Eddy-Diffusivity and Numerical Aspects

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Eddy-diffusivity (ED) approach

In ED closure the vertical sub-grid flux is parameterized as

$$\overline{w'\varphi'} = -k \frac{\overline{\varphi}}{z}$$

where *k* is an eddy-diffusivity (or eddy-viscosity) coefficient.

ED is virtually as old as the first modern studies of turbulence: Saint-Venant, Boussinesq – 1850s - 1870s

The mixing length approach (Taylor – 1915, Prandtl – 1925)

$$k_{\varphi} = c_{\varphi} l w_t$$

where w_t is a turbulent velocity and l is a mixing length.

Turbulent kinetic energy (TKE) closure was originally proposed <u>independently</u> by Kolmogorov (1942) and Prandtl (1945)

Eddy-Diffusivity

Turbulent Kinetic Energy

$$w_t = \sqrt{e} = \sqrt{\frac{1}{2}\left(\overline{u'u'} + \overline{v'v'} + \overline{w'w'}\right)} \quad \text{and} \quad \frac{e}{t} = \frac{}{z}\; k\frac{e}{z} + S + B - D$$

Where ***e*** is the Turbulent Kinetic Energy (TKE)
S is the shear production of TKE
B is the buoyancy production/consumption
D is the Dissipation of TKE

<u>Theoretically other closures are particular cases of TKE closure:</u>

1) Richardson number $\quad B + S = D$

2) K-profile (KPP) $\quad \frac{}{z}\;\frac{}{z}\; k\frac{e}{z} + B - D \;= 0$

ED in climate and weather prediction models

ED is used in virtually all weather and climate prediction models.

Typical flavours of ED:

- Ri-number closure: widespread in global models (Louis scheme)
- TKE closure: mostly in mesoscale models
- K-profile: becoming common (dry convective – Sc PBL)

ED is used with some success to represent:

- Neutral
- not-too-stable boundary layers
- Momentum mixing

Typical problems of ED in convective PBL:

Weak and unrealistic top-entrainment

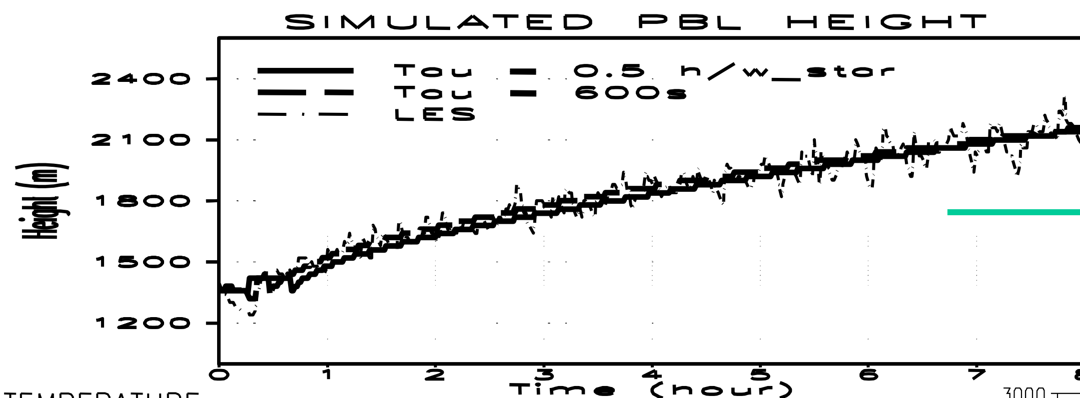
No counter-gradient fluxes

Unrealistic shallow moist convection

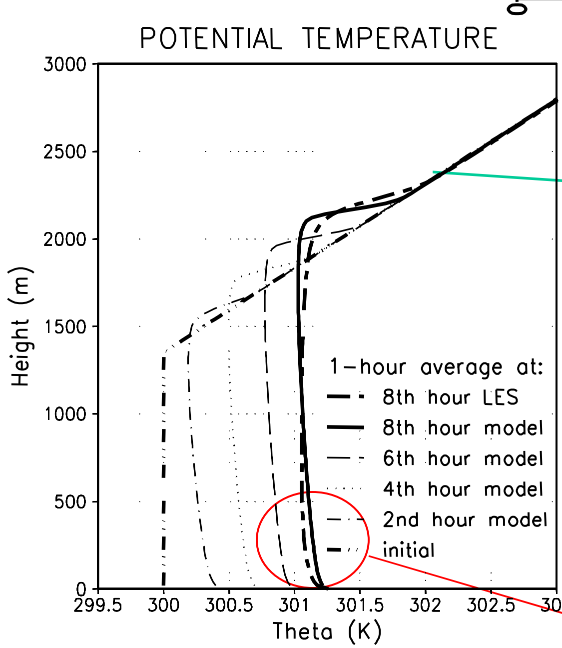
ED and the dry convective boundary layer

It is possible to obtain a realistic simulation with ED closure.

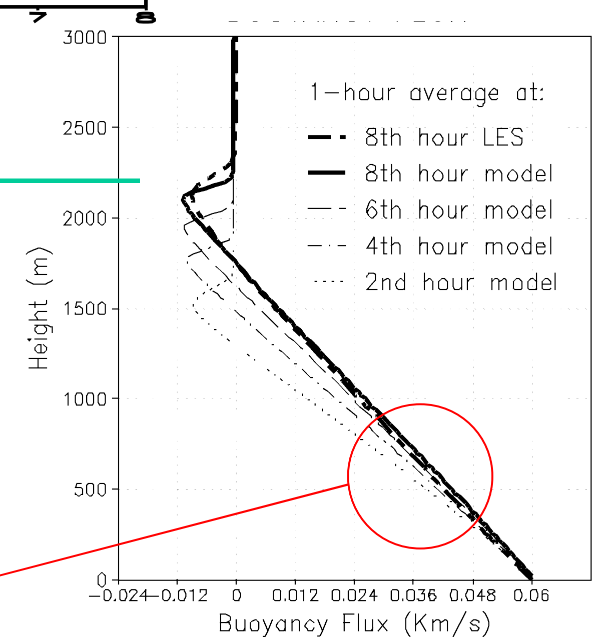
In this case: TKE equation + mixing length function of TKE



Boundary Layer height



Realistic top entrainment



Qs=60 Wm^{-2}

Counter-gradient problem: to maintain positive heat flux, ED $< \theta / z \quad 0$ needs

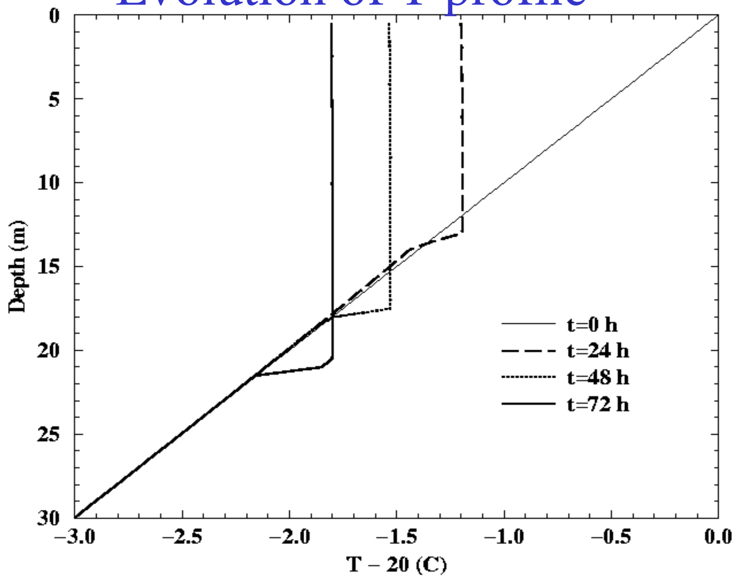
ED closure and ocean convection:

TKE equation + mixing-length function of TKE

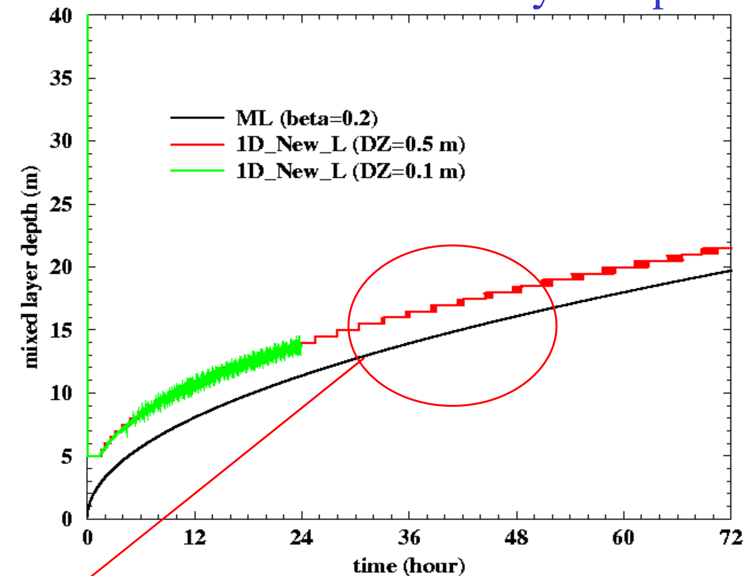
Ocean mixed layer cooled from above:

Qs=-200 Wm^{-2} , Δz=0.5 m, Δt=1 s, $\left(=T/\ \ z\right)_{t=0} \quad 0.1Km^{-1}$

Evolution of T profile



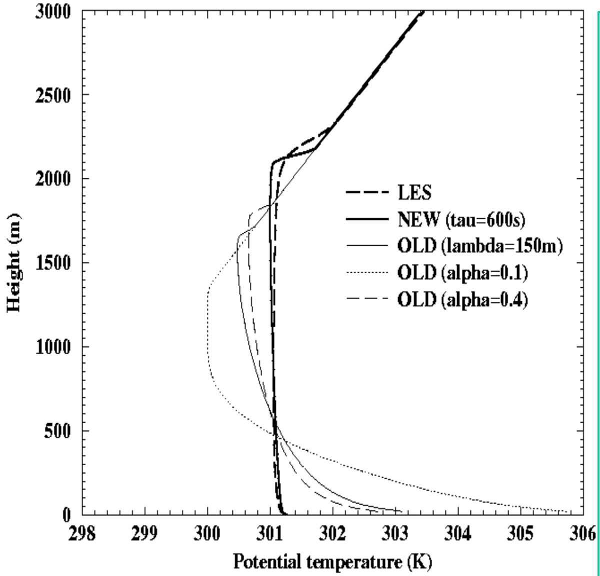
Evolution of mixed layer depth



$$D \quad \sqrt{t}$$

note: same parameters (e.g. *tau=0.5h/w$_*$*) for atmosphere and ocean.

Impact of mixing length formulation



OLD *l* is calculated using Blackadar(1962)

$$\frac{1}{l} = \frac{1}{kz} + \frac{1}{\lambda}$$

k is the von Karman constant and *λ* is calculated as

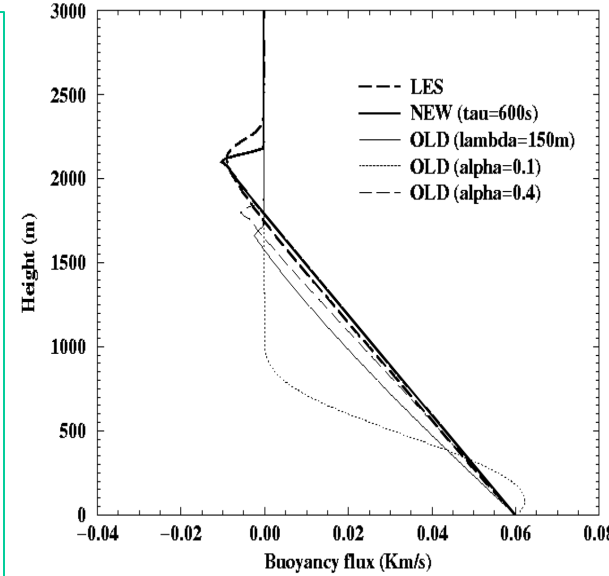
$$\lambda = \alpha \frac{zedz}{edz}$$

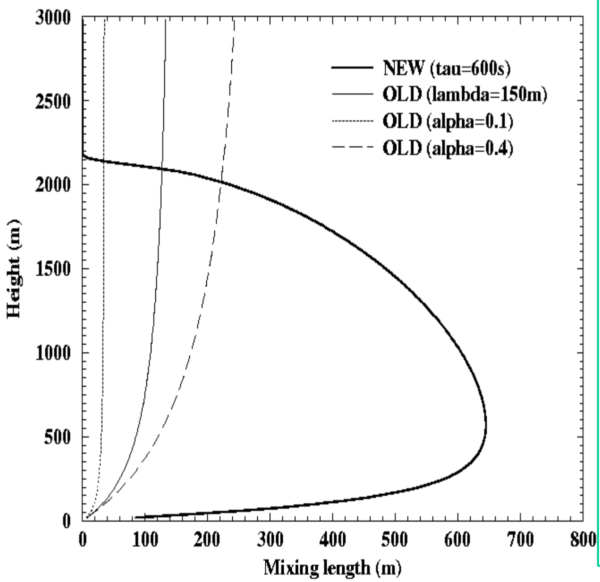
We test *α=0.1, α=0.4 and lambda=150 m.*

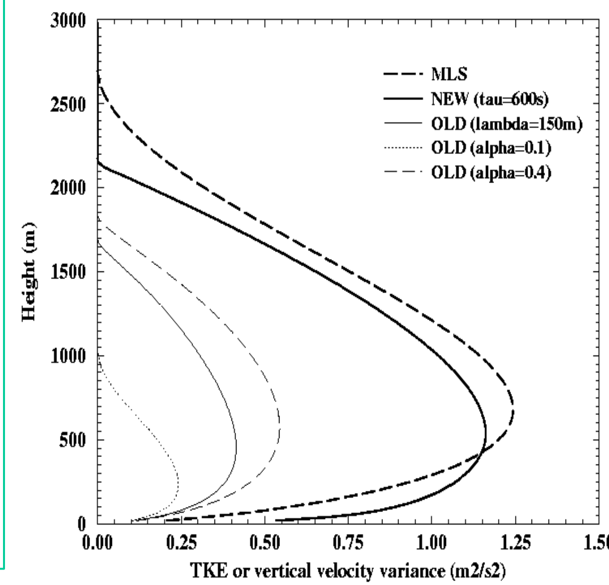
The NEW mixing length

$$l_h = \tau\sqrt{e}$$

with τ=600 s.

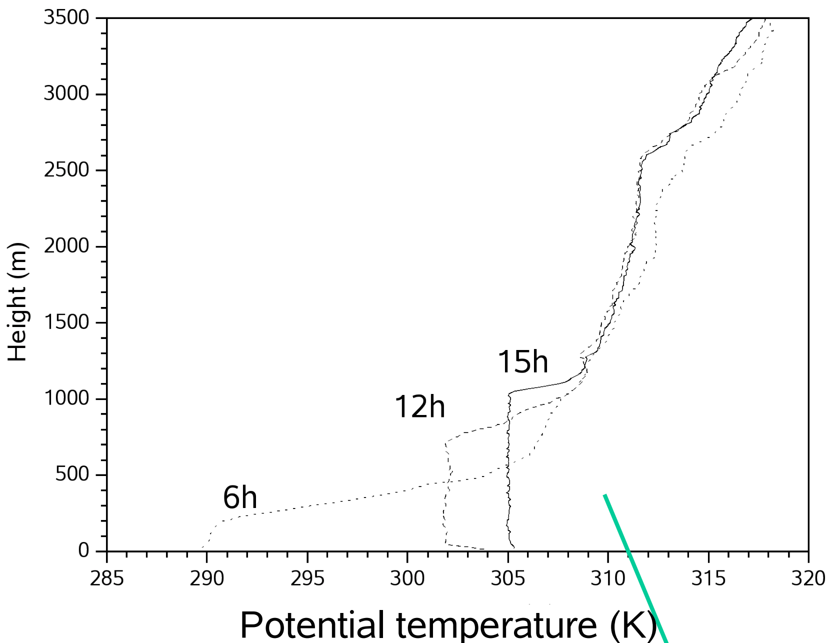


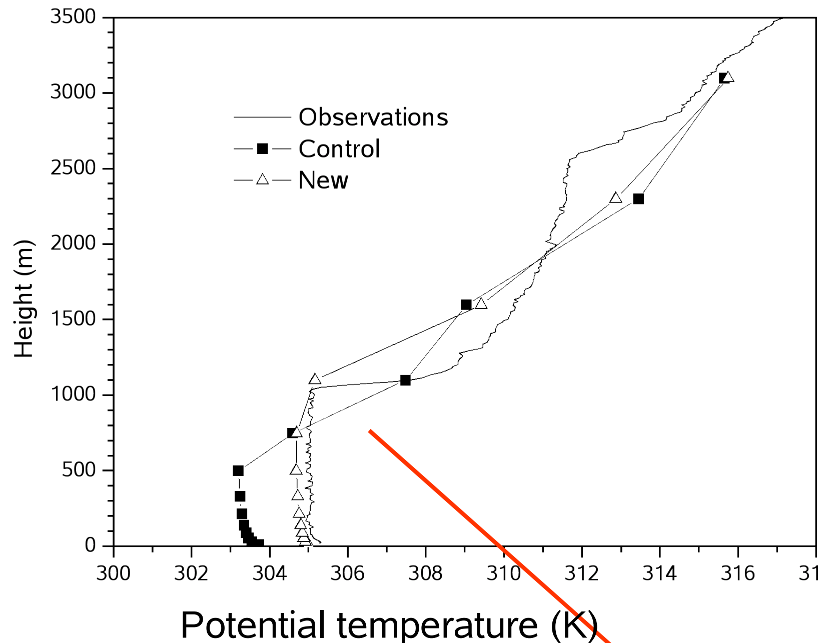




Dry convection over land

Evaluation of a mesoscale model against observations from the CICLUS campaign





Observations of potential temperature in Evora, Portugal, 24 July 1998

Observed PBL height ~1000m
Control PBL height ~ 500m
New PBL height ~ 1000m

Advection-diffusion nature of ED closure

Turbulent diffusion equation can be written as:

$$\frac{\theta}{t} = \frac{}{z} k \frac{\theta}{z} = \frac{k}{z}\frac{\theta}{z} + k\frac{^2\theta}{z^2}$$

In inversion region

$$\frac{\partial^2\theta}{\partial z^2} \simeq 0 \Rightarrow \frac{\partial\theta}{\partial t} \simeq -w\frac{\partial\theta}{\partial z}$$

1) Advection term dominates
2) gradient of k is important

Advection velocity:

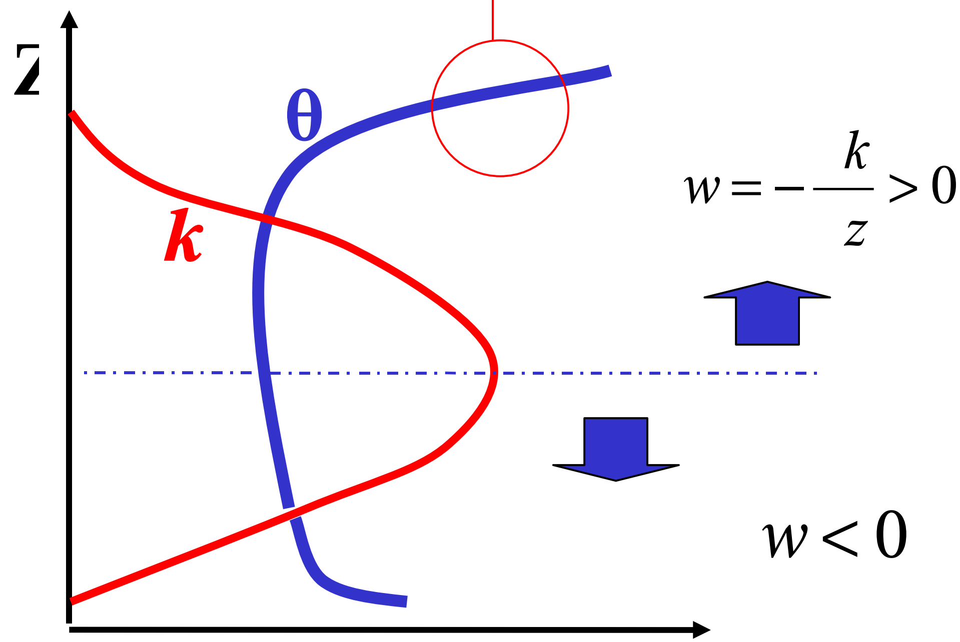
$$w = -\frac{k}{z}$$

Diffusion

ADV < 0

ADV > 0 DIFF > 0

ADV < 0



Advection component is crucial for simulation of convective PBL

ED and Stratocumulus boundary layer

Some success recently with ED in representing Sc PBL

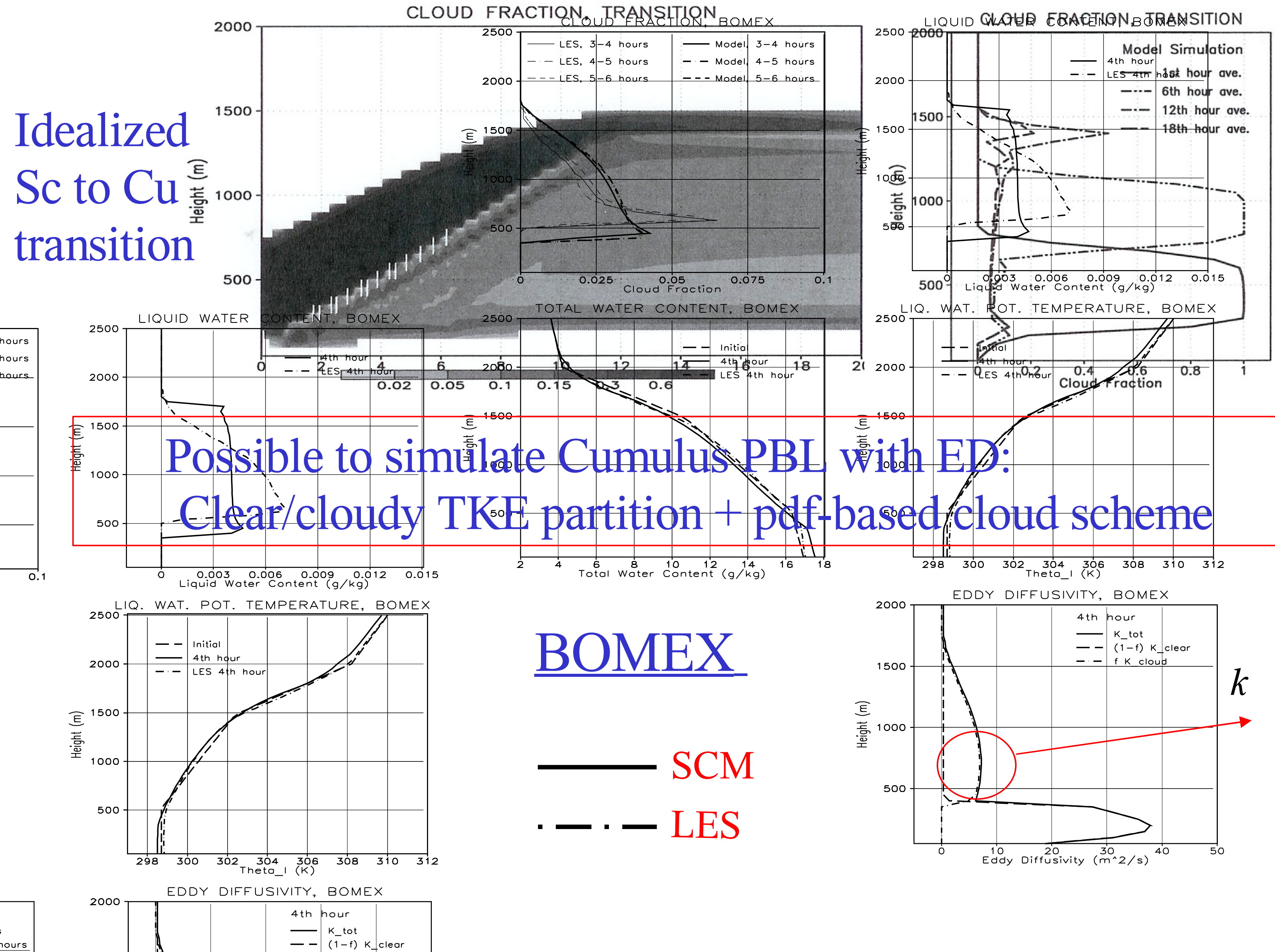
Different flavours:

1) ED TKE closure - mostly 1D
5) K-profile closure - positive impact in some models

7) But often with explicit entrainment parameterization
8) Still many problems:
    1) Treatment of the inversion
    2) Vertical resolution
    3) Interaction with radiation, subsidence

ED and the Cumulus PBL

Idealized Sc to Cu transition



Possible to simulate Cumulus PBL with ED:
Clear/cloudy TKE partition + pdf-based cloud scheme

BOMEX

SCM

LES

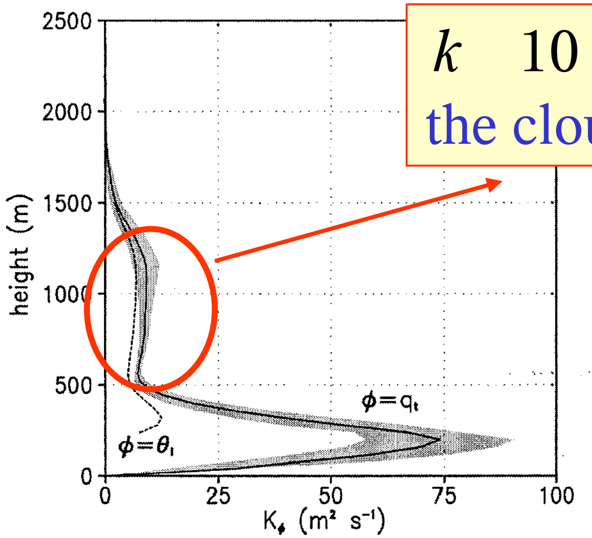
$k \quad 10 \ m^2 s^{-1}$

Why does ED work in shallow Cu PBL?

<u>BOMEX is close to a steady state</u>

$$\frac{\theta_l}{t} = -\frac{}{z}\left(\overline{w'\theta_l'}\right) \quad 0$$

$$\frac{}{z}\quad k\frac{\theta_l}{z} \qquad 0 \qquad \begin{cases}\theta_l = \alpha z + \beta \\ k = const.\end{cases}$$



$k \quad 10\ m^2 s^{-1}$ in the cloud layer

k coefficients based on BOMEX LES

Buoyancy flux is a function of the fluxes of q_t and θ_l

$$\overline{w'\theta_v'} = A\overline{w'\theta_l'} + B\overline{w'q_t'}$$

But A and B are different inside and outside a cloud

$$\left(\overline{w'\theta_v'}\right)_E \quad A\overline{w'\theta_l'}$$

$$\left(\overline{w'\theta_v'}\right)_C = B\overline{w'q_t'} > Bk\frac{q_t}{z} \quad 0$$

Positive source of TKE inside cloud => ED in cloud layer

Numerical Aspects

Highly non-linear system of equations (e.g. simple version of integro-differential temperature equation):

$$\frac{T}{t} = -w_c \frac{T}{z} + \frac{}{z} \; k_t \frac{T}{z} - \frac{1}{\rho C_p} \frac{}{z} \; {}_{0}^{z} \varepsilon \sigma T^4 dh + \frac{L}{C_p} C$$

convection

Turbulent diffusion

Thermal radiation

Clouds

Main numerical issues:

1) Coupling of different terms - fractional-steps methods

2) Non-linear numerical stability - Δt is controlled by large-scale

3) Low vertical resolution => poor accuracy

4) Coupling physics with dynamics (e.g. Semi-Lagrangian)

Stability of turbulent-diffusion equation

In PBL vertical diffusion parameterization:

1) k is not constant (neither in space nor in time)

2) k is a non-linear function of the mean variables

⇒fully implicit method is too expensive.

Note that what we are trying to solve is:

1) a system of coupled non-linear diffusion equations with

2) additional non-linear source/sink terms.

Typical method:

$$\frac{\varphi^{t+\Delta t} - \varphi^{t}}{\Delta t} = \frac{}{z}\ \gamma k^{t}\frac{\varphi^{t+\Delta t}}{z} + (1-\gamma)k^{t}\frac{\varphi^{t}}{z}$$

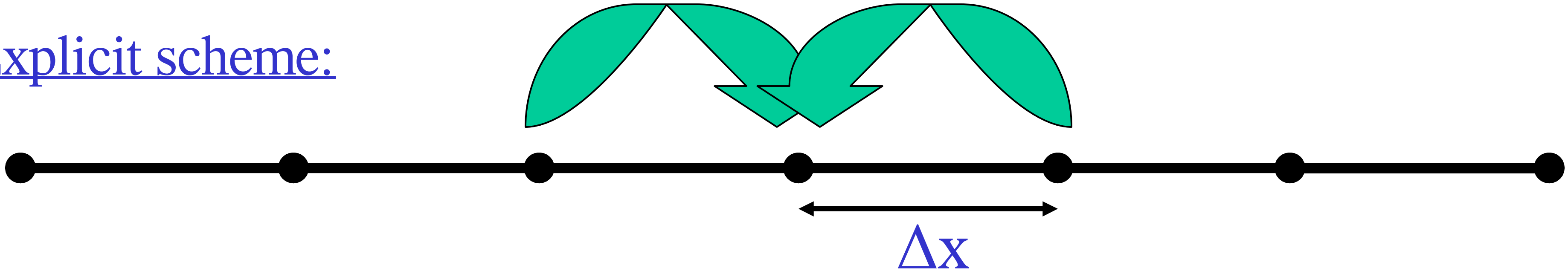
Over-implicit approach with γ>1 (e.g. 1.5 or 2)!

Not very accurate and not always stable (numerical oscillations)

A stable and explicit diffusion scheme

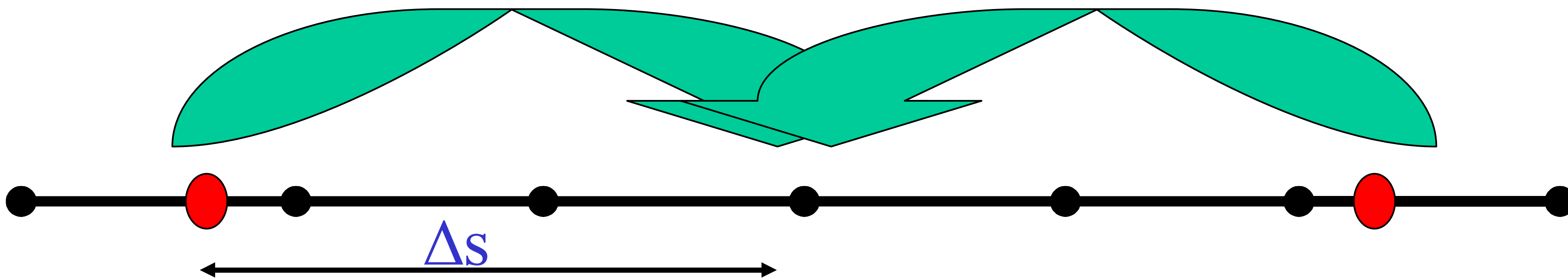
Fixed Stability Coefficient - FCS

Explicit scheme:



FCS scheme:

$$k\frac{\Delta t}{\Delta s^2} = \beta \quad \frac{1}{2} \qquad \Delta s = \sqrt{k\frac{\Delta t}{\beta}}$$



Used successfully in the context of 1D models, but not yet in a GCM

Eddy-Diffusivity/Mass-Flux solvers

An "implicit" approach

$$\frac{\varphi^{t+\Delta t}(z)-\varphi^{t}(z)}{\Delta t}=\frac{\partial}{\partial z}\left(K^{t}\frac{\partial\varphi^{t+\Delta t}}{\partial z}\right)+\frac{\partial}{\partial z}\left(M^{t}\left(\varphi^{t+\Delta t}-\varphi_{u}^{t}\right)\right)$$

Note: mass-flux + updraft variable are explicit => numerical oscillations

A possible solution

Mass-flux equations

$$\frac{\partial\overline{\varphi}}{\partial t}=-\frac{\partial}{\partial z}\left(M\left(\varphi_{u}-\overline{\varphi}\right)\right) \qquad \frac{\partial\varphi_{u}}{\partial z}=-\varepsilon\left(\varphi_{u}-\overline{\varphi}\right)$$

Can be written as

$$\frac{\partial\overline{\varphi}}{\partial t}=\frac{\partial}{\partial z}\left(\frac{M}{\varepsilon}\frac{\partial\varphi_{u}}{\partial z}\right)$$

A diffusion-type of equation

Solving this equation with a fixed stability coefficient method for diffusion could improve stability

A stable and explicit advection-diffusion scheme

$$\frac{\partial A}{\partial t}+u\frac{\partial A}{\partial x}=\frac{\partial}{\partial x}\left(k\frac{\partial A}{\partial x}\right)$$

1) traditional explicit scheme:

$$A_x^{t+\Delta t}=\tilde{\beta}A_{x+\Delta x}^t+\left(1-\tilde{\alpha}-2\tilde{\beta}\right)A_x^t+\left(\tilde{\beta}+\tilde{\alpha}\right)A_{x-\Delta x}^t$$

where $\tilde{\alpha}=\frac{u\Delta t}{\Delta x}$ $\tilde{\beta}=\frac{k\Delta t}{\Delta x^2}$ are the two stability coefficients

2) <u>new fixed stability coefficient scheme</u>:

$$A_x^{t+\Delta t}=\beta A_{x+\Delta s}^t+\left(1-\alpha-2\beta\right)A_x^t+\left(\beta+\alpha\right)A_{x-\Delta s}^t$$

with stability coefficients $\alpha=\frac{u\Delta t}{\Delta s}$ $\beta=\frac{k\Delta t}{\Delta s^2}$

Coefficients are fixed below stability limit => computation of Δs

Note: for k=0 we obtain the semi-Lagrangian scheme

A stable and explicit advection-diffusion scheme

Fixing the value of stability coefficients

$$(1-\alpha-2\beta)=\delta=0$$

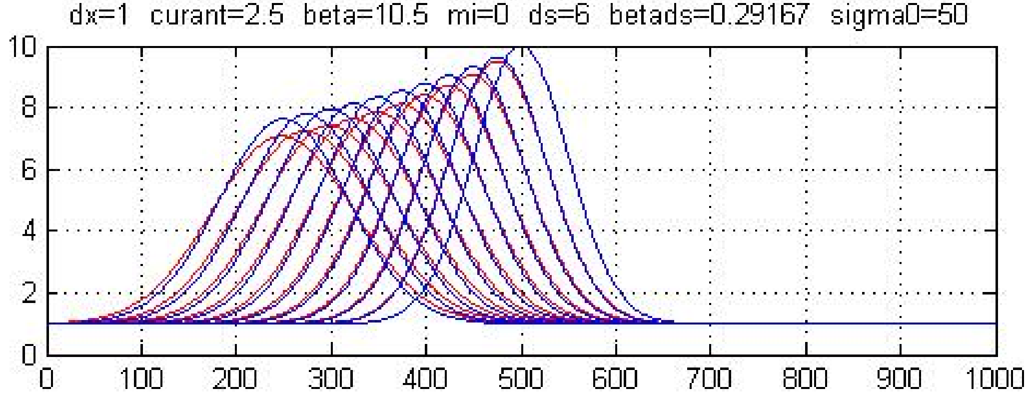
Leads to final algorithm

$$A_x^{t+\Delta t}=\beta A_{x\pm\Delta s}^{t}+(1-\beta)A_{x\mp\Delta s}^{t}$$

where '+' is for $u > 0$ and '-' is for $u < 0$ and

$$\Delta s=\frac{1}{2}\left(|u|\Delta t+\sqrt{|u|^2\Delta t^2+8k\Delta t}\right)$$

$$\beta=\frac{k\Delta t}{\Delta s^2}$$



Possibilities for coupling diffusive and advective processes in PBL

Vertical resolution and accuracy

Problems

b) Numerical convergence, stability

c) Sharp inversions versus low vertical resolution: even high-resolution models have layers of about 200m at 1500m

d) Inversions can be at different heights

e) Need to take into account: turbulent diffusion, non-linear advection, radiation, clouds, reaction (chemistry)

Possibilities

g) ED/mixed-layer approach, inversion reconstruction – but what about other regimes?

h) Special methods to deal with interfaces/fronts from CFD

i) Higher-order methods – but is it necessary?

j) Particle methods with turbulent diffusion included - complex problem of introducing diffusion into particle methods

k) Adaptive grids in vertical - but which variables to minimize? How to go back to original dynamics grid?

Numerical convergence of non-linear models

$$\frac{d\Phi}{dt} = F\left(\vec{\Phi}\right)$$ - Generic system of ODEs

$$\Phi^{t+\Delta t} = G\left(\Phi^{t}\right)$$ - Numerical solver

Gronwall's lemma can be used to show that, for $\left|\partial F_i / \partial \Phi_j\right| \quad L$ and $t \quad [0,T]$

$$\left\|\vec{\Phi}_n^{t+\Delta t} - \vec{\Phi}_a^{t+\Delta t}\right\| \quad D\Delta t^N \frac{\left(e^{LT}-1\right)}{L} + \left\|E_0\right\| e^{LT}$$

where N is the order of the scheme, D is a constant and $\left\|E_0\right\| = \left\|\Phi_n^0 - \Phi_a^0\right\|$

"Well-behaved" systems: $\Delta t \quad 0$, $\left\|E_0\right\| \quad 0$ ⇨ Uniform convergence (forever - any T)

Chaotic systems: $T_c\left(\Delta t\right) \quad -\lambda \log_{10}(\Delta t)$ ⇨ NO uniform convergence – T is finite!

In chaotic systems numerical convergence is NOT forever.

A sort of summary…

Advantages of Eddy-diffusivity (ED):

2) ED has been used for a while
(e.g. numerical/technical issues are relatively well-known)
3) Traditionally used for stable PBL, momentum
4) Can represent convective boundary layers as well
(dry, Sc and Cu boundary layers)

Numerical Aspects:

7) Non-linear stability issues still to be solved – some progress with methods similar to semi-Lagrangian for ED, EDMF
8) Vertical resolution and accuracy – some progress with inversion reconstruction approaches but still problematic
9) Coupling of different terms (more integrated approaches) – important implications also for aerosols/chemistry

A new mixing length formulation

Dry convective mixed layer

One-dimensional TKE model:

$$\frac{\theta}{t} = -\frac{}{z}\left(\overline{w\theta}\right) \qquad \frac{e}{t} = -\frac{}{z}\ \overline{we} + \frac{\overline{wp}}{\rho_0} + \frac{g}{\theta_0}\overline{w\theta} - \varepsilon$$

Eddy-diffusivity closure:

$$\overline{w\theta} = K_\theta \frac{\theta}{z} \qquad \overline{we} + \frac{\overline{wp}}{\rho_0} = - K_e \frac{e}{z}$$

with

$$K_\theta = C_\theta l \sqrt{e} \qquad \varepsilon = C_\varepsilon \frac{e^{3/2}}{l_\varepsilon} \qquad K_e = C_e l \sqrt{e}$$

A new mixing length: $l = \tau\sqrt{e}$

where *tau* is a time-scale. We use *tau=0.5h/w*$_*$

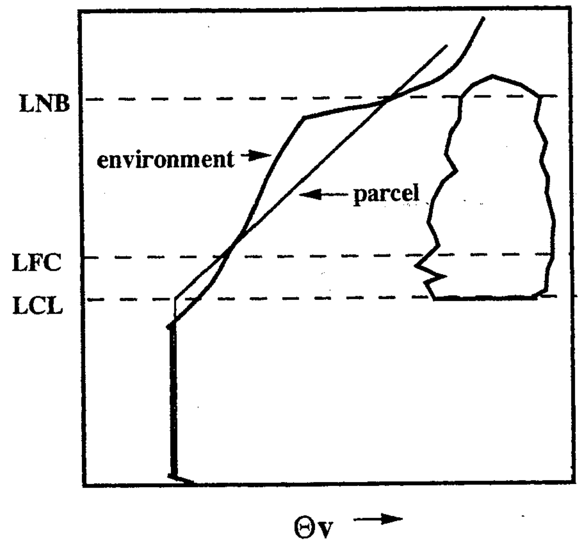
$$w_* = \left(\frac{g}{\theta_0}\overline{w'\theta'}_s h\right)^{1/3}$$

What is the problem for the Eddy-Diffusivity closure in shallow convection?

The Eddy-diffusivity closure usually produces a negative buoyancy flux in the cloud layer

The Mass-flux closure leads to a positive buoyancy flux in the cloud layer

$$\overline{w'\theta_v'} = -k\frac{\theta_v}{z} < 0$$



$$\overline{w'\theta_v'} = M\left(\theta_v^u - \overline{\theta}_v\right) > 0$$

The new mixing length formulation

Cloudy PBL: cumulus and stratocumulus

One-dimensional model:

$$\frac{\theta_l}{t} = -\frac{}{z}\left(\overline{w\,\theta_l}\right) - w\frac{\theta_l}{z} - R \qquad\qquad \frac{q_t}{t} = -\frac{}{z}\left(\overline{w\,q_t}\right) - w\frac{q_t}{z}$$

TKE partition (cloud and environment):

$$\frac{e_C}{t} = -\frac{}{z}\;\overline{w\,e} + \frac{\overline{w\,p}}{\rho_0}\;_C + \frac{g}{\theta_0}\left(\overline{w'\theta_v'}\right)_C - C_\varepsilon\frac{e_C^{3/2}}{l_\varepsilon}$$

$$\frac{e_E}{t} = -\frac{}{z}\;\overline{w\,e} + \frac{\overline{w\,p}}{\rho_0}\;_E + \frac{g}{\theta_0}\left(\overline{w'\theta_v'}\right)_E - C_\varepsilon\frac{e_E^{3/2}}{l_\varepsilon}$$

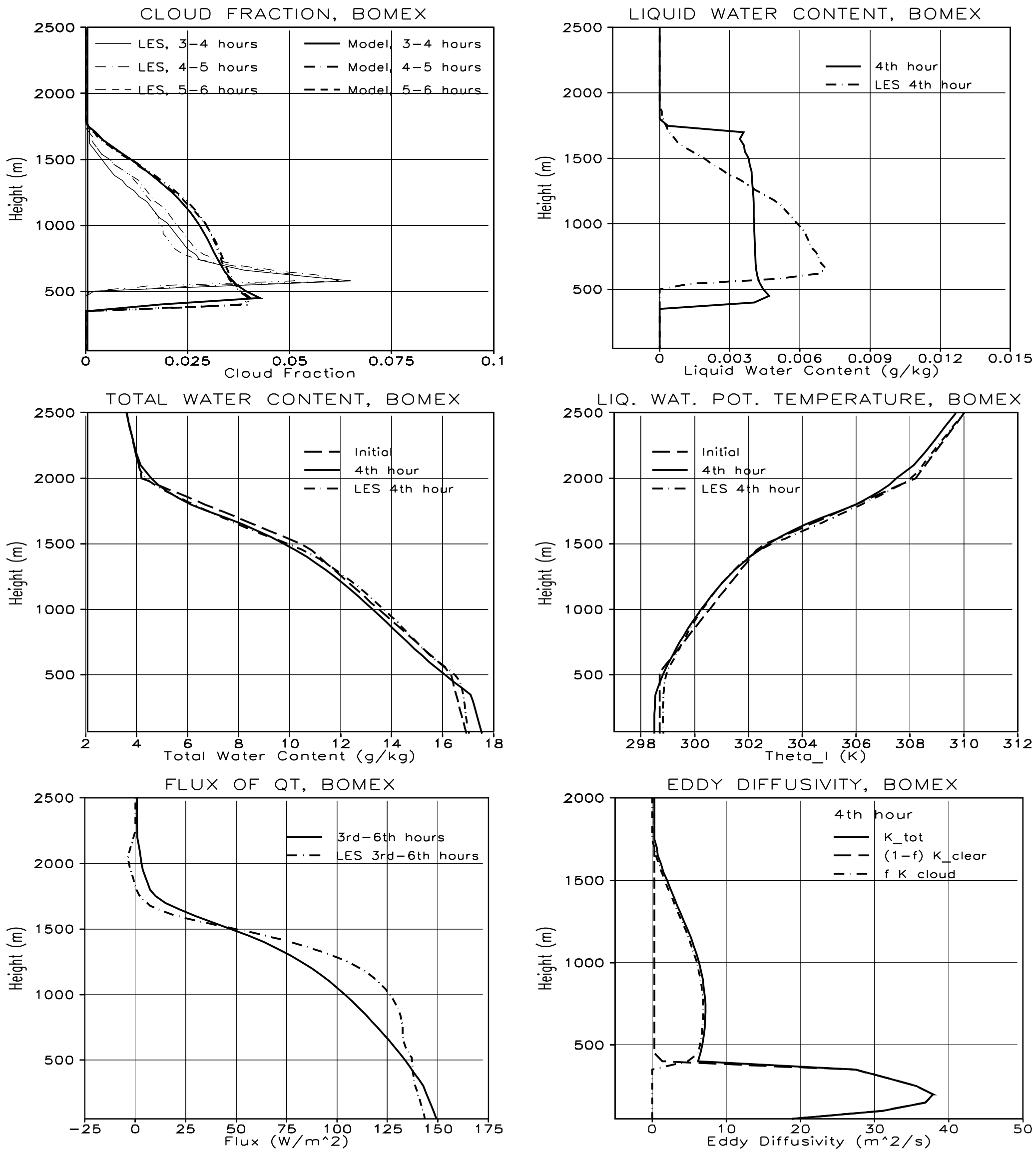
Eddy-diffusivity and new mixing length:

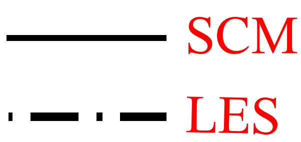
$$\overline{w\varphi} = - \quad aC_\varphi \tau e_C \;\frac{\varphi}{z} \;-(1 \;\; a)C_\varphi \tau e_E \;\frac{\varphi}{z}$$

Where *a* is the cloud fraction and *tau=600 s* is a time-scale.

ED and the shallow moist convection PBL

Intercomparison between single-column (SCM) and Large Eddy Simulation (LES) models based on BOMEX data





Non-linear numerical stability: example of the turbulent-diffusion equation

Consider the diffusion equation due to the ED parameterization:

$$\frac{\varphi}{t} = \frac{\quad}{z} \; k \frac{\varphi}{z}$$

An explicit discretization in time and space leads to

$$\varphi_z^{t+\Delta t} = \alpha \varphi_{z+\Delta z}^{t} + (1 - 2\alpha)\varphi_z^{t} + \alpha \varphi_{z-\Delta z}^{t} \;, \quad with \quad \alpha = k \frac{\Delta t}{\Delta z^2}$$

For $\alpha < 1/2$ the scheme is stable. But typical values:

$\Delta t \sim 1000$ s , $\Delta z \sim 100$ m , $k \sim 10\text{-}100\ m^2 s^{-1}$ => $\alpha \sim 1\text{-}10$

An implicit scheme

$$-\alpha \varphi_{z+\Delta z}^{t+\Delta t} + (1 + 2\alpha)\varphi_z^{t+\Delta t} - \alpha \varphi_{z-\Delta z}^{t+\Delta t} = \varphi_z^{t}$$

Is stable for a constant *k*.