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Two types of atmospheric models: Eulerian and Lagrangian are briefly described, followed by the introduction of Lagrangian Particle Dispersion Model (LPDM) NAME model as a primary tool used in this investigation. Reasons for choosing NAME are put forward in the end.

Atmospheric models: technical representation

Atmospheric models are used widely to calculate and predict physical processes and the transport within the atmosphere. Two main types of numerical models are distinguished: Eulerian and Lagrangian. These models differ with respect to the perspective of atmospheric motion.

Eulerian models define specific reference points in a gridded system that monitors atmospheric properties, including temperature, pressure, chemical concentration of tracers, over time. Being the representative of the Eulerian model, the Unified Model divides the world up into fixed grid cells [1, 2] which allows for modelling the interactive chemistry within the atmosphere, regarded as a three-dimensional single fluid, and applying well-developed convection parameterisation scheme to represent convective motions.

Unlike Eulerian models, Lagrangian models take the perspective of a finite element or so-called 'air parcel'. Over time both the position and properties of this air parcel are calculated according to the mean wind field data. The path along which air parcel travels is called its trajectory. It can be expressed as a differential equation (4.1). Advanced equation for the trajectory contains two components: mean winds and random turbulence.

In general, while particle is released at time t at prescribed rate, the new position is determined at time $(t+\Delta t)$ by relation:

$$(4.1) \quad \Delta X / \Delta t = A\,[X(t)]$$

with t - time, X - position vector and A - wind speed vector. For the initial position, X_0, at time, t_0, of the parcel, the path is determined through equation (4.2) [2,3]:

$$(4.2) \quad X_0\,(t=t_0) = X_0(X,t)$$

Thus, air parcels may be followed either forward (forward trajectories) or backward (backward trajectories) in time. These initial coordinates are called Lagrangian coordinates, which may be calculated through the following equations:

$$(4.3) \quad x(t+\Delta t)=x(t) + [u(t)+u_r(t)]\Delta t$$
$$(4.4) \quad y(t+\Delta t)=y(t) + [v(t)+v_r(t)]\Delta t$$
$$(4.5) \quad z(t+\Delta t)=z(t) + [w(t)+w_r(t)]\Delta t$$

These equations are enriched with new variables: u_r, v_r and w_r being the corresponding grid-scale velocity components. These grid-scale velocity components are iteratively determined as:

$$(4.6) \quad u_r(t) = u_r (t- \Delta t) R_u (\Delta t) + u_s(t-\Delta t)$$
$$(4.7) \quad v_r(t) = v_r (t- \Delta t) R_v (\Delta t) + v_s(t-\Delta t)$$
$$(4.8) \quad w_r(t) = w_r (t- \Delta t) R_w (\Delta t) + w_s(t-\Delta t)$$

Following variables: R_u, R_v and R_w stand for Lagrangian autocorrelation functions for each velocity component, and u_s, v_s and w_s are the random fluctuations of the velocity components. Lagrangian correlation functions are calculated from

$$(4.9) \quad R_u(\Delta t) = e^{-(\Delta t)/Tu}$$
$$(4.10) \quad R_v(\Delta t) = e^{-(\Delta t)/Tv}$$
$$(4.11) \quad R_w(\Delta t) = e^{-(\Delta t)/Tw}$$

These formulae (4.9, 4.10, 4.11) use variables: T_u, T_v and T_w, which are defined as the Lagrangian time scales for the corresponding velocity components. Once the calculations of Lagrangian time scale, autocorrelation functions, and the range of velocity fluctuations as Gaussian standard deviations from the mean are determined, a random velocity fluctuation is generated and used to calculate the new particle velocity, and hence the new particle position is established. [4]

NAME model: background and applications

Numerical Atmospheric Dispersion Modelling Environment (NAME) is a Lagrangian particle dispersion model developed by the UK Meteorological Office [42]. It relies on the motion of abstract particles through the model atmosphere subject to a combination of mean wind fields calculated by the Meteorological Office Unified Model and a random walk turbulence scheme [1, 3]. Meteorological input, including gridded winds, temperature and cloudiness, required for the running of NAME is calculated by incorporating a vast amount of observational data at three hourly intervals into a forecasting system. This process is continuously repeated to produce a three-dimensional analysis of the state of the atmosphere defined by meteorological variables. It is these UKMO meteorological data variables that are incorporated into NAME and are used to calculate particle positions and wind vectors.

Each particle released represents a mass of released substance [4]. It follows single steps, starting from the release of targeted species being simulated by a number of discrete particles. Then, each particle follows the individually computed path; specific parameterisation to include chemistry, diffusion, dynamics and decay can be applied at this stage. At the end of simulation, the density of particles, as one of the NAME output options, is calculated to obtain concentrations of released particles.

The first use of NAME was to monitor the emergency response of pollutant dispersion and air quality forecasting. The model was developed briefly after the Chernobyl explosion in 1986 and used to track the trajectory of radioactive dust plumes over Europe, resultant from the nuclear accident [1]. Since then, NAME model has been used widely to simulate dispersion of passive tracers, radionuclides and plumes mostly because they are well suited to problems in which high concentration gradients are involved. Giving fast response, as opposed to Eulerian models, is what makes NAME model a very useful predictive tool for assessment of emission releases [1]. NAME model applications will be exploited in the CAST 2014 campaign planning and the interpretative studies.

Assessment of turbulence and convection scheme in NAME

Multiple complex processes such as orographic lifts, winds experiencing friction along the Earth's surface, movement of unstable air masses are the reason why the atmosphere is in a constant state of turbulence (mixing). Regarding atmospheric models, turbulence is difficult to represent.

In NAME, the fundamental equation (4.3) for each particle trajectory can be expanded by adding more factors, which incorporate the advection scheme: wind speed, small-scale turbulence and low-frequency horizontal meandering. (Equation 4.12) [3]. This advection scheme shows how particles are advected at each time step, expressed as:

$$x(t+\Delta t)=x(t) + [u(x((t))+u'(x(t))+ u_l'(x(t))]\Delta t \quad (4.12)$$

where x is the particle position vector, u(x(t))the wind velocity vector, u'(x(t)) the turbulent velocity vector for small scale turbulence, ul'(x(t)) the velocity vector for low-frequency horizontal meandering, and Δt the timestep [2]. The turbulent velocity vector, u'(x(t)), is defined by a random walk formula which has horizontal and vertical components depending on velocity variances (σ_u^2 and σ_w^2), Lagrangian timescales (τ_u and τ_w) and a random Gaussian variable of zero mean and unit variance (r_t) (the standard random walk formulae for the turbulent velocity components in the horizontal (Equation 4.13) and vertical (Equation 4.14); first and second right-hand terms represent a memory of previous motion and a new random perturbation, respectively; 'drift velocity' which prevents particles from collecting at levels of small σ_w^2 is represented by the last term in 4.14 - for homogenous turbulence profiles, drift velocity term is negligible).

$$u'_{t+\Delta t} = u'_t(1-\frac{\Delta t}{\tau_u}) + (\frac{2\sigma_u^2 \Delta t}{\tau_u})^{1/2} r_t \quad (4.13)$$

$$w'_{t+\Delta t} = w'_t(1-\frac{\Delta t}{\tau_w}) + (\frac{2\sigma_w^2 \Delta t}{\tau_w})^{1/2} r_t + \frac{\Delta t}{\sigma_w}\frac{\delta \sigma_w}{\delta z}(\sigma_w^2 + w_t'^2)$$

(4.14)

Convection, defined as the latent heat driven vertical uplift of air, is another component of the atmosphere which is difficult to represent in the atmospheric models. Simulations made in this project had NAME convection scheme off, as previous NAME runs displayed similar results with convection scheme mode-on and mode-off. Convection component parameterisation was implicit within the Unified Model three-dimensional wind fields. UM wind fields treat convection as the averaged output of convective and descending motions over the grid box of certain resolution (in this case it is 25 km). This method does not represent the individual convective events which are responsible for the very rapid transport of tracers from the boundary layer to the TT in a hourly-up-to-daily timescale. Representation of convection scheme for NAME is currently under the UKMO research. In this project, convection component is averaged out in the 3D UM wind fields as the vertical velocity. Further in Results and Analysis section, data assessment is based on convection due to its well-known presence over the investigated Pacific region, though no statement on individual convective motions can be made. Convection stands as the main vertical transport mechanism for air masses and VSLSs over the Pacific Ocean area [4].

It is worth assessing how accurate the trajectory models are in general. Based on the Stohl et al, 1998, review paper on the accuracy of trajectory models, models which incorporated a three-dimensional wind fields and turbulent mixing scheme produce better representation of transportation, although errors of around 20% of the distance shall be anticipated [2]. However, Stohl did emphasise that trajectory error varied greatly on individual basis [2].

The most common way to assess how accurate the trajectory model is appears to be a comparison with a reference trajectory whose origin is known and whose quantity can be easily measured. Tracer experiments are usually carried out with tracers of opportunity rather than with artificially deployed tracers which require pre-planning and extra cost [2].

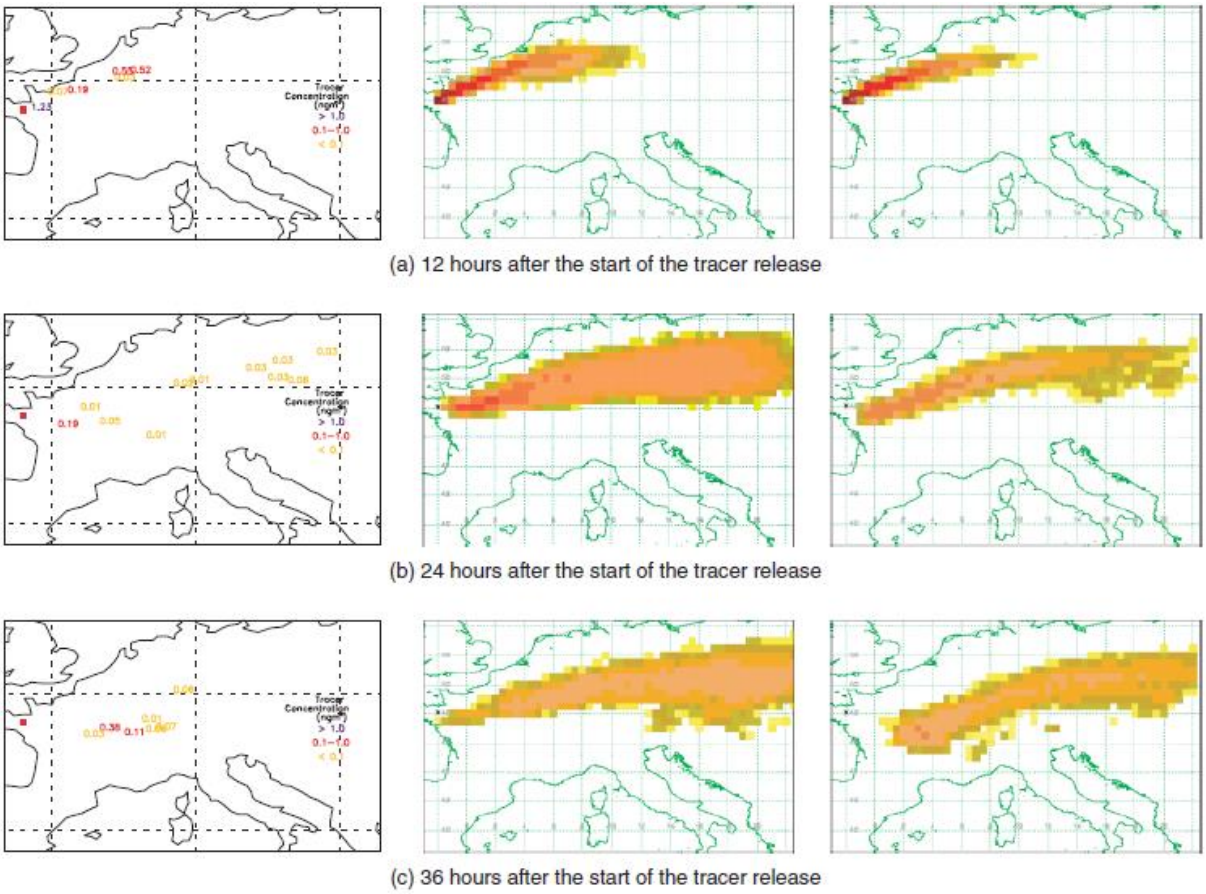

Figure 1. Surface tracer concentrations 12, 24 and 36 hours after the start of the tracer release. Left: observed surface concentrations (ngm^{-3}), the release dot indicated by red dot. Centre: model output of surface concentrations (ngm^{-3}) using a 0.442° spatial resolution. Right: model output of surface concentrations (ngm^{-3}) using a 0.110° spatial resolution. Both model outputs use a 30-minute temporal resolution and are plotted on a 0.5° resolution grid for comparison [5].

Based on the studies by Davis and Dacre, 2009 [5], NAME model as a dispersion model successfully predicted the transport simulations of emissions release species. Moreover, increasing the temporal and spatial resolution of the meteorological input data significantly led to improvements in the simulation (Figure 1). Another improvement involves the number of particles released - despite being more computationally demanding, the larger number of particles, the finer the resolution is [5].

Use of NAME model in flight planning

NAME model will be used specifically in the CAST campaign planning and the interpretative studies. Both forward and backward NAME modes will be exploited. NAME will be the primary tool suitable for coordinating the GH and BAe-146 flight tracks so GH will be flying through the air which ascended from the lower troposphere, from the region previously sampled by BAe-146. This will essentially be assumed to generate vertical profiles of the West Pacific troposphere, covering the entire troposphere and the TTL.

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