Turbulence modelling in large-eddy simulations of the cloud-topped atmospheric boundary layer

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1. Motivation and objectives

This paper discusses turbulence modelling in large-eddy simulations of the cloud-topped atmospheric boundary layer. While our primary focus is on simulations of stratocumulus clouds, most of the discussion is also relevant to other types of cloud. Stratocumulus clouds were chosen because of the important role they play in the Earth's climate, and because the fluid dynamics associated with these clouds has a number of features which researchers have found difficult to model accurately.

Marine stratocumulus clouds cover extensive areas off the west coasts of the large continents in the subtropics. Their presence in these regions is the result of strong static stability due to low sea-surface temperatures and to atmospheric subsidence associated with the descending branch of the Hadley circulation. Due to their high albedo, stratocumulus clouds have a significant effect on the Earth's radiative heat budget. From analysis of satellite data, Klein & Hartmann (1993) calculated top-of-the-atmosphere values of the order of -100 Wm^{-2} for the net cloud radiative forcing over stratocumulus decks. Randall *et al.* (1984) estimated that the global cooling resulting from a 4% increase in areal coverage by marine stratocumulus clouds would offset the expected warming from a doubling of atmospheric carbon dioxide. In addition to their role in the Earth's radiation budget, stratocumulus clouds also affect the dynamics of the atmosphere and oceans. Miller (1997), for example, found that stratocumulus clouds provide a negative-feedback mechanism which reduces the intensity of tropical convection and damps the tropical atmospheric circulation. Similarly, stratocumulus clouds over oceans in the subtropics reduce sea-surface temperatures in these regions by lowering the net surface heat flux. Most atmospheric general circulation models (GCMs) underpredict the amount of subtropical marine stratocumulus (Jakob 1999). In coupled atmosphere-ocean models, this can lead to positive sea-surface temperature biases of up to 5K. Such modelling errors have been shown to have a significant influence on both the predicted circulation (Nigam 1997) and the global radiation budget (Slingo 1990).

The use of large-eddy simulation (LES) to study the planetary boundary layer dates back to the early 1970s, when Deardorff (1972) used a three-dimensional simulation to determine velocity and temperature scales in the convective boundary layer. In 1974 he applied LES to the problem of mixing-layer entrainment (Deardorff 1974) and in 1980 to cloud-topped boundary layers (Deardorff 1980). Since that time the LES approach has been applied to planetary boundary layer problems by numerous authors (see for example Moeng 1986; Mason & Derbyshire 1990; Schumann & Moeng 1991*a*,*b*; Brown *et al.* 1994; Saiki *et al.* 2000; Stevens & Bretherton 1999; Stevens *et al.* 2001)

The popularity of the LES technique in atmospheric research is due in part to the difficulties involved with obtaining sufficient field data to develop and test theories concerning the structure and dynamics of the planetary boundary layer. Large-eddy simulations provide three-dimensional time-evolving velocity and scalar fields at a resolution limited only by computational resources. As such, LES is often used to isolate particular physical processes of interest such as entrainment across the inversion (Stevens *et al.* 2000) or transition from one type of cloud to another (Wyant *et al.* 1997). It is also used to generate databases of different atmospheric flow regimes in order to evaluate, refine and develop parameterisation schemes for use in large-scale models (eg. Lappen & Randall 2001). At the other end of the spectrum, LES is used as a platform on which to develop reliable models of cloud microphysics and radiation (Ackerman *et al.* 2000).

In spite of an increasing reliance on LES as a tool for developing and testing cloud theories and models, there is still considerable uncertainty concerning the fidelity of the simulations themselves. While LES has been shown to be relatively robust for simple cases such as simulations of a clear, convective boundary layer (Mason 1989), model intercomparisons for more complex cases have shown large variations in predictions of important statistics and bulk parameters. For example, in the 1995 Global Energy and Water Cycle Experiment (GEWEX) Cloud System Studies (GCSS) model intercomparison, Bretherton *et al.* (1999) compared simulations of a smoke cloud beneath a temperature inversion. Radiative cooling at the top of the cloud drives convection, which leads to entrainment across the inversion and to growth of the boundary layer. The authors found that the entrainment rates and other statistics predicted by the various LES codes differed by up to a factor of two. Similar entrainment processes occur at the top of stratocumulus clouds, although with the added complexity of latent-heat transfer due to condensation and evaporation of cloud droplets. A second example is the recent intercomparison of simulations of trade-wind cumuli by Stevens *et al.* (2001). Here again, important parameters such as stratiform cloud fraction and the variance of total-water mixing ratio were found to be highly sensitive to the choice of numerical method, spatial resolution and subgrid-scale turbulence model. Bulk parameters such as boundary-layer height, entrainment rate and cloud fraction are important variables in the parameterisations used in global circulation models. It is therefore essential that LES be made robust in its prediction of these variables if it is to be used as a tool for development and tuning of parameterisations for large scale models.

One of the main problem areas in large-eddy simulations of clouds is the accurate representation of processes occurring close to an inversion. Here, strong stable stratification reduces the size of the energetic eddies considerably, so that they are generally poorly resolved by simulations. Bretherton *et al.* (1999), for example, identify an "undulation" length scale given by $z_u = z_i/Ri$ (where z_i is the height of the inversion and Ri the Richardson number) which is of the order $5 - 10$ m in a strong inversion. Meanwhile, the grid-cell dimensions used for large-eddy simulations of the planetary boundary layer are typically 25 - 100 m, although, with advances in computer technology, highly-resolved simulations are now becoming possible. Stevens *et al.* (2000), for example, recently performed stratocumulus simulations at grid sizes down to 8 m in the horizontal directions by 4 m in the vertical direction. Even at this resolution, however, they found the predicted entrainment rate and entrainment efficiency to be sensitive to the subgrid model and numerics. A second reason for the difficulties encountered in modelling processes close to an inversion is that the stable stratification tends to damp vertical motions, making the turbulence in this region much more anisotropic than in an unstratified environment. Consequently turbulence models often use one or more corrections to account for the effects of stratification. In clouds, additional buoyancy sources result from energy transfer due to condensation and evaporation of water, and some authors (eg. MacVean & Mason (1990)) recommend applying further corrections to account for these processes.

An alternative to using such corrections is to adopt a dynamic approach, in which the parameters in the subgrid-scale turbulence model are computed at each point in space and time using information contained in the resolved velocity and scalar fields. This approach removes the need to make modelling decisions concerning the coefficients and length scales in the subgrid model. It also removes the need for corrections to account for buoyancy effects since all this information is obtained directly from the resolved flow field.

The dynamic approach, first proposed by Germano *et al.* (1991), has been used with considerable success for complex engineering flows (see Boivin *et al.* 2000; Branley & Jones 2001, for example), however its application to atmospheric flows has been limited. This is due in part to arguments by authors such as Mason & Brown (1999) to the effect that the dynamic procedure is inappropriate for atmospheric applications. These arguments are based on the premise that the dynamic procedure requires a filter cut-off wavenumber in the inertial subrange. This is incorrect. The theory behind the dynamic procedure assumes only that the same subgrid model can be used for both the resolved field and the test-filtered field. It is in fact the Smagorinsky model (Smagorinsky 1963), which is widely used for atmospheric simulations even at very coarse resolutions, whose derivation assumes resolution of the inertial subrange.

Bohnert (1993) tested the dynamic procedure in combination with the Smagorinsky model for simulations of clear and cloud-topped planetary boundary layers. The simulations were performed at a Reynolds number lower than that of a realistic atmospheric boundary layer and used simple parameterisations for cloud physics and radiation. In order to stabilise the model, it was necessary to average the calculated coefficient field over horizontal planes. Nevertheless, these results are encouraging. The dynamic model gave results comparable to, or better, than those obtained using the standard constant-coefficient Smagorinsky model with a Richardson-number correction.

The objective of the present study is to test the dynamic procedure in large eddy simulations of a marine stratocumulus cloud deck. The simulations will be performed at realistic Reynolds and Rayleigh numbers, with conditions matching those measured during the 2001 DYCOMS-II field experiment. This test case has a number of the features discussed above which typically cause difficulties in cloud simulations, namely strong stable stratification, and buoyancy sources within the cloud due to radiation, condensation and evaporation of water droplets. Following Zang *et al.* (1993), we use the mixed model as a base subgrid model, rather than the Smagorinsky model. The mixed model is a combination of the scale-similarity model of Bardina *et al.* (1980) and the Smagorinsky model. The dynamic mixed model of Zang *et al.* has been found to be more stable than the dynamic Smagorinsky model and it is hoped that its use will remove the need for averaging over horizontal planes. This is important in the present case, since horizontal planes close to the cloud-top contain both stably and unstably stratified regions. Horizontal averaging of the calculated model parameters would prevent the dynamic procedure from distinguishing between these two fundamentally different flow regimes.

The author is currently implementing the dynamic mixed model in the LES code, DHARMA, written by David Stevens. This code has performed well in model intercomparisons (see Bretherton *et al.* 1999; Stevens *et al.* 2001) and has also been used for a number of high-resolution simulations (Stevens & Bretherton 1999; Stevens *et al.* 2000, 2002) where it was shown to scale well on massively parallel architectures. In addition, the code has the option to use either standard parameterisations for radiation and cloud microphysics, or the more complex models of Ackerman *et al.* (1995), which treat the cloud microphysics explicitly and include a detailed treatment of radiative transfer.

In the following, we describe the governing equations, the numerical methods, and the parameterisations and models used in the DHARMA code. We rewrite the governing equations in filtered form and outline a turbulence closure based on the dynamic mixed model of Zang *et al.* Finally we discuss the test case and simulations which will be used to assess the performance of this approach to turbulence modelling in numerical simulations of clouds.

2. Governing equations

The basic equations governing the dynamics of the cloud-topped atmospheric boundary layer comprise equations for conservation of mass, momentum, energy and total water. In addition, radiative heat transfer and cloud microphysics must also be modelled. Cloud microphysics refers to the transitions between vapor, liquid and solid-phase water and the dynamics of the liquid and solid-phase components.

The governing equations are written in the anelastic form of Ogura & Phillips (1962) in which the thermodynamic variables such as pressure p are decomposed into an isentropic base state p_0 (corresponding to a uniform potential temperature θ_0) and a dynamic component. Following Clark (1979), the dynamic component is further decomposed into an initial environmental deviation in hydrostatic balance p_1 and a time-evolving dynamic perturbation p_2 to give

$$p(x, y, z, t) = p_0(z) + p_1(z) + p_2(x, y, z, t). \tag{2.1}$$

The resulting continuous equations written in Cartesian tensor notation are

$$\frac{\partial u_i}{\partial t} + \frac{1}{\varrho_0}\frac{\partial(\varrho_0 u_i u_j)}{\partial x_j} = -\frac{\partial \Pi}{\partial x_i} + g_i\frac{\theta_{v2}}{\theta_0} + H^{sub}_{u_i} + H^{gw}_{u_i} + H^{coriolis}_{u_i}, \tag{2.2}$$

$$\frac{\partial \theta_l^*}{\partial t} + \frac{1}{\varrho_0}\frac{\partial(\varrho_0 \theta_l^* u_j)}{\partial x_j} = H^{sub}_{\theta_l^*} + H^{LS}_{\theta_l^*} + H^{gw}_{\theta_l^*} + H^{rad}_{\theta_l^*}, \tag{2.3}$$

$$\frac{\partial q_t}{\partial t} + \frac{1}{\varrho_0}\frac{\partial(\varrho_0 q_t u_j)}{\partial x_j} = H^{sub}_{q_t} + H^{LS}_{q_t}, \tag{2.4}$$

$$\frac{\partial(\varrho_0 u_j)}{\partial x_j} = 0. \tag{2.5}$$

Here u_i is the velocity component in the i direction, ϱ is the density, Π is the perturbation pressure p_2/ϱ_0, g_i is the acceleration due to gravity, q_t the total water mixing ratio and $\theta_l^* = (\theta_l - \theta_0)/\theta_0$ is a scaled liquid-water potential temperature. Total-water mixing ratio is the sum of the liquid and vapour mixing ratios,

$$q_t = q_c + q_v = \frac{\varrho_c + \varrho_v}{\varrho_d}, \tag{2.6}$$

where ϱ_c, ϱ_v and ϱ_d are the density of the condensed water, the water vapour and the dry air respectively. Liquid-water potential temperature is defined as

$$\theta_l = \theta - \frac{L q_c}{C_{pd}\pi_0}. \tag{2.7}$$

Here L is the latent heat of vaporisation, C_{pd} is the specific heat at constant pressure for dry air and $\pi_0 = \left(\frac{p_0}{p_{ref}}\right)^{\frac{R_d}{C_p}}$ with p_{ref} a reference pressure and R_d the gas constant of dry air. The virtual potential temperature θ_v appearing in the buoyancy term of the momentum equations is given by

$$\theta_v = \theta + \theta_0 \left[\left(\frac{R_d}{R_v} - 1 \right) q_v - q_c \right], \tag{2.8}$$

where R_d and R_v are the gas constants of dry air and water vapor respectively.

The interior forcings H are body forces which parameterise the effects of: subsidence H^{sub}; horizontal large scale advective tendencies H^{LS}; and the Coriolis force $H^{coriolis}$. In addition, a Rayleigh damping term H^{gw} is applied to the top third of the domain to absorb gravity wave energy. The subsidence and large-scale advective tendencies result from the fact that the LES domain is not isolated, but is embedded within the global circulation. These forcings are generally specified as functions of z/z_i where z is the vertical height, and z_i is the height of the inversion. As an example, in the case of the trade-wind cumulus intercomparison of Stevens *et al.* (2001), the subsidence velocity w_{sub} was specified to vary linearly between 0 at the surface and 6.5 mm s^{-1} at z_i. The subsidence forcings then become,

$$H^{sub}_{u_i} = w_{sub} \frac{\partial u_i}{\partial z}, \tag{2.9}$$

$$H^{sub}_{\theta_l^*} = w_{sub} \frac{\partial \theta_l^*}{\partial z}, \tag{2.10}$$

$$H^{sub}_{q_t} = w_{sub} \frac{\partial q_t}{\partial z}. \tag{2.11}$$

The large-scale advective tendencies were specified as

$$\begin{aligned} \left[\frac{d\theta_l^*}{dt}\right]_{LS} &= -1.1575 \times 10^{-5} \left(3 - \frac{z}{z_i}\right) Ks^{-1}, \\ \left[\frac{dq_t}{dt}\right]_{LS} &= -1.58 \times 10^{-8} \left(1 - \frac{z}{z_i}\right) s^{-1}, \end{aligned} \tag{2.12}$$

for $z < z_i$. Above the inversion, the terms were linearly reduced to zero over a distance of 300 m. The Coriolis term is given by

$$H^{coriolis} = [fv, -fu, 0], \tag{2.13}$$

with the Coriolis parameter $f = 2\omega \sin\phi$, where ω is the angular velocity of the Earth and ϕ is the latitude.

3. Filtered equations

In LES, a spatial filter is applied to the governing equations. The application of a spatial filter G to a function f is defined as

$$\overline{f}(\mathbf{x}) = \int_\Omega G(\mathbf{x} - \mathbf{x}'; \overline{\Delta}(\mathbf{x})) f(\mathbf{x}') d\mathbf{x}', \tag{3.1}$$

where $\overline{\Delta}$ is the characteristic width of the filter. A box filter is used here as it fits naturally into the finite volume discretisation. The filter width is written in terms of the cell dimensions, $\overline{\Delta} = 2(\Delta_x \Delta_y \Delta_z)^{1/3}$.

Filtering the equations for conservation of momentum and mass yields

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{1}{\varrho_0}\frac{\partial(\varrho_0 \overline{u}_i \overline{u}_j)}{\partial x_j} = -\frac{\partial \overline{\Pi}}{\partial x_i} + g_i \frac{\overline{\theta}_{v2}}{\theta_0} - \frac{\partial \tau_{ij}}{\partial x_j} + \overline{H}^{sub}_{u_i} + \overline{H}^{gw}_{u_i} + \overline{H}^{coriolis}_{u_i}, \tag{3.2}$$

$$\frac{\partial(\varrho_0 \overline{u}_j)}{\partial x_j} = 0. \tag{3.3}$$

Here it is assumed that the isentropic fields ϱ_0 and θ_0, and the forcings H, vary slowly in space, so that extra moments resulting from the application of the filter to these terms may be neglected. The extra term in the momentum equations is the subgrid-scale stress or SGS tensor,

$$\tau_{ij} = \left(\overline{u_i u_j} - \overline{u}_i \overline{u}_j\right), \tag{3.4}$$

which represents transport of momentum by subgrid-scale turbulence. This term must be modelled to close the equations. The Smagorinsky eddy-viscosity model (Smagorinsky 1963) assumes that the anisotropic part of the SGS stress tensor is proportional to the large scale strain rate tensor,

$$\tau_{ij} - \frac{1}{3}\delta_{ij}\tau_{kk} = -2\nu_T \overline{S}_{ij}, \tag{3.5}$$

where

$$\overline{S}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right), \tag{3.6}$$

and that the eddy viscosity ν_T is itself a function of strain rate and filter size,

$$\nu_T = C\overline{\Delta}^2 \left|\overline{S}\right|. \tag{3.7}$$

Here $\left|\overline{S}\right| = \sqrt{2\overline{S}_{ij}\overline{S}_{ij}}$ and C is the dimensionless model coefficient. In the basic model, C is specified *a priori* and is often written as the Smagorinsky coefficient $C_s = \sqrt{C}$. For incompressible flows, the isotropic part of the SGS stress tensor, τ_{kk}, is absorbed into the pressure term.

For atmospheric simulations this basic model must be modified to account for the effects of stratification. This typically takes the form of a correction to the eddy viscosity to give

$$\nu_T = C\overline{\Delta}^2 \left|\overline{S}\right| \sqrt{1 - Ri/Pr_T}, \tag{3.8}$$

where $Ri = N^2/|S|^2$ is a gradient Richardson number and Pr_T is a turbulent Prandtl number. The buoyancy frequency N for dry air is defined as

$$N^2 = -\frac{g}{\theta}\frac{\partial \theta}{\partial z}. \tag{3.9}$$

In the DHARMA code, this formula is modified, following MacVean & Mason (1990), to include the effects of evaporation and condensation.

As discussed in the previous section, while these corrections have been shown to give good results for the relatively simple flows for which they were derived, in more complex flows the results are often highly sensitive to the choice of model coefficients and length scales. Apart from the need to set the model coefficient and length scale *a priori*, the Smagorinsky model has a number of other problems.

(a) The model assumes that the principal axes of the SGS stress tensor are aligned with

the resolved strain-rate tensor whereas analysis of DNS results has shown this not to be the case.
(b) The model does not predict the correct asymptotic behaviour near a solid boundary or in laminar/turbulent transitions.
(c) The model does not allow SGS energy backscatter to the resolved scales.

To overcome item (a) in this list, Bardina *et al.* (1980) proposed a model based on an assumption of similarity between the unresolved scales and the smallest resolved scales. In their "scale similarity model" the subgrid-scale stress is given by

$$\tau_{ij}^a = \left(\overline{\overline{u}_i \overline{u}_j} - \overline{\overline{u}}_i \overline{\overline{u}}_j\right)^a , \tag{3.10}$$

where superscript a specifies the anisotropic part of the tensors. Comparisons with DNS results show that the scale similarity model, which does not require alignment between the SGS stress tensor and the resolved strain-rate tensor, represents the structure of the SGS stress more accurately than does the Smagorinsky model. The model does not, however, dissipate sufficient energy and is usually combined with the Smagorinsky model to form a "mixed model".

Items (b) and (c) were addressed by Germano *et al.* (1991) who proposed a dynamic procedure that calculates the model coefficient dynamically at each point in space and time based on local instantaneous flow conditions. While the procedure can be used with any subgrid model, Germano *et al.* demonstrated the approach with the Smagorinsky model. The resulting dynamic Smagorinsky model has the correct asymptotic behaviour near solid boundaries and in laminar flow, and allows energy backscatter. Unfortunately, values of the predicted model coefficient tend to fluctuate considerably and some form of averaging, usually along homogeneous directions, is required to avoid numerical instability. In the present context, such averaging is problematic since there is no homogeneous direction. The stratocumulus cloud-top contains regions of both stable and unstable stratification within the same horizontal plane.

A number of variants of the dynamic procedure have been proposed to overcome the need for averaging. The localised dynamic models of Ghosal *et al.* (1992) and Piomelli & Liu (1995) are more stable but add to the complexity of the model. Instead, we have chosen to adopt the approach of Zang *et al.* (1993) who used the dynamic procedure with the mixed model as a base model, rather than with the Smagorinsky model. Zang *et al.* tested the dynamic mixed model for rotating stratified flow and reported a significant reduction in fluctuations of the coefficient compared with the dynamic Smagorinsky model. The dynamic mixed model has the added advantage that the scale similarity term removes the restriction of tensor alignment and provides better spectral representation of the subgrid-scale stress.

The mixed model for the subgrid-scale turbulent stress is written

$$\begin{aligned}\tau_{ij}^a &= -2C\overline{\Delta}^2 \left|\overline{S}\right| \overline{S}_{ij} + \left(\overline{\overline{u}_i \overline{u}_j} - \overline{\overline{u}}_i \overline{\overline{u}}_j\right)^a \\ &\equiv -2\nu_T \overline{S}_{ij} + \left(\overline{\overline{u}_i \overline{u}_j} - \overline{\overline{u}}_i \overline{\overline{u}}_j\right)^a ,\end{aligned} \tag{3.11}$$

where the first term on the right-hand side is the Smagorinsky component of the model while the second term represents the scale similarity component. The dynamic procedure involves the application of a test filter ($\widehat{\ }$) to the velocity field. By assuming that the same subgrid model can be used to represent the unresolved stresses for both the grid-filtered and test-filtered fields, an expression is derived for the required parameters,

$$C\overline{\Delta}^2 = -\frac{(L_{ij} - H_{ij})M_{ij}}{2M_{ij}M_{ij}}, \tag{3.12}$$

where

$$L_{ij} = \widehat{\overline{u}_i\overline{u}_j} - \widehat{\overline{u}}_i\widehat{\overline{u}}_j, \tag{3.13}$$

$$H_{ij} = \widehat{\overline{\overline{u}}_i\overline{\overline{u}}_j} - \widehat{\overline{\overline{u}}}_i\widehat{\overline{\overline{u}}}_j, \tag{3.14}$$

and

$$M_{ij} = \alpha^2|\widehat{\overline{S}}|\widehat{\overline{S}}_{ij} - \widehat{|\overline{S}|\overline{S}_{ij}}, \qquad \alpha = \widehat{\overline{\Delta}}/\overline{\Delta}. \tag{3.15}$$

Using these relations, the momentum equations become

$$\begin{aligned}\frac{\partial \overline{u}_i}{\partial t} + \frac{1}{\varrho_0}\frac{\partial(\varrho_0\overline{u}_i\overline{u}_j)}{\partial x_j} = &-\frac{\partial\overline{\Pi}}{\partial x_i} + g_i\frac{\overline{\theta}_{v2}}{\theta_0} + \frac{\partial}{\partial x_j}\left(2\nu_T\overline{S}_{ij} - \left(\overline{\overline{u}_i\overline{u}_j} - \overline{\overline{u}}_i\overline{\overline{u}}_j\right)^a\right)\\ &+ \overline{H}^{sub}_{u_i} + \overline{H}^{gw}_{u_i} + \overline{H}^{coriolis}_{u_i}.\end{aligned} \tag{3.16}$$

Following a similar argument the spatial filter is applied to the energy equation giving

$$\frac{\partial\overline{\theta}^*_l}{\partial t} + \frac{1}{\varrho_0}\frac{\partial(\varrho_0\overline{\theta}^*_l\overline{u}_j)}{\partial x_j} = -\frac{\partial\gamma}{\partial x_j} + \overline{H}^{sub}_{\theta^*_l} + \overline{H}^{LS}_{\theta^*_l} + \overline{H}^{gw}_{\theta^*_l} + \overline{H}^{rad}_{\theta^*_l}. \tag{3.17}$$

The SGS energy flux,

$$\gamma = \left(\overline{u_j\theta^*_l} - \overline{u}_j\overline{\theta}^*_l\right), \tag{3.18}$$

is approximated using a mixed model analogous to that used for the momentum equations,

$$\gamma = -\frac{\nu_T}{Pr_{\theta T}}\frac{\partial\overline{\theta}^*_l}{\partial x_j} + \left(\overline{\overline{u}_j\overline{\theta}^*_l} - \overline{\overline{u}}_j\overline{\overline{\theta}}^*_l\right), \tag{3.19}$$

with the eddy diffusivity computed using the eddy viscosity calculated for the velocities and a turbulent Prandtl number. Substituting into (3.17), the filtered energy equation becomes

$$\begin{aligned}\frac{\partial\overline{\theta}^*_l}{\partial t} + \frac{1}{\varrho_0}\frac{\partial(\varrho_0\overline{\theta}^*_l\overline{u}_j)}{\partial x_j} = &\ \frac{\partial}{\partial x_j}\left(\frac{\nu_T}{Pr_{\theta T}}\frac{\partial\overline{\theta}^*_l}{\partial x_j} - \left(\overline{\overline{u}_j\overline{\theta}^*_l} - \overline{\overline{u}}_j\overline{\overline{\theta}}^*_l\right)\right)\\ &+ \overline{H}^{sub}_{\theta^*_l} + \overline{H}^{LS}_{\theta^*_l} + \overline{H}^{gw}_{\theta^*_l} + \overline{H}^{rad}_{\theta^*_l}.\end{aligned} \tag{3.20}$$

Finally, by analogy, the filtered transport equation for total water is written

$$\begin{aligned}\frac{\partial\overline{q}_t}{\partial t} + \frac{1}{\varrho_0}\frac{\partial(\varrho_0\overline{q}_t\overline{u}_j)}{\partial x_j} = &\ \frac{\partial}{\partial x_j}\left(\frac{\nu_T}{Pr_{qT}}\frac{\partial\overline{q}_t}{\partial x_j} - \left(\overline{\overline{u}_j\overline{q}_t} - \overline{\overline{u}}_j\overline{\overline{q}}_t\right)\right)\\ &+ \overline{H}^{sub}_{q_t} + \overline{H}^{LS}_{q_t}.\end{aligned} \tag{3.21}$$

The turbulent Prandtl numbers, $Pr_{\theta T}$ and Pr_{qT}, in the subgrid models for the scalar variables are determined dynamically using the approach of Moin *et al.* (1991). This procedure is similar to that used to calculate the Smagorinsky coefficient outlined above. In this way, all coefficients and length scales in the subgrid-scale models for the flow variables are calculated dynamically, based on information in the resolved scalar and flow fields, and the need for *a priori* specification of parameters and corrections is removed.

4. Microphysics and radiation models

The DHARMA code has the option to use either a standard parameterisation for cloud microphysics, or the more complex explicit model of Ackerman *et al.* (1995). The code includes two standard parameterisations: a bulk-condensation model, in which cloud water q_c is found by inverting Wexler's expressions for saturated vapor pressure (Wexler 1976, 1977) using the method of Flatau *et al.* (1992); and the parameterised microphysics of Wyant *et al.* (1997) which includes a treatment of precipitation.

The cloud microphysics model of Ackerman *et al.* explicitly models the dynamics of two types of particle: condensation nuclei (CN) and water droplets. Particle size distributions are defined by $C(r, \mathbf{x}, t)$ where Cdr is the mean number concentration (per unit volume) of particles with radius between r and $r + dr$. A filtered particle-continuity equation is solved for each particle size,

$$
\begin{aligned}
\frac{\partial \overline{C}}{\partial t} + \frac{\partial (\overline{C}\overline{u}_j)}{\partial x_j} = \quad & \frac{\partial (v_f \overline{C})}{\partial z} + S_n - R_n \overline{C} + \frac{\partial (g_r \overline{C})}{\partial r} \\
& + \frac{1}{2} \int_{r_{min}}^{r} K_c(r, (r^3 - r'^3)^{1/3}) \overline{C}(r') \overline{C}((r^3 - r'^3)^{1/3}) dr' \\
& - \overline{C} \int_{r_{min}}^{r_{max}} K_c(r, r') \overline{C}(r') dr' \\
& + \overline{H}_C^{sub} + \overline{H}_C^{LS} + \frac{\partial}{\partial x_j} \left(\frac{\varrho_0 \nu_T}{Pr_{CT}} \frac{\partial (\overline{C}/\varrho_0)}{\partial x_j} - \left(\overline{\overline{u}_j \overline{C}} - \overline{\overline{u}}_j \overline{\overline{C}} \right) \right).
\end{aligned} \tag{4.1}
$$

Here v_f is the particle sedimentation velocity, S_n represents particle creation, R_n is the particle removal rate, g_r is the condensational growth rate and K_c is a coalescence kernel. The first term on the right hand side is the particle flux divergence due to sedimentation. This flux is modelled using the Stokes-Cunningham expression for $Re < 10^{-2}$ and the interpolation of Beard (1976) for higher Re. The second and third terms on the right hand side represent particle creation and transitions between CN and droplets. The fourth term is the divergence in radius-space due to condensation and evaporation. The first integral represents creation of particles due to collisions of smaller particles while the second integral represents the loss of particles due to collisions with other particles. $\overline{H}_C^{sub}$ and $\overline{H}_C^{LS}$ are the subsidence and large-scale advective tendencies similar to those appearing in the gas phase equations. The final term is a turbulent diffusion flux representing the subgrid-scale stresses resulting from the filtering operation. The turbulent Prandtl number Pr_{CT} is set equal to that calculated dynamically for q_t.

Ackerman *et al.* (1995) give further details on modelling of condensation growth, CN activation, total evaporation of droplets, particle collisions and new particle creation. Particle size distributions for CN and droplets are each typically divided into 20 bins with geometrically increasing size such that the particle volume doubles between successive bins.

Because time scales for the cloud microphysics are typically smaller than those for the large-scale dynamics, the microphysics equations are integrated over a series of smaller substeps within each time step of the flow-dynamics model. Also, while the flow-dynamics model uses total-water mixing ratio q_t and liquid-water potential temperature θ_l^* as the thermodynamic variables (see (2.3) and (2.4)), the microphysical model uses the concentration of water vapour G and the potential temperature θ. The equations for these variables are written

$$\frac{\partial \overline{G}}{\partial t} + \frac{\partial (\overline{G}\overline{u}_j)}{\partial x_j} = -4\pi\varrho_w \int_{r_{min}}^{r_{max}} r'^2 g_r(r')\overline{C}(r')dr' + \frac{\partial}{\partial x_j}\left(\frac{\varrho_0 \nu_T}{Pr_{qT}}\frac{\partial(\overline{G}/\varrho_0)}{\partial x_j} - \left(\overline{\overline{u}_j\overline{G}} - \overline{\overline{u}}_j\overline{\overline{G}}\right)\right) + \overline{H}_G^{sub} + \overline{H}_G^{LS}, \tag{4.2}$$

$$\frac{\partial(\varrho_0\overline{\theta})}{\partial t} + \frac{\partial(\varrho_0\overline{\theta}\overline{u}_j)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\varrho_0\nu_T}{Pr_{\theta T}}\frac{\partial\overline{\theta}}{\partial x_j} - \left(\overline{\overline{u}_j\overline{\theta}} - \overline{\overline{u}}_j\overline{\overline{\theta}}\right)\right) + \overline{H}_\theta^{sub} + \overline{H}_\theta^{LS}. \tag{4.3}$$

Here ϱ_w is the density of liquid water and the integral in (4.2) represents vapour exchange with the droplets. The turbulent Prandtl numbers are those calculated for the corresponding variables in the flow-dynamics model.

The fluxes of particles and water vapour across the lower boundary are calculated using Monin-Obukhov similarity functions. Here, the model integrates the surface-layer flux-profile relations of Businger *et al.* (1971) following the method of Benoit (1977). Lateral boundaries are periodic and at the upper boundary the flux divergence is set to zero.

Radiation is modelled in different ways depending on the requirements of the particular study at hand. A simple approach, often used for model intercomparisons, is to parameterise radiation as the sum of two components: a clear-sky radiative-cooling component, typically taken to be a fixed -2 K/day everywhere below the inversion; and a cloud-associated "Beer's Law" component. In the latter, long-wavelength radiative cooling is assumed to be proportional to the liquid-water content and is exponentially attenuated as the overlying liquid-water path increases. The resulting radiative heat flux F_r is then given by

$$F_r(z) = F_r(H)exp\left(-K_a \int_z^H \varrho_0 q_c dz\right), \tag{4.4}$$

where H is the height of the domain.

A more complex approach models radiative heat transfer following the method of Toon *et al.* (1989). The model computes multiple scattering over 26 solar wavelengths ($0.26\ \mu\text{m} < \lambda < 4.3\mu\text{m}$) and absorption and scattering over 14 infrared wavelengths ($4.4\ \mu\text{m} < \lambda < 62\mu\text{m}$). Blackbody energy beyond those wavelength domains is included to agree with the Stefan-Boltzmann law. An exponential-sum formulation is used to treat gaseous absorption coefficients while the optical properties of particles are determined through Mie calculations in which the complex refractive index for liquid water is used as interpolated from the datasets of Painter *et al.* (1969), Palmer & Williams (1974) and Downing & Williams (1975). The model uses a value for carbon dioxide concentration appropriate to the year of the study. Measurements of the present global annual mean carbon dioxide concentration give a value of approximately 370 ppm by volume ($\approx 10\%$ higher than in the early 1980's). The ozone profile is taken from the *U.S. Standard Atmosphere* (NOAA 1976).

5. Numerical method

The numerical method is described in detail by Stevens & Bretherton (1996). The equations are integrated using a forward-in-time projection method based on a 2nd-order Runge-Kutta scheme similar to that of Bell & Marcus (1992). The integration proceeds as follows:

– advance velocities to $t = n + 1/2$ using explicit Euler
– solve a Poisson equation and do pressure correction at $t = n + 1/2$
– advance scalars to $t = n + 1$
– advance velocity to $t = n + 1$ using a modified trapezoid rule
– solve Poisson equation and do pressure correction at $t = n + 1$

The projection procedure is described in detail by Almgren *et al.* (1998).

The spatial discretisation is performed on a staggered grid (Arakawa C). Second-order central differences are used for diffusion terms and pressure gradients while the advection terms use a modified version of the "Uniform Third-Order Polynomial Interpolation Algorithm" (UTOPIA) of Leonard *et al.* (1993). The modified scheme developed by Stevens & Bretherton (1996) includes additional transverse correction terms which improve the stability of the scheme while maintaining its accuracy. For the scalar equations, the 3D flux limiter of Zalesak (1979) is used to ensure a monotonic solution. Source terms are computed using the second-order accurate method of Smolarkiewicz & Pudykiewicz (1992) and Smolarkiewicz & Margolin (1993). Stevens and Bretherton show that the overall scheme is second-order accurate in space and time, energy-conserving and stable up to a CFL number of 1.0.

At the lower boundary, surface fluxes of momentum, θ_l^* and q_t are calculated using the same similarity relations as those used for water vapour and particle fluxes (see Section 4). The lateral boundaries are periodic while the top boundary uses a rigid lid. As discussed above, numerical problems due to gravity waves reflecting from the top boundary are prevented by using a Rayleigh damping layer in the upper third of the domain.

6. Future plans

The performance of the dynamic mixed model will be tested using a series of simulations of a nocturnal marine stratocumulus cloud deck. The particular test case chosen is the DYCOMS-II field experiment which took place off the coast of San Diego in July, 2001. DYCOMS-II is an acronym for "Dynamics and Chemistry of Marine Stratocumulus – Phase II: Entrainment". The purpose of the experiment was to collect data for use in testing large-eddy simulations of nocturnal stratocumulus. In particular, the experiment focused on cloud-top processes involved in entrainment.

The domain to be used for the simulations has size 3.2 km $\times$ 3.2 km $\times$ 1.5 km and is periodic in the horizontal directions. Two sets of simulations will be performed: one set using the dynamic mixed model and the other using the classical Smagorinsky model with the standard corrections. Each set comprises a series of simulations at grid resolutions ranging from coarse resolution (32 m horizontal by 16 m vertical grid size) to very fine resolution (4 m horizontal by 2 m vertical). Previous studies (eg. Stevens *et al.* 2000) indicate that all energetic scales will be resolved in the very fine resolution simulations, so that these simulations can reasonably be used as a benchmark for comparing the performance of the subgrid-scale turbulence models.

Comparisons will be made with a view to answering the following questions:

1) Does the dynamic mixed model more accurately represent the subgrid-scale turbulence,

in the sense that it reduces the difference between the coarser grid solutions and the benchmark solution?

2) How do the subgrid-scale stresses predicted by the dynamic model compare with those of the standard model? Does the dynamic model, for example, predict a Richardson-number dependence in regions of stable stratification similar to that used in the standard model?

3) How does the dynamic model perform for simulations in which the inertial subrange is not well resolved?

For coarser simulations in which the inertial subrange is not resolved, Stevens *et al.* (1999) found that the turbulent kinetic energy equation approach gives results which are less dependent on grid resolution than those obtained using a Smagorinsky model. A possible future study would test the performance of a turbulence closure scheme in which the dynamic procedure is used to determine the coefficients in the turbulent kinetic energy equation.

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