SHOC Technical Document

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1 Introduction

Simplified Higher Order Closure (SHOC; Bogenschutz and Krueger, 2013) is a parameterization of subgrid-scale (SGS) clouds and turbulence. It is formulated to parameterize SGS shallow cumulus, stratiform cloud, and boundary layer turbulence in models that can either resolve deep convection or has an existing deep convection parameterization. SHOC is an assumed-PDF based parameterization and uses a double Gaussian PDF to diagnose cloud fraction, cloud water, and higher-order turbulence moments. SHOC is only a liquid cloud parameterization, thus it is assumed that any model SHOC is implemented in can treat the ice cloud phase.

Table 1 describes the SHOC prognostic variables and their nomenclature to be used throughout this document.

The liquid water potential temperature, θ_l, is defined as:

$$\theta_l \approx \theta - \frac{L_v}{c_{pd}} q_l \tag{1.1}$$

where θ is potential temperature, L_v is the latent heat of vaporization, c_{pd} the specific heat of dry air at constant pressure, q_l the liquid water mixing ratio. The turbulent kinetic energy ($\overline{e}$) is defined as

$$\overline{e} = 0.5(\overline{u'^2} + \overline{v'^2} + \overline{w'^2}), \tag{1.2}$$

where $\overline{u'^2}$, $\overline{v'^2}$, and $\overline{w'^2}$ represent the SGS zonal, meridional, and vertical wind variances, respectively.

In the SHOC parameterization, all prognostic variables are defined vertically at the midpoint of the grid box.

Table 2 describes key diagnostic variables used throughout the SHOC parameterization, and their respective locations on the vertical grid. Note that many diagnostic variables are defined at the interfaces of the grid box. This is because many diagnostic variables are the result of centered vertical differences of the prognostic variables.

The code for SHOC breaks down each process into a separate subroutine. Briefly, the order of operations of SHOC is described below. Each process is then expanded upon with its own section.

SHOC order of operations:

1. **Diagnose Turbulence Length Scale** (section 2): The length scale represents the

Table 1: Prognostic Variables in SHOC

variable	description	units
θ_l	Liquid water potential temperature	K
q_t	Total water mixing ratio (vapor + cloud liquid)	kg/kg
e	Turbulent kinetic energy	m^2/s^2
u	Zonal wind component	m/s
v	Meridional wind component	m/s
c	Tracer constituent	varies

Table 2: Key Diagnostic Variables in SHOC. M in the location column indicates that the variable is located vertically in the mid-point of the grid box, while I indicates that the variable is located at the grid interfaces.

variable	description	units	location
L	Turbulent Length Scale	m	M
$\overline{\theta_l'^2}$	Temperature variance	K^2	I
$\overline{q_t'^2}$	Moisture variance	kg^2/kg^2	I
$\overline{w'^2}$	Vertical velocity variance	m^2/s^2	M
$\overline{w'\theta_l'}$	Vertical temperature flux	K m/s	I
$\overline{w'q_t'}$	Vertical moisture flux	m/s kg/kg	I
$\overline{q_t'\theta_l'}$	Temperature and moisture covariance	K kg/kg	I
$\overline{w'^3}$	Third moment of vertical velocity	m^3/s^3	I
$\overline{w'\theta_v'}$	Buoyancy flux	K m/s	M
K_m	Eddy diffusivity for momentum	m^2/s	M
K_h	Eddy diffusivity for heat	m^2/s	M

size of unresolved large eddies in a column. This is needed to close the TKE equation and to diagnose several second order moments.

2. **Solve the Turbulence Kinetic Energy Equation** (section 3): Advance the TKE equation (due to shear production, buoyant production, and dissipation processes) one time step. Note that advection of TKE is performed by the host model, while turbulent transport of TKE is done by SHOC turbulence diffusion.

3. **Perform Turbulence Diffusion** (section 4): Using eddy coefficients derived from TKE, advance $\overline{u}$, $\overline{v}$, $\overline{\theta_l}$, $\overline{q_t}$, $\overline{e}$, and any tracers ($\overline{c}$) one time step using an implicit diffusion solver.

4. **Diagnose the Second Order Moments** (section 5): Diagnose $\overline{q_t'^2}$, $\overline{\theta_l'^2}$, $\overline{q_t'\theta_l'}$, $\overline{w'^2}$, $\overline{w'\theta_l'}$, and $\overline{w'q_t'}$. These are the second order moments needed to close the assumed PDF.

5. **Diagnose the Third Order Moment** (section 6): Diagnose the third moment of vertical velocity ($\overline{w'^3}$), needed to parameterize vertical velocity skewness in the assumed PDF

6. **Compute Assumed PDF** (section 7): Use the Assumed PDF to compute SGS cloud water, cloud fraction, and the buoyancy flux ($\overline{w'\theta_v'}$).

In SHOC the order of operations is chosen deliberately so that the prognostic variables are updated first and the clouds are diagnosed last. This is to prevent supersaturation from occurring when SHOC is complete, to avoid any potential conflicts with a microphysics scheme which may be called in the host model.

2 Turbulence Length Scale

2.1 Mixing Length Formulation in the Sub-Cloud Region

The empirical formulation is based on the finding that the turbulent length scale in the sub-cloud region is highly correlated with the distance from the wall, strength of the turbulence, boundary layer depth, and local thermal stability (Bogenschutz et al. 2010). Within the turbulent boundary layer, the length scale definition is set equal to an asymptotic shape, similar to that of Blackadar (1962). However it is weighted more strongly by the strength of the turbulence. This reflects the behavior that as the grid size increases, the SGS TKE increases and so does the mixing length. The effects of thermal stability are also included to reduce the length scale where the local stability is large.

The formulation in (2.1) is empirically determined from LES data and essentially represents a geometric average between the strength of the SGS TKE (as suggested by Texieria et al. 2004) and an asymptote length scale, with a contribution due to stability effects. The geometric average assures that in close proximity to the surface, the length scale will be small. This is not guaranteed in the formulation of Texieria et al. 2004 (where $L \propto \tau\sqrt{e}$) because SGS TKE is often very large near the surface due to large variances of the horizontal winds due to downdrafts.

$$L = \sqrt{8\left[\frac{1}{\tau_l\sqrt{e}kz} + \frac{1}{\tau\sqrt{e}D_b} + 0.01\delta\frac{N^2}{\overline{e}}\right]^{-1}} \tag{2.1}$$

Above, k is the von Karman constant and τ_l represents a timescale empirically set as 400 s (Texieria et al. 2004). D_b is a measure of the boundary layer depth, which is different than L_∞ used in the Blackadar formulation as it only includes integration up a model column until a cloud is detected (Xu and Krueger 1991)

$$D_b = 0.1\frac{\int_0^{z(q_l>0)} \overline{e}^{1/2} z dz}{\int_0^{z(q_l>0)} \overline{e}^{1/2} dz}, \tag{2.2}$$

where $z(q_l > 0)$ is the first vertical grid level where a cloud is detected (where $z(q_l(k) > 0)$ but no clouds are detected below k). Finally, in equation 2.1 δ is defined as:

$$\delta = \begin{cases} 1 & \text{if} \quad N^2 > 0 \\ 0 & \text{if} \quad N^2 \leq 0 \end{cases}$$

where N^2 is the moist Brunt Vaisala Frequency. In SHOC N^2 is defined as:

$$N^2 = \frac{g}{\overline{\theta_v}}\frac{\partial\overline{\theta_v}}{\partial z} \tag{2.3}$$

where θ_v is the virtual potential temperature defined as:

$$\theta_v = \theta(1 + 0.61q_v - q_l), \tag{2.4}$$

where q_v is the water vapor mixing ratio.

2.2 Mixing Length Formulation for Clouds

Based on similarity analysis from high resolution LES of several regimes (including stratocumulus, cumulus, and deep convection), it is determined that the length scale in clouds is strongly related to cloud depth and strength of the SGS TKE. Therefore, the formulation within clouds is

$$L = \sqrt{8\left[\frac{\overline{e}}{(w_*/D_c)^2} + 0.01\delta\frac{N^2}{\overline{e}}\right]^{-1}}, \tag{2.5}$$

where D_c is the cloud depth, defined simply as

$$D_c = z_{top} - z_{base}, \tag{2.6}$$

where z_{top} represents the height of cloud top and z_{base} represents the height of cloud base.

In (2.5), τ is another timescale that is needed. Unlike equation 2.1, I do not assume that τ_c in the clouds is a constant. Therefore I set τ_c equal to an eddy turnover timescale within the cloud. That is

$$\tau_c = \frac{D_c}{w_*}, \tag{2.7}$$

where w_* is the convective velocity scale for the cloud ensemble which is defined by Khairoutdinov and Randall (2002) as

$$w_*^3 = 2.5\frac{g}{\overline{\theta}_v}\int_{z_{base}}^{z_{top}} \overline{w'\theta_v'}dz. \tag{2.8}$$

3 Turbulent Kinetic Energy Equation

In SHOC, the turbulent kinetic energy (TKE) equation to be solved is given by:

$$\frac{\partial\overline{e}}{\partial t} = \underbrace{-\overline{u_j}\frac{\partial\overline{e}}{\partial x_j}}_{\text{advection}} + \underbrace{\frac{g}{\overline{\theta}_v}\left(\overline{w'\theta_v'}\right)}_{\text{buoyant production}} - \underbrace{P_s}_{\text{shear production}} - \underbrace{\frac{\partial\overline{w'e}}{\partial z}}_{\text{turbulent transport}} - \underbrace{C_{ee}\frac{\overline{e}^{3/2}}{L}}_{\text{dissipation}}. \tag{3.1}$$

The first term on the RHS of equation 3.1 is advection, which is performed by the host model (i.e. SCREAM dynamics) and not SHOC.

The second term is the buoyant production of TKE. The buoyancy flux term $(\overline{w'\theta_v'})$ is closed by integrating over the assumed PDF (see section 7) using equation 7.15. Thus, $\overline{w'\theta_v'}$ from the previous SHOC time step is used to close this term.

The shear production term is computed according to Bretherton and Park (2009):

$$-P_s = -\overline{w'u'}\frac{\partial\overline{u}}{\partial z} - \overline{w'v'}\frac{\partial\overline{v}}{\partial z} = K_M S^2, \tag{3.2}$$

where

$$S^2 = \left(\frac{\partial\overline{u}}{\partial z}\right)^2 + \left(\frac{\partial\overline{v}}{\partial z}\right)^2. \tag{3.3}$$

Since $\overline{u}$ and $\overline{v}$ are located vertically in the mid-points, S^2 is computed on the interface grid while K_m is linearly interpolated to the interface grid. After the shear production term is calculated on the interface grid, it is interpolated to the mid-point grid to be consistent with the location of $\overline{e}$.

The boundary surface value of $K_M S^2$ is set to zero as the boundary fluxes for TKE are applied in the diffusion solver.

The fourth term on the RHS of equation 3.1 represents the turbulent transport of TKE. This term is computed in the turbulent diffusion (section 4) of SHOC.

The last term on the RHS of equation 3.1 represents the turbulent dissipation of TKE. Here C_{ee} is a turbulent constant, which is defined in Deardorff (1980) as $C_{ee} = C_{e1} + C_{e2}$, where $C_{e1} = C_e/0.133$ and $C_{e1} = C_e/0.357$ and $C_e = C_k^3/C_s^4$. Finally, $C_k = 0.1$ and $C_s = 0.15$.

After TKE is updated due to buoyant production, shear production, and dissipation processes, the eddy diffusivity parameters for heat and momentum, to be used in turbulence diffusion, are respectively defined in the TKE module as:

$$K_H = C_{Kh} \tau_v \overline{e} \tag{3.4}$$

$$K_M = C_{Km} \tau_v \overline{e} \tag{3.5}$$

where C_{Kh} and C_{Km} are tunable constants. C_{Kh} and C_{Km} could be tuned independently, but as a starting point we set them equal to 0.1. In equations 3.4 and 3.5 τ_v represents a damped return to isotropic timescale where $\tau = 2\overline{e}/\epsilon$ and

$$\tau_v = \tau \left[1 + \lambda_0 N^2 \tau^2\right]^{-1} \tag{3.6}$$

where $\lambda_0 = 0$ if $N^2 < 0$ and ϵ is the turbulence dissipation rate (last term of equation 3.1). If $N^2 > 0$ then λ_0 is set as a ramp function in terms of the integrated column stability in the lower troposphere (N_∞^2):

$$\lambda_0 = \lambda_{min} + \lambda_{slope} * (\frac{N_\infty^2}{g} - N_{low}), \tag{3.7}$$

$$N_\infty^2 = \int_{1000hPa}^{800hPa} N^2 dz. \tag{3.8}$$

Where $\lambda_{min} = 0.001$, $\lambda_{slope} = 0.35$, and $N_{low} = 0.037$. Here, λ_{slope} is an adjustable parameter. λ_0 has a minimum threshold of 0.001 and a maximum threshold of 0.04.

4 Turbulence Diffusion

The prognostic variables for SHOC (table 1) are updated due to turbulence diffusion via:

$$\frac{\partial \overline{\chi}}{\partial t} = -\frac{\partial \overline{w'\chi'}}{\partial z}. \tag{4.1}$$

Where χ represents any of SHOC's prognostic variables (θ_l, q_t, u, v, e, or c). SHOC uses downgradient diffusion to represent the vertical flux of turbulence using:

$$\overline{w'\chi'} = -K_\chi \frac{\partial \chi}{\partial z}, \tag{4.2}$$

where K_χ represents either K_H or K_M.

To preserve numerical stability equations 4.1 and 4.2 are solved using an implicit backward Euler scheme for the diffusion of θ_l, q_t, u, v, e, or c. Given an input state χ^* and diffusivity profile:

$$\frac{\chi(t+\Delta t) - \chi^*}{\Delta t} = \frac{\partial}{\partial z}\left(K_\chi(z)\frac{\partial}{\partial z}\chi(t+\Delta t)\right). \tag{4.3}$$

In SHOC the surface fluxes for heat, moisture, TKE, and tracers are explicitly deposited into the lowest model layer and then implicit diffusion is performed. For TKE the bottom surface flux is defined as

$$u_*^3 = max(\sqrt{((\overline{u'w'}_{sfc} + \overline{v'w'}_{sfc})^{0.5})}, 0.01). \tag{4.4}$$

However, the method of explicit surface fluxes results in a numerically unstable solution for momentum since such explicit adding can flip the direction of the lowest model layer wind ($\overline{u}_s^*$, $\overline{v}_s^*$), especially when the lowest model layer is thin. Thus, the surface momentum fluxes ($\tau_x^* = \overline{u'w'}_s, \tau_y^* = \overline{v'w'}_s$) in SHOC are added in an implicit way. This is done by computing the total momentum surface stress and applying this as a boundary condition in equation 4.3:

$$k_{tot} = max[\sqrt{((\tau_x^*)^2 + (\tau_y^*)^2)}/max(\sqrt{((\overline{u}_s^*)^2 + (\overline{u}_s^*)^2)}, 1), 10^{-4}]. \tag{4.5}$$

The procedure for the solution of the implicit equation 4.3 follows that of Richtmeyer and Morton (1967, pp 198-200).

5 Diagnosis of Second Order Moments

In order to close the assumed PDF (section 7) we need to diagnose several second order moments. Namely, we need to determine, $\overline{w'\theta_l'}$, $\overline{w'q_t'}$, $\overline{q_w'\theta_l'}$, $\overline{q_t'^2}$, $\overline{\theta_l'^2}$, and $\overline{q_w'\theta_l'}$.

The expression we use to determine $\overline{w'\theta_l'}$ and $\overline{w'q_t'}$ is based on downgradient diffusion as:

$$\overline{w'C'} = -K_H \frac{\partial \overline{C}}{\partial z} \tag{5.1}$$

where C is interchanged for θ_l and q_t.

For the scalar variances and covariances, SHOC diagnoses these terms as:

$$\overline{q_t'^2} = C_{q_t} S_m \left(\frac{\partial \overline{q_t}}{\partial z}\right)^2 \tag{5.2}$$

$$\overline{\theta_l'^2} = C_{\theta_l} S_m \left(\frac{\partial \overline{\theta_l}}{\partial z}\right)^2 \tag{5.3}$$

$$\overline{q_t'\theta_l'} = C_{q_t\theta_l} S_m \frac{\partial \overline{q_t}}{\partial z}\frac{\partial \overline{\theta_l}}{\partial z}, \tag{5.4}$$

where $S_m = \tau_v K_H$. C_{q_t}, C_{θ_l}, and $C_{q_t\theta_l}$ are tunable coefficients to adjust the strength of diagnosed variances and covariances. Default setting for these coefficients are C_{q_t}, C_{θ_l}, and $C_{q_t\theta_l} = 1.0$.

Note that $\overline{w'\theta_l'}$, $\overline{w'q_t'}$, $\overline{q_w'\theta_l'}$, $\overline{q_t'^2}$, $\overline{\theta_l'^2}$, and $\overline{q_t'\theta_l'}$ are all computed on the interface grid. Thus, before the computation of these terms K_H and τ_v are linearly interpolated to the interface grid.

The expression for $\overline{w'^2}$ is:

$$\overline{w'^2} = \frac{2}{3}\bar{e} \tag{5.5}$$

6 Third Moment of Vertical Velocity

The final term needed to close the assumed PDF is the third order moment of vertical velocity ($\overline{w'^3}$), which is parameterized following that of Canuto et al. (2001). Canuto et al. (2001) provides expressions for several third-order moments, but we are only interested in $\overline{w'^3}$.

The expressions provided by Canuto et al. (2001) were originally derived for the dry convective boundary layer and we simply replace potential temperature with liquid water potential temperature ($\overline{\theta_l}$) to make the expressions valid in moist convection. The original dynamic equations for the third order moment can be found in Canuto (1992) and these equations entail fourth-order moments that can be written as

$$\overline{a'b'c'd'} = \left(\overline{a'b'}\;\overline{c'd'} + \overline{a'c'}\;\overline{b'd'} + \overline{a'd'}\;\overline{b'c'}\right) F. \tag{6.1}$$

If function F is taken to be unity then the above expression reduces to the quasi-normal approximation. This was done in Canuto et al. (1994) but the results of some of their third-order moments were not satisfactory when compared to LES data.

The expression for $\overline{w'^3}$ is as follows:

$$\overline{w'^3} = \left(\Omega_1 - 1.2X_1 - \frac{3}{2}f_5\right)\left(c - 1.2X_0 + \Omega_0\right)^{-1}, \tag{6.2}$$

with the functions X and Ω_0 defined as

$$\begin{aligned}
X_0 &= \gamma_2 \tilde{N}^2\left(1 - \gamma_3\tilde{N}^2\right)\left[1 - (\gamma_1 + \gamma_3)\tilde{N}^2\right]^{-1} \\
X_1 &= \left[\gamma_0 f_0 + \gamma_1 f_1 + \gamma_2\left(1 - \gamma_3\tilde{N}^2\right) f_2\right]\left[1 - (\gamma_1 + \gamma_3)\tilde{N}^2\right]^{-1} \\
\Omega_0 &= \omega_0 X_0 + \omega_1 Y_0 \\
\Omega_1 &= \omega_o X_1 + \omega_1 Y_1 + \omega_2.
\end{aligned} \tag{6.3}$$

The ω function's are given by

$$\begin{aligned}\omega_0 &= \gamma_4\left(1-\gamma_5\tilde{N}^2\right)^{-1}\\ \omega_1 &= (2c)^{-1}\,\omega_0\\ \omega_2 &= \omega_1 f_3 + \frac{5}{4}\omega_0 f_4.\end{aligned}\tag{6.4}$$

The γ's are constants which depend on the adjustable parameter c. Canuto et al. (2001) and previous work found that $c = 7$, although small variations are allowed. The γ constants are given by:

$$\begin{aligned}\gamma_0 &= 0.52c^{-2}\,(c-2)^{-1}\\ \gamma_1 &= 0.87c^{-2}\\ \gamma_2 &= 0.5c^{-1}\\ \gamma_3 &= 0.60c^{-1}\,(c-2)^{-1}\\ \gamma_4 &= 2.4\,(3c+5)^{-1}\\ \gamma_5 &= 0.6c^{-1}\,(3c+5)^{-1}.\end{aligned}\tag{6.5}$$

Finally, the functions are introduced which incorporate the second-order moments of $\overline{w'^2}$, $\overline{w'\theta_l'}$, $\overline{\theta_l'}$, and $\overline{e}$. These are defined as follows:

$$\begin{aligned}f_0 &= (g\alpha)^3\,\tau_v^4\overline{w'\theta_l'}\frac{\partial\overline{\theta_l'^2}}{\partial z}\\ f_1 &= (g\alpha)^2\,\tau_v^3\left(\overline{w'\theta_l'}\frac{\partial\overline{w'\theta_l'}}{\partial z}+\frac{1}{2}\overline{w'^2}\frac{\partial\overline{\theta_l'}}{\partial z}\right)\\ f_2 &= g\alpha\tau_v^2\overline{w'\theta_l'}\frac{\partial\overline{w'^2}}{\partial z}+2g\alpha\tau_v^2\overline{w'^2}\frac{\partial\overline{w'\theta_l'}}{\partial z}\\ f_3 &= g\alpha\tau_v^2\left(\overline{w'^2}\frac{\partial\overline{w'\theta_l'}}{\partial z}+\overline{w'\theta_l'}\frac{\partial\overline{e}}{\partial z}\right)\\ f_4 &= \tau_v\overline{w'^2}\left(\frac{\partial\overline{w'^2}}{\partial z}+\frac{\partial\overline{e}}{\partial z}\right)\\ f_5 &= \tau_v\overline{w'^2}\frac{\partial\overline{w'^2}}{\partial z}.\end{aligned}\tag{6.6}$$

All of the above f functions have the dimensions of velocity cubed. In addition, we define $\tilde{N}^2 = \tau_v^2 N^2$.

Once $\overline{w'^3}$ is determined we perform clipping to ensure that this calculation does not produce unrealistically large values. $\mid \overline{w'^3} \mid$ is constrained by $w3_{clip}\sqrt{2.0\overline{w'^2}}$. Where $w3_{clip}$ is an adjustable parameter with a default value of 1.2.

7 Assumed PDF

Here details of the Analytic Double Gaussian (ADG) 1 PDF (as referred to in Larson et al. 2002), which is the PDF used in SHOC, are presented. The input moments for this PDF are $\overline{\theta_l}$, $\overline{q_t}$, $\overline{w'^2}$, $\overline{w'\theta_l'}$, $\overline{w'q_t'}$, $\overline{q_w'\theta_l'}$, $\overline{q_t'^2}$, $\overline{\theta_l'^2}$, $\overline{q_w'\theta_l'}$, and $\overline{w'^3}$. Note that at the beginning of this module $\overline{w'\theta_l'}$, $\overline{w'q_t'}$, $\overline{q_w'\theta_l'}$, $\overline{q_t'^2}$, $\overline{\theta_l'^2}$, $\overline{w'^3}$ are interpolated to the mid-point grid.

This PDF, as the name suggests, is based on the double Gaussian form as

$$P_{adg1}(w', \theta_l', q_t') = aG_1(w', \theta_l', q_t') + (1-a)G_2(w', \theta_l', q_t'). \tag{7.1}$$

Here G_1 and G_2 are the individual Gaussians and the parameters for the ADG 1 can be found analytically. To do this, some assumptions have to be made. The first assumption is that the subplume variations in w are uncorrelated with those in q_t and θ_l. Letting $i = 1$ or 2, the individual Gaussians in equation 7.1 are then given by

$$\begin{aligned}
G_i(w', \theta_l', q_t') = {} & \frac{1}{(2\pi)^{3/2}\sigma_{wi}\sigma_{q_t i}\sigma_{\theta_l i}(1 - r^2_{q_t\theta_l i})^{1/2}} \exp\left[-\frac{1}{2}\left(\frac{w' - (w_i - \overline{w})}{\sigma_{wi}}\right)^2\right] \\
& \times \exp\left(-\frac{1}{2(1 - r^2_{q_t\theta_l i})}\left\{\left[\frac{q_t' - (q_{ti} - \overline{q_t})}{\sigma_{q_t i}}\right]^2 + \left[\frac{\theta_l' - (\theta_{li} - \overline{\theta_l})}{\sigma_{\theta_l i}}\right]^2\right.\right. \\
& \left.\left. - \; 2r_{q_t\theta_l i}\left[\frac{q_t' - (q_{ti} - \overline{q_t})}{\sigma_{q_t i}}\right]\left[\frac{\theta_l' - (\theta_{li} - \overline{\theta_l})}{\sigma_{\theta_l i}}\right]\right\}\right).
\end{aligned} \tag{7.2}$$

Now we must define the PDF parameters. The PDF parameters are based on the equations of Lewellen and Yoh (1993) and are found by integrating over the 12 relevant input moments over the double Gaussian PDF. Four of these equations are (the rest are analogous):

$$\begin{aligned}
\overline{w} &= aw_1 + (1-a)w_2 \\
\overline{w'^2} &= a[(w_1 - \overline{w})^2 + \sigma^2_{w1}] + (1-a)[(w_2 - \overline{w})^2 + \sigma^2_{w2}] \\
\overline{w'^3} &= a[(w_1 - \overline{w})^3 + 3(w_1 - \overline{w})\sigma^2_{w1}] + (1-a)[(w_2 - \overline{w})^3 + 3(w_2 - \overline{w})\sigma^2_{w2}] \\
\overline{w'q_t'} &= a[(w_1 - \overline{w})(q_{t1} - \overline{q_t}) + r_{wq_t1}\sigma_{w1}\sigma_{q_{t1}}] + (1-a)[(w_2 - \overline{w})(q_{t2} - \overline{q_t}) + r_{wq_t2}\sigma_{w2}\sigma_{q_{t2}}].
\end{aligned} \tag{7.3}$$

with the relative amplitude of the Gaussian a is defined as

$$a = \frac{1}{2}\left\{1 - Sk_w\left[\frac{1}{4(1 - \tilde{\sigma}_w^2)^3 + Sk_w^2}\right]^{1/2}\right\}. \tag{7.4}$$

This is obtained by assuming that the standard deviations of the two Gaussins are equal in w and integrating over the PDF. Here $Sk_w \equiv \overline{w'^3}/(\overline{w'^2}^{3/2})$, represents the skewness of vertical velocity. In the case of $\overline{w'^2}$=0 it is assumed that the PDF reduces to a single delta function. The parameters for w_1 and w_2 are given by:

$$\tilde{w}_1 \equiv \frac{w_1 - \overline{w}}{\sqrt{\overline{w'^2}}} = \left(\frac{1-a}{a}\right)^{1/2}(1 - \tilde{\sigma}_w^2)^{1/2} \tag{7.5}$$

and

$$\tilde{w}_2 \equiv \frac{w_2 - \overline{w}}{\sqrt{\overline{w'^2}}} = \left(\frac{a}{1-a}\right)^{1/2} (1 - \tilde{\sigma}_w^2)^{1/2}. \tag{7.6}$$

To avoid numerical instabilities in the model a threshold for a must be defined as $0.01 \leq a \leq 0.99$. We also have the definitions of $\tilde{\sigma}_w \equiv \sigma_{w1}/\sqrt{\overline{w'^2}} = \sigma_{w2}/\sqrt{\overline{w'^2}}$ and $\tilde{\sigma}_w^2 = 0.4$.

Now to define terms for θ_{l1} and θ_{l2} we get:

$$\tilde{\theta}_{l1} \equiv \frac{\theta_{l1} - \overline{\theta_l}}{\sqrt{\overline{\theta_l'^2}}} = -\frac{\overline{w'\theta_l'}/(\sqrt{\overline{w'^2}}\sqrt{\overline{\theta_l'^2}})}{\tilde{w}_2} \tag{7.7}$$

and

$$\tilde{\theta}_{l2} \equiv \frac{\theta_{l2} - \overline{\theta_l}}{\sqrt{\overline{\theta_l'^2}}} = -\frac{\overline{w'\theta_l'}/(\sqrt{\overline{w'^2}}\sqrt{\overline{\theta_l'^2}})}{\tilde{w}_1}. \tag{7.8}$$

Should there be no variability in θ_l then the means of the Gaussians are set equal so that $\theta_{l1} = \theta_{l2} = \overline{\theta_l}$ and the widths of the Gaussians in the θ_l direction are set to zero.

Unlike vertical velocity, the widths in the θ_l direction are allowed to differ. These are found by integrating over the PDF and defined as:

$$\frac{\sigma_{\theta_l 1}^2}{\overline{\theta_l'^2}} = \frac{3\tilde{\theta}_{l2}[1 - a\tilde{\theta}_{l1}^2 - (1-a)\tilde{\theta}_{l2}^2] - [Sk_{\theta_l} - a\tilde{\theta}_{l1}^3 - (1-a)\tilde{\theta}_{l2}^3]}{3a(\tilde{\theta}_{l2} - \tilde{\theta}_{l1})} \tag{7.9}$$

and

$$\frac{\sigma_{\theta_l 2}^2}{\overline{\theta_l'^2}} = \frac{3\tilde{\theta}_{l1}[1 - a\tilde{\theta}_{l1}^2 - (1-a)\tilde{\theta}_{l2}^2] - [Sk_{\theta_l} - a\tilde{\theta}_{l1}^3 - (1-a)\tilde{\theta}_{l2}^3]}{3(1-a)(\tilde{\theta}_{l2} - \tilde{\theta}_{l1})}. \tag{7.10}$$

To prevent unrealistic solutions the following condition is set

$$0 \leq \frac{\sigma_{\theta_l 1,2}^2}{\overline{\theta_l'^2}} \leq 100. \tag{7.11}$$

Analogous equations are used to find $\tilde{q}_{t1,2}$ and $\sigma_{qt1,2}^2$.

The equations above make clear that SHOC is dependent on the skewness of θ_l and q_t. For the ADG 1 PDF, neither $\overline{\theta_l'^3}$ and $\overline{q_t'^3}$ are input moments, therefore diagnostic assumptions must be made. Sk_{θ_l} is simply set to zero for the ADG 1 PDF as it is found that this value prevents numerical instabilities from being introduced. To represent skewness in cumulus layers the following conditions are set for Sk_{q_t}: When $|\tilde{q}_{t2} - \tilde{q}_{t1}| > 0.4$ we set $Sk_{q_t} = 1.2 Sk_w$. When $|\tilde{q}_{t2} - \tilde{q}_{t1}| \leq 0.2$ we set $Sk_{q_t} = 0$. Between these two extremes Sk_{q_t} is linearly interpolated.

The within-plume correlations are computed by setting $r_{q_t\theta_l 1} = r_{q_t\theta_l 2}$ and integrating over the PDF to obtain an equation for $\overline{q_t'\theta_l'}$ and hence:

$$r_{q_t\theta_l 1,2} = \frac{\overline{q_t'\theta_l'} - a(q_{t1} - \overline{q_t})(\theta_{l1} - \overline{\theta_l}) - (1-a)(q_{t2} - \overline{q_t})(\theta_{l2} - \overline{\theta_l})}{a\sigma_{q_t 1}\sigma_{\theta_l 1} + (1-a)\sigma_{q_t 2}\sigma_{\theta_{l2}}} \tag{7.12}$$

with the condition that

$$-1 \leq r_{q_t\theta_l 1,2} \leq 1 \tag{7.13}$$

because correlations must lie between -1 and 1.

Now that we have defined the PDF parameters, we can now diagnose SGS cloud and turbulence terms. Cloud fraction, liquid water content, and liquid water flux are all given by:

$$\begin{aligned} C &= a(C)_1 + (1-a)(C)_2 \\ \overline{q_l} &= a(\overline{q_l})_1 + (1-a)(\overline{q_l})_2 \\ \overline{w'q_l'} &= a[(w_1 - \overline{w})(\overline{q_l}) + (\overline{w'q_l'})_1] + (1-a)[(w_2 - \overline{w})(\overline{q_l})_2 + (\overline{w'q_l'})_2]. \end{aligned} \tag{7.14}$$

In addition, the buoyancy flux can be closed using the expression:

$$\overline{w'\theta_v'} = \overline{w'\theta_l'} + \frac{1-\epsilon_o}{\epsilon_o}\theta_o \overline{w'q_t'} + \left[\frac{L_v}{c_p}\left(\frac{p_o}{p}\right)^{R_d/c_p} - \frac{1}{\epsilon_o}\theta_o\right]\overline{w'q_l'} \tag{7.15}$$

The individual cloud fraction C and mean specific liquid water content $\overline{q_l}$ are calculated by linearizing the variability in θ_l and q_t (with analogous expressions for the Gaussian 1 and 2 for equations 7.16 though 7.23):

$$C = \frac{1}{2}\left[1 + \mathrm{erf}\left(\frac{s}{\sqrt{2}\sigma_s}\right)\right] \tag{7.16}$$

and

$$\overline{q_l} = sC + \frac{\sigma_s}{\sqrt{2\pi}}\exp\left[-\frac{1}{2}\left(\frac{s}{\sigma_s}\right)^2\right]. \tag{7.17}$$

Here erf is the error function and σ_s is the standard deviation of s, which is equal to the liquid water content when s is greater than zero, but can also be negative and is conserved under condensation. These two terms are defined as (Lewellen and Yoh 1993):

$$\begin{aligned} s &= q_t - q_s(T_l, p)\frac{(1+\beta q_t)}{[1+\beta q_s(T_l,p)]} \\ \sigma_s^2 &= c_{\theta_l}^2\sigma_{\theta_l}^2 + c_{q_t}^2\sigma_{q_t}^2 - 2c_{\theta_l}\sigma_{\theta_l}c_{q_t}\sigma_{q_t}r_{q_t\theta_l} \end{aligned} \tag{7.18}$$

where q_s is the saturation mixing ratio with respect to either water or ice or a hybrid of the two depending on the temperature, and β is defined as:

$$\beta = \beta(T_l) = \frac{R_d}{R_v}\left(\frac{L_v}{R_d T_l}\right)\left(\frac{L_v}{c_p T_l}\right). \tag{7.19}$$

Also defined are the following terms:

$$c_{q_t} = \frac{1}{1 + \beta(T_l)q_s(\overline{T_l}, p)} \tag{7.20}$$

and

$$c_{\theta_l} = \frac{1 + \beta(\overline{T_l})\overline{q_t}}{[1 + \beta(\overline{T_l})q_s(\overline{T_l}, p)]^2}\frac{c_p}{L_v}\beta(\overline{T_l})q_s(\overline{T_l}, p)\left(\frac{p}{p_o}\right)^{R_d/C_p} \tag{7.21}$$

Finally, the flux of liquid water is given by:

$$\overline{w'q_l'} = C\overline{w's'} \tag{7.22}$$

where

$$\overline{w's'} = c_{q_t}\sigma_w\sigma_{q_t}r_{wq_t} - c_{\theta_l}\sigma_w\sigma_{\theta_l}r_{w\theta_l}. \tag{7.23}$$

In the above expressions q_s and β are defined as:

$$q_s(T_l, P) = \frac{R_d}{R_v}\frac{e_s(T_l)}{p - [1 - (R_d/R_v)]e_s(T_l)} \tag{7.24}$$

and

$$\beta = \beta(T_l) = \frac{R_d}{R_v}\left(\frac{L_v}{R_dT_l}\right)\left(\frac{L_v}{c_pT_l}\right). \tag{7.25}$$

Here q_s is the saturation specific humidity, e_s is the saturation vapor pressure over liquid, p is pressure, c_p is the specific heat at constant pressure, and R_d and R_v are the gas constants for dry air and water vapor. In addition, we define T_l as the liquid water temperature:

$$T_l = T - \frac{L_v}{c_p}q_l \tag{7.26}$$

where T is temperature. In SHOC, e_s is computed based on Flatau et. al (1992).

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