

# Large-eddy simulation of stratocumulus-topped atmospheric boundary layers with dynamic subgrid-scale models

By Inanc Senocak

## 1. Motivation and objectives

Earth's climate and its geographical variation is strongly influenced by cloud coverage. It is estimated that about 50% of the earth is covered by clouds at any given time, providing a shield from solar radiation. Radiative energy transfer and its interaction with clouds play an important role in the thermal structure and stratification of the atmosphere. For instance, clouds have high reflectivity in the visible wavelengths, thus providing relative cooling of the atmosphere. They also absorb strongly in the infrared wavelengths, resulting in heating of the atmosphere (Salby 1996).

Condensation is the major physical process that is responsible for cloud formation. Clouds can be classified into four broad categories, namely: cumulus, cirrus, nimbus and stratus (Rogers & Yau 1989). Many other classifications can be derived from combinations of these four broad categories. A comprehensive description can be found in Scorer & Wexler (1967). Among various types of clouds, marine stratocumulus clouds have received increased attention because of the important role they play in the global radiation budget. Marine stratocumulus clouds cover about 25% of the Earth's ocean at any instant. These are low-level clouds that exist below 1.5 km with several hundred meters in thickness and they rarely produce precipitation. Their horizontal coverage is extensive and more homogeneous than other type of clouds. Their appearance is grey and a wavy undersurface is typical (Kantha & Clayson 2000; Heymsfield 1993; Mason 1975).

The structure of the marine stratocumulus cloud-topped atmospheric boundary layer is driven by both cloud-top radiative cooling and positive buoyancy flux from the surface that maintains the atmospheric boundary layer in a well-mixed turbulent state. Above the cloud layer, negative buoyancy flux has a stabilizing effect, suppressing the turbulence there (Kantha & Clayson 2000). The entrainment of dry air from above the cloud layer induces evaporative cooling and entrained air parcel can sink further down enhancing the turbulent mixing within the clouds, known as cloud top entrainment instability (Deardorff 1980*a*). Clearly, the structure of cloud-topped atmospheric boundary is more complicated than a cloud-free atmospheric boundary layer due to strong interactions among cloud microphysics, turbulent motions and the radiative energy transfer.

In large-eddy simulation (LES), three-dimensional, large unsteady flow structures are resolved and the effects of the unresolved scales are modeled. A filtering operation is applied to the governing equations to distinguish between the resolved scales that are computed and smaller scales that are modeled. LES has been widely applied to simulate atmospheric boundary layers, partly because of the difficulties involved in observational studies and field experiments (Stevens & Lenschow 2001). An extensively studied topic is LES of cloud-free convective atmospheric boundary layers. The salient features of these boundary layers have been compared to observations and well documented (Kantha

& Clayson 2000). The presence of clouds complicates the problem due to additional physics and reliable numerical simulations of cloud-topped boundary layer is still an active research area. In the following, several representative studies are briefly mentioned to help describe the current state of the knowledge.

An early study on three-dimensional modeling of cloud-topped atmospheric boundary layer is by Deardorff (1980*b*). He studied the structure of turbulence and entrainment within stratocumulus layers with and without cloud-top radiative cooling and suggested that simulations need high resolution at the inversion. It was also found that a functional dependence on Richardson number helps correlate the entrainment rate. Deardorff (1980*a*) has defined a criterion for the cloud top entrainment instability. It was found that entrainment rate increases decisively when the equivalent potential temperature gradient across the cloud top drops below a critical value. It was also shown that a strong instability can lead to stratocumulus breakup leading to a scattered cumulus layer. Tag & Payne (1987) indicated that in addition to Deardorff's criterion, the vertical motions should exceed a threshold for the cloud breakup to occur.

Moeng (1986) studied the structure of a stratus-topped boundary layer using LES. It was found that the vertical component of the turbulent kinetic energy is generated by buoyancy and a portion of this energy is redistributed in the horizontal directions due to pressure effects. It was also shown that turbulence is generated more effectively by surface heating than cloud-top cooling.

Bohnert (1993) tested the dynamic procedure for LES of cloud-topped boundary layer. Simple parametrization for cloud microphysics and radiation were adopted. The dynamic model results were compared to the results of SGS model that were optimized in an ad-hoc fashion. The results were found to be comparable. The importance of SGS modeling in predicting cloud breakup was also highlighted.

Stevens *et al.* (2000) investigated the dependence of an LES model on mesh resolution, numerical schemes and SGS model. They provided simulations of varying resolutions for the simulation of stratocumulus topped marine boundary layer. Different SGS models and advection schemes were tested. It was found that thickness of the inversion layer, depth of entraining eddies and shape of the vertical velocity spectra is influenced by mesh resolution. Motions at the inversion were found to be underresolved even for the finest resolution. The entrainment rate was found to depend on both numerical and SGS dissipation.

Duynkerke, Zhang & Jonker (1995) performed an observational study to describe the microphysical and turbulent structure of stratocumulus observed during the Atlantic Stratocumulus Transition Experiment (ASTEX). The turbulence kinetic energy budget, velocity and temperature variance, and vertical fluxes were calculated. The entrainment was found to be very efficient, which resulted in reduction of turbulent kinetic energy production due to buoyancy. It was also shown that water vapor flux, liquid water flux, and drizzle rate have the same magnitude.

Stevens *et al.* (1998) presented an LES study of the ASTEX case. They adopted a drop-size resolving cloud microphysics model that enabled them to perform simulations with and without drizzle. It was found that inclusion of drizzle in modeling leads to sharp decrease in entrainment and turbulent kinetic energy generation by buoyancy. The authors have hypothesized that shallow, well-mixed radiatively driven stratocumulus cannot persist in the presence of heavy drizzle.

Duynkerke *et al.* (1999) did a comparison of actual ASTEX observations with computations obtained from LES and one-dimensional single column models. The buoyancy

flux obtained from LES agrees well with the observations. The authors concluded that drizzle has small influence on the buoyancy flux, although significant uncertainty exists in its parametrization.

The objective of the present study is to evaluate the dynamic procedure in LES of stratocumulus topped atmospheric boundary layer and assess the relative importance of subgrid-scale modeling, cloud microphysics and radiation modeling on the predictions. The simulations will also be used to gain insight into the processes leading to cloud top entrainment instability and cloud breakup. In this report we document the governing equations, numerical schemes and physical models that are employed in the Goddard Cumulus Ensemble model (GCEM3D). We also present the subgrid-scale dynamic procedures that have been implemented in the GCEM3D code for the purpose of the present study.

## 2. Numerical formulation

The numerical model used in this study to simulate cloud-topped atmospheric boundary layers is the Goddard Cumulus Ensemble model(GCEM3D). Its main features are described in Tao & Simpson (1993), Simpson & Tao (1993) and Tao *et al.* (2003).

### 2.1. Governing equations

Acoustic waves are part of the solution of the compressible Navier-Stokes equations and very small time steps are needed to resolve them. On the other hand, acoustic waves do not impact the dynamics of thermal convection for low Mach number flows. Therefore, the governing equations of motion are simplified by filtering out the sound waves from them. The resulting set of equations is known as the anelastic equations (Ogura & Phillips 1962). In deriving these equations the basic assumption is to decompose the thermodynamic state variables into a horizontally averaged base quantity, which only depends on altitude, and a perturbation quantity, which depends on both time and space, as follows

$$\begin{aligned} p(x, y, z, t) &= p_o(z) + p'(x, y, z, t), \\ \rho(x, y, z, t) &= \rho_o(z) + \rho'(x, y, z, t), \\ T(x, y, z, t) &= T_o(z) + T'(x, y, z, t), \end{aligned} \quad (2.1)$$

where  $p$  is the pressure,  $\rho$  is the density of moist air and  $T$  is the temperature. The following moist equation of state is used in deriving the momentum equations

$$p = \rho RT(1 + 0.61q_v), \quad (2.2)$$

where  $R$  is the gas constant for dry air and  $q_v$  is the mixing ratio of water vapor. The pressure is nondimensionalized according to a reference pressure ( $p_o$ ) value

$$\pi = \left(\frac{p}{p_o}\right)^{R/C_p}, \quad (2.3)$$

where  $C_p$  is the specific heat of dry air at constant pressure. The potential temperature is defined as

$$\theta = \frac{T}{\pi}. \quad (2.4)$$

The anelastic form of the filtered continuity equation reads as follows

$$\frac{\partial(\rho_o \bar{u}_i)}{\partial x_i} = 0. \quad (2.5)$$

The filtered momentum equations, using the f-plane approximation, are written as

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{1}{\rho_o} \frac{\partial(\rho_o \bar{u}_i \bar{u}_j)}{\partial x_j} = -C_p \theta_o \frac{\partial \pi'}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + g_i \left( \frac{\theta'}{\theta_o} + 0.61 q'_v - q_l \right) + F_{coriolis}, \quad (2.6)$$

where  $g_i$  is the gravitational acceleration. The Coriolis term that appears in the momentum equations is written as

$$F_{coriolis} = [2\omega \sin \phi u_2, -2\omega \sin \phi u_1, 0], \quad (2.7)$$

where  $\omega$  is the angular velocity of the Earth and  $\phi$  gives the latitude.  $\tau_{ij}$  represents the subgrid scale stress tensor and its particular form is described in section 2.3. The primed variables represent deviation from horizontally averaged quantities.

The equations for potential temperature  $\theta$  and the water vapor mixing ratio  $q_v$  are written as follows

$$\begin{aligned} \frac{\partial \bar{\theta}}{\partial t} + \frac{1}{\rho_o} \frac{\partial(\rho_o \bar{\theta} \bar{u}_i)}{\partial x_i} = & -\frac{\partial \gamma_i^\theta}{\partial x_i} + \frac{L_v}{C_p} (c - e_c - e_r) + \frac{L_f}{C_p} (f_s + f_g - m_s - m_g) \\ & + \frac{L_s}{C_p} (d_{ice} - s_{ice}) + Q_{rad}, \end{aligned} \quad (2.8)$$

$$\frac{\partial \bar{q}_v}{\partial t} + \frac{1}{\rho_o} \frac{\partial(\rho_o \bar{q}_v \bar{u}_i)}{\partial x_i} = -\frac{\partial \gamma_i^{q_v}}{\partial x_i} + (c - e_c - e_r) + (d_{ice} - s_{ice}), \quad (2.9)$$

where  $L_v$ ,  $L_f$  and  $L_s$  are the latent heats of condensation, fusion and sublimation, respectively. The quantities  $c$ ,  $e_c$ ,  $e_r$ ,  $f$ ,  $m$ ,  $d_{ice}$ ,  $s_{ice}$  represent the rates of condensation, evaporation of cloud droplets, evaporation of rain drops, freezing of rain drops, melting of snow and graupel/hail, deposition of ice particles and sublimation of ice particles, respectively. The particular forms for these phase change rates are not explicitly formulated. Instead, a saturation adjustment scheme is adopted that calculates the amount of phase change rate in order to remove any supersaturated vapor and/or subsaturation of cloud water. The saturation adjustment scheme is described in Soong & Ogura (1973) and Tao, Simpson & McCumber (1989).  $\gamma_i^\phi$  is the subgrid scale flux of the scalar, which is explained in section 2.3.  $Q_{rad}$  is the source due to radiative heat transfer. It is described in section 2.4.

## 2.2. Cloud microphysics model

The formulation of the cloud microphysical processes is based on solving scalar transport equations for each hydrometeor species. The transport equations for cloud water ( $q_c$ ), cloud ice ( $q_{ice}$ ), rain ( $q_r$ ), snow ( $q_s$ ), graupel/hail ( $q_g$ ) are written as

$$\frac{\partial \bar{q}_c}{\partial t} + \frac{1}{\rho_o} \frac{\partial(\rho_o \bar{q}_c \bar{u}_i)}{\partial x_i} = -\frac{\partial \gamma_i^{q_c}}{\partial x_i} + (c - e_c) + T_{q_c}, \quad (2.10)$$

$$\frac{\partial \bar{q}_{ice}}{\partial t} + \frac{1}{\rho_o} \frac{\partial(\rho_o \bar{q}_{ice} \bar{u}_i)}{\partial x_i} = -\frac{\partial \gamma_i^{q_{ice}}}{\partial x_i} + (d_{ice} - s_{ice}) + T_{q_{ice}}, \quad (2.11)$$

$$\frac{\partial \bar{q}_r}{\partial t} + \frac{1}{\rho_o} \frac{\partial(\rho_o \bar{q}_r \bar{u}_i)}{\partial x_i} - \frac{1}{\rho_o} \frac{\partial(\rho_o \bar{q}_r U_r)}{\partial x_3} = -\frac{\partial \gamma_i^{q_r}}{\partial x_i} + (m_s + m_g - f_s - f_g - e_r) + T_{q_r}, \quad (2.12)$$

$$\frac{\partial \bar{q}_s}{\partial t} + \frac{1}{\rho_o} \frac{\partial(\rho_o \bar{q}_s \bar{u}_i)}{\partial x_i} - \frac{1}{\rho_o} \frac{\partial(\rho_o \bar{q}_s U_s)}{\partial x_3} = -\frac{\partial \gamma_i^{q_s}}{\partial x_i} + (d_s - s_s - m_s + f_s) + T_{q_s}, \quad (2.13)$$

$$\frac{\partial \bar{q}_g}{\partial t} + \frac{1}{\rho_o} \frac{\partial(\rho_o \bar{q}_g \bar{u}_i)}{\partial x_i} - \frac{1}{\rho_o} \frac{\partial(\rho_o \bar{q}_g U_g)}{\partial x_3} = -\frac{\partial \gamma_i^{q_g}}{\partial x_i} + (d_g - s_g - m_g + f_g) + T_{q_g}, \quad (2.14)$$

where  $V_r$ ,  $V_s$  and  $V_g$  are the fall speeds of rain, snow and graupel, respectively. Their values are obtained from parameterizations.  $\gamma_i^\phi$  is the subgrid-scale flux of the scalar.  $T_\phi$  represents the microphysical transfer rates between the hydrometeor species. A total of 27 different processes are considered and the reader is referred to Lin, Farley & Orville (1983) for details of their formulation. To illustrate the parameterizations of these processes, only the microphysical transfer rate of rain  $T_{q_r}$  is described in this report. For instance, if the temperature is above  $0^\circ\text{C}$ , then the production term for rain is given by the following equation

$$T_{q_r} = P_{RACW} + P_{RAUT} + P_{SACW} + P_{GACW} - P_{GMLT} - P_{SMLT} + P_{REVP}(1 - \delta_1). \quad (2.15)$$

The terms on the right hand side of the above equation are the accretion of cloud water by rain, autoconversion of cloud water to form rain, accretion of cloud water by snow, accretion of cloud water by graupel, melting of graupel to form rain, melting of snow to form rain, evaporation of rain, respectively. The accretion of rain by cloud water  $P_{RACW}$  is written as

$$P_{RACW} = \frac{\pi E_{rw} n_{0r} a q_c \Gamma(3 + b)}{4 \lambda_r^{3+b}}, \quad (2.16)$$

where  $E_{rw}$  is the collection efficiency, which is assumed to be 1,  $n_{0r}$  is the intercept parameter of the rain drop size distribution,  $\Gamma$  is the gamma function,  $\lambda_r$  is the slope parameter in rain size distribution and  $a, b$  are empirical constants. Exponential size distributions are assumed for rain, snow and graupel/hail. The explicit forms of other transformation rates are documented in Lin *et al.* (1983).

### 2.3. Subgrid-scale turbulence models

Three turbulence closure models will be considered for comparison. These are the subgrid-scale kinetic energy model of Klemp & Wilhelmson (1978), which is the base turbulence model in the GCEM3D code, the dynamic Smagorinsky model of Germano *et al.* (1991) and the localized dynamic Smagorinsky model of Piomelli & Liu (1995). The implementation of dynamic turbulence models by Kirkpatrick (2002) has been coupled to the GCEM3D code. In the following sections these models are briefly explained.

#### 2.3.1. Subgrid-scale kinetic energy model

A transport equation for subgrid-scale turbulent kinetic energy is solved, which is then used to specify the eddy viscosity. The influence of buoyancy on the turbulent motions is also modeled. The equation for subgrid-scale turbulent kinetic energy is written as

$$\frac{\partial E}{\partial t} + \frac{1}{\rho_o} \frac{\partial(\rho_o E \bar{u}_i)}{\partial x_j} = \overline{gw'(\frac{\theta'}{\theta_o} + 0.61q'_v - q'_l)} - \tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial}{\partial x_j} (K_m \frac{\partial E}{\partial x_j}) - \frac{C_e}{\Delta} E^{3/2}, \quad (2.17)$$

$$\begin{aligned} \Delta &= (\Delta x \Delta y \Delta z)^{1/3}, \\ K_m &= C_m \Delta E^{1/2}, \\ \tau_{ij} &= \frac{2}{3} E \delta_{ij} - K_m \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right), \end{aligned} \quad (2.18)$$

where  $K_m$  is the turbulent eddy viscosity,  $\Delta$  is the filter width. The empirical constants  $C_e$  and  $C_m$  have the values of 0.7 and 0.2, respectively. The subgrid-scale scalar fluxes

are modeled as

$$\gamma_i^\phi = K_h \frac{\partial \phi}{\partial x_i}, \quad (2.19)$$

where  $K_h/K_m = 3$  is used. The buoyancy flux in a saturated area is computed as

$$\overline{w' \left( \frac{\theta'}{\theta_o} + 0.61q'_v - q'_l \right)} = -AK_h \frac{\partial \theta_e}{\partial z} + K_h \frac{\partial q_t}{\partial z}, \quad (2.20)$$

where

$$A = \frac{1}{\theta_o} \frac{1 + \frac{1.61\varepsilon L q_v}{R_d T}}{1 + \frac{\varepsilon L^2 q_v}{C_p R_d T^2}}, \quad (2.21)$$

and  $\varepsilon = 0.622$ .

In an unsaturated area, the buoyancy flux is computed as follows:

$$\overline{w' \left( \frac{\theta'}{\theta} + 0.61q'_v - q'_l \right)} = -K_h \left( \frac{1}{\theta} \frac{\partial \theta}{\partial z} + 0.61 \frac{\partial q_v}{\partial z} \right). \quad (2.22)$$

### 2.3.2. Dynamic Smagorinsky model

Smagorinsky model (Smagorinsky 1963) is commonly used in LES to model the subgrid scale stresses. It is based on eddy viscosity assumption and can be written as

$$\tau_{ij} - \frac{1}{3} \delta_{ij} \tau_{kk} = -2C \Delta^2 |\bar{S}| \bar{S}_{ij}, \quad (2.23)$$

where  $C$  is a dimensionless parameter and  $|\bar{S}| = \sqrt{2\bar{S}_{ij}\bar{S}_{ij}}$ . The filtered strain rate is defined as

$$\bar{S}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right). \quad (2.24)$$

Germano *et al.* (1991) have introduced the dynamic procedure that offers advantages over the original Smagorinsky model. In this model the parameter  $C$  is computed at each time step from the information already available in the resolved velocity field. The basic formalism behind the dynamic Smagorinsky model is explained in the following.

The dynamic model involves filters of different sizes. In addition to the grid filter, a test filter is introduced. The subgrid scale stress tensor based on the grid filter and the test filter are written respectively as

$$\begin{aligned} \tau_{ij} &= \overline{u_i u_j} - \bar{u}_i \bar{u}_j, \\ T_{ij} &= \widehat{\overline{u_i u_j}} - \hat{u}_i \hat{u}_j, \end{aligned} \quad (2.25)$$

where the symbols overbar and the hat represent the grid and test filtering operations, respectively. Applying the test filter to  $\tau_{ij}$  and subtracting it from  $T_{ij}$  yields the following identity (Germano, 1992)

$$L_{ij} = T_{ij} - \hat{\tau}_{ij} = \widehat{\overline{u_i u_j}} - \hat{u}_i \hat{u}_j. \quad (2.26)$$

The significance of this identity is that it can be computed from the large eddy field. Germano *et al.* (1991) have utilized this identity to dynamically compute the coefficient of the Smagorinsky model as follows.

$$L_{ij} - \frac{1}{3} \delta_{ij} L_{kk} = \alpha_{ij} C - \widehat{\beta_{ij} C}, \quad (2.27)$$

where

$$\begin{aligned}\alpha_{ij} &= -2\widehat{\Delta}^2\widehat{S}\widehat{S}_{ij}, \\ \beta_{ij} &= -2\Delta^2\bar{S}\bar{S}_{ij}.\end{aligned}\quad (2.28)$$

For atmospheric boundary layers, where the horizontal directions are assumed to be homogeneous, the filtering operation is applied only in the horizontal direction and  $C$  is assumed to be independent of the homogeneous directions and taken out of the filtering operator. Equation (2.27) is rearranged to the following form

$$L_{ij} - \frac{1}{3}\delta_{ij}L_{kk} = CM_{ij}, \quad (2.29)$$

where

$$M_{ij} = \alpha_{ij} - \widehat{\beta}_{ij}. \quad (2.30)$$

Following the method described in Lilly (1992), the coefficient  $C$  is computed so as to minimize the sum of the squares of the residuals of equation (2.29). The numerator and the denominator are averaged over the horizontal (x,y)-plane.

$$C(z, t) = \frac{\langle M_{ij}L_{ij} \rangle_{xy}}{\langle M_{kl}M_{kl} \rangle_{xy}}. \quad (2.31)$$

Once  $C$  is calculated, the subgrid scale stress tensor, given in equation (2.23) is computed. In a similar approach, the subgrid-scale flux of a scalar  $\phi$  can be computed dynamically Moin *et al.* (1991). If we consider the following eddy diffusivity subgrid-scale model

$$\gamma_i = -\frac{\nu_t}{Pr_t} \frac{\partial \bar{\phi}}{\partial x_i}, \quad (2.32)$$

where the kinematic eddy viscosity is computed with the dynamic Smagorinsky model as  $\nu_t = C\Delta^2|\bar{S}|$ . The dynamic procedure can also be applied to compute the turbulent Prandtl number  $Pr_t$ . The subgrid-scale scalar flux based on the test filter scale is written as

$$G_i = -\frac{C\widehat{\Delta}^2}{Pr_t}|\widehat{S}|\frac{\partial \widehat{\phi}}{\partial x_i} \quad (2.33)$$

The test and grid scale fluxes are related to each other by the following identity

$$P_i = G_i - \widehat{\gamma}_i = \widehat{\phi}\widehat{u}_i - \widehat{\phi}\widehat{u}_i = -C\frac{\widehat{\Delta}^2|\widehat{S}|}{Pr_t}\frac{\partial \widehat{\phi}}{\partial x_i} + C\frac{\Delta^2|\widehat{S}|}{Pr_t}\frac{\partial \bar{\phi}}{\partial x_i}. \quad (2.34)$$

The above equation can be recast into the following form

$$P_i = -\frac{C}{Pr_t}R_i. \quad (2.35)$$

Following the suggestion of Lilly (1992), a least squares procedure is applied to compute the value of  $Pr_t$ . Note that the value of  $C$  is determined earlier.

$$\frac{1}{Pr_t} = -\frac{1}{C} \frac{\langle P_i R_i \rangle_{xy}}{\langle R_m R_m \rangle_{xy}} \quad (2.36)$$

After calculating the  $Pr_t$ , equation (2.31) is used to compute the subgrid scale flux of a scalar.

### 2.3.3. Approximate localized dynamic Smagorinsky model

The dynamic Smagorinsky model is not general for flows with no homogeneous direction, because of the need for averaging in the homogeneous directions. Ghosal *et al.* (1995) have addressed the mathematical inconsistencies and proposed a new formulation for the dynamic procedure that makes it applicable to arbitrary inhomogeneous flows. They have also provided formal justifications for the ad-hoc procedures that have been adopted in the early versions of the dynamic model.

The mathematical inconsistency in previous versions comes from the fact that space and time dependent coefficient  $C$  is simply taken out of the filtering operation. In the variational formulation of Ghosal *et al.* (1995),  $C$  is kept inside and an integral equation needs to be solved at each time step to determine  $C$ . This method is referred to as the dynamic localization model.

The solution of an integral equation is costly. Piomelli & Liu (1995) have followed a simpler approach and proposed the approximate localized dynamic model. In the following this method is briefly described.

Equation (2.27) is recast in the following form.

$$-C\alpha_{ij} = L_{ij}^a + \widehat{C^*}\beta_{ij}, \quad (2.37)$$

where

$$L_{ij}^a = L_{ij} - \frac{1}{3}\delta_{ij}L_{kk}. \quad (2.38)$$

An estimated value  $C^*$  is assumed, which is the value of  $C$  from the previous time step. Along with this approximation, a least squares procedure is applied to compute  $C$  as given below

$$C = -\frac{(L_{ij}^a + \widehat{C^*}\beta_{ij})\alpha_{ij}}{\alpha_{mn}\alpha_{mn}}. \quad (2.39)$$

The same iterative idea applies to equation (2.31) to compute the  $Pr_t$  of the subgrid-scale flux of a scalar quantity.

## 2.4. Radiation model

In an effort to describe the physical models in GCEM3D code in a single document, we briefly summarize the basic formalism of the radiation modeling.

The plane parallel assumption is typically adopted to model the radiative energy transfer. The convenience of the assumption comes from the fact that the properties of the atmosphere vary sharply with height due to its stratification, hence, the medium is regarded as horizontally homogeneous (Salby 1996).

The intensity of a radiation pencil, traversing a distance  $ds$  along the direction of its propagation, changes due to absorption, scattering and emission, which can be described by the following equation (Liou 2002).

$$dI_\lambda = -K_\lambda\rho I_\lambda ds + j_\lambda\rho ds, \quad (2.40)$$

where  $k_\lambda$  is the mass extinction cross section due to absorption and scattering and  $j_\lambda$  is the source function due to emission and scattering. In plane-parallel assumption, it is convenient to define an optical thickness as

$$\tau = \int_{z'}^{\infty} k_\lambda dz, \quad dz = \mu ds, \quad \mu = \cos\theta, \quad (2.41)$$

where  $z$  is the vertical direction and  $\theta$  is the angle between the path of radiation and the



vertical, which is specifically called the zenith angle. The basic equation, describing the radiative energy transfer in plane-parallel atmospheres is written as

$$\mu \frac{dI(\tau; \mu, \phi)}{d\tau} = I(\tau; \mu, \phi) - J(\tau; \mu, \phi). \quad (2.42)$$

The source function  $J$  is defined as

$$J(\tau; \mu, \phi) = \frac{\tilde{\omega}}{4\pi} \int_0^{2\pi} \int_{-1}^1 I(\tau; \mu', \phi') P(\mu, \phi; \mu', \phi') d\mu' d\phi' + \frac{\tilde{\omega}}{4\pi} F_o P(\mu, \phi; -\mu_0, \phi_0) e^{-\tau/\mu_0} - (1 - \tilde{\omega}) B[T(\tau)], \quad (2.43)$$

where  $P(\mu, \phi; \mu', \phi')$  is the phase function, which gives the angular distribution of scattered energy as a function of direction,  $\phi$  is the azimuthal angle,  $\tilde{\omega}$  is the single scattering albedo,  $B[T(\tau)]$  is the Planck's function representing the blackbody emission of the medium, and  $F_o$  is the solar irradiance at the top of atmosphere. Upon solution of equation (2.43), the flux density  $F_\lambda$  and the total flux density  $F$  are computed based on the following definitions

$$F_\lambda^{\uparrow\downarrow}(\tau) = 2\pi \int_0^1 I_\lambda^{\uparrow\downarrow}(\tau, \pm\mu) \mu d\mu \quad , F = \int_0^\infty F_\lambda d\lambda. \quad (2.44)$$

The heating rate due to radiation that appears in the potential temperature equation,  $Q_{rad}$ , is then computed as

$$Q_{rad} = -\frac{1}{\rho_0 C_p} \frac{dF(z)}{dz}. \quad (2.45)$$

Equation (2.43) is an integrodifferential equation and its numerical solution is quite involved due to sharp variation of the atmospheric properties with height. The computation of radiation fluxes involves spectral, vertical and directional integrations. Because the absorption coefficient varies sharply with wave number, the spectral integration is the most CPU intensive part. However, the major difficulty comes from the dependence of the absorption coefficient on pressure and temperature. Hence, effective parametrization is an important part in the numerical solution of equation (2.42). Different approaches are adopted depending on the nature of the radiation problem. A detailed account of atmospheric radiation modeling can be found in Liou (2002).

The radiative transfer model that is incorporated into the GCEM code is documented in Chou & Suarez (1996a,b). The radiation scheme can model the absorption due to water vapor,  $CO_2$ ,  $O_3$ , and  $O_2$ , and scattering by clouds, aerosols and molecules. Fluxes are integrated almost over the full spectrum, ranging from  $0.175 \mu m$  to  $10 \mu m$ . The radiation field is divided into three distinct regions. In the ultraviolet and photosynthetically active regions, the spectrum is divided into 8 bands, in which single  $O_3$  absorption coefficient and Rayleigh scattering coefficient is used for each band. The infrared region is divided into three bands and the k-distribution method is applied with ten absorption coefficients in each band. The  $\delta$ -Eddington approximation is used to compute the reflection and transmission of a cloud and aerosol-laden layer. Two-stream adding method is then used to compute the fluxes.

## 2.5. Numerical schemes

In GCEM3D code, the governing equations are discretized on a staggered grid. The momentum equations are solved using the second order central difference scheme for the

spatial derivatives and the second order accurate leap-frog scheme for temporal derivatives. A time smoother is adopted to avoid the time splitting problem associated with the leap-frog scheme. Forward time differencing and the multi-dimensional positive definite advection transport algorithm (MPDATA) of Smolarkiewicz & Grabowski (1990) are used to solve the scalar transport equations. A direct solver (FFT) is utilized for the solution of the pressure Poisson equation. The GCEM3D code has been parallelized to run on the SGI Origin clusters using OpenMP (Jin *et al.* 2003).

Lateral boundary conditions are periodic and free slip boundary conditions are imposed on the top and bottom boundaries for all the variables except the vertical velocity that vanishes at the top and bottom boundary.

### 3. Future work

The sugrid-scale turbulence models described in the previous section will be tested with progressively refined mesh resolutions, adopting the ASTEX field experiment as the test case. The relative influence of subgrid-scale modeling, cloud microphysics and radiation modeling on the predictions will be investigated. The simulations will also be used to gain insight into the processes leading to the cloud top entrainment instability and cloud breakup. Additionally, the dynamic modeling subroutine will be parallelized to speed up the overall computation.

Preliminary computations produced comparable results of wind speeds, soundings of cloud water and potential temperature among the subgrid-scale models considered. However, the computations also indicated problems with the top boundary resulting in spurious cloud formation and unstable stratification. A possible cure to the problem might be to use a Rayleigh absorbing layer, which is commonly used in atmospheric simulations, in the proximity of the top boundary to damp the vertically propagating gravity waves.

In this report we have briefly documented the governing equations and physical models that are employed in the GCEM3D code. We have also described the subgrid-scale dynamic procedures that have been introduced to the GCEM3D code in this study. We are in the process of double checking the implementation and the results. The findings of the present study will be published in the open literature.

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