

# P1.38 A STRATEGY FOR IMPROVEMENT OF LES PREDICTION OF STRATOCUMULUS ENTRAINMENT USING THE 'ONE-DIMENSIONAL TURBULENCE' SIMULATION METHOD

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## 1. STRATOCUMULUS ENTRAINMENT: A MODELING CHALLENGE

The phenomenology of stratocumulus (Sc) entrainment challenges the precepts on which atmospheric flow modeling and simulation are based. Here, we adopt the terminology of Wyngaard (1998): simulations resolve most of the energy-containing motions on the computational mesh but models do not resolve the turbulent motion. Spatial and temporal resolution of turbulent motions is of greatest importance in situations that involve strong influence of localized microphysics on large scale motions. Sc entrainment is a salient example of such a scenario. The governing microphysics is localized in the sense that its mean state, as well as its fluctuations, vary significantly over a short vertical distance (order 1 m) at cloud top. The challenge in this regard is to capture the influence of cloud-top microphysics on large scales either by resolving the relevant spatial scales or by sub-grid-scale (SGS) modeling that parameterizes this influence.

At this time it is difficult to formulate a suitable SGS model because the dynamical process that conditions the air in the entrainment interface layer (EIL) above cloud top is not well understood. This process is governed by the interaction of detrainment of cloudy air into the EIL, turbulent mixing of cloudy and clear air in the EIL, evaporative and radiative cooling, subsidence, and the entrainment process itself. Laboratory and field measurements and direct numerical simulations (DNS) do not, individually or collectively, provide the needed empirical guidance for SGS modeling of the EIL.

These considerations motivate efforts to push large-eddy simulations (LES) of Sc to progressively finer vertical mesh resolution at cloud top. Recent work indicates that the 5 m resolution that is now achievable, in conjunction with present capability to model SGS processes, is not sufficient and there is no clear path to significant improvement in the foreseeable future (Stevens et al., 2005). In the face of this challenge, what possi-

bility is there for modeling or simulation to contribute further to physical understanding and prediction of Sc entrainment?

To establish context for the approach outlined here, it is useful to note that Sc entrainment is one example of a variety of situations in which microscale physics and chemistry strongly influence large scale motions. Combustion is analogous in this regard, and the analogy is multi-faceted. Combustion is strongly influenced by turbulent mixing, phase change, and associated radiative couplings. Buoyancy is often inconsequential, but the effects of chemically induced thermal expansion are almost always important. The crucial microscale phenomenology occurs in a thin flame front whose evolution is largely controlled by heat transport.

Recognizing then that microscale feedback to large scales is a generic challenge, a generic strategy for addressing this challenge should be sought. Here, such a strategy is outlined, with emphasis on progress toward its application to Sc entrainment.

To introduce the strategy described here, it is useful to compare LES and single-column modeling (SCM), both of which have been applied to Sc. In Wyngaard's terminology, LES is simulation and SCM is modeling, because the former but not the latter resolves individual turbulent motions. Note that this distinction between simulation and modeling is not directly tied to the difference between the spatial dimensionalities of LES and SCM. For example, a 3D Reynolds-averaged Navier-Stokes (RANS) method is a model rather than a simulation by this definition. Also, lower-dimensional formulations can be simulations, as in 2D implementations of LES. Accordingly, a 1D formulation can be a simulation rather than a model if a method can be devised to represent individual turbulent motions in 1D.

This raises two questions. First, is it feasible to do this in a manner that provides useful predictive capability? Second, if this is feasible, in what way would it be advantageous?

The first question is addressed in what follows. Sc entrainment is a useful context for answering the second question. As noted, the computational cost of 3D LES precludes adequate resolution of EIL dynamics in the near future. 2D LES of Sc, though less costly than

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3D LES, is subject to artifacts that limit its predictive capability to a degree that may counteract its computational cost advantages (Stevens et al., 1998). In this context, what is needed but not yet available is an affordable method for capturing the leading order effects and their locally resolved, coupled dynamics in a manner that provides at least an idealized representation of the underlying physics. A 1D formulation, denoted ‘one-dimensional turbulence’ (ODT), is described here that has the potential to fill this need. Progress toward realization of this potential is described.

## 2. MODELING APPROACH

To introduce ODT, a Boussinesq formulation is outlined that simulates the time evolution of velocity components  $u$ ,  $v$ , and  $w$  and density  $\rho$  defined on a 1D domain representing the vertical ( $z$ ) coordinate. This evolution involves two processes: (1) a sequence of eddy events, which are instantaneous transformations that represent turbulent stirring, and (2) intervening time advancement of conventional form. Each eddy event may be interpreted as the model analog of an individual turbulent eddy. The locations, sizes, and frequency of eddy events are governed by a stochastic process.

During the time interval between each eddy event and its successor, the time evolution of property profiles is governed by the equations

$$(\partial_t - \nu \partial_z^2) u(z, t) = 0 \quad (1)$$

$$(\partial_t - \nu \partial_z^2) v(z, t) = 0 \quad (2)$$

$$(\partial_t - \nu \partial_z^2) w(z, t) = 0 \quad (3)$$

$$(\partial_t - \gamma \partial_z^2) \rho(z, t) = 0. \quad (4)$$

Here  $\nu$  is viscosity and  $\gamma$  is diffusivity of the scalar, temperature, that controls the density. In laboratory-scale applications of ODT, resolution of molecular transport is affordable so the molecular transport coefficients are used. For domain sizes comparable to the depth of the atmospheric boundary layer (ABL), this degree of resolution is unaffordable, so SGS closure analogous to closures used in LES is employed (see Sec. 3).

To illustrate the approach, consider convection between horizontal surfaces at  $z = 0$  and  $H$ , with unstable stratification maintained by boundary conditions. (1)-(4) are solved on  $[0, H]$ . Boundary conditions applied to the velocity at  $z = 0$  and  $H$  are  $u = v = w = 0$ . Density boundary conditions are  $\rho(0, t) = \rho_1$  and  $\rho(H, t) = \rho_2$ , where  $\rho_2 > \rho_1$  to enforce unstable stratification, which drives the flow.

Each eddy event consists of two mathematical operations. One is a mapping operation representing the

fluid displacements associated with a notional turbulent eddy. The other is a modification of the velocity profiles in order to implement pressure-induced energy redistribution among velocity components and net kinetic-energy gain or loss due to equal-and-opposite changes of the gravitational potential energy. These operations are represented symbolically as

$$\begin{aligned} \rho(z) &\rightarrow \rho(M(z)) \\ u(z) &\rightarrow u(M(z)) + c_u K(z) \\ v(z) &\rightarrow v(M(z)) + c_v K(z) \\ w(z) &\rightarrow w(M(z)) + c_w K(z). \end{aligned} \quad (5)$$

According to this prescription, fluid at location  $M(z)$  is moved to location  $z$  by the mapping operation, thus defining the map in terms of its inverse  $M(z)$ . This mapping is applied to all fluid properties. The additive term  $c_s K(z)$ , where  $s = u, v$ , or  $w$ , affects only the velocity components. It implements the aforementioned kinetic-energy changes. Potential-energy change is inherent in the mapping-induced vertical redistribution of the  $\rho$  profile; see (9).

The map used to represent turbulent eddy motion, termed the ‘triplet map’ (see Kerstein, 1991 for an illustration and motivational discussion), is defined as

$$M(z) \equiv z_0 + \begin{cases} 3(z - z_0) & \text{if } z_0 \leq z \leq z_0 + \frac{1}{3}l, \\ 2l - 3(z - z_0) & \text{if } z_0 + \frac{1}{3}l \leq z \leq z_0 + \frac{2}{3}l, \\ 3(z - z_0) - 2l & \text{if } z_0 + \frac{2}{3}l \leq z \leq z_0 + l, \\ z - z_0 & \text{otherwise.} \end{cases} \quad (6)$$

This mapping takes a line segment  $[z_0, z_0 + l]$ , shrinks it to a third of its original length, and then places three copies on the original domain. The middle copy is reversed, which maintains the continuity of advected fields and introduces the rotational folding effect of turbulent eddy motion. Property fields outside the size- $l$  segment are unaffected.

In (5),  $K$  is a kernel function that is defined as  $K(z) = z - M(z)$ , i.e., its value is equal to the distance the local fluid element is displaced. It is non-zero only within the eddy interval, and it integrates to zero so that the process does not change the total ( $z$ -integrated) momentum of individual velocity components. It provides a mechanism for energy redistribution among velocity components, enabling the model to simulate the tendency of turbulent eddies to drive the flow toward isotropy, constrained by the requirement of total (kinetic plus potential) energy conservation during the eddy event (which is non-dissipative).

To quantify these features of eddy energetics, and thereby specify the coefficients  $c_s$  in (5), it is convenient to introduce the quantities

$$s_K \equiv \frac{1}{l^2} \int s(M(z)) K(z) dz, \quad (7)$$

where  $s = u, v, w$ , or  $\rho$ . Substitution of the definition of  $K(z)$  into (7) yields

$$s_K = \frac{1}{l^2} \int [zs(M(z)) - M(z)s(M(z))] dz \quad (8)$$

$$= \frac{1}{l^2} \int [s(M(z)) - s(z)]z dz.$$

Because  $M(z)$  is a measure-preserving map of the  $z$  domain onto itself, the domain integral of any function of  $M(z)$  is equal to the domain integral of the same function with argument  $z$ . This allows the substitutions of  $z$  for  $M(z)$  that yield the final result in (8). For  $s = \rho$ , this expression is proportional to the potential-energy change induced by the triplet map. The energy change  $\Delta$  caused by an eddy event can then be expressed as

$$\Delta = \rho_0 l^2 (c_u u_K + c_v v_K + c_w w_K) + \frac{2}{27} \rho_0 l^3 (c_u^2 + c_v^2 + c_w^2) + gl^2 \rho_K, \quad (9)$$

where a reference density  $\rho_0$  (defined here as mass per unit height, based on a nominal column cross-section) is introduced (i.e., the standard Boussinesq prescription), as well as the gravitational acceleration  $g$ .

The representation of both the potential and kinetic energy contributions in (9) using (7) is a consequence of the definition chosen for  $K$ . Based on this definition, another equivalent form of (7),

$$s_K \equiv \frac{4}{9l^2} \int_{z_0}^{z_0+l} s(z)[l - 2(z - z_0)] dz, \quad (10)$$

which is useful for numerical implementation, is readily obtained.

Overall energy conservation requires  $\Delta = 0$ . Two additional conditions are required to specify the coefficients  $c_s$ . These are based on a representation of the tendency for eddies to induce isotropy. For this purpose, it is noted that there is a maximum amount  $Q_s = \frac{27}{8} \rho_0 l s_K^2$  of kinetic energy that can be extracted from a given velocity component  $s$  during an eddy event (Kerstein et al., 2001). (The amount of energy actually extracted or deposited depends on  $c_s$ .)  $Q_s$  is thus the 'available energy' in component  $s$  prior to event implementation. The tendency toward isotropy is introduced by requiring the available energies of the three velocity components to be equal upon completion of the eddy event. This provides the additional needed conditions and yields the following expression determining  $c_s$ :

$$c_s = \frac{27}{4l} \left[ -s_K \pm \sqrt{\frac{1}{3} \left( u_K^2 + v_K^2 + w_K^2 - \frac{8gl}{27} \frac{\rho_K}{\rho_0} \right)} \right]. \quad (11)$$

The physical criterion that resolves the sign ambiguity is explained in Kerstein et al. (2001). Note that the

last term in (11) is the square root of a quantity proportional to the net available energy  $Q_u + Q_v + Q_w - P$ , where the quantities  $Q_s$  are the component available energies prior to event implementation and  $P$  is the gravitational potential energy change caused by triplet-mapping of the  $\rho$  profile, requiring equal-and-opposite change of available energy during eddy implementation, as enforced by the condition  $\Delta = 0$ . If  $P$  is positive (stable stratification) and larger than the available energy, then the eddy is energetically prohibited. In this case, the argument of the square root in (11) is negative and the eddy event is not implemented (see below).

Although the formulation of an individual eddy event incorporates several important features of turbulent eddies (Kerstein, 1991), the key to the overall performance of the model is the procedure for determining the sequence of eddy events during a simulated flow realization. The expected number of eddies occurring during a time interval  $dt$ , whose parameter values are within  $dz$  of  $z_0$  and within  $dl$  of  $l$ , is denoted the 'eddy rate distribution'  $\lambda(z_0, l; t) dz_0 dl dt$ , which has units of  $(\text{length}^2 \times \text{time})^{-1}$ . Eddies are randomly sampled from this distribution. Mathematically, this generates a marked Poisson process (Snyder and Miller, 1991) whose mean rate as a function of the 'mark' (parameter) values  $z_0$  and  $l$  varies with time. The physical content of the eddy selection process is embodied in the expression for  $\lambda$  that is adopted,

$$\lambda = \frac{C\nu}{l^4} \sqrt{\left(\frac{u_K l}{\nu}\right)^2 + \left(\frac{v_K l}{\nu}\right)^2 + \left(\frac{w_K l}{\nu}\right)^2 - \frac{8gl^3}{27\nu^2} \frac{\rho_K}{\rho_0} - Z}. \quad (12)$$

$\lambda$  is set equal to zero if the argument of the square root is negative, indicating an energetically prohibited event; see the discussion of (11).

(12) involves two free parameters,  $C$  and  $Z$ .  $C$  scales the eddy event rate, and hence the simulated turbulence intensity, for a given flow configuration. The role of  $Z$  is to impose a threshold eddy Reynolds number that must be exceeded to allow eddy occurrence (Kerstein and Wunsch, 2006). In near-wall flow, the transition from the viscous layer to the buffer layer is sensitive to this threshold and hence to  $Z$  (Schmidt et al., 2003). For  $Z > 0$ , eddies are suppressed entirely when local values of the eddy Reynolds number are sufficiently small.

For  $Z = 0$ , the argument of the square root is a scaled form of the net available energy. Thus, for given  $z_0$  and  $l$ , (12) with  $Z = 0$  is simply the dimensionally consistent relation between the net available energy and the length and time scales of eddy motion, where the associated time scale is the inverse of the (appropriately normalized) eddy rate  $\lambda$ . (12) may therefore

be viewed as a representation of mixing-length phenomenology within the ODT framework. This phenomenology is the basis of many turbulence modeling approaches, including SGS closure of LES (see Sec. 3). However, the present approach, which does not involve averaging, differs from the typical use of mixing-length concepts to close averaged equations in several respects:

1. Rather than assigning a unique  $l$  value at each spatial location, ODT allows eddies of all sizes throughout the spatial domain, with location-dependent frequencies of occurrence that are specified by (12).
2. Quantities on the right-hand side of (12) depend on the instantaneous flow state rather than an average state, so eddy occurrences are responsive to unsteadiness resulting from transient forcing or from statistical fluctuations inherent in the eddy-sampling process.
3. Eddy occurrences thus depend on the effects of prior eddies and affect future eddy occurrences. These dependencies induce spatio-temporal correlations among eddy events, leading to a physically based representation of turbulence intermittency.

These attributes of ODT are the basis of its detailed representation of turbulent cascade dynamics coupled to boundary conditions, shear and buoyant forcing, etc. In particular, the stochastic variability of simulated ODT realizations arises from a physically based representation of turbulent eddy statistics, and thus enables a conceptually sound and mathematically consistent assessment of the effects of stochastic variability on the variability of, and correlations among, output statistics. In these respects, ODT is a simulation rather than a model in the terminology of Wyngaard (1998).

The formulation outlined above combines features introduced in previous ODT formulations. If two of the three velocity components are removed from the model, (12) reduces to the eddy rate distribution used in Wunsch and Kerstein (2001). If the buoyancy term is omitted, (12) resembles a previous expression for  $\lambda$  (Kerstein et al., 2001), except that here,  $\lambda$  is based on the total available energy (including contributions from all three velocity components) rather than the available energy associated with vertical motion. Use of the total available energy is advantageous here because the onset of instability (in the present context, eddy events) then occurs at the correct critical value,  $Ri_c = \frac{1}{4}$ , of the gradient Richardson number (Turner, 1979).

The unsteadiness of the rate distribution  $\lambda$  suggests the need to reconstruct this distribution continuously

as the flow state evolves. This prohibitively costly procedure is avoided by an application of the rejection method (L'Ecuyer, 2004), involving eddy sampling based on an arbitrary sampling distribution that is designed to over-sample all eddies. True rates are computed only for sampled eddies, and are used to determine eddy acceptance probabilities. The resulting procedure adequately approximates the desired sampling from  $\lambda$  (Kerstein, 1999a), and is exact in the limit of infinite over-sampling. The choice of the arbitrary sampling distribution affects the efficiency of the sampling procedure, but not the statistics of the eddies that are selected for implementation.

Given an eddy-sampling time-step  $\Delta t_s$  and an arbitrary joint probability density function  $h(z_0, l)$  used to sample  $z_0$  and  $l$ , time advancement of the ODT simulation is implemented as follows:

1. Advance (1)-(4) for a time interval  $\Delta t_s$ .
2. Sample  $z_0$  and  $l$  values from  $h(z_0, l)$ .
3. For these values, compute  $\lambda(z_0, l)$  based on the current flow state.
4. Compute the ratio  $P$  of the rate  $\lambda(z_0, l)$  of occurrence of an eddy with these  $z_0$  and  $l$  values as given by the model to the rate  $h(z_0, l)/\Delta t_s$  based on the sampling procedure.
5. Implement the selected eddy with probability  $P$  based on a Bernoulli trial, i.e., implement the eddy if  $P = \lambda(z_0, l)\Delta t_s/h(z_0, l)$  is larger than a random variable sampled from the uniform distribution over  $[0, 1]$ .

$\Delta t_s$  must be assigned a value small enough so that  $P$  never exceeds unity. For numerical accuracy,  $P \ll 1$  should be obeyed with at most rare exceptions. For an evolving flow, it is efficient to adjust  $\Delta t_s$  during advancement in order to direct the  $P$  values toward a target range, typically of order 0.01.

### 3. ADAPTATION FOR ABL APPLICATION

For application to the ABL, the formulation of Sec. 2 is modified in several ways. First, an SGS closure is introduced. Second, instead of density, an appropriate adiabatically conserved thermodynamic variable is used. For moist thermodynamics, two conserved variables are needed. Third, radiative flux divergence is introduced. Fourth, Coriolis and subsidence effects are introduced. Fifth, an empirically motivated modification of the eddy selection process is proposed to improve its entrainment representation.

The second through fourth modifications are closely analogous to standard treatments in LES, so they are not elaborated here. They were implemented for dry conditions, with radiation omitted, by Kerstein and Wunsch (2006). The other modifications are explained briefly.

LES momentum closures typically evaluate the SGS stresses in terms of the resolved strain field (Sagaut, 2006). Although all velocity components are evolved in ODT, their spatial variation is captured only in the  $z$  direction, so the strain tensor is not fully known. This prevents SGS closure of ODT that is formally identical to LES closure.

There is also a more fundamental consideration. Except for imposed subsidence, advection along the ODT domain is not implemented by displacing fluid as prescribed by the vertical velocity  $w$ . Rather, it consists of a sequence of vertical fluid displacements by triplet maps. The velocity profiles are inputs to the stochastic process that governs the selection of eddy events, but this connection between velocity and advection is less direct than in the exact governing equations.

An ODT SGS closure intended to model the effects of unresolved transport should be based on an estimate of the transport that would have occurred if the model had been better resolved. Therefore it should be based on the stochastic process governing eddy events. On this basis, an SGS momentum closure for constant-property ODT has been formulated (McDermott et al., 2005). It evaluates the SGS transport by ensemble averaging the stochastic evolution of the unresolved scales given the current resolved flow state, approximated by local linearization of velocity profiles. An adaptation of this closure was used for ODT simulation of a stably stratified ABL configuration (Kerstein and Wunsch, 2006). The closure used in that application lacked features analogous to SGS closure of LES of this variable-property flow (Kosovic and Curry, 2000). In particular, it is anticipated that implementation of an ODT analog of the subgrid turbulent kinetic energy equation will have a beneficial effect on closure performance.

In addition to this ABL application, ODT has been applied to a variety of buoyant stratified flows and results have been compared to laboratory and field measurements (Kerstein, 1999a; Kerstein, 1999b; Dreeben and Kerstein, 2000; Wunsch and Kerstein, 2001; Wunsch, 2003; Wunsch and Kerstein, 2005). These applications include entrainment of overlying stable fluid driven by either convection or shear (Kerstein, 1999a). This and subsequent unpublished studies of penetrative convection using various ODT formulations indicate a model discrepancy that illustrates both the capabilities and limitations of ODT and suggests a strategy for

further improvement.

A common feature of laboratory and geophysical penetrative convection is a reversal from positive to negative buoyancy flux as  $z$  increases within the mixed layer (Conzemius and Fedorovich, 2006). This reflects the nonlocality of transport associated with the entrainment of overlying stable fluid. If the mixed-layer eddies scour small parcels of overlying fluid and mix them at the top of the layer (i.e., localized transport and mixing), then the observed sign change is not expected.

ODT involves nonlocal transport due to the occurrence of a wide range of eddy sizes during the simulation. Nevertheless, simulations of penetrative convection using ODT formulations to date yield much less than the observed magnitude of negative buoyancy flux near the top of the mixed layer. Apparently, these formulations do not entrain enough overlying fluid deep enough into the mixed layer to reproduce this feature. Comparison of ODT to convective flow structure explains this deficiency and suggests a remedy.

In the mixed layer, rising plumes encounter the stable overlying fluid and are energetically prohibited from rising further. Due to their inertia, their motion continues but is redirected horizontally, resulting in a splat pattern and consequent strong localized shear near the top of the mixed layer. This shear induces turbulence that engulfs overlying fluid. In addition, wisps of overlying fluid are pulled downward in regions of convergence and consequent downward re-direction of these horizontal flows.

In ODT, eddy occurrence is determined energetically, as indicated by (12). The energy penalty associated with downward displacement of buoyant overlying fluid must be compensated by energy available from other sources. Near the top of the mixed layer, these sources are kinetic energy fluctuations (quantified by the shear metric based on the function  $K$ ) and displacements within the mixed layer that reduce the gravitational potential energy of the eddy. In general, an eddy must extend farther into the mixed layer than into the overlying stable layer in order to provide sufficient compensatory energy. This is qualitatively reasonable but does not capture entrainment augmentation due to the concentration of shear near the top of the mixed layer caused by plume splat. As a result, ODT does not displace enough of the overlying stable fluid far enough downward to reproduce the observed vertical profile of buoyancy flux.

ODT cannot capture the kinematics of plume splat, but the following modification of eddy selection and implementation can emulate the associated energetics. In addition to the usual eddy sampling, assume that there is also sampling of sets of three vertically adja-

cent eddies, identical in size. A selection criterion is formulated that determines that either all or none of these eddies are implemented. The sum of the available energies of the three eddies prior to eddy implementation is computed, and sum of the energy changes that would be caused by implementation of these eddies is also computed. Adding these two quantities, net available energy after implementation of all eddies is obtained. This energy is distributed equally among the three eddies, and is used to decide, in the usual manner, whether or not one of the three eddies should be implemented. (Now they all have the same available energy and hence the same likelihood of implementation.) This decision determines the implementation of either all or none of the eddies.

This additional eddy sampling qualitatively emulates the splat scenario in the following sense. The downward displacement of overlying fluid scales as the size of a single eddy (the topmost eddy) within the set of three (assuming that, typically, the other two are entirely within the mixed layer), but the  $z$  range corresponding to the set of three eddies contributes to the energy required for this displacement to occur. This provides a mechanism for redistributing the energy within this  $z$  range in order to drive entraining motions that would otherwise be unlikely or energetically forbidden. This energy-based mechanism emulates the outcome of plume splat without replicating the kinematics of plume splat. Specifically, it does not replicate the splat-induced horizontal shear that mediates the conversion of plume kinetic energy into the gravitational potential energy associated with downward displacement of stable fluid.

It remains to be determined, in future studies, whether this modification of eddy sampling improves the ODT treatment of penetrative convection quantitatively. Even if it does, it may not capture all the relevant phenomenology. Consider the meteorologically important regime of sheared convective boundary layer entrainment. There is evidence that shear can reduce entrainment by disrupting rising plumes (Conzemius and Fedorovich, 2006). In ODT, the persistence of plume motion is not represented, so no analog of shear-induced plume disruption is anticipated. The absence of persistent plume motion in ODT is compensated by adjustment of the parameter  $C$  that scales eddy transport. Therefore a value of  $C$  for which ODT simulation of penetrative convection without shear is accurate could be too high when shear is present.

These considerations illustrate subtleties of ABL phenomenology that might not be fully captured by ODT. Nevertheless, the various applications of ODT to date indicate that ODT has predictive capabilities that are comparable in many instances to multidimen-

sional flow simulations, though much less costly computationally. This motivates ongoing efforts, described next, to develop an ODT simulation of the  $Sc$ -topped ABL.

#### 4. A STRATEGY FOR IMPROVED ENTRAINMENT MODELING

The ODT formulation described in Sec. 3 is central to a strategy that is being pursued to improve the accuracy of LES prediction of  $Sc$  entrainment:

1. Using ODT, simulate flows that reproduce portions of EIL phenomenology.
2. Based on these simulations, validate the ODT formulation, with improvements as needed, and set model parameters.
3. Run  $Sc$ -topped ABL cases comparable to available field data and LES to evaluate the complete ODT representation of  $Sc$  entrainment.
4. Use ODT to perform an extensive parameter study of EIL structure and dynamics.
5. On this basis, formulate a free-standing physics model of the EIL.
6. Configure this model as a cloud-top SGS closure for LES of  $Sc$ .

A longer-term strategy that is also being pursued is to incorporate ODT itself into LES as an SGS closure or as an autonomous process that dispenses with the need for advancement of filtered LES quantities. This strategy is not discussed here, but progress to date is reported elsewhere (Kerstein, 2002; Schmidt et al., 2003; McDermott, 2005; Schmidt et al., 2005). The current strategy, as enumerated above, is explained briefly.

To establish the performance of ODT as a convective boundary layer model, it must first be validated as a model of turbulent convective transport. This has been done through comparisons of ODT mean transport and fluctuation properties for the configuration defined below (4) to convection-cell measurements over a wide range of Rayleigh and Prandtl numbers (Wunsch and Kerstein, 2005). As noted in Sec. 3, the performance of ODT as a convective boundary layer model is deficient in some respects, but the strategy outlined there to remedy these deficiencies is being implemented. ODT will then be evaluated as a model of dry convective boundary layers with and without shear.

An important feature of the EIL is buoyancy reversal resulting from evaporative cooling of detrained cloudy

air. Buoyancy reversal has been studied experimentally as a single-phase mixing process by Shy and Breidenthal (1990). ODT simulations of the experimental configuration reproduced the salient parameter dependencies that were observed (Wunsch, 2003). On this basis, an algebraic model was formulated that idealizes the physical content of the ODT representation of the experimental configuration. In this model, molecular diffusion of species in the stable layer above the mixed layer preconditions this overlying layer, reducing its stability and thereby facilitating entrainment. As a result, molecular diffusivity appears as a parameter in the algebraic expression for the entrainment rate. The algebraic model successfully correlates both the measurements and ODT simulation results over a broad parameter range including many experimentally inaccessible conditions (such as unattainable ratios of species diffusivity to viscosity).

These results sharpen the analogy between single-phase buoyancy-reversing systems and Sc entrainment. The main distinction between the two is that molecular diffusion conditions the overlying fluid in the former (as inferred from the comparisons of models and measurements), but the coupled processes of detrainment, radiative flux divergence, and phase change govern the conditioning of the EIL. Therefore, in an algebraic model representing Sc interaction with the EIL (in effect a Sc entrainment model), the analog of the molecular diffusion coefficient in the single-phase buoyancy reversal model will be a representation of the coupled multi-process dynamics of the EIL.

ODT will provide a highly resolved representation of EIL dynamics. ODT simulations with order  $10^4$  mesh cells are routine and some applications involve order  $10^5$  mesh cells, so sub-meter resolution in a Sc simulation is readily achieved. In recent work, an adaptive mesh scheme has been developed that will enable resolution of a few cm where needed in the EIL.

To validate the ODT representation of EIL processes, the ODT treatment of phase change in cloud aerosols and of radiative coupling must be tested. Phase change in clouds and its dynamical effects have been studied using the linear-eddy model (LEM), based on both bulk (Krueger, 1993; Krueger et al., 1997) and explicit-droplet (Su et al., 1998) microphysics. Like ODT, LEM utilizes map-based advection as specified by (6), but eddy selection in LEM is based on sampling from prescribed distributions rather than from the internally computed ODT distribution (12). These studies demonstrate the efficacy of map-based advection for simulation of mixing and associated phase change. Radiative coupling within ODT will be tested by comparison to a smoke-cloud experiment in which convection is radiatively driven (Sayler and Breidenthal, 1998).

That experiment exhibited an unexplained sensitivity to molecular diffusivity. This sensitivity will be investigated using ODT.

These preliminary studies will establish the ODT formulation and parameter assignments for Sc application. Sc cases comparable to available LES and field measurements will then be simulated. In addition, a wide-ranging parameter study will be performed. Analogous to the ODT study of buoyancy reversal, these results will enable the development of an EIL physics model of algebraic form.

It will be straightforward to configure such a model as an LES closure, but it is challenging to couple it to LES in a way that does not swamp the physical model by numerical transport. An LES intended for application to Sc evolution for a period of many hours or days must be run at coarser resolution than the codes that resolve 5 m vertically for brief periods. In such a coarse LES, the EIL is so narrow that its physics representation reduces, as a practical matter, to a set of jump conditions. A front tracking scheme can be used to implement the jump conditions without introducing excessive numerical artifacts.

The prospective EIL model governing these jump conditions may be of algebraic form, analogous to the algebraic model of buoyancy reversal. Alternatively, it may involve one or more ordinary differential equations, or a more elaborate treatment. In turbulent combustion simulations, models determining the jump conditions across an evolving flame front vary widely in complexity, in one case involving implementation of LEM within the simulation to evaluate jump conditions on the fly (Schmidt and Klein, 2003). The combustion application involves fronts that are more tortuous on large scales than the EIL, but EIL dynamics are more sensitive to front inclination than are flame dynamics.

In the present context, the common features of combustion and Sc entrainment are more relevant than the differences. Both involve localized frontal dynamics whose coupling to large scale evolution strongly influences that evolution. The localized dynamics cannot be resolved in a simulation of the full system. The level of complexity of SGS modeling required to represent these dynamics adequately, let alone the details of the SGS model, cannot be gleaned from general or heuristic considerations. A detailed, albeit idealized, simulation of the localized dynamics is an essential tool for development of the needed SGS model, or as noted, the simulation tool itself can be the SGS model. Here, a strategy has been outlined for development of an SGS model for LES of Sc entrainment based on the identification of ODT as an appropriate simulation tool.

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