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A fluctuations scheme in NAME III

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Report on the development of a scheme for predicting concentration fluctuations in NAME III.

Introduction

This report discusses a fluctuations scheme for predicting concentration fluctuations within the framework of the NAME III dispersion model. The NAME III fluctuations scheme is based on the scheme developed by David Thomson for use in the ADMS modelling system (see ADMS documentation [1, 2, 3] and related literature [4]). However, there are some significant differences between the two implementations of the scheme which essentially arise out of the contrast between the Eulerian approach of the ADMS model and the Lagrangian setting of the NAME III particle-puff trajectory model. Owing to such differences in the two implementations, we should not expect the fluctuations scheme to produce identical results in NAME III and ADMS for any particular dispersion scenario, although we would anticipate that any discrepancies between the two schemes should be small.

1 What does the NAME III fluctuations scheme predict?

The fluctuations scheme in NAME III aims to predict two aspects of the concentration fluctuations: (a) the standard deviation of concentration at each 'receptor' grid-point, and (b) the probability distribution at each grid-point (expressed either as probabilities of exceeding specified concentration thresholds or as percentiles of concentration). Strictly speaking here, constructing the probability distribution in (b) is an extension of the calculation in (a) since modelling the probability distribution requires an estimate of the mean concentration and standard deviation at each location.

The standard deviation σ_c of the concentration fluctuations is processed as a 4-d field in NAME III. That is, it is requested (either by the user or internally) using a field requirement (Type :: FieldReq_) and constructed as a function of x, y, z (spatial position) and t (time) with the values stored in a 4-d array (Type :: Field_). The calculation requires several extra fields to be available on the same grids, viz. mean concentration, average travel time and X-Stats (particle displacement statistics as a function of travel time). The fluctuations code separately calculates an estimate of σ_c at each individual grid-point location at each time; further details of the calculation are presented later.

Two special derived types have been introduced to allow the processing of probability distributions in NAME III. A probability distribution (constructed as exceedence probabilities or percentiles) is requested by the user as a pdf requirement (Type :: PdfReq_). It is constructed as a function of x, y, z (spatial position), t (time) and p (threshold) with the values stored in a 5-d array within the pdf output (Type :: Pdf_). The calculation of a pdf requires the mean concentration $\overline{c}$ and standard deviation σ_c fields to be available on the necessary spatial and temporal grids. For each individual grid-point location, the fluctuations scheme calculates the parameters of a clipped Gaussian distribution which matches these predicted values of $\overline{c}$ and σ_c at each time. Then exceedence probabilities or percentiles are constructed as appropriate.

Currently the NAME III fluctuations scheme can only predict concentration statistics for a *single continuous point source*. It should be possible to extend this to consider finite-duration releases from a point source, or continuous releases from more complex source geometries and multiple sources. The present scheme produces estimates of the fluctuations statistics of the instantaneous concentrations and, in principle, is also able to model the time-averaged concentrations (although, in practice, other parts of the NAME III code do not support the time-averaging option yet).

2 Code structure of the NAME III fluctuations scheme

The NAME III fluctuations scheme makes some use of version 3.0 of the ADMS fluctuations code (specifically, it uses the version submitted by David Thomson to CERC for inclusion in ADMS 3.0 as opposed to the actual source code of the ADMS 3.0 model maintained by CERC). The original procedures were written in fixed-format Fortran 77 and hence some amendments have been necessary (mainly to the formatting of the routines) in order to compile them as Fortran 90 procedures. Note that any material changes (i.e. not just formatting issues) to the existing code are stated in the comments section at the start of each procedure.

The routines required by our new fluctuations scheme are contained in a module, the *fluctuations module*, stored in the file *Fluctuation.F90*. These include some new 'front-end' procedures that provide an interface between the NAME III environment and the ADMS-style routines. Note that some inputs to the scheme are calculated differently in NAME III from the approach used by ADMS; for example, using estimates of the plume spread σ_y and σ_z calculated directly from particle trajectories (X-Stats information) rather than via the mean concentration field.

The detailed structure of the fluctuations module is summarised by the tree diagram in Figure 1. From the viewpoint of the overall NAME III structure, there are three routines that are called from outside the fluctuations module:

CalculatePlumeSigmas (calculates estimates of the standard deviations σ_y and σ_z of particle displacements at a given travel time)

CalculateSigmaC (calculates an estimate of the standard deviation σ_c of the concentration fluctuations at one grid-point location at a given time)

CalculatePdf (calculates estimates of exceedence probabilities or percentiles of the concentration pdf given a mean and standard deviation of the probability distribution)

These top-level procedures have been declared public and are available to the wider NAME III code; all other procedures in the fluctuations module are private to that module and cannot be accessed externally (this means any changes to these routines will be transparent to the rest of the code). The top-level routines listed above are called from the Output module during processing/outputing of the fluctuation requirements.

3 Future developments

At the time of writing this document, the fluctuations scheme in NAME III has not been tested or tuned in any way. It is recommended that the next phase of development should consider an extensive testing programme for our new scheme. There is also a need to provide fuller documentation of the scheme (such as a user guide).

References

[1] Thomson, D.J., 'The fluctuations module', *ADMS Technical Specification paper P13/01E/92*, CERC, 1992.

[2] Thomson, D.J., 'Averaging time and fluctuations in ADMS versions 1 and 2', *ADMS Technical Specification paper P13/03C/96*, CERC, 1996.

[3] Thomson, D.J., 'Concentration fluctuations in ADMS 3, including fluctuations from anisotropic and multiple sources', *ADMS Technical Specification paper P13/07D/00*, CERC, 2000.

[4] Thomson, D.J., 'A practical model for predicting the fluctuation statistics of dispersing material', in preparation.

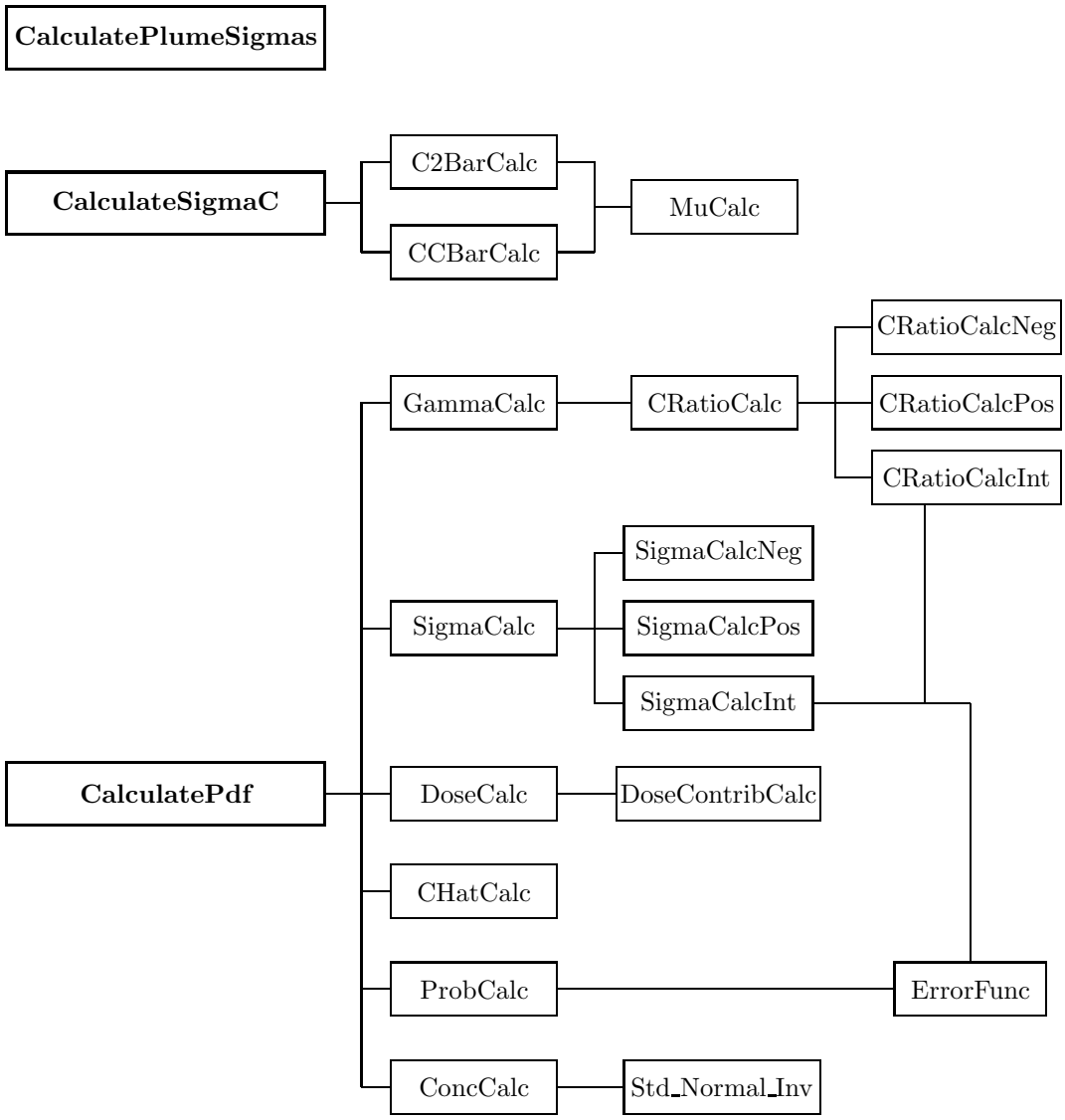

Figure 1: the structure of the fluctuations module in *Fluctuation.F90*