

A REVIEW OF PARAMETERIZATION SCHEMES FOR TURBULENT BOUNDARY-LAYER PROCESSES

Roland B. Stull

Dept. of Atmospheric & Oceanic Sciences
University of Wisconsin, Madison, Wisconsin, USA

Abstract: When the equations of motion are averaged over a grid-cell volume in a numerical weather forecast model, extra turbulence terms appear that must be approximated or parameterized. Such parametrizations, known as closure assumptions, can be classified by their statistical order (S) and the degree of nonlocality (N). While no parameterization is perfectly accurate, they offer a range of physical details and computation economies from which to choose.

1. THE CLOSURE PROBLEM

When the equations of motion are averaged over a grid-cell volume within a numerical weather prediction (NWP) model, turbulence terms appear such as those for divergence of turbulent flux (Stull, 1988):

$$\begin{aligned} \frac{\partial \bar{\theta}}{\partial t} &= \dots (\text{advection, radiation, conduction, etc.}) \dots - \frac{\partial \overline{w'\theta'}}{\partial z} \\ \frac{\partial \bar{q}}{\partial t} &= \dots (\text{advection, condensation, diffusion, etc.}) \dots - \frac{\partial \overline{w'q'}}{\partial z} \\ \frac{\partial \bar{U}}{\partial t} &= \dots (\text{advection, pressure - grad., Coriolis, etc.}) \dots - \frac{\partial \overline{w'u'}}{\partial z} \\ \frac{\partial \bar{V}}{\partial t} &= \dots (\text{advection, pressure - grad., Coriolis, etc.}) \dots - \frac{\partial \overline{w'v'}}{\partial z} \end{aligned}$$

$\underbrace{\hspace{10em}}_{\text{storage}} = \dots \underbrace{\hspace{10em}}_{\text{(other physics)}} \dots - \underbrace{\hspace{10em}}_{\text{vertical flux divergence}}$

where (U, V) are horizontal wind components, θ is potential temperature, q is humidity, primed quantities $(\cdot)'$ represent a local (unresolved) deviations from the grid-cell-mean $(\bar{\cdot})$, and where correlations such as $\overline{w'\theta'}$ represent vertical fluxes (heat flux in this case, see Fig 1). These terms represent the resolvable effect of unresolved (subgrid) motions or eddies. To accurately forecast mean, winds temperature, humidity, and pollutant concentrations, it is necessary to properly account for these turbulence terms.

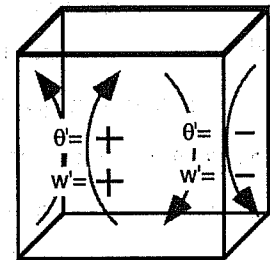


Fig. 1. Example of subgrid turbulent motions within single NWP grid cell, which causes a positive heat flux $\overline{w'\theta'}$.

Attempts to write equations for these new turbulence unknowns lead to even more unknowns — a dilemma known as the **closure problem**. Using heat flux for example, an infinite number of equations result:

$$\begin{aligned} \frac{\partial \bar{\theta}}{\partial t} &= \dots - \frac{\partial \overline{w' \theta'}}{\partial z} \\ \frac{\partial \overline{w' \theta'}}{\partial t} &= \dots - \frac{\partial \overline{w' w' \theta'}}{\partial z} \\ \frac{\partial \overline{w' w' \theta'}}{\partial t} &= \dots - \frac{\partial \overline{w' w' w' \theta'}}{\partial z} \end{aligned}$$

etc.

In NWP models it is necessary to approximate or parameterize some of unknowns to yield a finite set of equation. Such parameterizations are called **closure assumptions**.

Parameterizations do not come from first principles. Instead, they involve the creativity and imagination of the researcher to approximate nature. Parameterizations must be:

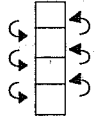
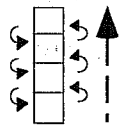
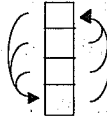
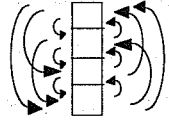
- physically reasonable
- dimensionally correct
- invariant under coordinate transformations
- consistent with budgets and constraints (e.g., non-negative humidities, etc.)

While the first quality is the most important, it is also the most subjective. As a result there tend to be as many parameterizations as researchers.

2. A CLOSURE CLASSIFICATION

An attempt to organize closure assumptions is presented in Table 1. One measure of the closure is the highest statistical order (S) for which a forecast equation is retained. Another measure is the degree of nonlocalness (N) represented. This latter measure is particularly important for convective mixed layers, where coherent structures such as thermals can transport air between the surface layer and the top of the mixed layer via an advective-like process.

Table 1 is presented as a grid, and the various closures are identified by their grid coordinates. For example, the turbulence kinetic energy (TKE) closure is type $S_{1.5}N_0$, because statistically it is a one-and-a-half order, and it utilizes purely local approximations. Transilient turbulence theory (T3) is closure type S_1N_3 , because it is statistically first-order closure and is fully nonlocal. Some grid coordinates are empty, such as S_2N_3 , which indicate that either the closure has not yet been invented, or I accidentally missed it during my literature search. A bibliography of many closure schemes is given by Stull (1988) is not reproduced here.

Table 1. A classification of turbulence closures.		Nonlocalness (N)			
		N ₀	N ₁	N ₂	N ₃
Statistical Order (S) symbol sample equations		none or local mixing 	bulk or non-local corrected 	2-stream 	fully nonlocal 
S ₀	$\bar{\theta} = param.$ or $\partial(\bar{\theta})/\partial t = param.$	similarity theory (e.g.: log wind profile)	bulk slab integrated	mass-flux	
S ₁	$\frac{\partial \bar{\theta}}{\partial t} = \dots - \frac{\partial \overline{w' \theta'}}{\partial z}$ $\overline{w' \theta'} = param.$	1 st -order closure	modified gradient	top-down/ bottom-up	spectral diffusivity
		K-theory mixing-length theory	horizontal rolls	2-stream	transient integral turbulent adjustment direct interaction approx. orthonormal expansions
S _{1.5}	$\frac{\partial \bar{\theta}}{\partial t} = \dots - \frac{\partial \overline{w' \theta'}}{\partial z}$ $\frac{\partial(TKE)}{\partial t} = param.$ $\overline{w' \theta'} = param.$	TKE k-ε Yamada level 2.5			
S ₂	$\frac{\partial \bar{\theta}}{\partial t} = \dots - \frac{\partial \overline{w' \theta'}}{\partial z}$ $\frac{\partial \overline{w' \theta'}}{\partial t} = \dots - \frac{\partial \overline{w' w' \theta'}}{\partial z}$ $\overline{w' w' \theta'} = param.$	2 nd -order closure		2nd-order mass flux	
S ₃	$\frac{\partial \bar{\theta}}{\partial t} = \dots - \frac{\partial \overline{w' \theta'}}{\partial z}$ $\frac{\partial \overline{w' \theta'}}{\partial t} = \dots - \frac{\partial \overline{w'^2 \theta'}}{\partial z}$ $\frac{\partial \overline{w'^2 \theta'}}{\partial t} = \dots - \frac{\partial \overline{w'^3 \theta'}}{\partial z}$ $\overline{w'^3 \theta'} = param.$	3 rd -order closure			

3. ZERO-ORDER CLOSURES

These closures do not include prognostic equations for mean variables vs height. Instead, they either prescribe the vertical profile of mean variables diagnostically, or they prescribe a generic profile shape for the profile but forecast the parameters in the shape equation. In the subsections that follow, an attempt is made to illustrate the various types of closure. These discussions are not meant to be exhaustive.

3.1 Closure type S_0N_0

Similarity theory gives S_0N_0 diagnostic equations for profiles of mean and turbulent quantities. The equation form and parameter values are found empirically. These equations are made dimensionless by variables that describe constraints or forcings on the flow. The equations are hopefully universal, because it is assumed that changes in the flow are driven by changes in the forcings and constraints. Similarity theories are usually valid for a vary narrow range of atmospheric conditions. For example, different similarity relationships are give for different static stabilities.

A classic example is the log wind profile for neutral static stability:

$$\frac{\bar{M}}{u_*} = \frac{1}{k} \cdot \ln\left(\frac{z}{z_0}\right)$$

where \bar{M} is mean wind speed (the desired dependent variable) and z is height (the independent variable). Two forcings are the friction velocity, u_* , and roughness length, z_0 . An empirical parameter is the von Karman constant, $k = 0.4$. The only way for the wind speed \bar{M} to change with time is if the forcings change with time, which indeed they can do.

For non-neutral static stability, different empirical equations must be used that include the surface heat flux $\overline{w'\theta'_s}$ as an additional forcing. The Obukhov length, L , is designed to incorporate this flux, giving new dimensionless height of $z/L = k \cdot z \cdot (g/T) \cdot \overline{w'\theta'_s} / u_*^3$. Thus, for diabatic conditions:

$$\frac{\bar{M}}{u_*} = f\left(\frac{z}{z_0}, \frac{z}{L}\right)$$

Högström (1988) has suggested an improved flux-profile relationship for this log wind profile based on $k = 0.4$, and Wieringa (1992) has provided updated tables of roughness length for various landscapes.

While the similarity relationships above apply to the bottom of the surface layer, they were not designed to fit the top of the surface layer in convective conditions. Some recent research (Santoso and Stull, 1994) suggest that a better fit to the surface layer in convective conditions is given by

$$\frac{\bar{M}}{M_{ML}} = \left(\frac{z}{z_s}\right)^A \cdot \exp\left[A \cdot \left(1 - \frac{z}{z_s}\right)\right]$$

where the mixed-layer wind speed M_{ML} is a forcing, constraint z_s is the height of the top of the surface layer, and empirical parameter $A = 0.0975$.

Similarity relationships have been proposed for the vertical profiles of $U, V, M, \theta, q, \overline{u'^2}, \overline{v'^2}, \overline{w'^2}, \overline{\theta'^2}, \overline{q'^2}, TKE, \varepsilon$ (= TKE dissipation rate), and many other variables. An updated catalog of similarity relationships is in a technical report (Stull, 1990).

3.2 Closure type S_0N_1

Bulk closures prescribe a profile shape, but allow parameters of the shape equation to be forecast. The simplest bulk closure is the **slab** model of the mixed layer (ML), which assumes constant potential temperature, humidity, and wind speed with height. Thus, the only parameters that need to be forecast are the average ML temperature $\langle\theta(t)\rangle$, the depth $z_i(t)$ of the ML, and the temperature discontinuity $\Delta\theta(t)$ across the top of the ML (Fig 2a).

At night, an exponential equation is sometimes used as the specified profile shape (Fig 2b). For this case, only the inversion strength $\Delta\theta$ and depth h need be forecast.

3.3 Closure type S_0N_2

Mass flux models prescribe the fraction of area σ covered by updrafts within convective MLs. (Penc and Albrecht, 1986, Randall et al, 1992). If the updraft and downdraft speeds w_u and w_d are specified as a function of height, then a mass flux M_c can be defined as

$$M_c \equiv \rho \cdot \sigma \cdot (1 - \sigma) \cdot (w_u - w_d)$$

This mass flux can be thought of as the amount of vertical stirring in the convective ML.

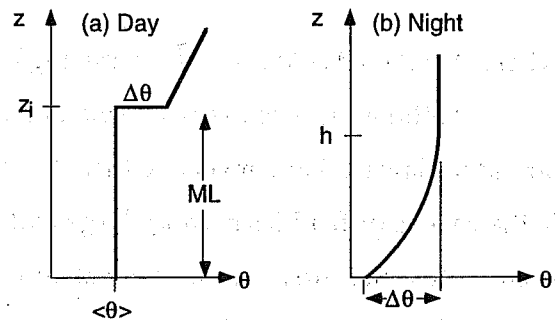


Fig. 2. Bulk models for the (a) convective mixed layer and the (b) stable boundary layer.

If the states within updrafts and downdrafts are also specified as a function of height, , then grid-volume mean values and fluxes can be parameterized. Using heat for example, specification of updraft and downdraft values of θ_u and θ_d allow:

$$\bar{\theta} = \theta_u \cdot \sigma + \theta_d \cdot (1 - \sigma)$$

$$\overline{w' \theta'} \approx M_c \cdot (\theta_u - \theta_d)$$

4. FIRST-ORDER CLOSURES

4.1 Closure type S₁N₀

Boussinesq (1877) suggested that turbulent fluxes can be approximated analogous to molecular fluxes; namely, as flowing down the local gradient. For turbulence, however, he suggested that an eddy diffusivity K should be used instead of a molecular diffusivity. Prandtl (1925) refined this approximation by allowing K to vary with wind shear, under the assumption the stronger shears create more-vigorous turbulence that causes greater turbulent transport. For example, for heat:

$$\overline{w' \theta'} \approx -K \cdot \frac{\partial \bar{\theta}}{\partial z}$$

where $K = l^2 \cdot |\Delta M / \Delta z|$, and l is a mixing length representing the average eddy size.

K-theory is essentially a "small-eddy" theory, which works fine for neutral and stable boundary layers. For convective MLs, however, K-theory has difficulties because large eddies such as thermals are active in the real atmosphere. These difficulties appear in the observations as countergradient fluxes (implying negative values of K) and as fluxes in regions of zero gradient (implying infinite or undefined values of K , see Fig 3). In mixing-length approaches, the difficulties appear as mixing lengths that are much larger than than the vertical grid increment across which local mixing is computed (an apparent contradiction).

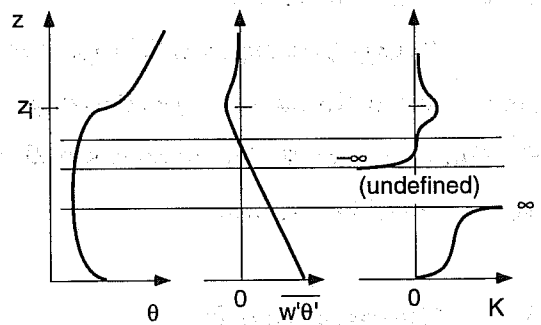


Fig. 3. Measured values of potential temperature θ and heat flux $\overline{w' \theta'}$ yield "measured" values of K that are problematic within the interior of the convective mixed layer.

4.2 Closure type S₁N₁

K-theory gained widespread use and acceptance because of its success in laboratory flows and within atmospheric surface layers. When the anomalous behavior within the convective ML was discovered, a variety of improved parameterizations were proposed that remained within the paradigm of local diffusion.

One such example is the “modified gradient” approach, where the fluxes are still assumed to flow down a local gradient, but where an artificial gradient γ is added to the true measured gradient during convective conditions (Deardorff 1966, Holtslag and Moeng 1991). This approach avoids the necessity of negative or infinite values of K .

$$\overline{w'\theta'} \approx -K \cdot \left[\frac{\partial \bar{\theta}}{\partial z} - \gamma \right]$$

4.3 Closure type S₁N₂

An alternative improvement to K-theory is to split the true gradient into two artificial gradients of opposite sign, and assume that there is small-eddy diffusion down each of these separate gradients (Fig 4). This results in **two streams** of turbulent flux, one diffusing from the **bottom up**, and the other from the **top down** (see review by Stull, 1988, plus more recent papers by Chatfield and Brost 1987, and Moeng and Wyngaard 1989). Weil (1990) discusses some of the difficulties of the top-down/bottom-up approach.

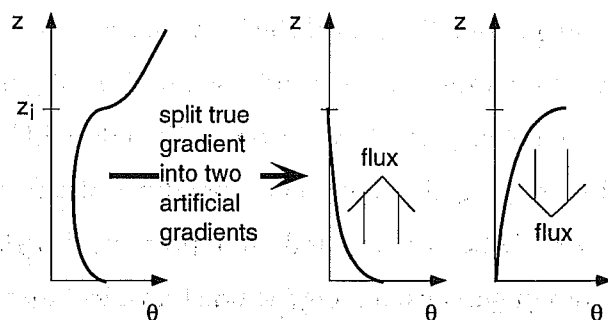


Fig. 4. Top-down/bottom-up approach.

4.4 Closure type S₁N₃

This class of closure marks a break from small-eddy K-theories. For this situation, eddies of a whole spectrum of sizes are parameterized as causing advective-like transport between every possible pair of grid-cell heights within the turbulent domain.

The concept is illustrated in Fig 5. Picture a stack of grid cells, with initial potential temperatures as sketched in Fig 5a. Conceptually split each layer can into a series of air parcels (Fig 5b). Next, turbulence rearranges the air parcels, as indicated with the curved arrows in Fig 5b. Some of the motions are caused by large eddies (e.g. thermals) that transport air from the surface to the top of the layer, while other eddies have medium and small sizes.

After a short period of time, the air parcels are rearranged as sketched in Fig 5c. The final average potential temperatures in each layer are shown in Fig 5d, based on simple averages of the air parcels ending in the various destination layers.

The net result is a change in resolved temperatures between states (5a) and (5d), caused by unresolved eddies and parcel movement. In Fig 5a, note the middle level indicated by an arrow at right. Across this level, there is zero local gradient, because the temperature above and below that level are 10°C. However, nonlocal eddies in Fig 5b moved some 15°C up across that level, while air of only 10°C moved down across that level. As a result, there is a net flux across the level, in spite of the zero gradient.

Models of such nonlocal transport have been proposed under a range of names, although they essentially share the same physics. Direct interaction approximation was one of the first models, although its apparent complexity precluded wide-spread application. Spectral diffusivity theory was one of the first applications of fully nonlocal mixing to the atmosphere, which was modeled by eddy diffusivities having different values for eddies of different sizes. Other simpler and more practical descriptions of nonlocal mixing include transient turbulence theory, integral closure theory, and turbulent adjustment. Orthonormal expansions approach nonlocal mixing as an exercise in applied mathematics. Nonlocal closures are reviewed by Stull (1992).

The amount of mixing between various heights is described by a transient matrix, which indicates for each destination height the fraction of air that came from various source heights. Fig 6 shows an example matrix corresponding to Fig 5, which is asymmetric for convective MLs. As a first-order closure, the elements in this matrix can be parameterized as a function of the wind and temperature profiles.

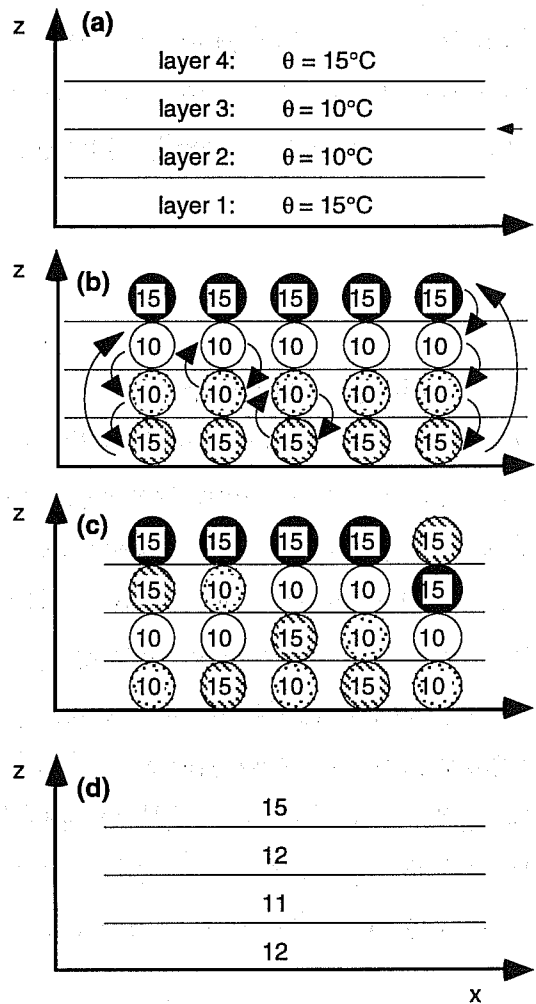


Fig. 5. Nonlocal mixing concept.

source layer =	4	3	2	1	
destination layer 4	0.8	0	0	0.2	= c
3	0.2	0.4	0.2	0.2	
2	0	0.6	0.2	0.2	
1	0	0	0.6	0.4	

Fig. 6. Transient matrix, c. Each row and each column sum to 1, to conserve mass.

5. ONE-AND-A-HALF ORDER CLOSURE – Closure type $S_{1.5}N_0$

As an extension of Prandtl's mixing length hypothesis, one might suppose that eddy diffusivities are greater when the flow is more turbulent. While Prandtl considered only mechanically-generated (wind-shear induced) turbulence, the turbulence kinetic energy (TKE) approach can also include buoyantly-generated turbulence and turbulence that is transported in from other locations.

Within this approach, one needs a forecast equation for TKE. Knowing the TKE as well as the mean gradients, it is then possible to parameterize the fluxes. While this method allows K to vary in a more realistic manner, it still assumes the flux flows down the local gradient. Hence this approach can still be problematic in regions of zero gradient such as the interior of the ML.

The TKE equation contains many higher-order turbulence terms, which also must be approximated. One of those terms is the dissipation rate, ϵ . An improved 1.5-order closure carries forecast equations for both TKE and ϵ . This latter approach is often called the k - ϵ closure.

6. SECOND-ORDER CLOSURES

6.1 Closure type S_2N_0

Second-order closure carries forecast equations for not only all the mean variables ($\bar{\theta}$, \bar{U} , \bar{V} , \bar{q}), but also for all the second order terms ($\overline{v'^2}$, $\overline{w'^2}$, $\overline{\theta'^2}$, $\overline{q'^2}$, $\overline{u'v'}$, $\overline{u'w'}$, $\overline{v'w'}$, $\overline{u'\theta'}$, $\overline{u'q'}$, $\overline{v'\theta'}$, $\overline{v'q'}$, $\overline{w'\theta'}$, $\overline{w'q'}$, $\overline{\theta'q'}$). Some also include forecast equations for dissipation rate.

Third and higher-order correlations and pressure-correlation terms must be parameterized. Most such parameterizations utilize down-gradient local diffusion, for example:

$$\overline{w'w'\theta'} = -K_1 \frac{\partial \overline{w'\theta'}}{\partial z}$$

These approaches have the greater burden of more prognostic equations and variables, but they give forecasts of some useful higher-order turbulence statistics which might not be available from lower-order closures.

Virtually all of these higher-order local closures are based on the premise that forecasts of mean variables ($\bar{\theta}$, \bar{U} , \bar{V} , \bar{q}) are improved as the closure approximations are pushed to higher and higher orders. This premise has for the most part been confirmed via the forecasts that have been produced. One reason for such success is that more physics is included when more equations are retained. This also implies that as the higher orders make lesser contributions to the mean flow.

6.2 Closure type S_2N_2

Randall et al (1992) proposed a mass flux parameterization that utilized second-order closure to determine updraft and downdraft characteristics. For example, updraft area and mass flux can be found in terms of vertical velocity skewness S_w and vertical velocity variance $\overline{w'^2}$:

$$\sigma = \frac{1}{2} - \frac{S_w}{2 \cdot \sqrt{4 + S_w^2}} \quad \text{and} \quad M_c = \rho \cdot \left(\frac{\overline{w'^2}}{4 + S_w^2} \right)^{1/2}$$

Thus, if prognostic equations are carried for vertical velocity variance (a second-order term) and vertical-velocity skewness (a third-order term), then the updraft area and mass flux can be found.

As it turns out, Randall et al (1992) did not use the model in this higher-order mode. Instead used LES to "measure" higher-order statistics, and then held fixed the resulting σ and M_c values in a closure type of S_0N_2 .

7. THIRD-ORDER CLOSURE – Closure type S_3N_0

This type of closure is similar to second-order closure, except that forecast equations for third-order terms are retained. Fourth-order terms as parameterized as local diffusion down the local gradient of the third and second-order terms. For example:

$$\overline{w' w' w' \theta'} = -K_2 \cdot \frac{\partial \overline{w' w' \theta'}}{\partial z} \quad \text{or} \quad \overline{w' w' w' \theta'} = fnt \left(\frac{\partial \overline{w'^2}}{\partial z}, \frac{\partial \overline{w' \theta'}}{\partial z} \right)$$

Higher-order statistics are more difficult to measure in the real atmosphere, and the resulting signal-to-noise ratio is very poor. As a result, we have little knowledge of the actual behavior of this very-high order terms, and thus have little basis upon which to guide and validate our parameterizations. Never-the-less, the inclusion of additional physics in the third-order equations ensures an improved forecast regardless of any crude parameterizations that might be made in the fourth-order terms.

8. RECOMMENDATIONS

Generally, those closures toward the upper left of Table 1 are more **economical**, while those toward the bottom or right provide more **detail**. Within the limitations of the closure, the **accuracy** of the upper left closure can be just as great as those toward the bottom or right.

By **economical**, we mean that fewer equations must be solved, allowing quicker computer execution times. However, most of the economical closures are designed for special subsets of boundary-layer behavior, such as for the convective mixed layer. This means that additional code must be incorporated into the NWP model to switch between the special closures, such as to decide when to use unstable-mixed-layer parametrizations vs stable-boundary-layer parametrizations. Also, there are many real situations (such as strong surface heating WITH strong winds) which do not fall into any special-case categories.

Detail means that additional flow information is available. For example, increasing values of S or N give more information about higher-order turbulence statistics, including: mixing lengths and nonlocal transport distances, fluxes (local or nonlocal), variances or nonlocal transport velocities, skewness or asymmetry, spectra (local Fourier spectra or nonlocal transport spectra). Also, these more-sophisticated closures can mimic a wider range of arbitrary boundary-layer situations.

Parameterization beauty is in the eye of the beholder. Each type of closure has unique strengths and weaknesses. Hence, there can be no recommendation of a "best" closure. As computer power increases, it will be more affordable and perhaps beneficial to utilize the more sophisticated and generally-applicable closures.

9. THE FUTURE

While it might seem esoteric to forecast the future of weather-forecast models, it is often wise to plan ahead. My personal opinion is that the quality of weather forecasts will improve when the grid size becomes sufficiently small. The reason is that parameterizations will not be needed for many meteorological phenomena such as thermals, clouds, and the effects of surface heterogeneities. Fewer parameterizations will allow fewer errors, because the physics and dynamics will be calculated deterministically rather than arbitrarily approximated.

Limited-domain large-eddy simulation (LES) models have already demonstrated such potential. They have been used to "foretell" many atmospheric characteristics that have later been verified with atmospheric observations.

For global NWP models to take advantage of this approach, the grid size over the whole globe must be reduced to that of present-day LES models ($\Delta x \approx \Delta y \approx \Delta z \approx 100$ m). Such evolution is throttled by computer storage and computational speeds, which would need a many-fold increase. If recent-past computer evolution is any indicator, we might reach the needed computer power in about ten to twenty years, which is well within the career-span of many researchers.

10. ACKNOWLEDGEMENTS

This paper was prepared by invitation from the European Centre for Medium-Range Weather Forecasts (ECMWF) for presentation at their seminar on Parameterization of Sub-Grid Scale Physical Processes, Reading, England, 5-9 September 1994. Their support is gratefully appreciated.

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