give the true separation between horizontal and vertical motion.

The use of θ coordinates can help reduce the effects of numerical diffusion, i.e. give better effective resolution. Chipperfield *et al.* [1997] showed that a θ-coordinate model gave a much better simulation of polar ClONO2 than a p-coordinate version (which had excessive spurious mixing between air rich in ClO and air rich in NO_2). Also, θ-coordinate transport models can do a better representation of the tropical 'tape recorder' signal and age of stratospheric air than p-coordinate models which typically have the tape- recorder signal moving too fast and the air too young. As explained in Gregory and West [2002] in p coordinates variations in ascent can be two orders of magnitude greater than the mean ascent, and the advection scheme has to 'jiggle' the tracers back and forth; in θ coordinates the CTM is closer to just dealing with the mean ascent (see Thuburn, this issue).

3.2 Vertical Transport

In TOMCAT the vertical mass flux between model levels is diagnosed from the divergence of the horizontal mass fluxes. The divergence is integrated from the top of the model (usually 0 hPa) with the boundary condition that the mass flux is zero here. This procedure ensures mass balance between the horizontal and vertical winds. Care is taken to ensure that if the TOMCAT levels do not coincide with the analysis levels (e.g. ECMWF) the different vertical grid spacing does not affect the mass flux across any particular surface - i.e. the mass flux divergences are mapped on to the CTM grid in a way which preserves the integral.

In SLIMCAT the vertical transport can also be diagnosed from the integral of the horizontal mass flux divergence (though this time using the model θ coordinates). However, a prime motivation for developing

SLIMCAT was to allow the estimate of vertical transport in theta coordinates by diagnosing diabatic heating rates. SLIMCAT uses a radiation scheme (e.g. MIDRAD [Shine, 1987]) to calculate heating rates using the analysis temperatures and trace gas fields (e.g. O_3, H_2O, CO_2..) either from climatology or calculated by the model. In principle, this approach should then be able to diagnose the diabatic vertical transport contained in the analyses.

In practice there are some difficulties with this approach. Net heating rates diagnosed in this way do not preserve vertical mass balance (see Shine [1989]), i.e. the net vertical mass flux across a pressure surface is not zero. Therefore, some correction is needed to ensure this. As the only constraint is a global mass balance there are an infinite ways of achieving this which will lead to different local corrections to heating rates. Moreover, this approach of calculating the vertical mass flux in this way is not constrained by the horizontal (analysed) winds, which will also lead to a mass balance problem. If the net heating rates were available from the ECMWF model this could ensure the consistency between vertical and horizontal motion calculated in this way.

3.3 Mass Balance

It is a very desirable property of an atmospheric chemical transport model to conserve mass. For example, studies of the fate pollutant emissions where a fixed mass is emitted will be degraded if some of the pollutant mass is lost (or created!) through model artefacts. The term 'mass conservation' is used to cover alot of elements in an atmospheric model.

In SLIMCAT/TOMCAT the default Prather [1986] advection scheme conserves mass, although the alternative semi-Lagrangian scheme does not. However, a model which has a 'mass conserving' advection scheme may still not conserve mass overall because of errors in other processes. All-in-all, to ensure a 3D CTM conserves tracer mass a large number of individual processes need to be mass conserving.

At a given timestep the CTM reads in the analyses containing the horizontal winds (vorticity and divergence) and the surface pressure (p_s). Mass conservation is best addressed by using 'mass fluxes' rather than winds. Hence the analyses contain the information on the mass of atmosphere in a column (from p_s) and its rate of change (integral of mass flux divergence). By carefully ensuring that the conversion from analysed winds to the mass fluxes on the model grid are done in a conservative way, at a given time the CTM's mass transport can be in balance. (This is the correction addressed in Bregman *et al*. [2003] which has always been included in TOMCAT).

However, even the above is not enough to ensure full 'mass conservation' during a simulation because of the time discretisation. Typically analyses are available every 6 hours with no information at times in between. Although there will be global mass conservation the local mass in a box as a result of advection by the 6-hourly winds will not necessarily balance that diagnosed from the instantaneous p and T fields. Because of this there is a 'mass correction' in TOMCAT (and SLIMCAT). Every meteorological cycle (e.g. 6 hours) the mass of a model grid box is adjusted to that diagnosed from the analyses at that time, and the tracer masses scaled accordingly. This is the correction referred to in Stockwell and Chipperfield [1999] (and which is not addressed by Bregman *et al*. [2003]).

Finally, the mass of the atmosphere in the meteorological model used to produce the analyses (e.g. ECMWF) will not necessarily be conserved. Some changes are expected, e.g. due to changing H_2O content of the atmosphere, but other changes can occur to do model/parametrisation changes.

3.4 Subgridscale

Though not the specific subject of this workshop, it is worth noting that off-line CTMs may also include parameterisations of tropospheric ’sub-gridscale’ processes. (There is no additional transport terms needed in the stratosphere apart from advection by resolved winds). In the case of these tropospheric parameterisations (e.g. convection, boundary layer mixing) the off-line model should ideally be as consistent as possible with the meteorological model used to produce the forcing winds, i.e. it is desirable to also have fields such as convective mass fluxes from the meteorological model.

4 Data Assimilation

Section 3 outlined how on off-line CTM should use meteorological analyses. Even if the model uses these winds in an optimum way, the CTM simulations may still be unrealistic due to errors in the winds themselves. While the analyses can be expected to give a good representation of the rapid horizontal winds (e.g. location of the polar vortex on a given day) this may be a particular problem for simulating the slow meridional ’Brewer Dobson’ circulation. Chemical data assimilation can be used to correct the CTM for errors in the transport.

The technique of data assimilation is used routinely in numerical weather prediction to create meteorological analyses. Over the past 5 years or so, there has been increasing interest in applying similar techniques to observations of chemical species in the atmosphere. The assimilation of such observations, and the creation of ‘chemical analyses’ is expected to lead to better use of observations and to improvements in chemical models. The methods used for the assimilation of chemical observations can be divided into variational and sequential.

Chipperfield *et al.* [2002] included the sequential data assimilation scheme of Khattatov *et al.* [2000] into the SLIMCAT CTM. The nature of the species treated (e.g. long-lived tracers and members of chemical families) meant that it was necessary to impose constraints on the assimilation to ensure self-consistency (and to ensure consistency with the non-assimilated fields).

Chipperfield *et al.* [2002] showed that by assimilating HALOE CH_4, and using tracer-tracer correlations, the CTM simulation of long-lived tracers can be improved. A particular area of improvement is the representation of the sub-tropical barrier where the forcing winds (UKMO in this case) appeared to overestimate isentropic mixing. This procedure, of course, does not improved the analysed winds but simply corrects the model tracer fields. A better approach in the future would be to assimilate the long-lived tracers in the meteorological model.

5 Summary

The off-line chemical transport modelling community relies totally on the provision of high quality analyses, such as those from the ECMWF. When they have the analyses, such modellers then perform a wide range of comparisons between their models and observations which reveals important information about the quality of the winds and temperatures. This information should be available to the meteorological agencies.

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