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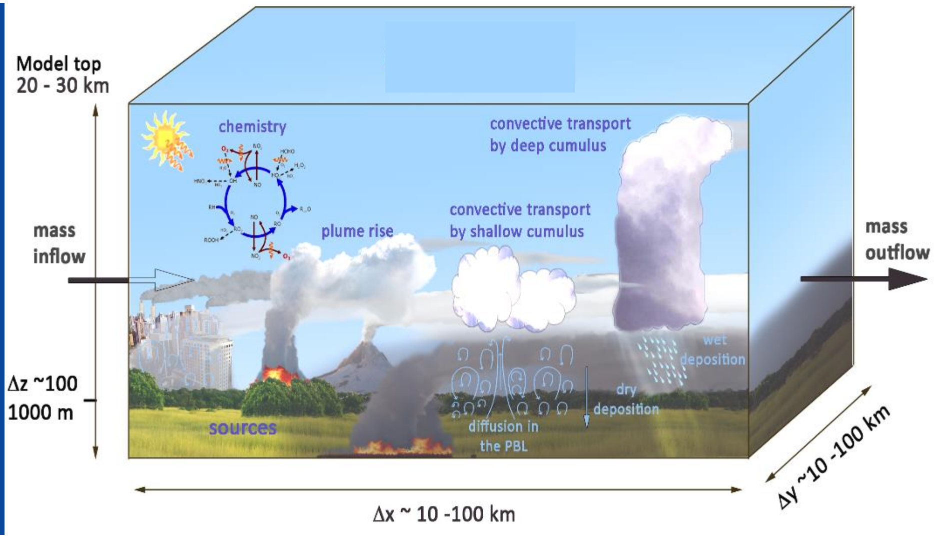

Grid and sub-grid scale processes in atmospheric tracer transport modeling

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CPTEC

GMAI
Grupo de Modelagem da Atmosfera e Interfaces
Modeling of the Atmosphere and its Interfaces Group

Contents

- Motivation
- Fundamental Equations
- Mass continuity Equation
- Grid and sub-grid scale transports
- Emissions
- WGNE NWP-Aerosol project

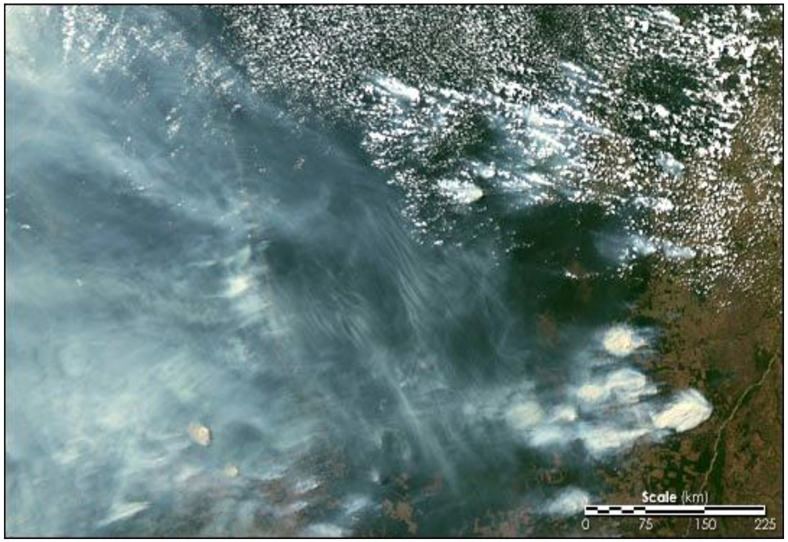
Atmospheric Tracer Modelling

- Air pollution / air quality forecast
- Greenhouse gases
- Aerosol interaction with radiation and clouds
- Biogeochemical cycles
- Volcanic Ash forecast

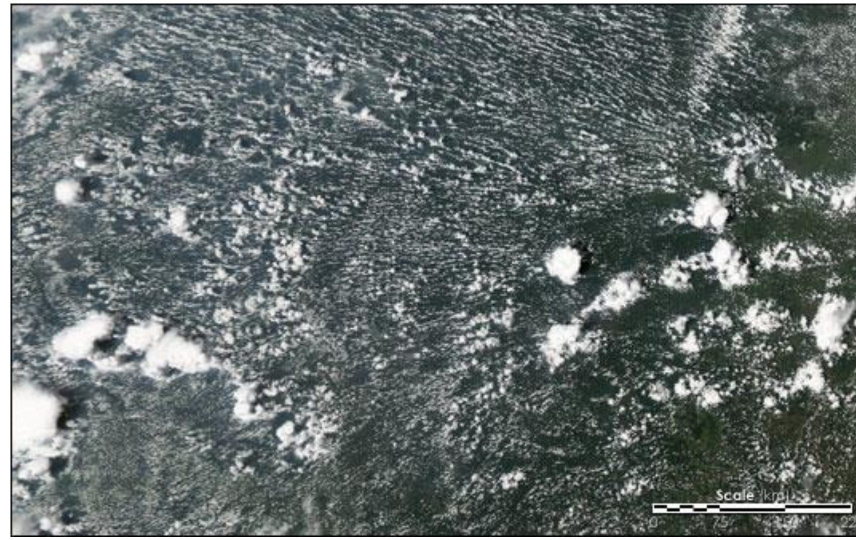
Effect of smoke on inhibition of cloud formation

Satellite images of the Amazon rainforest rarely show **smoke and cumulus clouds together**.

11/August/2002 – Brazilian Amazon



15/November/2002 – Brazilian Amazon

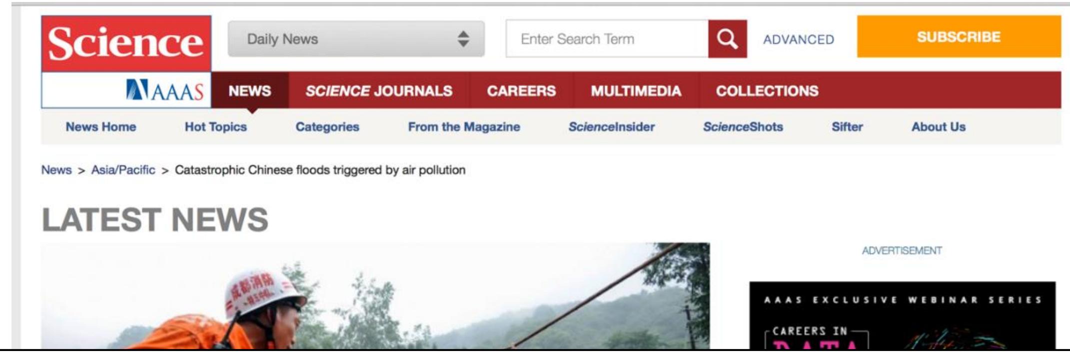


Satellite images of the Amazon rainforest rarely show smoke and cumulus clouds together. Smoke, mainly from agricultural fires, displaces the cumulus clouds that normally form above the forest each afternoon. (NASA image by Jesse Allen and Robert Simmon)

A uniform layer of scattered cumulus clouds is typically present, along with some thunderstorms, over the Amazon rainforest. Compare this image of a day with little smoke, with the image above. Both images were acquired by the Moderate Resolution Imaging Spectroradiometer aboard NASA's Aqua satellite, on August 11 (top) and November 15 (bottom), 2002.

Koren et al., 2004 - Science

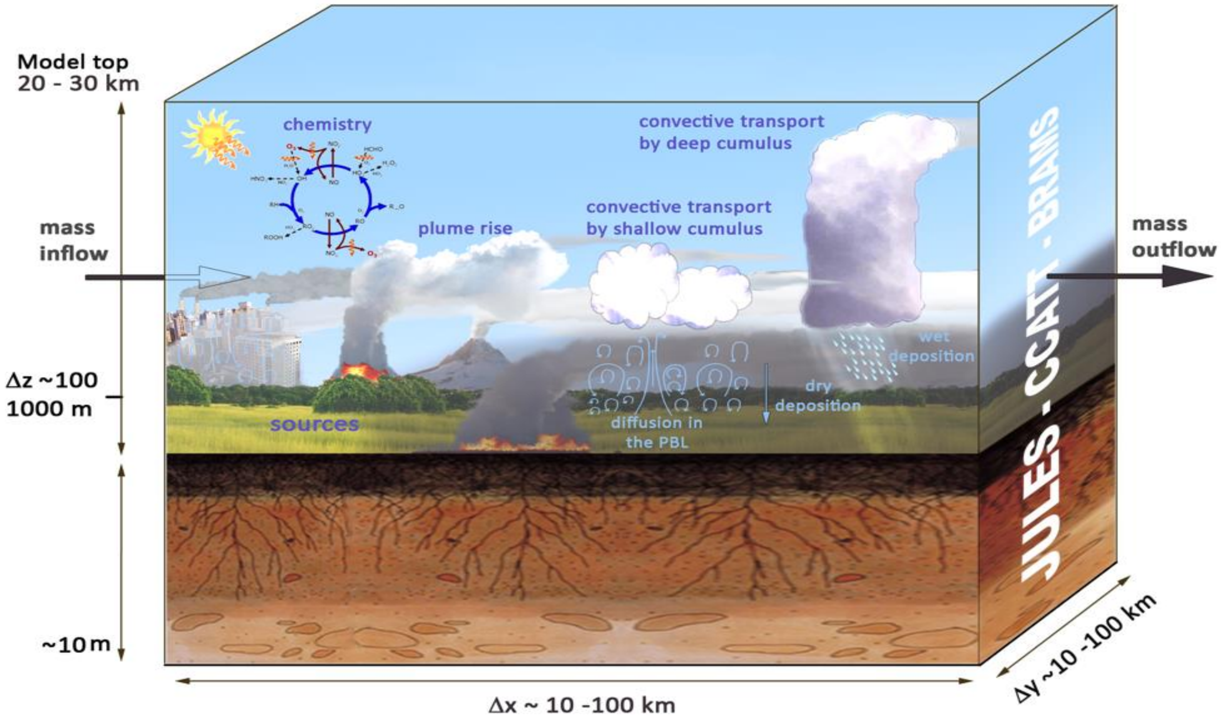
PNNL/USA: *Air Pollution Amplified Extreme Weather, Floods in China in 2013*



- *Even though the flood was the worst in 50 years in, the weather forecast missed it, potentially because the pollution effect discovered in this study is not included in weather forecast models.*
- *The significance of human-caused pollution emissions to modify weather and climate is the important finding of this study.*
- *Understanding that reducing pollution locally in the Sichuan Basin would substantially alleviate downwind floods has important socioeconomic implications and is especially useful for policy-makers.*

http://news.sciencemag.org/asiapacific/2015/07/catastrophic-chinese-floods-triggered-air-pollution

CPTEC/INPE developments on integrated atmospheric modeling:



Brazilian developments on the Regional Atmospheric Modeling System BRAMS (v. 5.1 - 2015)

www.brams.cptec.inpe.br

Freitas et al., ACP 2009, Moreira et al., GMD 2013, Longo et al., GMD 2013

Fundamental Equations Governing the Evolution of the Atmosphere

$$\frac{\partial \vec{v}}{\partial t} = -\vec{v}\cdot\nabla\vec{v} - \frac{1}{\rho_a}\nabla p - g\vec{k} - 2\vec{\Omega}\times\vec{v} + \vec{F}_{visc}$$

$$\frac{\partial \rho_a}{\partial t} = -\nabla\cdot\rho_a\vec{v}$$

$$\frac{\partial r_n}{\partial t} = -\vec{v}\cdot\nabla r_n + Q_{r_n}(s_{[1]},\dots,s_{[\mu]};\dots),\ n=1,\eta$$

$$\frac{\partial \theta}{\partial t} = -\vec{v}\cdot\nabla\theta + Q_\theta(s_{[1]},\dots,s_{[\mu]};\dots)$$

Equation of state (perfect or ideal gas)

$$\frac{\partial s_{[1]}}{\partial t} = -\vec{v}\cdot\nabla s_{[1]} + Q_{s_{[1]}}(s_{[1]},\dots,s_{[\mu]};\theta,p,r_n,R\dots)$$

$$\frac{\partial s_{[2]}}{\partial t} = -\vec{v}\cdot\nabla s_{[2]} + Q_{s_{[2]}}(s_{[1]},\dots,s_{[\mu]};\theta,p,r_n,R,\dots)$$

...

$$\frac{\partial s_{[\mu]}}{\partial t} = -\vec{v}\cdot\nabla s_{[\mu]} + Q_{s_{[\mu]}}(s_{[1]},\dots,s_{[\mu]};\theta,p,r_n,R,\dots)$$

(1) Fundamental equations:

- Navier-Stokes,
- Mass conservation for air and water,
- 1st Law of Thermodynamics,
- Eq. of state.

(2) mass continuity equations for tracers (gases/aerosols)

**For double-moment cloud microphysics, number concentration continuity equations are also solved. The same for some aerosol models.

"Pure" meteorological and off-line, on-line or coupled atmospheric-chemistry models

- If only the system of eq. (1) is solved using prescribed set of $[s_{[1]},...,s_{[\mu]}]$

$\Rightarrow$ "pure" meteorological model.

- If only the system of eq. (2) is solved using prescribed set of $[u,v,w,\theta,p,r_n,...]$

$\Rightarrow$ off-line chemistry transport model.

- If both systems are solved simultaneously (the same dynamics)

but using a prescribed set of $[s_{[1]},...,s_{[\mu]}]$.

$\Rightarrow$ on-line chemistry transport model.

- If both systems are solved simultaneously (the same dynamics) but system

(1) uses the solution $[s_{[1]},...,s_{[\mu]}]$ of system (2):

$\Rightarrow$ coupled atmospheric-chemistry transport model.

Mass continuity equation:

Mathematically describes the dynamical and chemical processes that determine the distribution of chemical species.

Flux form : $\frac{\partial \rho_{[\eta]}}{\partial t} + \underbrace{\nabla \cdot (\rho_{[\eta]} \vec{v})} = Q_{[\eta]}$

transport — sources / sinks / chemical forcing

Advective form : $\frac{\partial s_{[\eta]}}{\partial t} + \overbrace{\vec{v} \cdot \nabla s_{[\eta]}} = \frac{Q_{[\eta]}}{\rho_a}$ **or** $\frac{ds_{[\eta]}}{dt} = \frac{Q_{[\eta]}}{\rho_a}$

where,

$\rho_{[\eta]}$ is the mass (or number) density of species η

ρ_a is the air mass (or number) density

$s_{[\eta]} = \frac{\rho_{[\eta]}}{\rho_a}$ is the mass (or volume) mixing ratio

$Q_{[\eta]}$ is the source (E) / sink (R) and / or chemical production / loss (P - L) rate of species η

$\vec{v}$ is the wind velocity vector

One important propertie : if $Q_\eta = 0 \Rightarrow$ no forcing

$\frac{ds_\eta}{dt} = 0 \Rightarrow s_\eta = cte \therefore$ following the air parcel (the Lagrangian point of view)

The Reynolds decomposition applied to the mass continuity equation

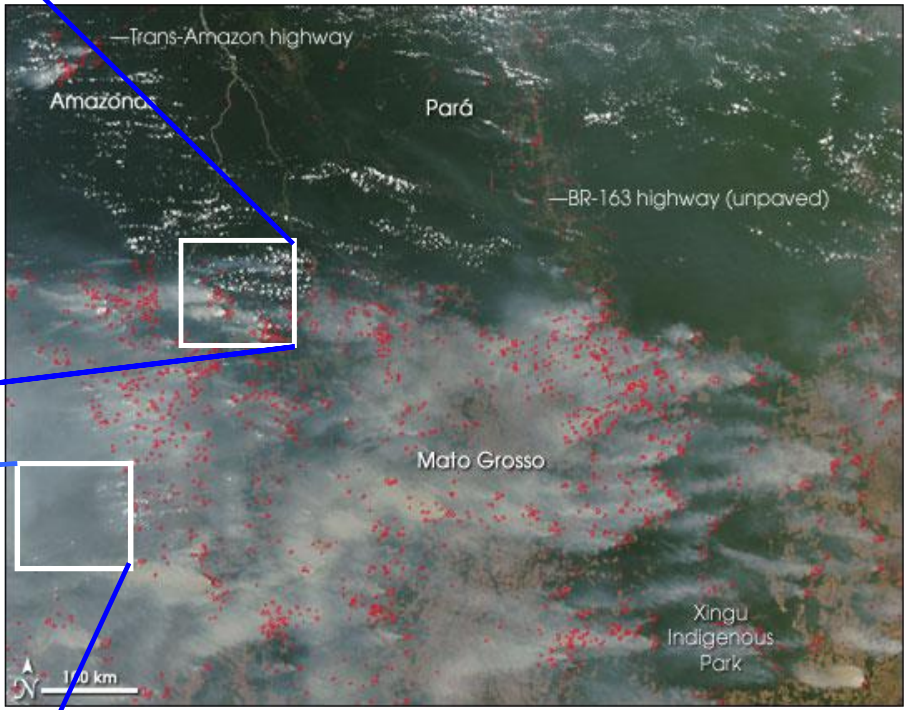
$$\frac{\partial \bar{s}}{\partial t} + \underbrace{\bar{u}\frac{\partial \bar{s}}{\partial x} + \bar{v}\frac{\partial \bar{s}}{\partial y} + \bar{w}\frac{\partial \bar{s}}{\partial z}}_{\text{transport of tracer by the mean wind or grid-scale advection term}} = \underbrace{-\frac{1}{\rho_0}\left(\frac{\partial \rho_0 \overline{u's'}}{\partial x} + \frac{\partial \rho_0 \overline{v's'}}{\partial y} + \frac{\partial \rho_0 \overline{w's'}}{\partial z}\right)}_{\text{sub-grid transport by the un-resolved flows (turbulence, cumulus convection, e.g.)}} + \overline{Q_s} \quad *$$

To solve the mass conservation equation:

- We need parameterizations and closures to determine the turbulent or un-resolved fluxes: $\left(\overline{u's'}, \overline{v's'}, \overline{w's'}\right)$
- We need to define the sources/sinks and the chemical forcing at grid scale: $\overline{Q_s}$
- We need the grid scale wind field: $(\bar{u}, \bar{v}, \bar{w})$
- We need numerical methods and initial and boundary conditions.
- The solution will provide us the 4d **mean tracer mixing ratio** field at the grid points (x_i, y_j, z_k) and discrete time levels t_n: $\bar{s} = \bar{s}(x_i, y_j, z_k, t_n)$
- However, remember that the model will provide the **grid box mean**, and so, you must take this into account when comparing model solution with field observations.

* Derivation at the end of this presentation / background section

Comparison between model and local observation



Numerical solution of the mass continuity equation: using splitting operator

$$\left(\frac{\partial s}{\partial t}\right) = \left(\frac{\partial s}{\partial t}\right)_{adv} + \left(\frac{\partial s}{\partial t}\right)_{\substack{turb\\CLP}} + \left(\frac{\partial s}{\partial t}\right)_{conv} + \ldots + \left(\frac{\partial s}{\partial t}\right)_{chem}$$

- Current computational resources do not allow numerical solution of the continuity equation with all terms simultaneously (the transport term couples the 3 space dimensions with N species = Nx Ny Nz Nspecies ~ 10^4 – 10^5 equations)

- The splitting operator methodology is commonly used to solve each process independently and then couple the various changes resulting from the separate partial calculations (Yanenko 1971, Seinfeld and Pandis 1998, Lanser and Verwer 1998).

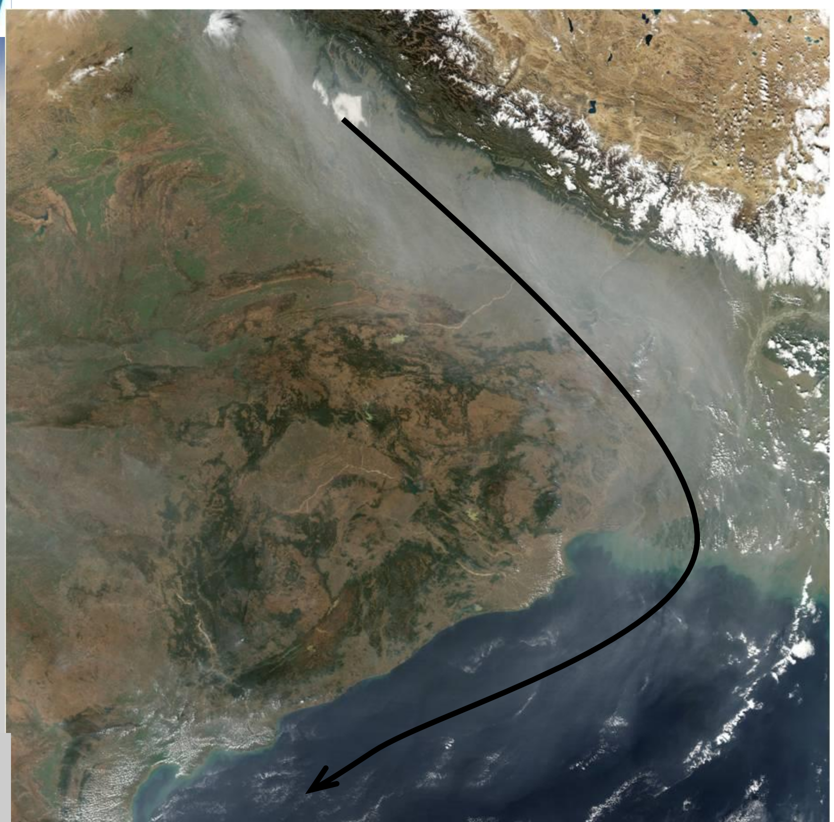
- The final solution can be achieved by the parallel or sequential (direct, symmetrical, weighted) techniques.

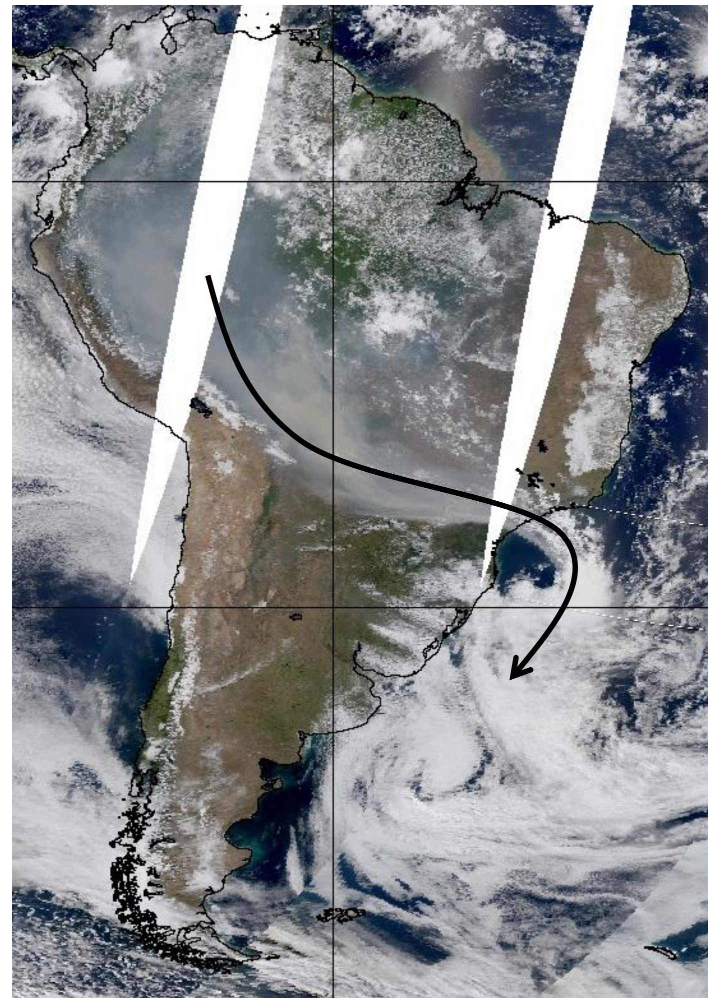
$$\begin{cases}
\left(\frac{\partial \bar{s}}{\partial t}\right)_{adv} = -\sum_i \bar{u}_i \frac{\partial \bar{s}}{\partial x_i} \\
\left(\frac{\partial \bar{s}}{\partial t}\right)_{\substack{turb\\CLP}} = -\frac{1}{\rho_0} \sum_i \frac{\partial \rho_0 \left(\overline{u_i' s'}\right)_{turb}}{\partial x_i} \\
\left(\frac{\partial \bar{s}}{\partial t}\right)_{conv} = -\frac{1}{\rho_0} \sum_i \frac{\partial \rho_0 \left(\overline{u_i' s'}\right)_{conv}}{\partial x_i} \\
\ldots \\
\left(\frac{\partial \bar{s}}{\partial t}\right)_{emissions} = E \\
\left(\frac{\partial \bar{s}}{\partial t}\right)_{chem} = P - L
\end{cases}$$

The mass continuity equation after the Reynolds decomposition

$$\frac{\partial \bar{s}}{\partial t} + \underbrace{\bar{u}\frac{\partial \bar{s}}{\partial x} + \bar{v}\frac{\partial \bar{s}}{\partial y} + \bar{w}\frac{\partial \bar{s}}{\partial z}}_{\text{transport of tracer by the mean wind or grid-scale advection term}} = \underbrace{-\frac{1}{\rho_0}\left(\frac{\partial \rho_0 \overline{u's'}}{\partial x} + \frac{\partial \rho_0 \overline{v's'}}{\partial y} + \frac{\partial \rho_0 \overline{w's'}}{\partial z}\right)}_{\text{sub-grid transport by the un-resolved flows (turbulence, cumulus convection, e.g.)}} + \overline{Q_s}$$

How to solve this term (the grid scale transport) ?





Desired properties of numerical schemes for advection

The advection equation for tracers / pollutants η :

$$\frac{\partial \rho_\eta}{\partial t} + \nabla \cdot (\rho_\eta \vec{v}) = 0$$ the flux form.

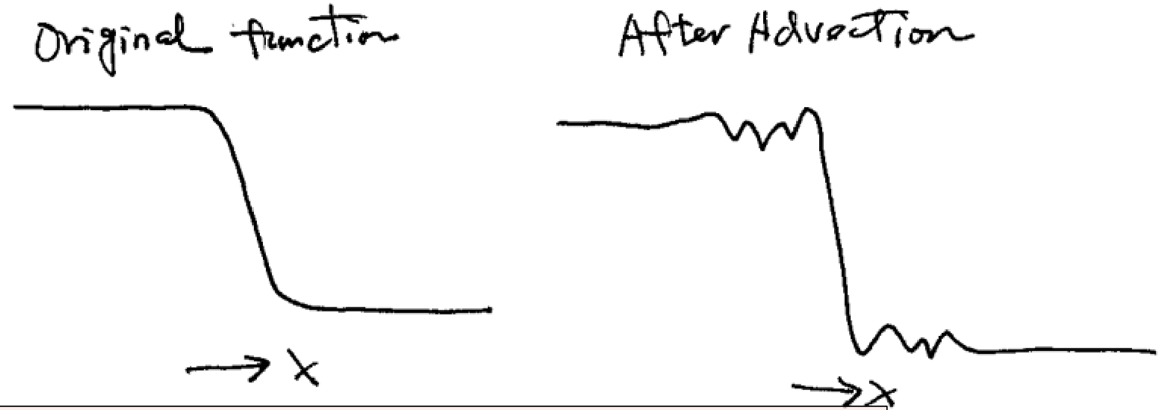
$$\frac{\partial s_\eta}{\partial t} + \vec{v} \cdot \nabla s_\eta = 0$$ the advective form.

Desired properties:

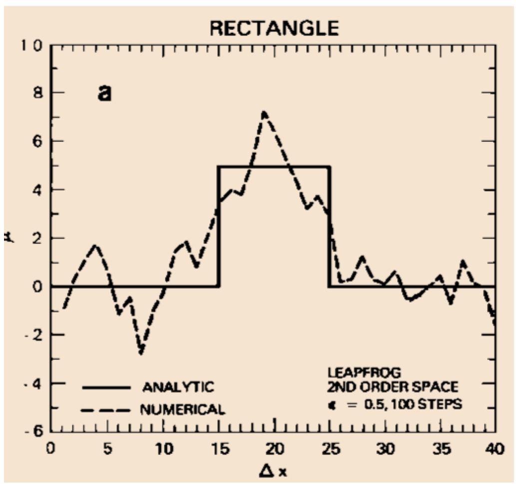
- mass conserving
- monotonicity and shape preserving
- positive definite
- local
- accurate
- stable
- efficient from computational point of view
- multi-tracer computational efficiency (re-use of repeated calculations)
- keeps tracers non-linear correlation
- multi component mass conserving (mainly for aerosol and cloud microphysics models)

For a comprehensive review:
Lauritzen et al.: Atmospheric transport schemes: desirable properties and a semi-Lagrangian view on finite-volume discretizations. Numerical Techniques for Global Atmospheric Models, 2011.

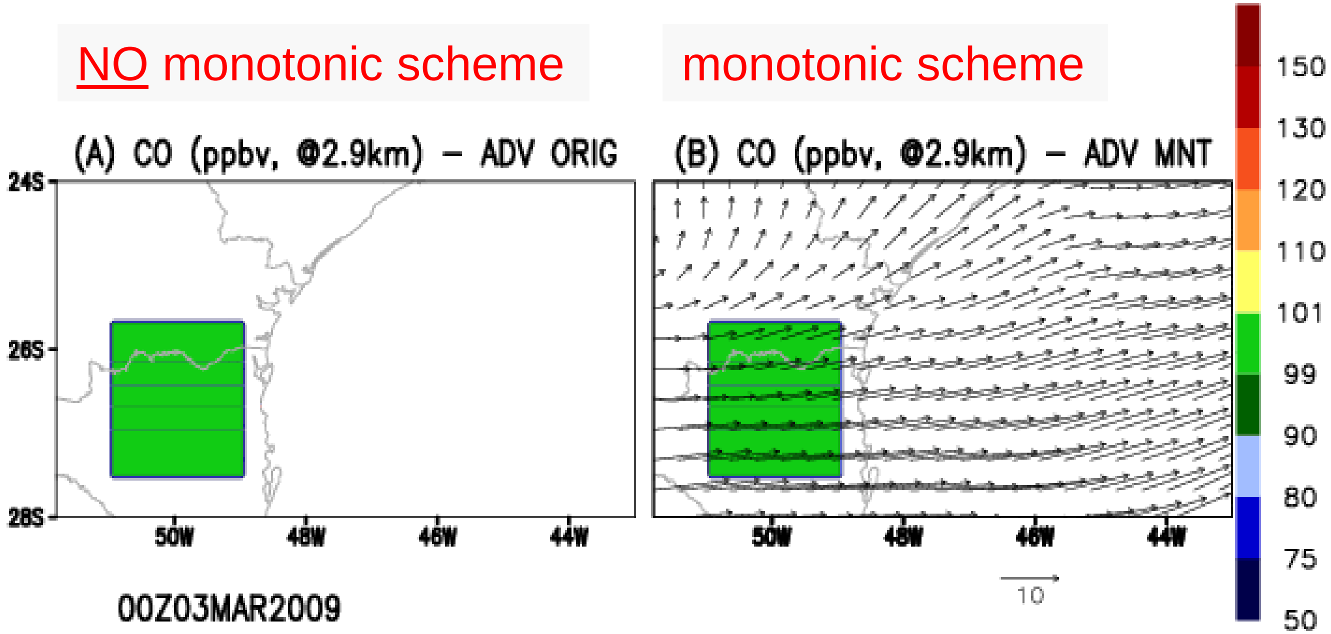
Monotonicity of Advection Schemes



- Monotonic numerical schemes are ones which, given an initial distribution which is monotonic before advection, produce a monotonic distribution after advection.
- A consequence of this property is that monotonic schemes neither create new extrema in the solution nor amplify existing extrema.
- The spurious oscillations can cause positive-definite fields, such as mass and water, to turn negative.
- Even small negative oscillations may make unstable chemical solvers
- Monotonic schemes are necessary for transporting fields with sharp gradients:
    - emissions from urban areas, volcanoes, fires
    - Clouds fields
    - Temperature in cold fronts



Advection of a square in a divergent wind

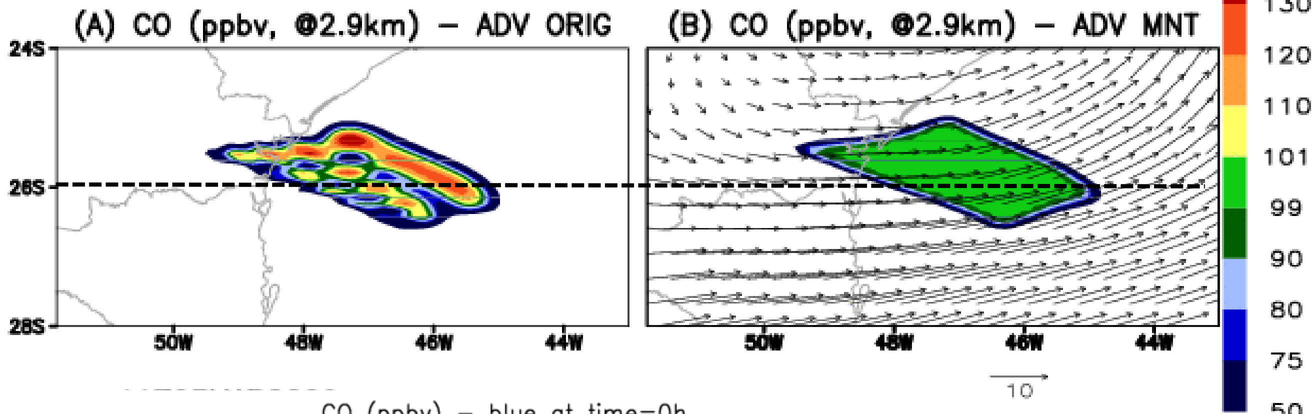


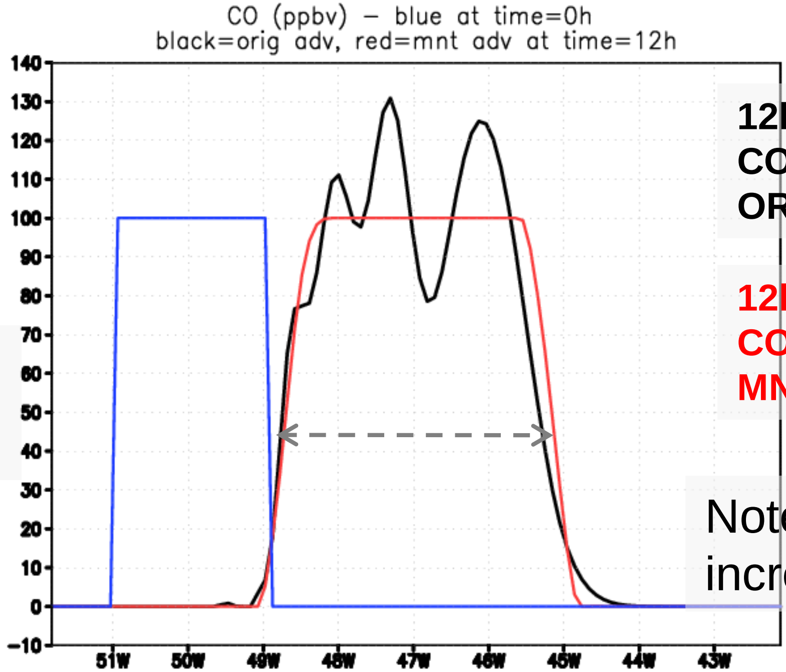
Tracer with initial mixing ratio = 100 ppbv
12 hours integration

Simulation with no numerical or physical based diffusion

Advection of a square in a divergent wind

NO monotonic scheme | monotonic scheme





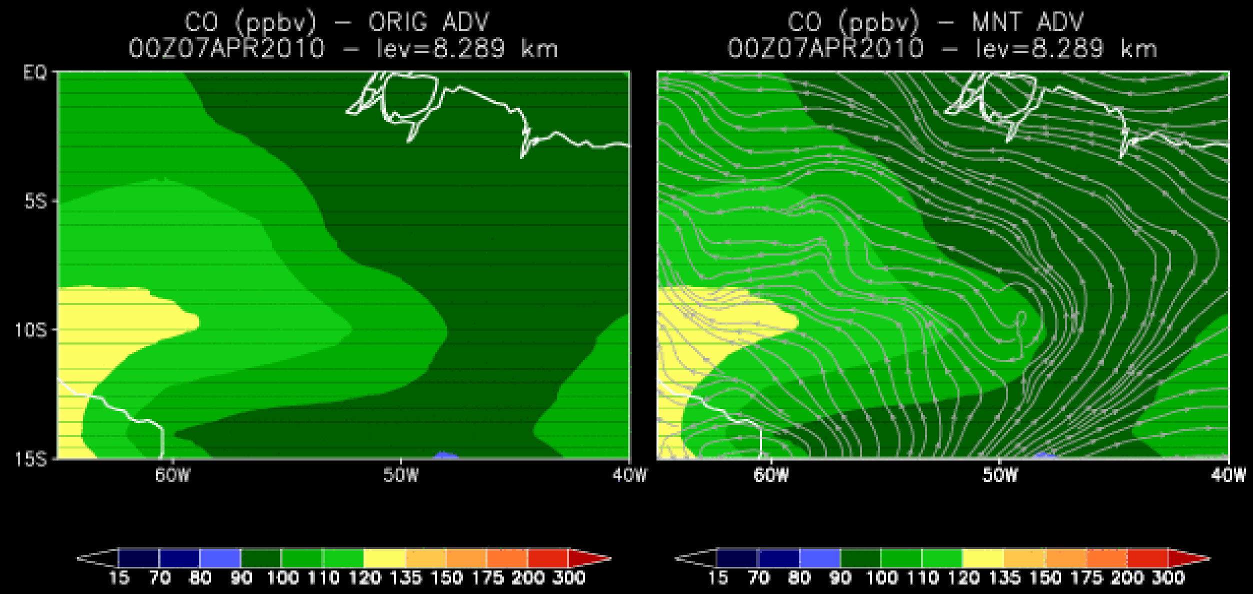
TRACER (CO) INITIAL DISTRIBUITION

12h after CO DISTRIBUITION ORIG advection

12h after CO DISTRIBUITION MNT advection

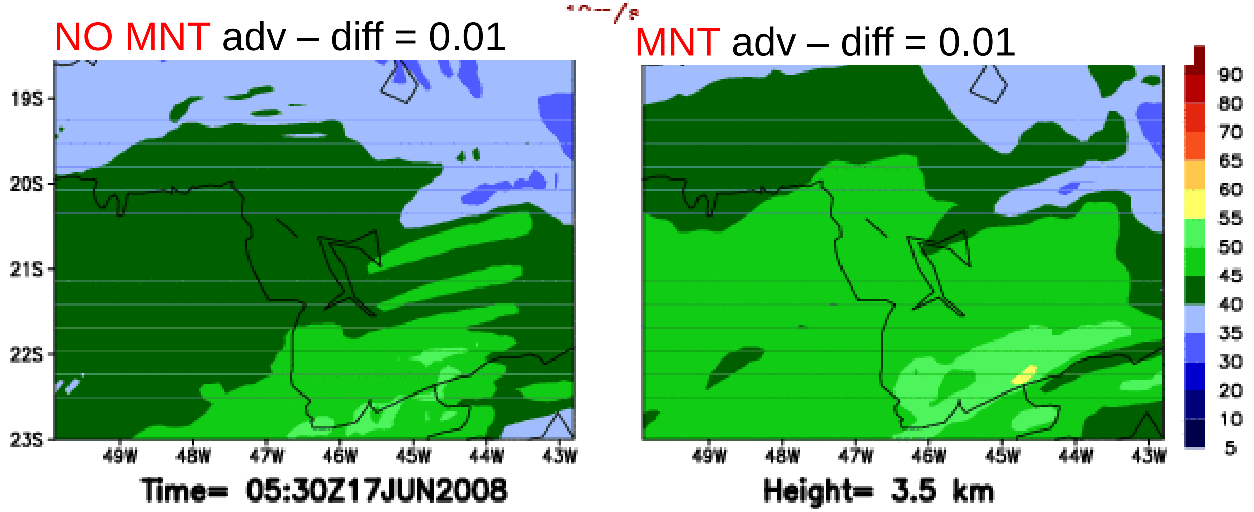
Note the wind divergence increasing the plume size

Impact of a monotonic advection scheme on the transport of isolated biomass burning smoke plumes in Amazon basin



Simulation of a ozone plume

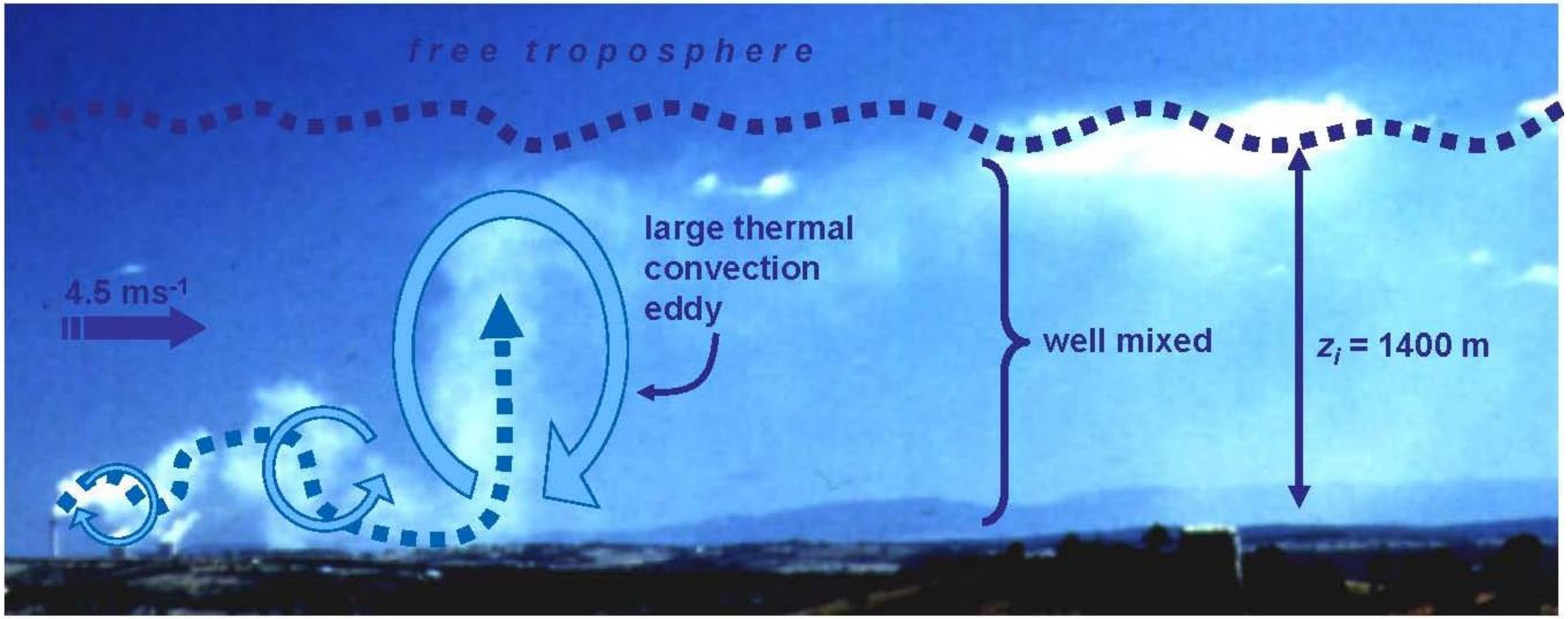
From 14 to 24 UTC 17 June 2008 and at vertical level of 3.5 km



The mass continuity equation after Reynolds decomposition

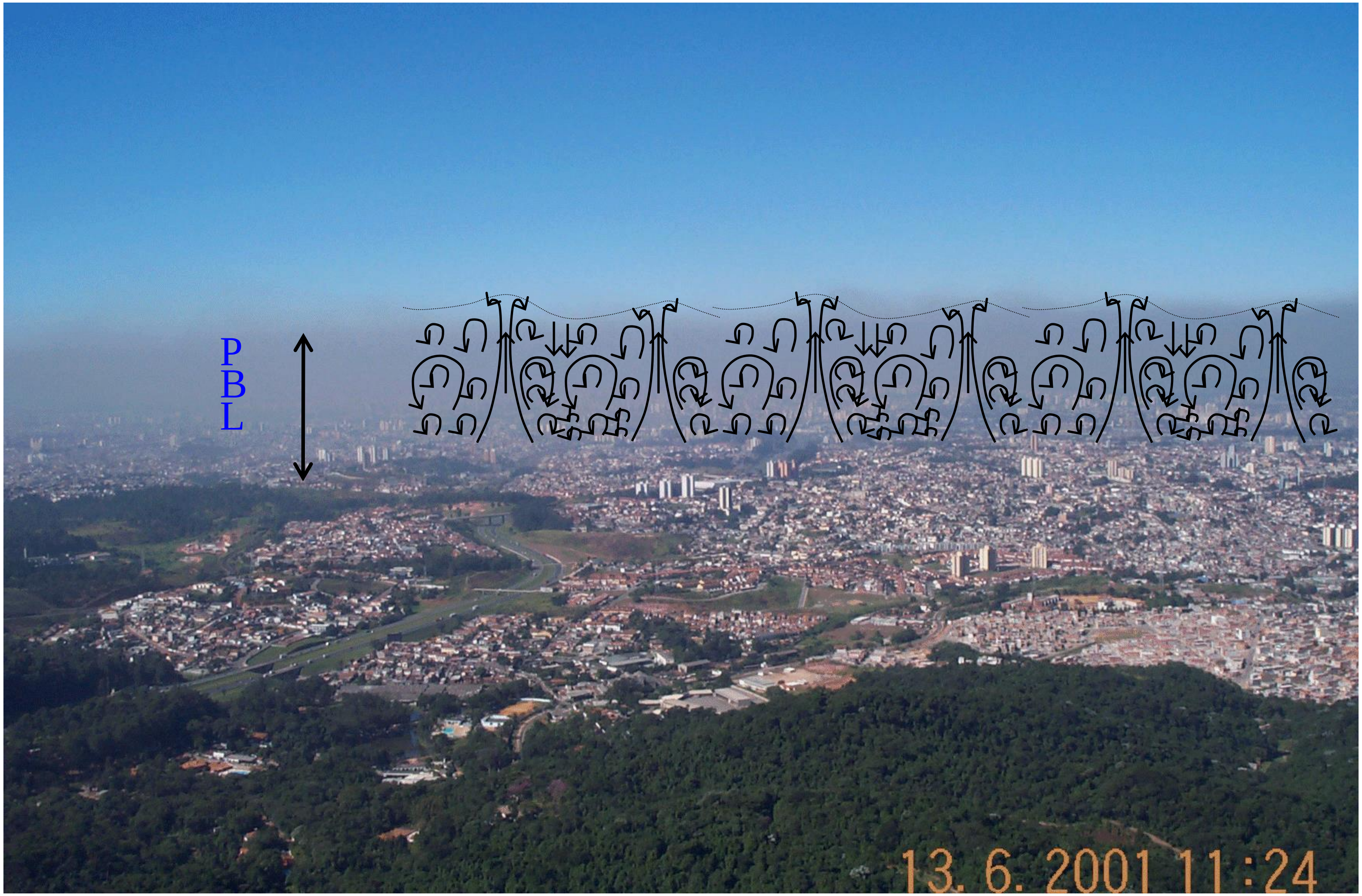
$$\frac{\partial \bar{s}}{\partial t} + \underbrace{\bar{u}\frac{\partial \bar{s}}{\partial x} + \bar{v}\frac{\partial \bar{s}}{\partial y} + \bar{w}\frac{\partial \bar{s}}{\partial z}}_{\text{transport of tracer by the mean wind or grid-scale advection term}} = \underbrace{-\frac{1}{\rho_0}\left(\frac{\partial \rho_0 \overline{u's'}}{\partial x} + \frac{\partial \rho_0 \overline{v's'}}{\partial y} + \frac{\partial \rho_0 \overline{w's'}}{\partial z}\right)}_{\text{sub-grid transport by the un-resolved flows (turbulence, cumulus convection, e.g.)}} + \overline{Q_s}$$

How to solve this term (sub-grid scale transport) ?



Tarong, Queensland (AUS), stack height: 210 m, z_i = 1400 m, w* = 2.5 ms^{-1}. Photo: Geoff Lane, CSIRO (AUS)

Sub-grid scale diffusive transport (daytime)



Planetary boundary layer over Sao Paulo city and trapped air pollution

Sub-grid scale diffusive transport

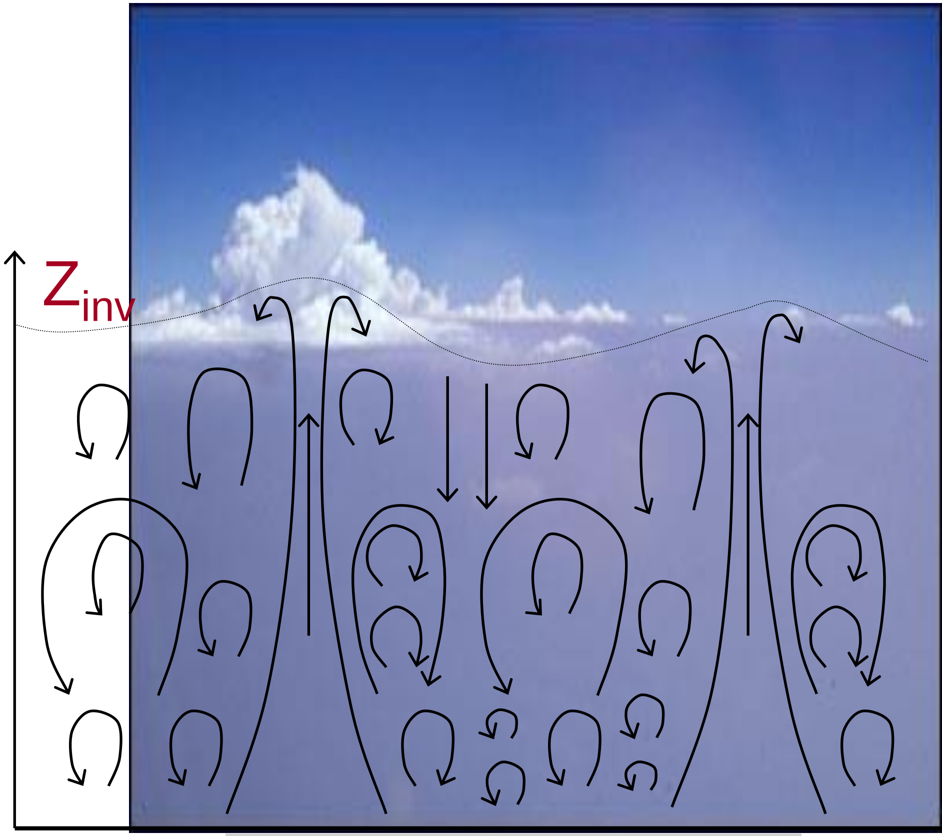
Diffusive transport:

$$\left(\frac{\partial \overline{s}}{\partial t}\right)_{\substack{PBL\\turb}} = -\frac{1}{\rho_0}\sum_i \frac{\partial(\rho_0 \overline{u_i' s'})}{\partial x_i}$$

A simple approach to the unresolved transport is by using K-theory in which the covariances are evaluated as the product of an eddy mixing coefficient and the gradient of the transported mean quantity:

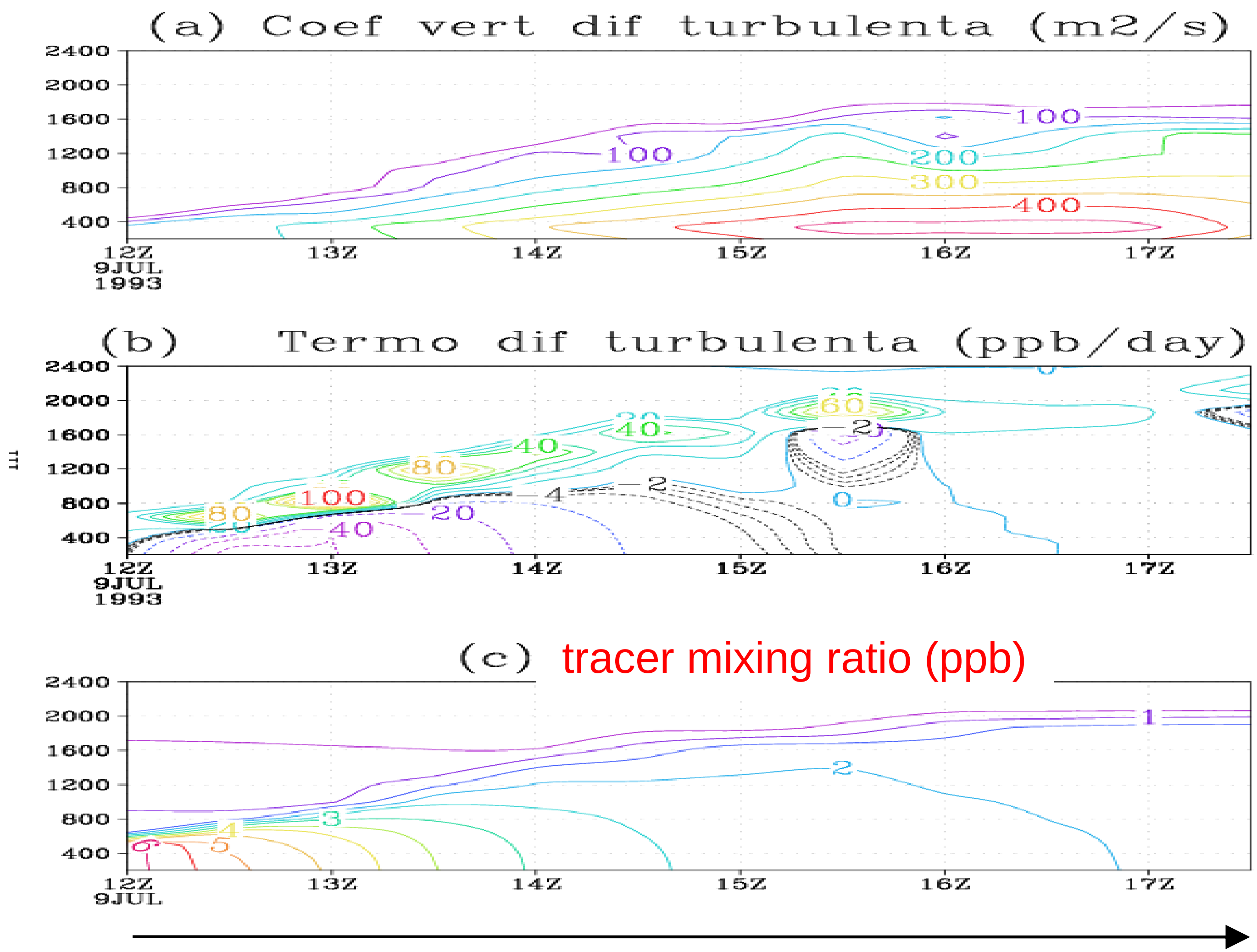
$$\overline{u_i' s'} = -K_{h_i}\frac{\partial \overline{s}}{\partial x_i}$$

Diffusion coefficients need to be specified as a function of flow characteristics (e.g. shear, stability, length scales).



boundary layer eddies

Sub-grid scale transport by diffusion in the PBL



K_{h_i}

$\left(\frac{\partial \overline{s}}{\partial t}\right)_{turb}^{PBL}$

$\overline{S}$

diurnal time (cbl)

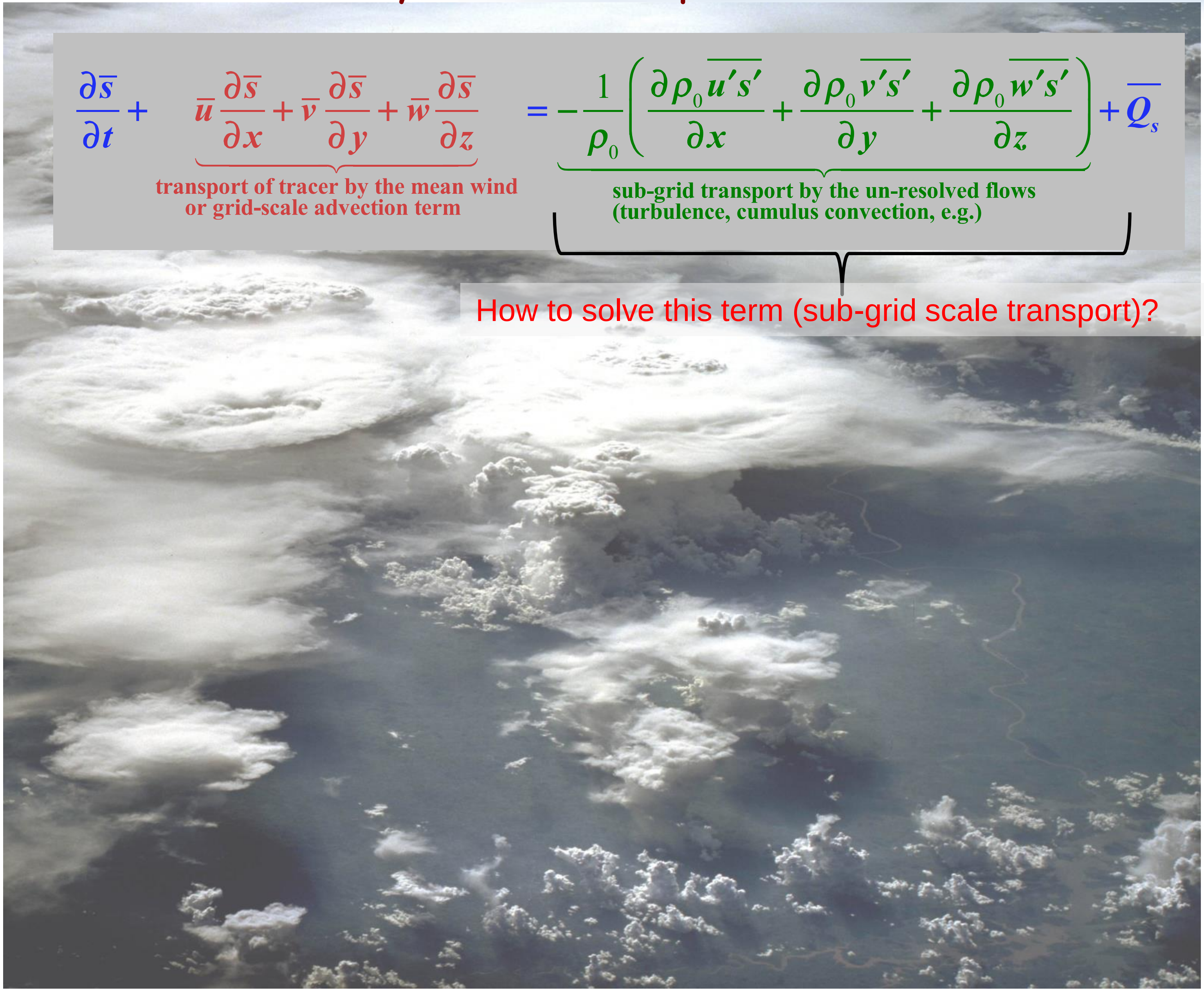
The mass continuity equation after Reynolds decomposition

$$\frac{\partial \bar{s}}{\partial t} + \underbrace{\bar{u}\frac{\partial \bar{s}}{\partial x} + \bar{v}\frac{\partial \bar{s}}{\partial y} + \bar{w}\frac{\partial \bar{s}}{\partial z}}_{\text{transport of tracer by the mean wind or grid-scale advection term}} = \underbrace{-\frac{1}{\rho_0}\left(\frac{\partial \rho_0 \overline{u's'}}{\partial x} + \frac{\partial \rho_0 \overline{v's'}}{\partial y} + \frac{\partial \rho_0 \overline{w's'}}{\partial z}\right)}_{\text{sub-grid transport by the un-resolved flows (turbulence, cumulus convection, e.g.)}} + \overline{Q_s}$$

transport of tracer by the mean wind or grid-scale advection term

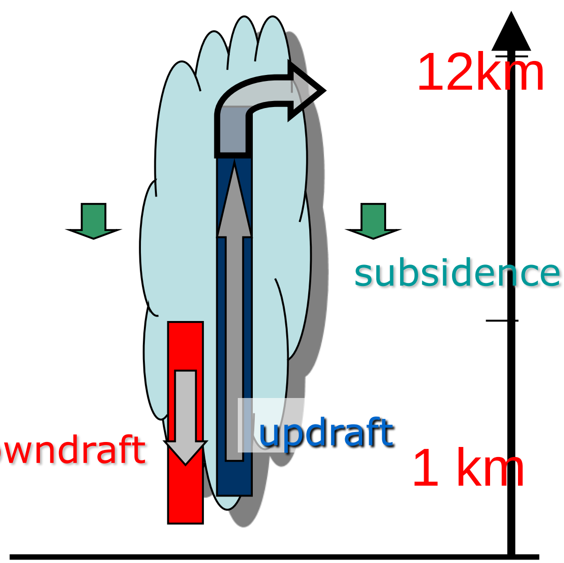
sub-grid transport by the un-resolved flows (turbulence, cumulus convection, e.g.)

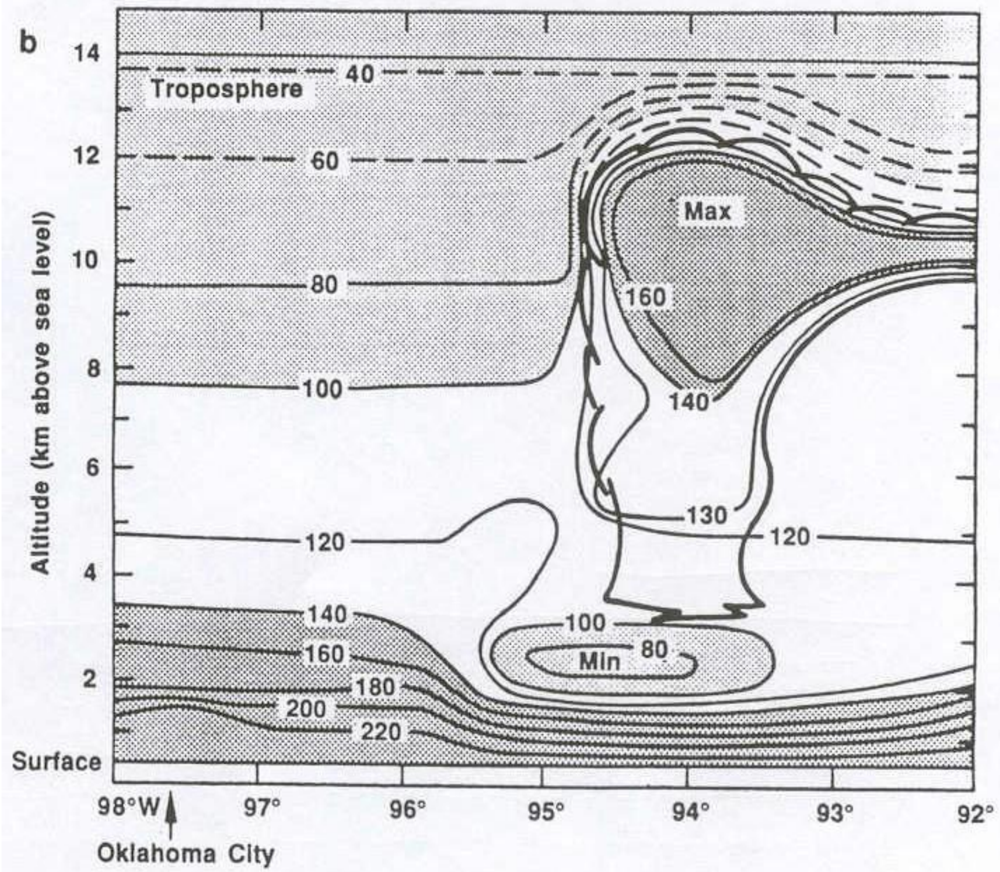
How to solve this term (sub-grid scale transport)?



Convective tracer transport by deep clouds

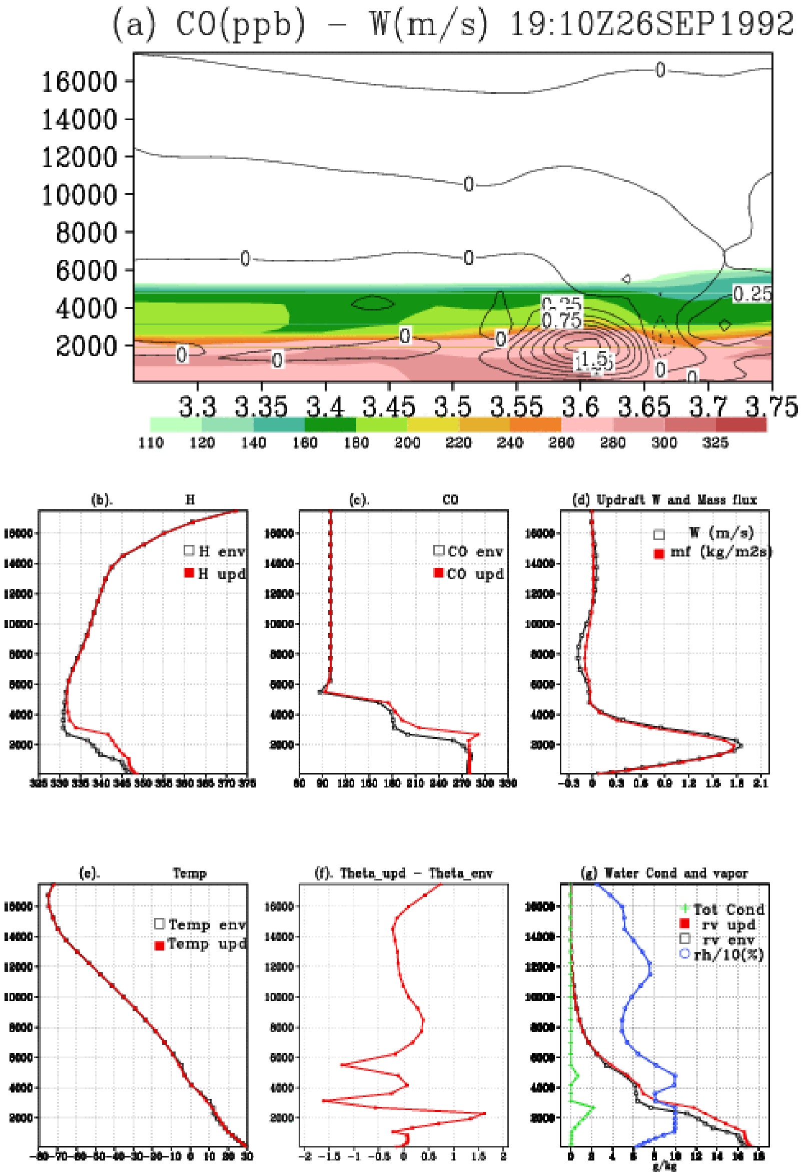
Cloud venting is a very important mechanism transporting pollutants from the PBL to the upper levels, affecting the chemistry of troposphere and the biogeochemical cycles.

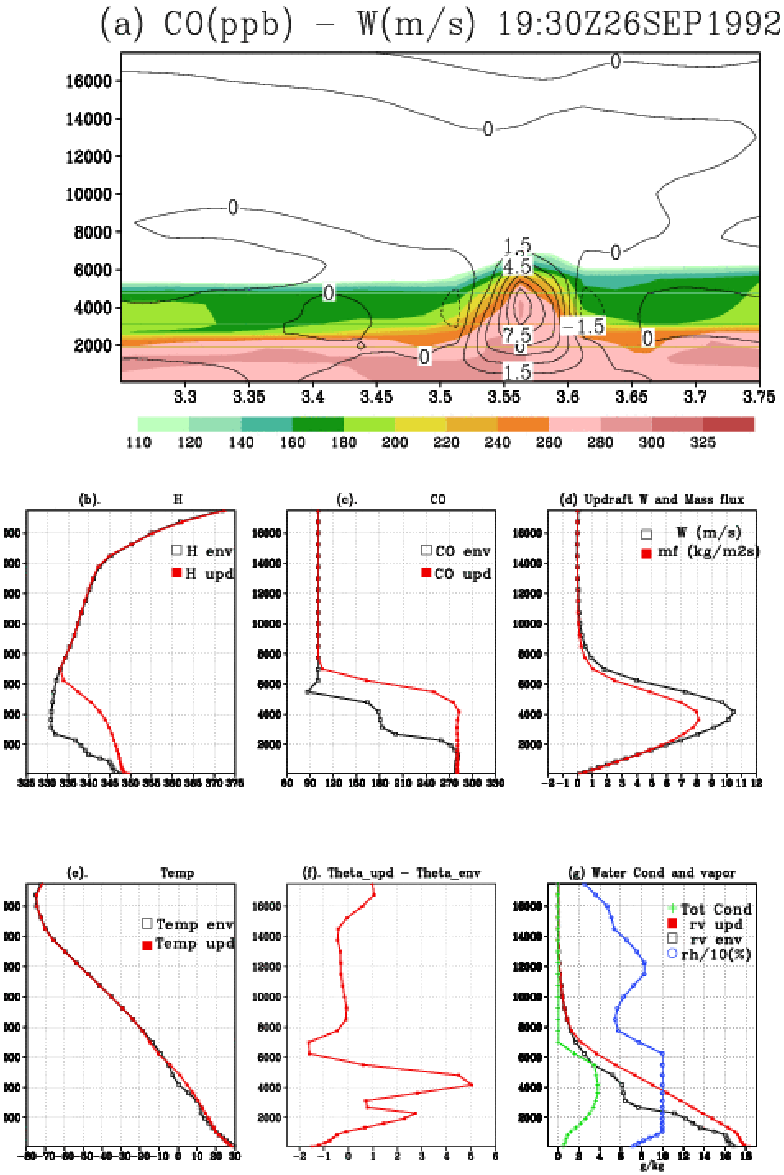




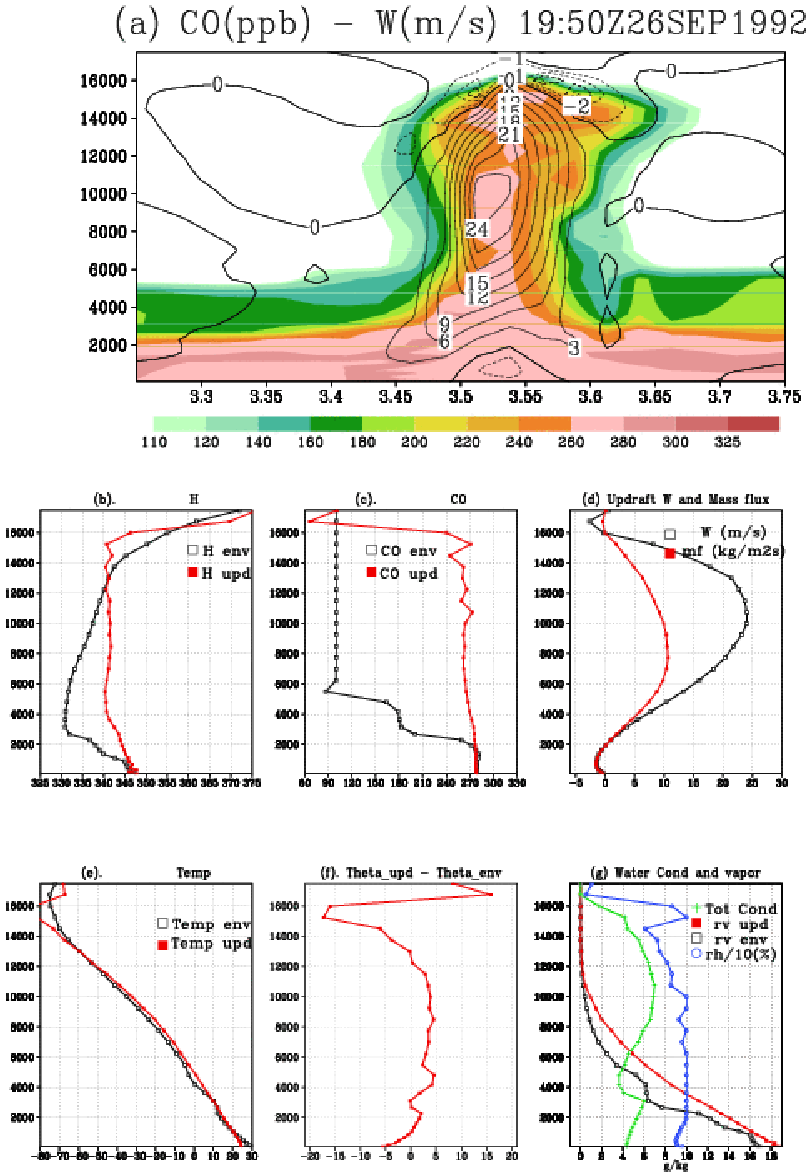
CO mixing ratio (ppbv) observed on 06/14/1985 nearby Oklahoma City (US). Dashed isolines refer to climatological values (Dickerson et al., 1987).

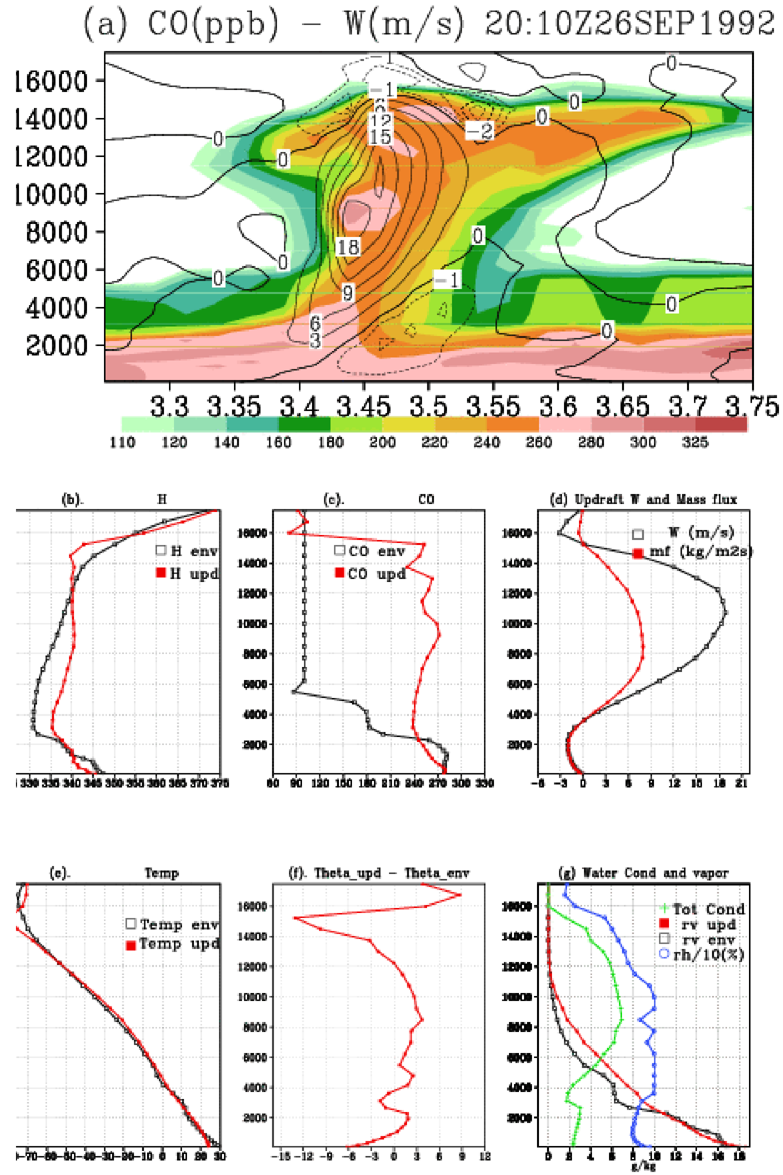
Simulation at 2.5 km horizontal grid length





Simulation at 2.5 km horizontal grid length





Sub-grid scale transport processes

$$\frac{\partial \bar{f}}{\partial t} + \underbrace{\bar{u}\frac{\partial \bar{f}}{\partial x} + \bar{v}\frac{\partial \bar{f}}{\partial y} + \bar{w}\frac{\partial \bar{f}}{\partial z}}_{\text{transport of scalar by the mean wind or grid-scale advection term}} = \underbrace{-\frac{1}{r_0}\left(\frac{\partial r_0 \overline{u'f'}}{\partial x} + \frac{\partial r_0 \overline{v'f'}}{\partial y} + \frac{\partial r_0 \overline{w'f'}}{\partial z}\right)}_{\text{sub-grid transport by the un-resolved flow (turbulence, cumulus convection, e.g.)}} + \overline{Q_f}$$

$$\left(\frac{\partial \bar{f}}{\partial t}\right)_{\text{convective transport}} = -\frac{1}{r_0}\left(\frac{\partial r_0 \overline{u'f'}}{\partial x} + \frac{\partial r_0 \overline{v'f'}}{\partial y} + \frac{\partial r_0 \overline{w'f'}}{\partial z}\right)$$

$$\left(\frac{\partial \bar{f}}{\partial t}\right)_{\text{convective transport}} \approx -\frac{1}{r_0}\frac{\partial r_0 \overline{w'f'}}{\partial z}$$

sub-grid scale transport associated with the cumulus convection

$\overline{w'f'}$ is the eddy convective flux

How to estimate ?

with some algebra:

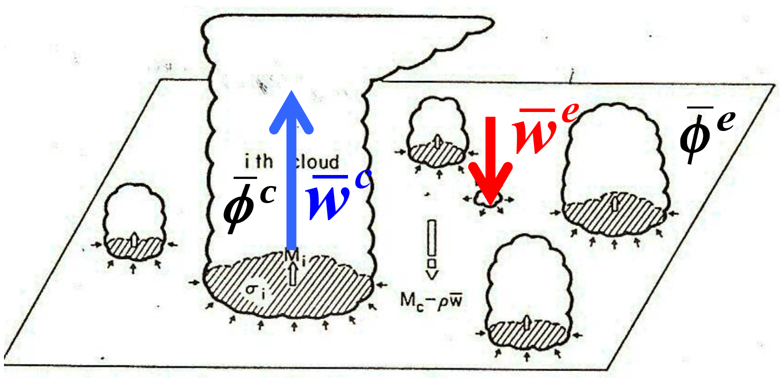
$$\overline{w'\phi'} = \overline{w\phi} - \bar{w}\bar{\phi} = \sigma(1-\sigma)(\bar{w}^c - \bar{w}^e)(\bar{\phi}^c - \bar{\phi}^e)$$ *

$\overline{w'\phi'}$: the vertical eddy transport of ϕ per unit horizontal area and air density.

$\sigma = \frac{a}{A}$ fraction of active cumulus area

ϕ^c, ϕ^e scalar quantity in cloud and in the environment

w^c, w^e the same for vertical velocity



total area ***A*,**

cumulus area ***a*,**

* Derivation at the end of this presentation / background section

The Vertical Eddy Transport:
the approximation of small area covered by cumulus

Vertical eddy transport:

$$\overline{w'\phi'} = \overline{w\phi} - \bar{w}\bar{\phi} = \sigma\left(1-\sigma\right)(\bar{w}^c - \bar{w}^e)(\bar{\phi}^c - \bar{\phi}^e)$$

Assume the small area approximation:

$$\sigma << 1 \Rightarrow (1-\sigma) \approx 1; \quad \bar{w}^c >> \bar{w}^e \, and \; \bar{\phi}^e \approx \bar{\phi}$$

$$\therefore \overline{w'\phi'} = \sigma \bar{w}^{c*}(\bar{\phi}^c - \bar{\phi})$$

Define convective mass flux : $m_c = \bar{\rho}_{air}\sigma\bar{w}^{c*}$

$$\therefore \overline{w'\phi'} = \frac{m_c(\bar{\phi}^c - \bar{\phi})}{\bar{\rho}_{air}} \rightarrow \frac{\text{aproximation used by the most conven-}}{\text{tional mass-flux based parameterizations}}$$

Here m_c is determined using a 'closure' formulation.

See at the background section, the formulation with scale dependence following the unified parameterization approach of Arakawa et al., (2011)

Parameterized deep/shallow convective transport

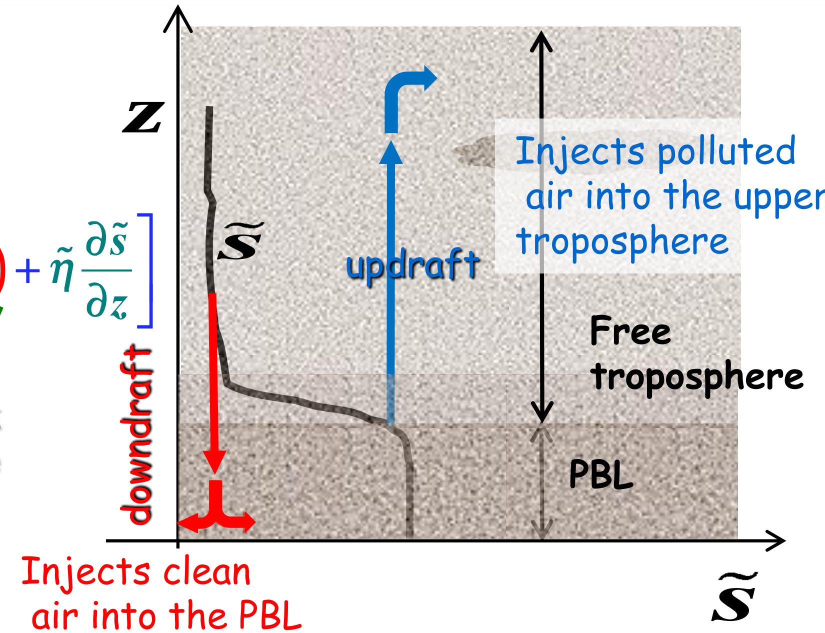
$$\left(\frac{\partial \bar{s}}{\partial t}\right)_{deep\ conv} = \frac{1}{\rho_0}\frac{\partial}{\partial z}(\rho_0 \overline{w's'})$$

$$\left(\frac{\partial \bar{s}}{\partial t}\right)_{deep\ conv} = \frac{m_u(z_b)}{\rho_0}\left[\delta_u \eta_u (s_u - \tilde{s}) + \delta_d \varepsilon \eta_d (s_d - \tilde{s}) + \tilde{\eta}\frac{\partial \tilde{s}}{\partial z}\right]$$

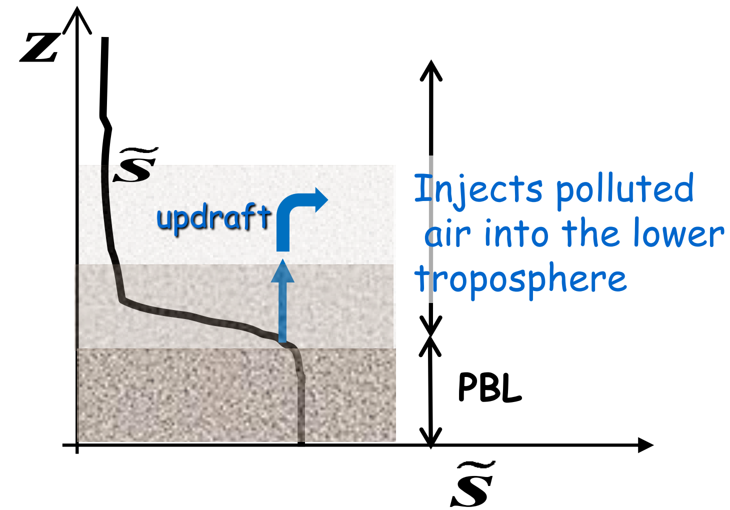
Updraft detrainment

downdraft detrainment

environment subsidence

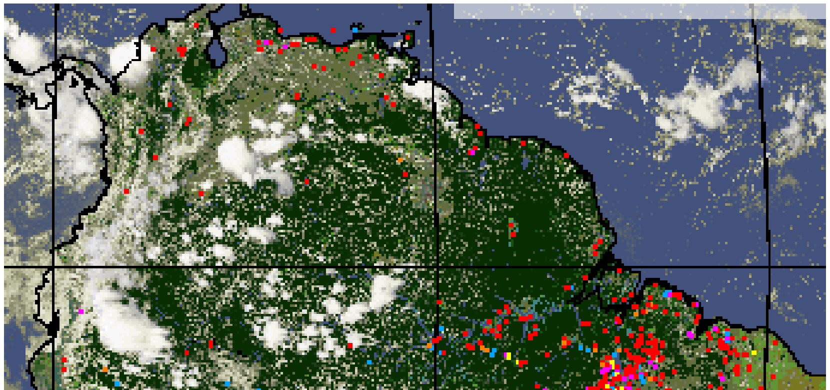


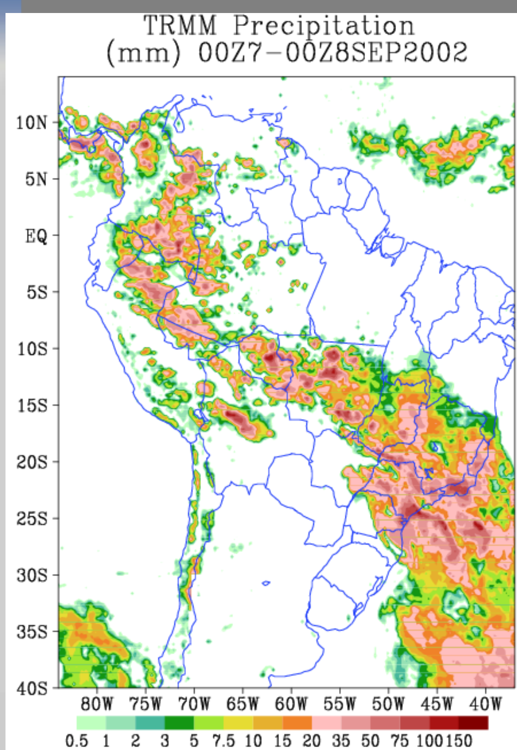
$$\left(\frac{\partial \bar{s}}{\partial t}\right)_{shallow\ conv} = \frac{m_b}{r_0}\left[d_u h_u (s_u - \tilde{s}) + \tilde{h}\frac{\partial \tilde{s}}{\partial z}\right]$$

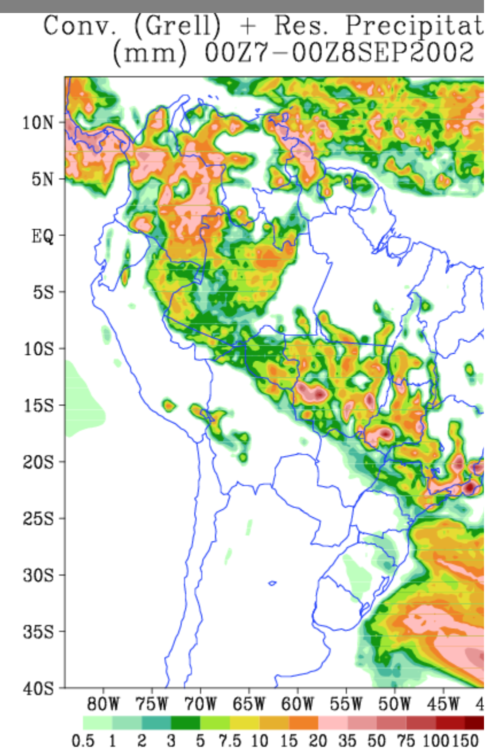


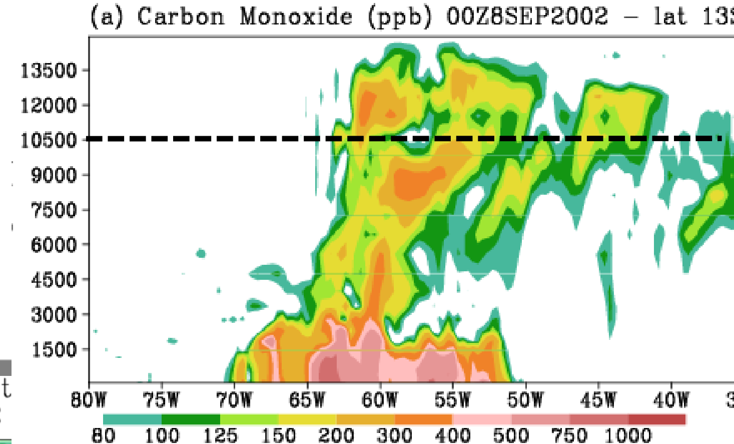
Deep Convective Transport of CO

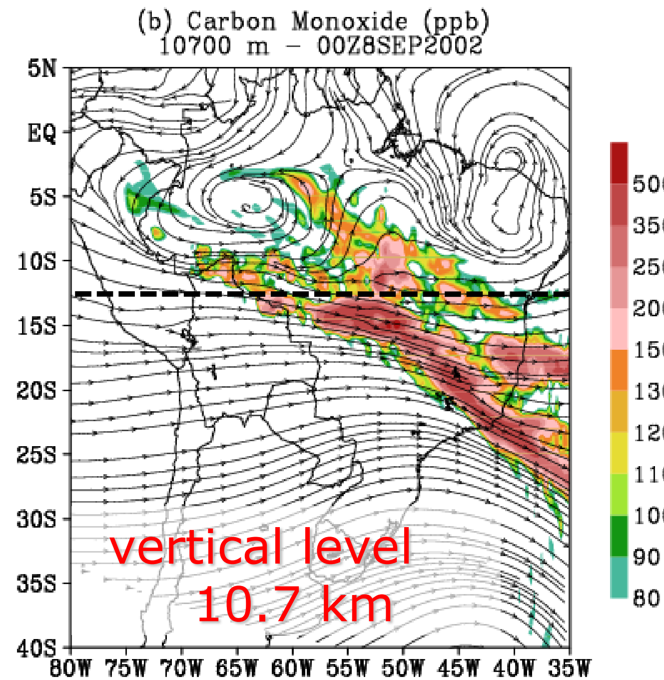
07 Sep 2002 - Cold front approach



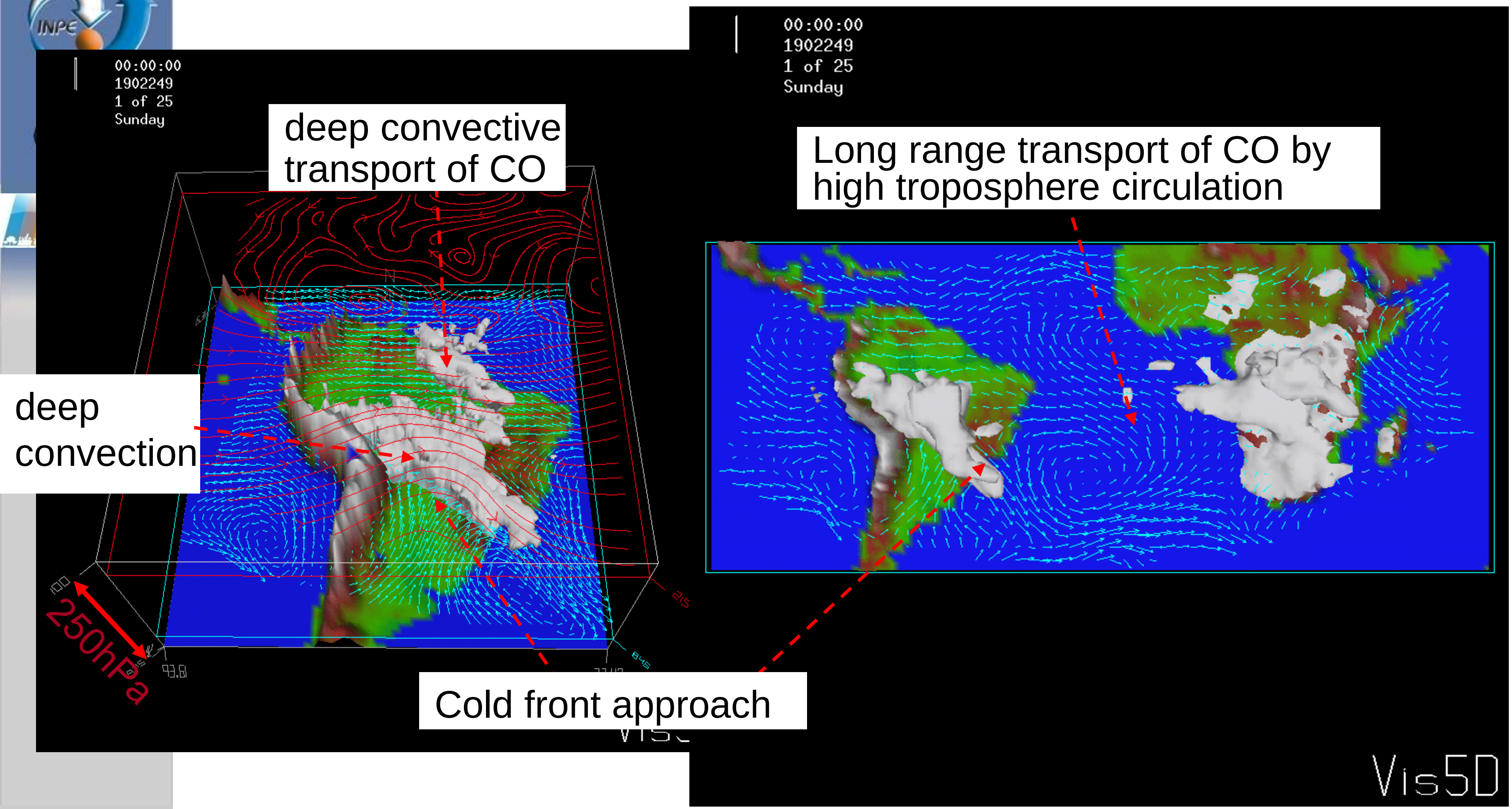






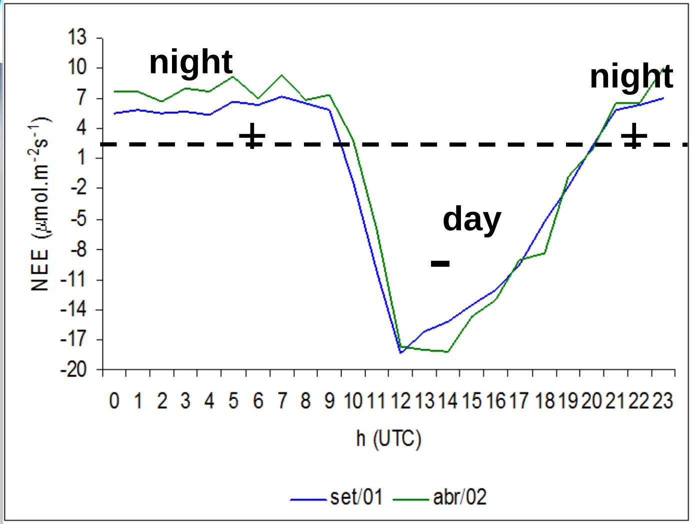


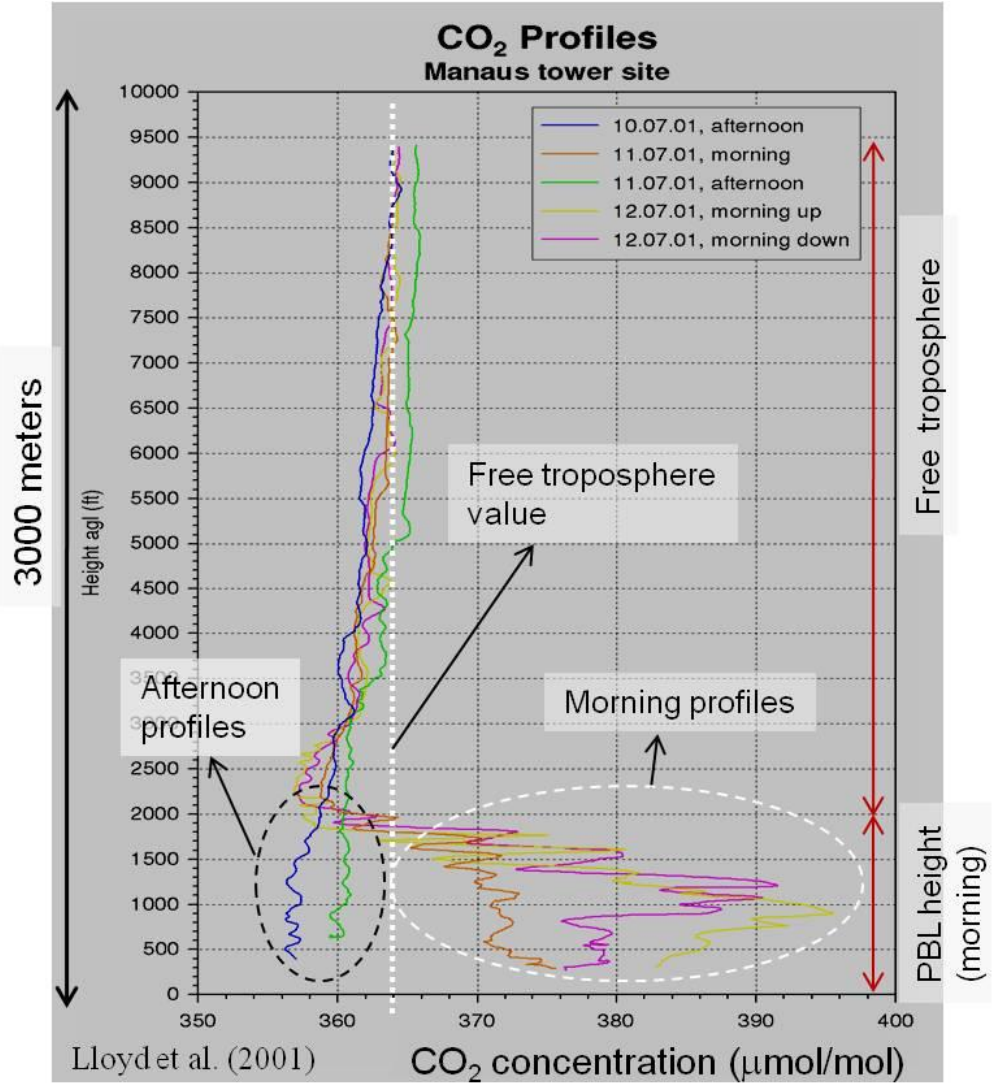
High Troposphere and Long Range Transport of CO



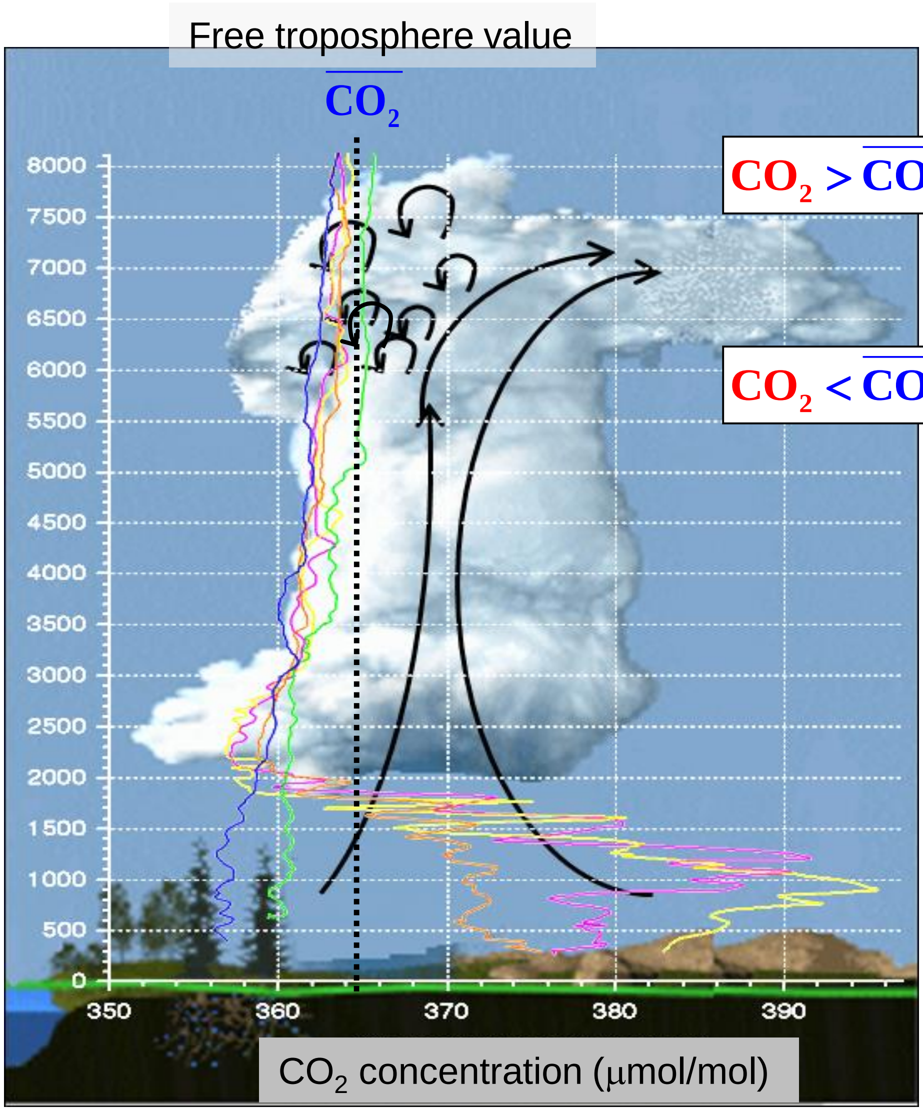
The CO_2 profile: diurnal variation and the rectifier effect

CO_2 surface flux on Amazon





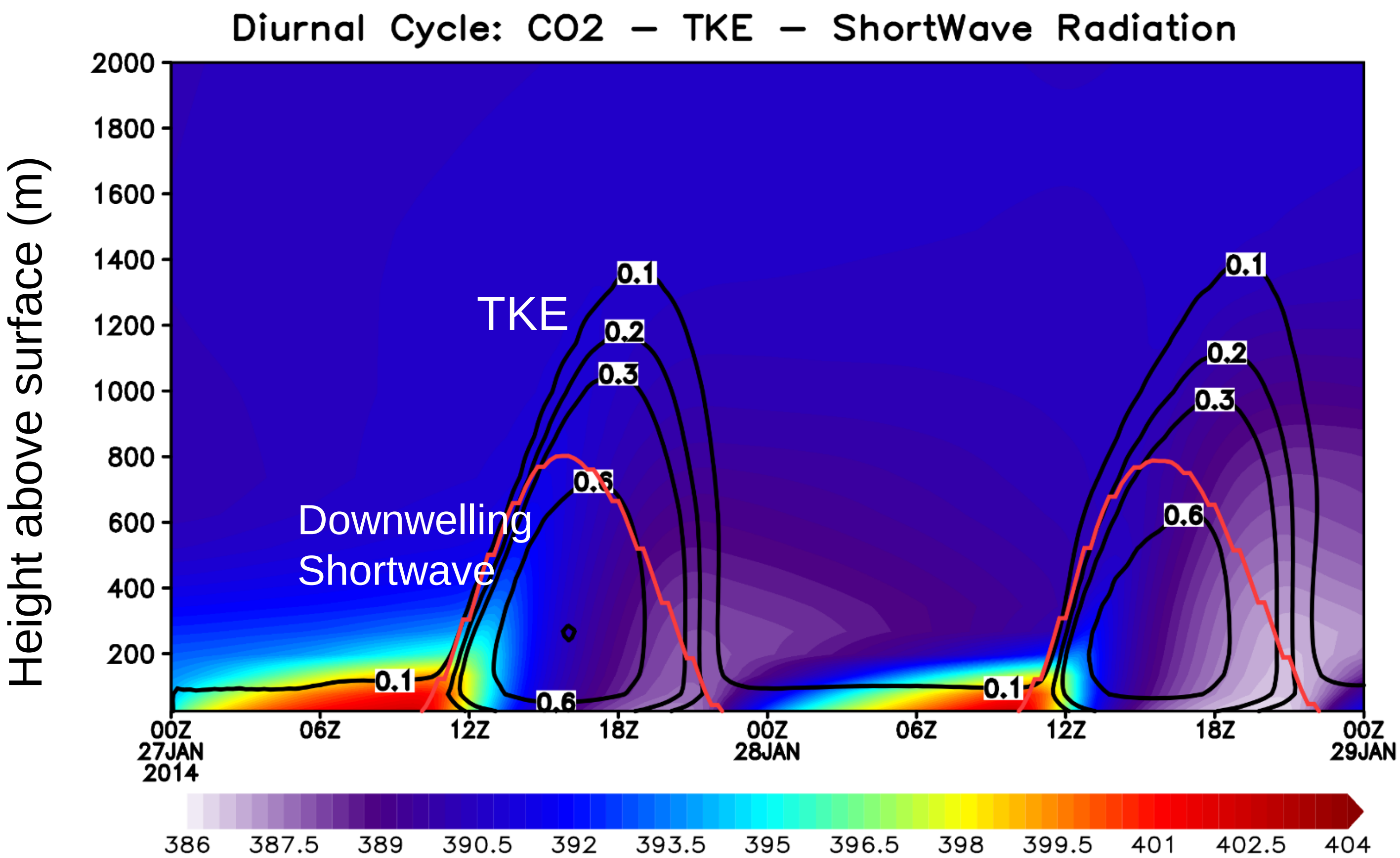
The CO_2 profile: diurnal variation and the rectifier effect



$CO_2 > \overline{CO_2}$ Morning => CO_2 enriched detrainment air mass.

$CO_2 < \overline{CO_2}$ Afternoon =>CO_2 depleted detrainment air mass.

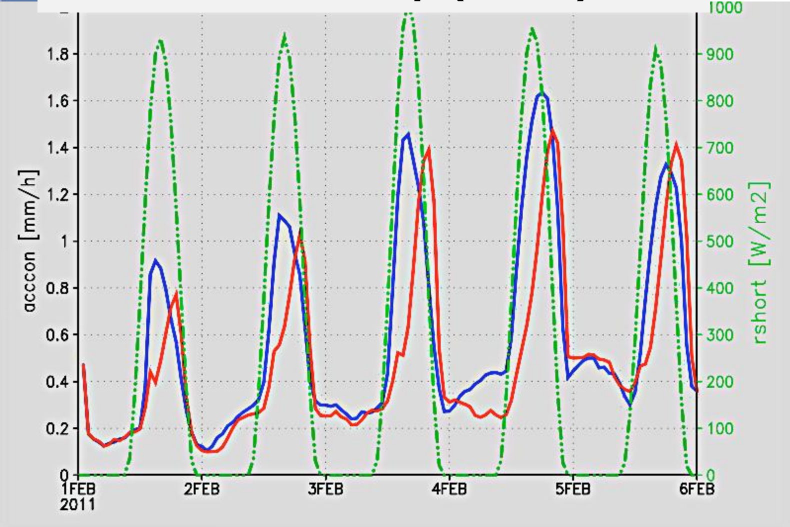
Diurnal Cycle of CO_2 over the Amazon Basin



Simulation with BRAMS + JULES-UK surface scheme

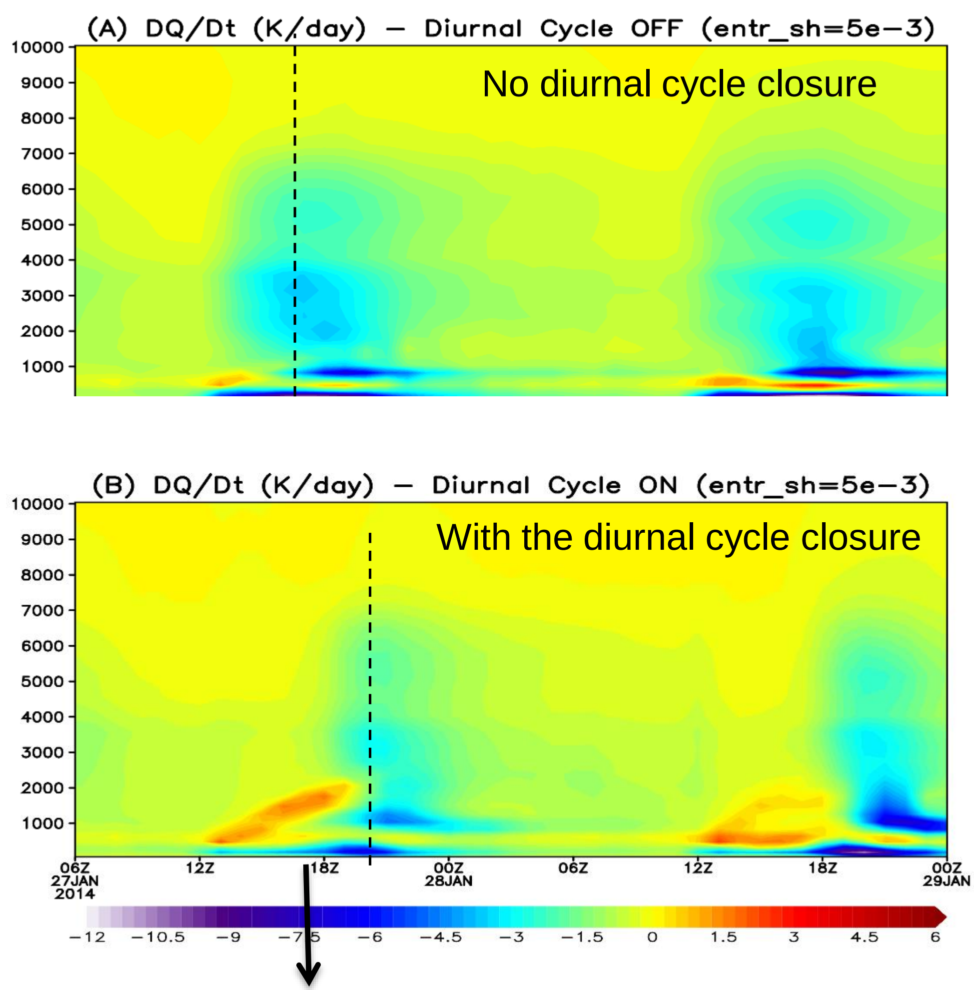
Improved diurnal cycle of deep convection with Bechtold et al new closure for non-equilibrium convection

Conv Precip (mm/h)



- 5 days forecast of CP precip (mm/h)
- Model grid spacing 27km
- Area average over Amz. Basin
- BLUE = diurnal cycle closure OFF
- RED = diurnal cycle closure ON
- GREEN= sfc solar radiation

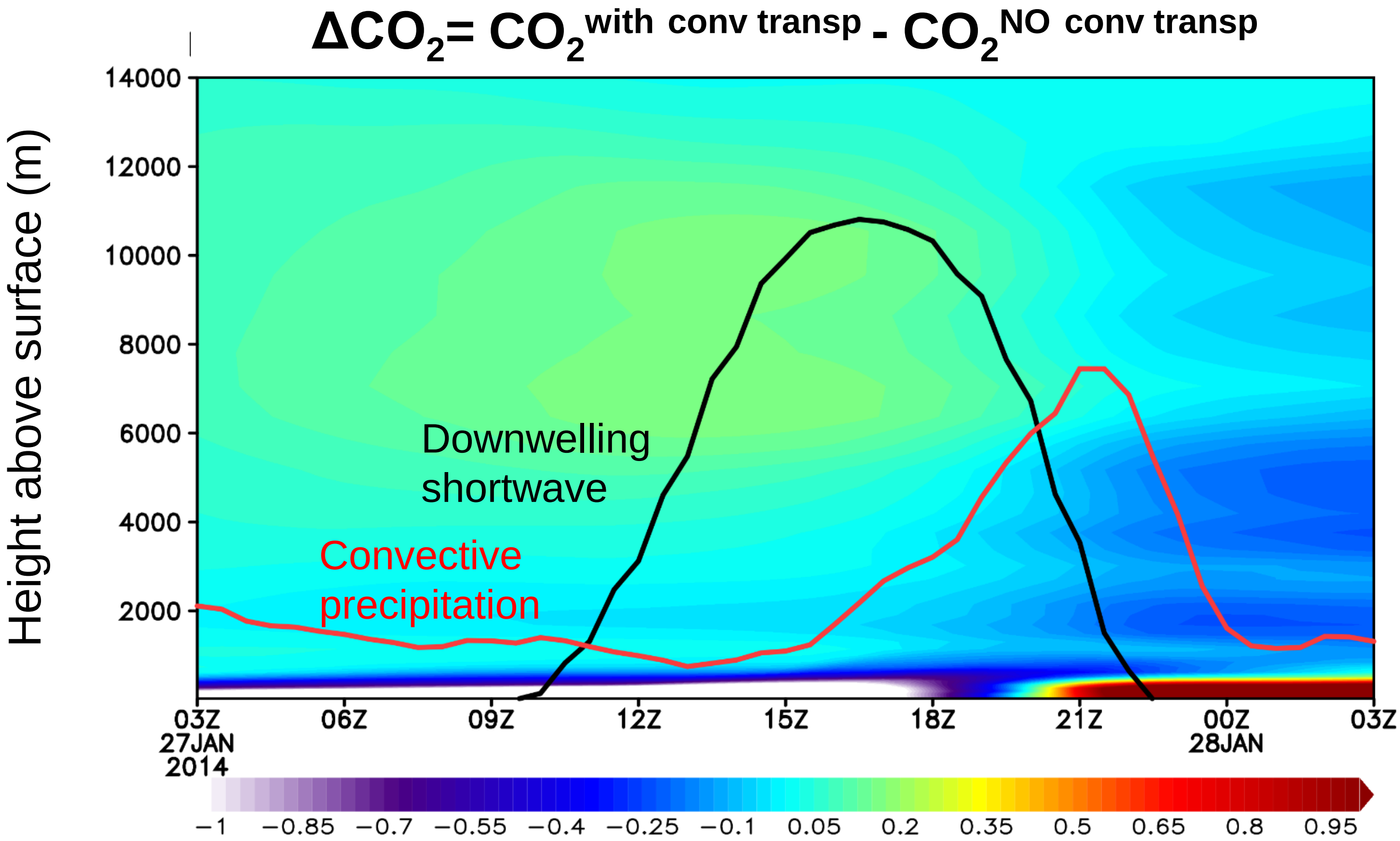
water vapor tendency



Better transition from shallow to deep convection

Bechtold et al., 2014 JAS.

Diurnal Cycle of the Precipitation over the Amazon and impacts on the convective transport of CO2



Convective scheme (in collaboration w/ G. Grell - NOAA/GSD) Scale-aware/Aerosol-aware

- **Stochastic approach adapted from the Grell-Devenyi (2002) scheme**
- **Deep and shallow (non-precipitating) plumes**
- **Scale awareness through Arakawa approach (2011) or spreading of subsidence.**

$$\overline{w\psi} - \bar{w}\bar{\psi} = (1-\sigma)^2(\overline{w\psi} - \bar{w}\bar{\psi})_{adj}$$

Eddy transport

Fractional area covered by active updraft and downdraft plumes.

Given by a conventional CP for a full adjustment to a quasi-equilibrium state

σ = f (entrainment rate), σ ➔ 1 when Δx➔ O (km)

- **Aerosol dependence (experimental) :**

Autoconversion rate: Berry formulation

$$\left(\frac{\partial r_{rain}}{\partial t}\right) = \frac{(\rho r_c)^2}{60\left(5 + \frac{0.0366\ CCN}{\rho r_c m}\right)}$$

Modified evaporation of raindrops (Jiang and Feingold, 2010) based on empirical relationship

$$PE \sim (I_1)^{\alpha_s - 1}(CCN)^{\zeta} = C_{pr}(I_1)^{\alpha_s - 1}(CCN)^{\zeta}$$

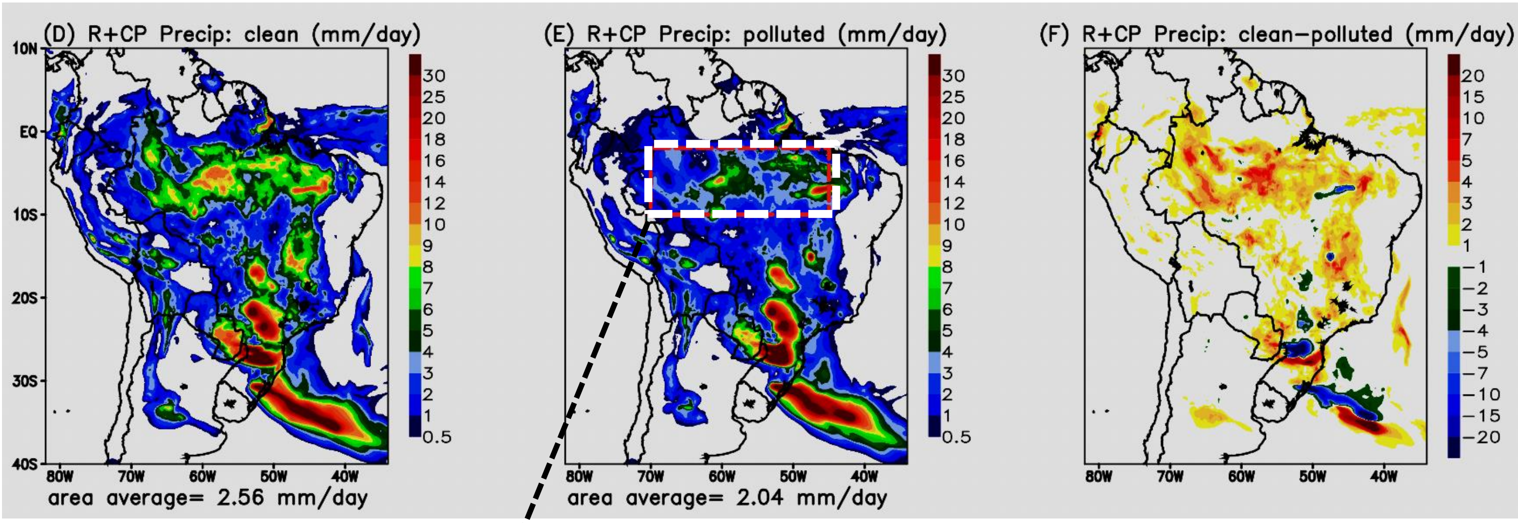
Proportionality between precipitation efficiency (**PE**) and total normalized condensate (**I_1**), requiring determination of the proportionality constant **C_{pr}**

- **Transport of momentum**
- **Convective (deep and shallow) transport of tracers, including scavenging**
- **Fully mass conservative, including water and tracers**
- **New closure from P. Bechtold et al (2014) => improved the diurnal cycle**

(Grell and Freitas, 2014, ACP)

BRAMS simulations for South America
clean / polluted – dx 20 km – 24h accumulated (mm)

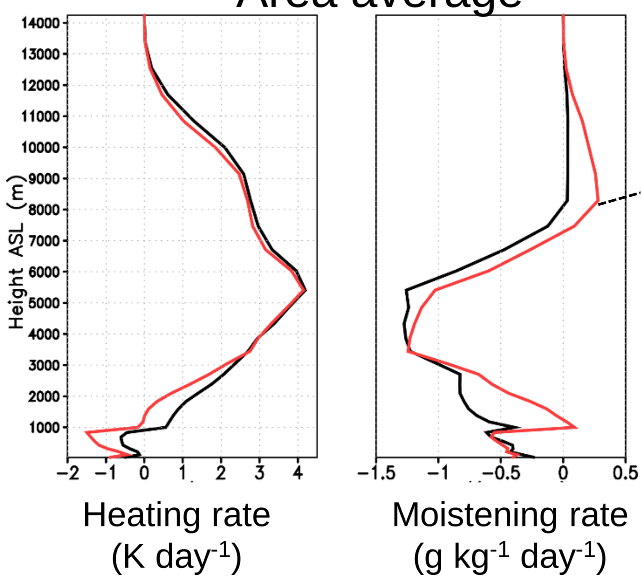
total rainfall: clean — **total rainfall: polluted** — **clean - polluted**



Area average

Clean:
CCN 150 cm^{-3}

Polluted
CCN 3000 cm^{-3}



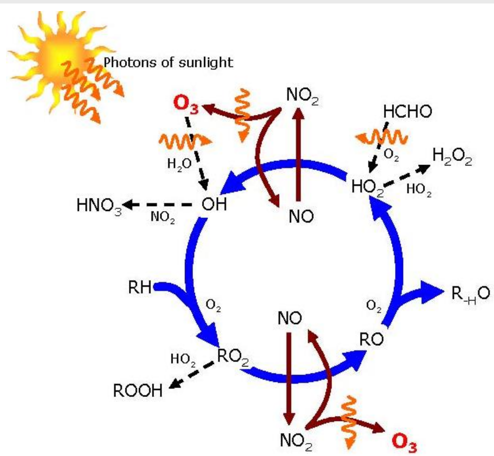
(Grell and Freitas, 2014, ACP)

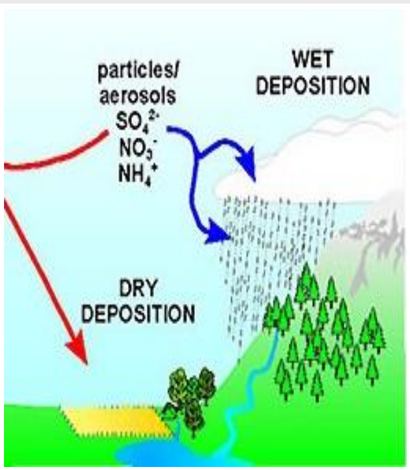
Mass continuity equation: the forcing term

$$\underbrace{\frac{\partial \bar{s}}{\partial t}}_{\text{mixing ratio tendency}} + \underbrace{\bar{u}_i \frac{\partial \bar{s}}{\partial x_i}}_{\text{grid-scale advection term}} = \underbrace{-\frac{1}{\rho_0}\left(\frac{\partial \rho_0 \overline{u_i' s'}}{\partial x_i}\right)}_{\text{sub-grid scale transport by the un-resolved flows}} + \underbrace{\overline{Q_s}}_{\text{forcing}}$$

$$\overline{Q_s} = E + PL + R$$

- E : emission (biomass burning, urban-industrial processes ...)
- PL : chemical reactions $\left(\frac{\text{photodissociation - kinetics}}{\text{homogeneous - heterogeneous}}\right)$
- R : sink (dry and wet deposition)



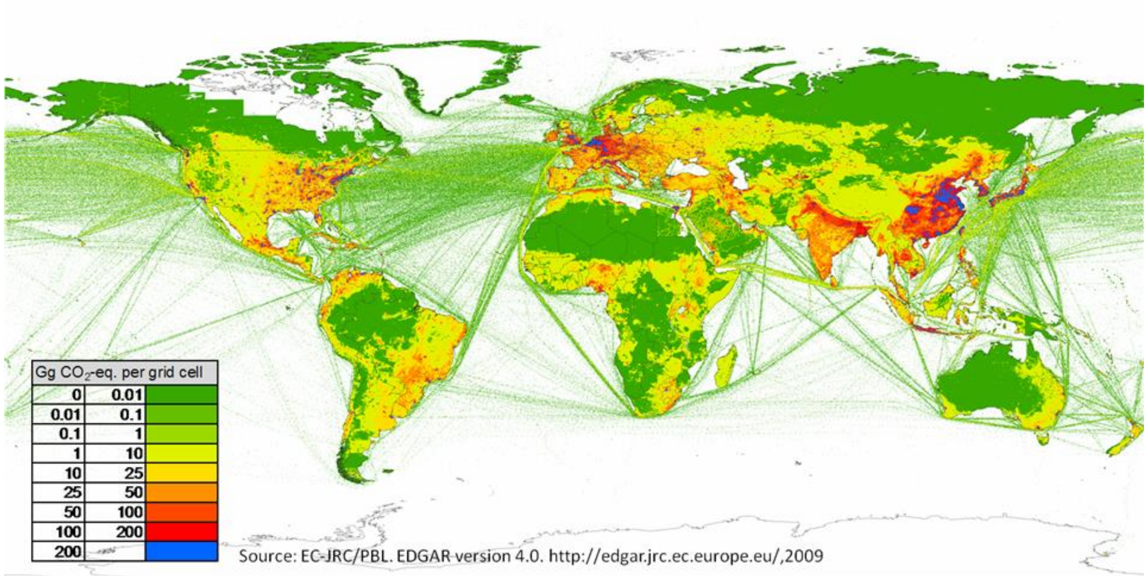


Including source emissions

- Anthropogenic sources (urban-industrial-transport)
- Biogenic
- Charcoal production, waste agric. burning
- Biomass burning
- Volcanoes
- Soil dust (mineral aerosol)
- Sea salt

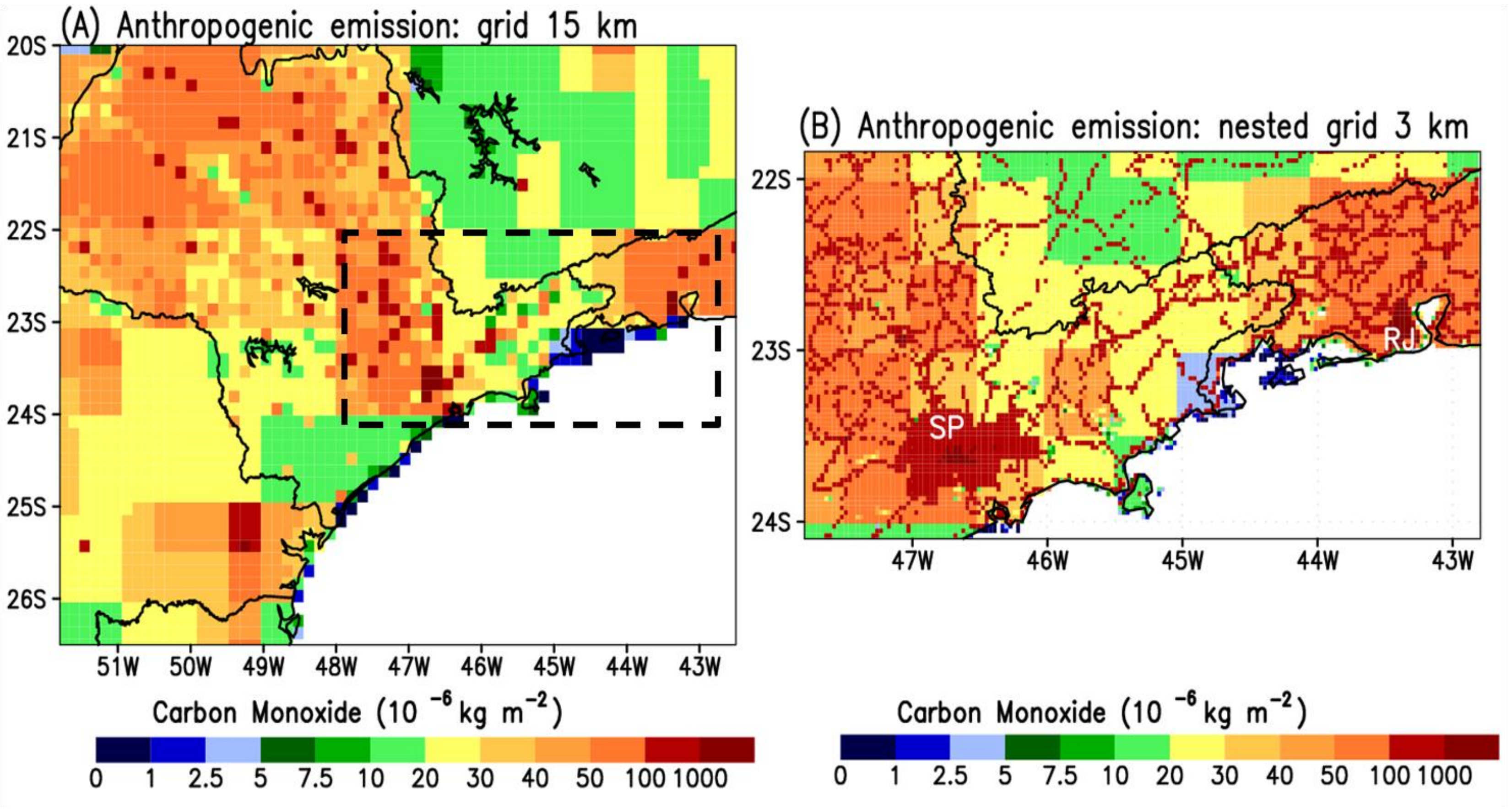
Anthropogenic sources - global inventories:
Emissions Database for Global Atmospheric Research (EDGAR)

1970-2005
1x1, 0.5x0.5, 0.1x0.1 degree
Species:
1. CO
2. NOX
3. CO2
4. CH4
5. SO2
6. N2O
7. SF6
8. NMVOC



http://edgar.jrc.ec.europa.eu/index.php

Global - Regional – Local Emissions Inventories



Including emissions in the model

urban-industrial-transportation (land-ocean)
charcoal prduction, wast agric. burning
biogenic

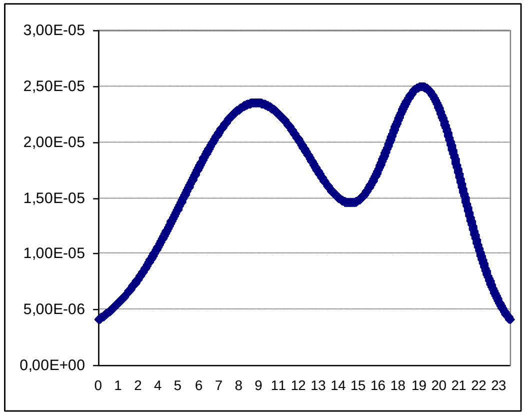
$\Rightarrow$ surface emission

emission flux: F_η, units: $kg[\eta]\,m^{-2}$

source term (mass mixing ratio): $E_\eta = \dfrac{F_\eta}{\rho_{air}\Delta z_{\text{first phys. model layer}}}$, units: $\left(\dfrac{kg[\eta]}{kg[air]}\right)$

Diurnal cycle of the urban emission:

$r(t)$



Time

mass mixing ratio tendency:

$E_\eta(t) = r(t) E_\eta$, units: $\left(\dfrac{kg[\eta]}{kg[air]\,s}\right)$

Biomass Burning Emissions

- Fundamental reaction and primary emissions:

$$[CH_2O]+O_2 \rightarrow CO_2+H_2O+heat$$

- Secondary emissions: CO, NO_x, hydrocarbons (CH_4, e.g.), particulate material, etc.

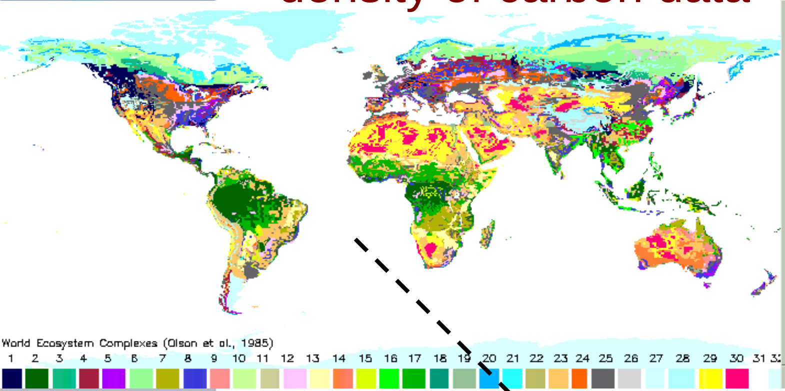
- Greenhouse gases: CO_2, N_2O, CH_4

- CO is an ozone precursor.

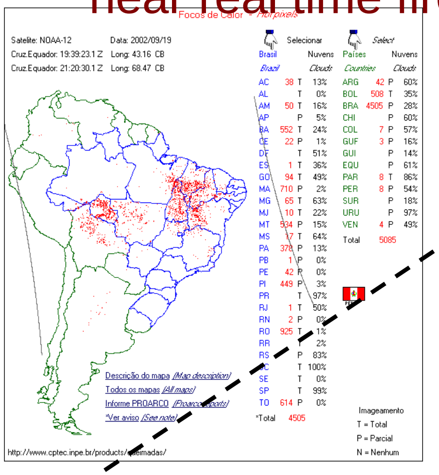
- Particulate material has also radiative and microphysics effects with potential impact on the hydrological cycle.

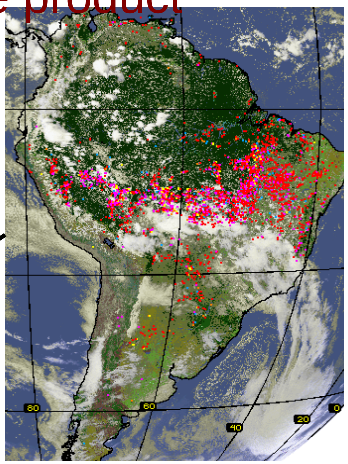
Biomass burning emissions inventory: regional scale - daily basis

density of carbon data

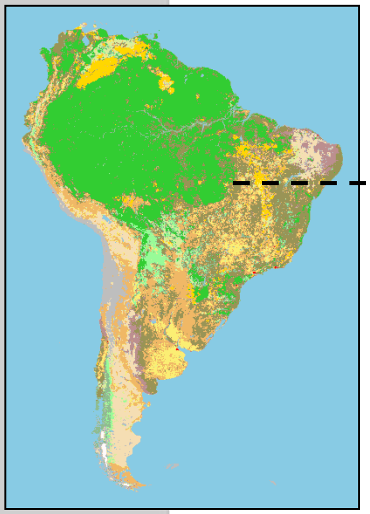


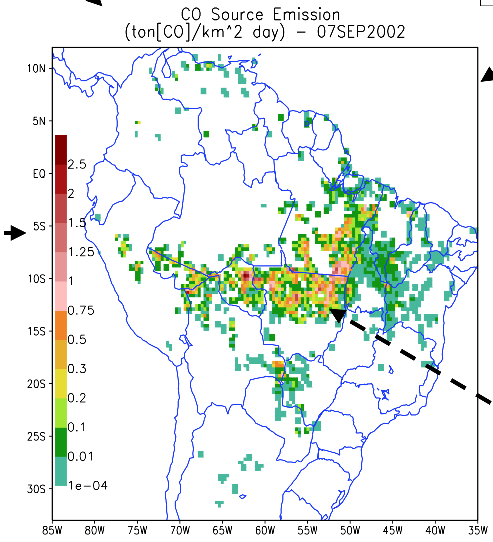
near real time fire product





land use data





emission & combustion factors

Biome category	Emission Factor for CO (g/kg)	Emission Factor for PM2.5 (g/kg)	Aboveground biomass density (α, kg/m²)	Combustion factor (β, fraction)
Tropical forest[1]	110.	8.3	20.7	0.48
South America savanna[2]	63.	4.4	0.9	0.78
Pasture[3]	49.	2.1	0.7	1.00

[1] Average values for primary and second-growth tropical forests, [2] Average values for campo cerrado (C3) and cerrado sensu stricto (C4), [3] value for campo limpo (C1). All numbers are from Ward et al.,

mass estimation

$$M_{[h]} = a_{veg} . b_{veg} . E_{f_{veg}}^{[h]} . a_{fire} ,$$

CO source emission (kg m^{-2}day^{-1})

Using the Fire Radiative Power (FRP) to estimate fire emissions (the up-down approach)

Boreal forest (USA)

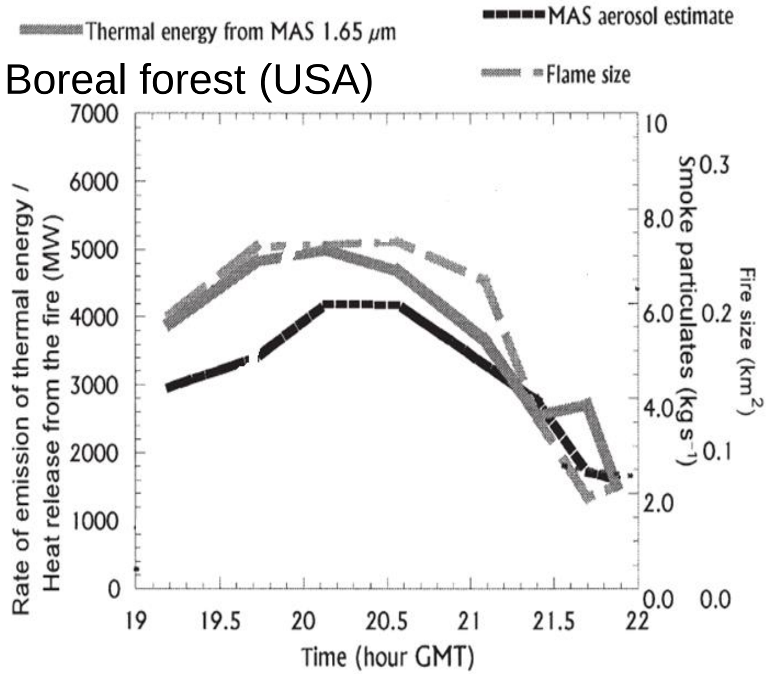
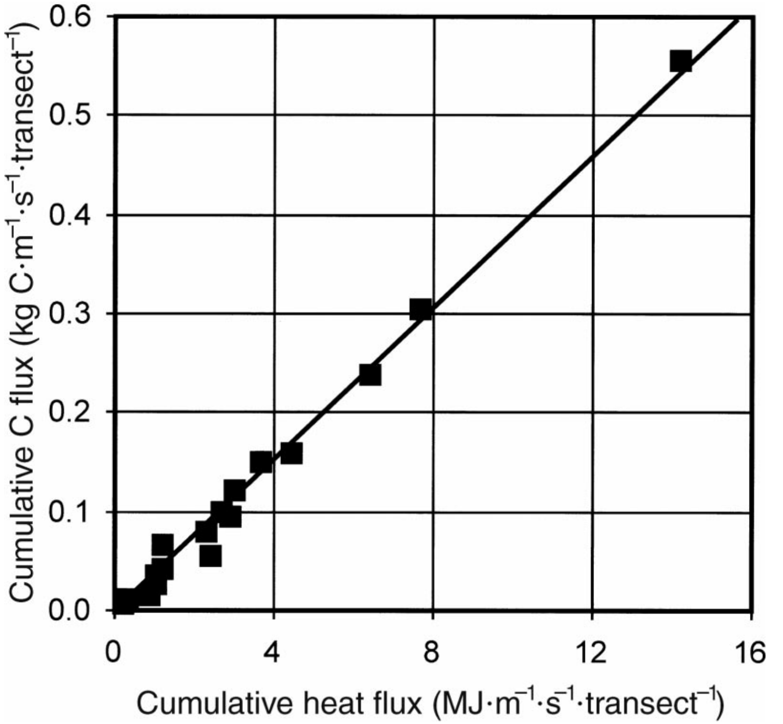


Figure 1. Relationship between the rate of emission of thermal radiative energy and smoke particulates from a prescribed fire in Oregon in 1994, based on MODIS Airborne Simulator (MAS) measurements aboard the ER-2 aircraft.

Note the strong similarity between the time dependence of the rate of emission of radiative energy, the fire size and the rate of emission of smoke as obtained from the remote sensing data (after Kaufman *et al.* 1998a).

Adapted from Kaufman et al., 1998

Carbon flux X sensible heat flux from fire

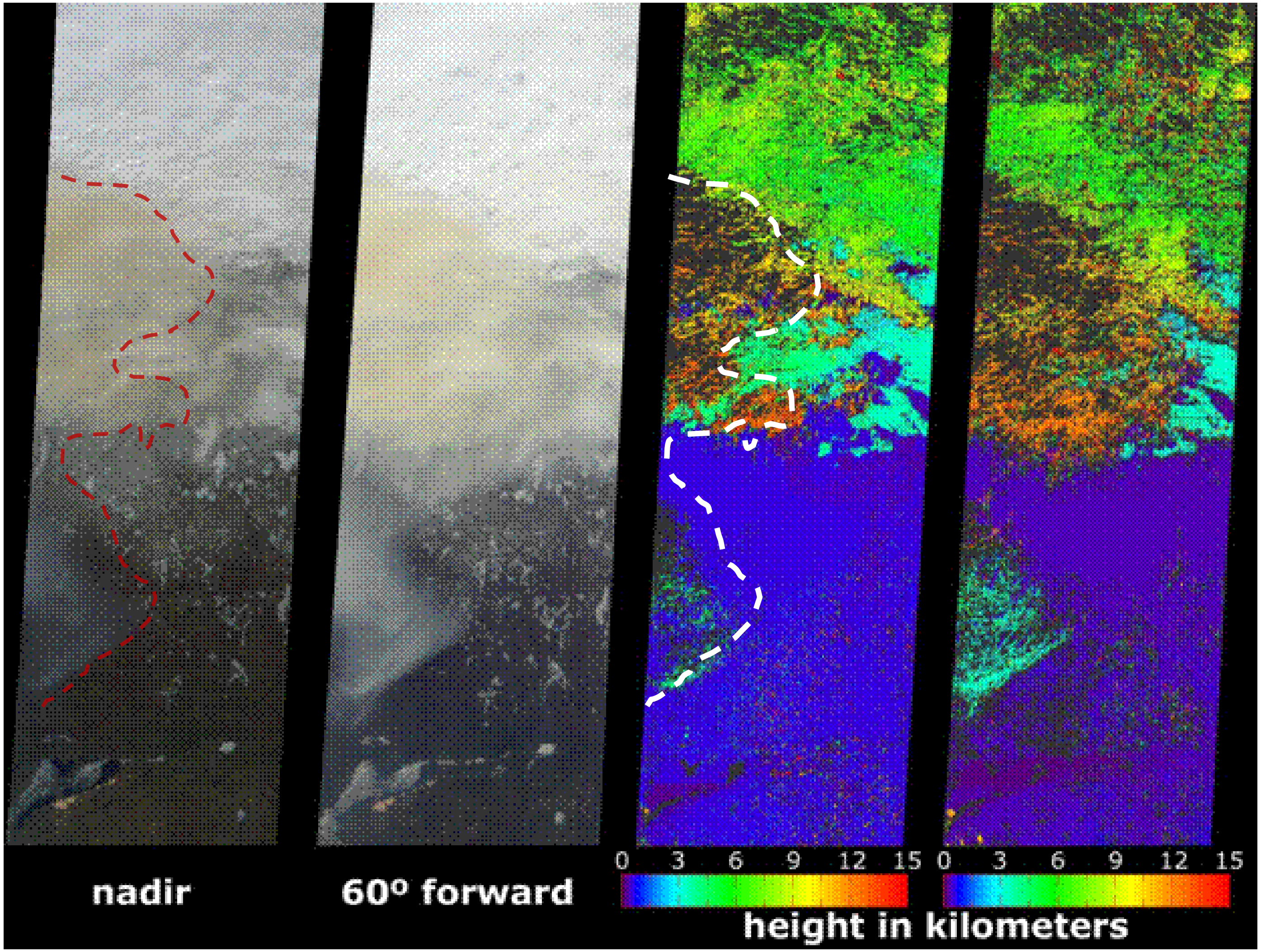


Tropical forest and cerrado area (Brazil)

Adapted from Riggan et al., 2004

Smoke plume rise in the lower troposphere

Smoke injected into the upper troposphere and lower stratosphere: the Chisholm forest fire case



Chisholm forest fire (May 23, 2001, Canada) provides confirming evidence that dense smoke can reach the upper troposphere and lower stratosphere. Source: Multi-angle Imaging SpectroRadiometer (MISR), JPL.

How to determine the actual height of the injection layer associated with the plume rise from vegetation fires ?

Deforestation fires in Rondônia, Brazil, 2002

Plume-rise of vegetation fires due to the strong initial buoyancy produced by the combustion process.

How to include this sub-grid scale transport \in large scale models?

A simple way:

$$Q = \frac{hbA}{\Delta t} \begin{cases} h = 15500\sim20000\text{kJ/kg} \\ b = \text{biomass burned} \\ A = \text{burned area} \\ \Delta t = \text{duration of the fire(flaming phase)} \end{cases}$$

$$E_c = (0.4 - 0.8)Q \quad \text{(McCarter\&Brido, 1965)}$$

use Manins (1985) formula (stably stratified atmosphere):

$$z = 1434(E_c)^{1/4} \begin{cases} E_c \text{ in gigaWatts} \\ z \text{ in meters} \end{cases}$$

How to include this sub-grid scale transport in large scale models?

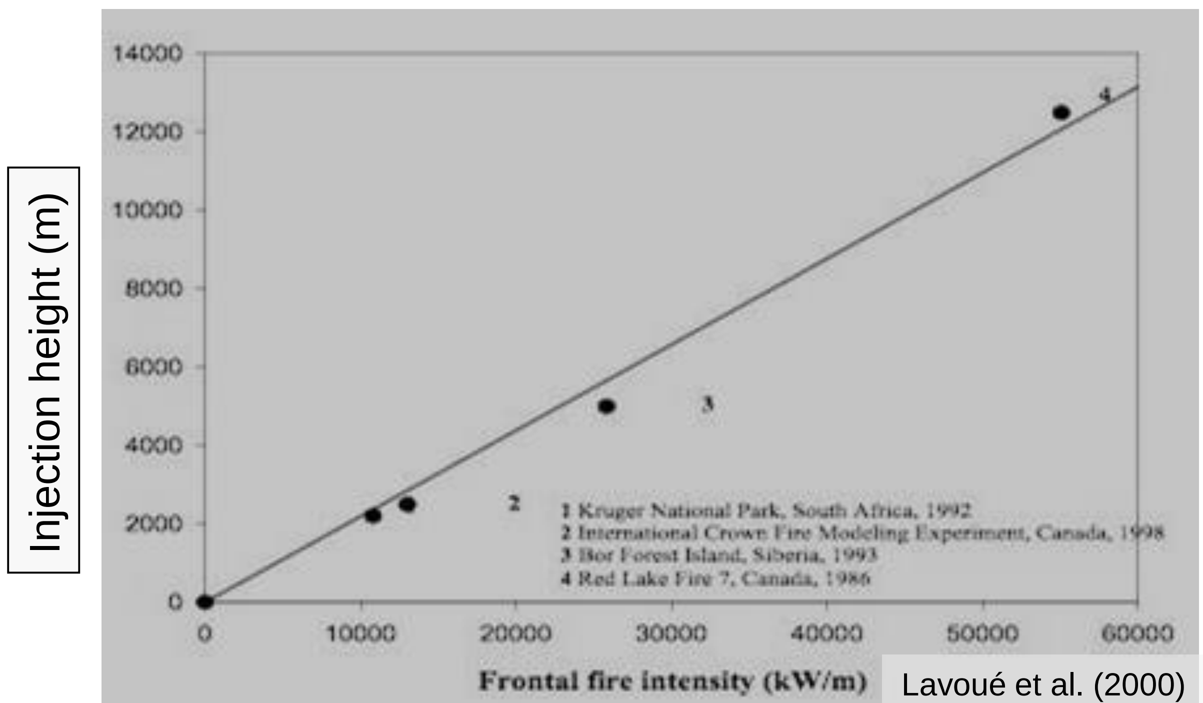
Another way:

Injection height in terms of the frontal fire intensity: ***Fi = H w r***

where:

- H is the combustion heat of the fuel
- w is the rate of fuel consumption
- r is the rate of fire propagation.

Lavoué et al. (2000) proposes the following relationship between the fire intensity and the injection height for boreal forest : ***InjectionH=0.23 Fi***

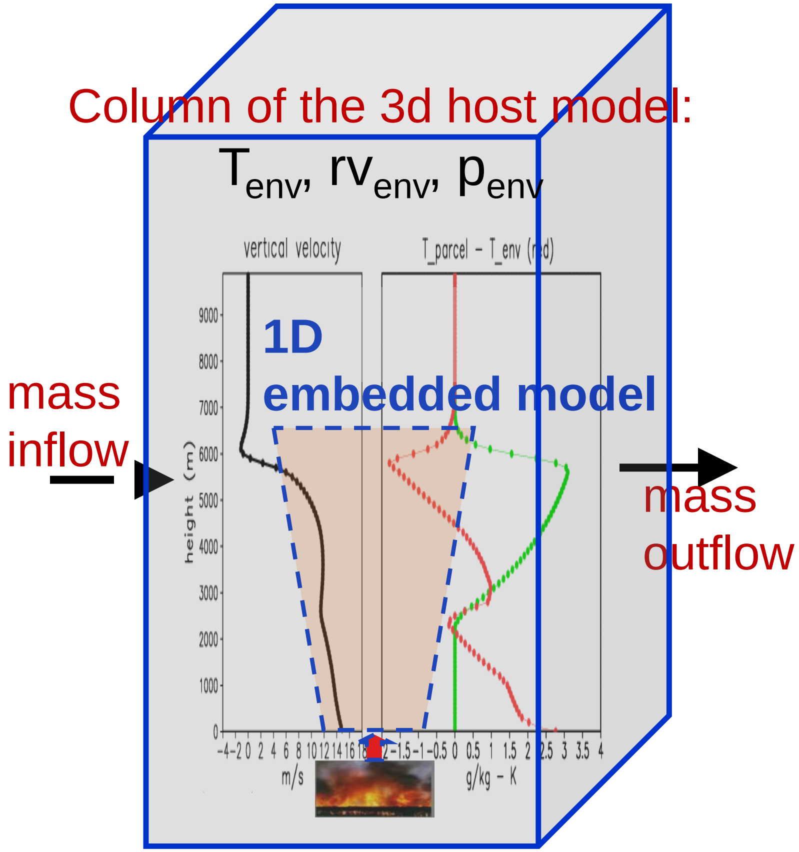


Lavoué et al. (2000)

How to include this sub-grid transport in large scale models?

1D cloud model (CM)

- Use a 1D CM embedded in each column of the large-scale atmospheric-chemistry transport model;
- Each grid box with fires, pass the large-scale condition of the host model to the 1D CM and the Morton et al. (1956) lower boundary condition for the vertical velocity and temperature excess of the in-plume air parcels;
- Resolve explicitly the motion of the plume;
- Return to the host model with the final rise of the plume (or the injection layer);
- Take account final rise of the plume at the source emission, releasing material emitted at flaming phase at this layer.



Cartoon describing the methodology

The 1-d in-line cloud model: governing equations

- W equation
- U equation
- 1st thermod law
- water vapor conservation
- cloud water conservation
- rain/ice conservation
- equation for plume size

$$\frac{\partial w}{\partial t}+w\frac{\partial w}{\partial z}=\gamma gB-\frac{2\alpha}{R}w^2-\delta_{entr}w$$

$$\frac{\partial u}{\partial t}+w\frac{\partial u}{\partial z}=-\frac{2\alpha}{R}|w|(u-u_e)-\delta_{entr}(u-u_e)$$

$$\frac{\partial T}{\partial t}+w\frac{\partial T}{\partial z}=-w\frac{g}{c_p}-\frac{2\alpha}{R}|w|(T-T_e)+\left(\frac{\partial T}{\partial t}\right)_{\substack{micro-\\physics}}-\delta_{entr}(T-T_e)$$

$$\frac{\partial r_v}{\partial t}+w\frac{\partial r_v}{\partial z}=-\frac{2\alpha}{R}|w|(r_v-r_{ve})+\left(\frac{\partial r_v}{\partial t}\right)_{\substack{micro-\\physics}}-\delta_{entr}(r_v-r_{ve})$$

$$\frac{\partial r_c}{\partial t}+w\frac{\partial r_c}{\partial z}=-\frac{2\alpha}{R}|w|r_c+\left(\frac{\partial r_c}{\partial t}\right)_{\substack{micro-\\physics}}-\delta_{entr}r_c$$

$$\frac{\partial r_{ice,rain}}{\partial t}+w\frac{\partial r_{ice,rain}}{\partial z}=-\frac{2\alpha}{R}|w|r_{ice,rain}+\left(\frac{\partial r_{ice,rain}}{\partial t}\right)_{\substack{micro-\\physics}}+\text{sedim}-\delta_{entr}r_{ice,rain}$$

$$\frac{\partial R}{\partial t}+w\frac{\partial R}{\partial z}=+\frac{6\alpha}{5R}|w|R+\frac{1}{2}\delta_{entr}R$$

$$\left(\frac{\partial \xi}{\partial t}\right)_{\substack{micro-\\physics}}\quad(\xi=T,r_v,r_c,r_{rain},r_{ice}),\ \text{sedim}\left\{\begin{array}{l}\textit{bulk microphysics:}\\ \textit{Kessler, 1969; Berry, 1967}\\ \textit{Ogura \& Takahashi, 1971}\end{array}\right.$$

The lower boundary condition

$$F=\frac{g\Re}{\pi c_p}\frac{E}{p_e}A$$ buoyancy flux

$$R=\frac{6\alpha}{5}z$$ plume radius

The closure

A º plume area » instantaneous fire size

E º convective energy from fire (Wm^{-2})

E @0.4 - 0.8 X_{flux} (McCarter & Broido, 1965)

X_{flux} (heat flux) - from FRP (MODIS, GOES, etc)

Freitas et al., GRL 2006, ACP 2007, 2010, Paugam et al., ACPD 2015

Including plume rise sub-grid scale transport in low resolution atmospheric models

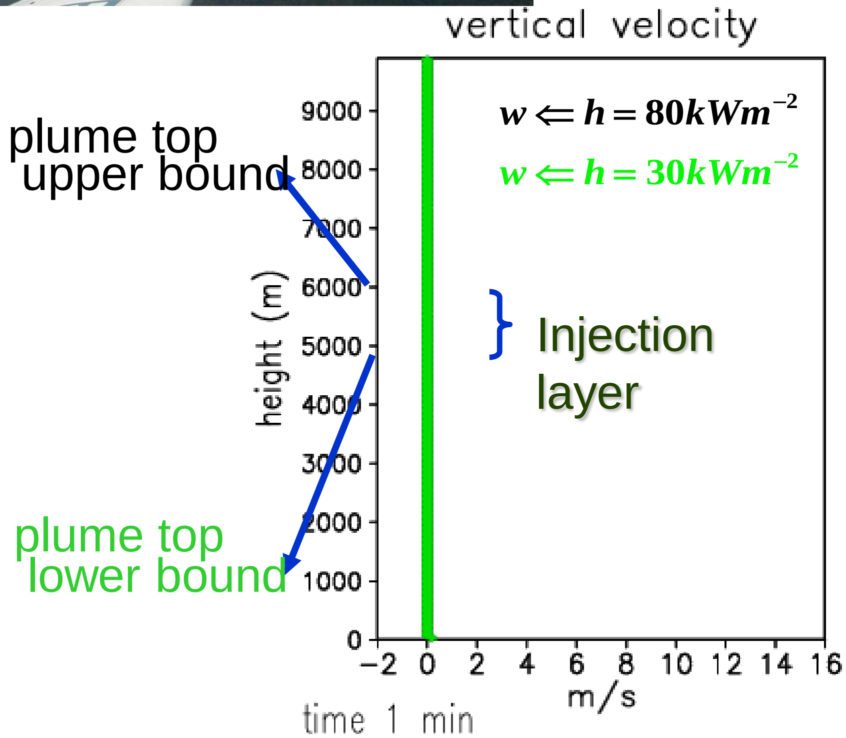
1D in-line cloud model for vegetation fires

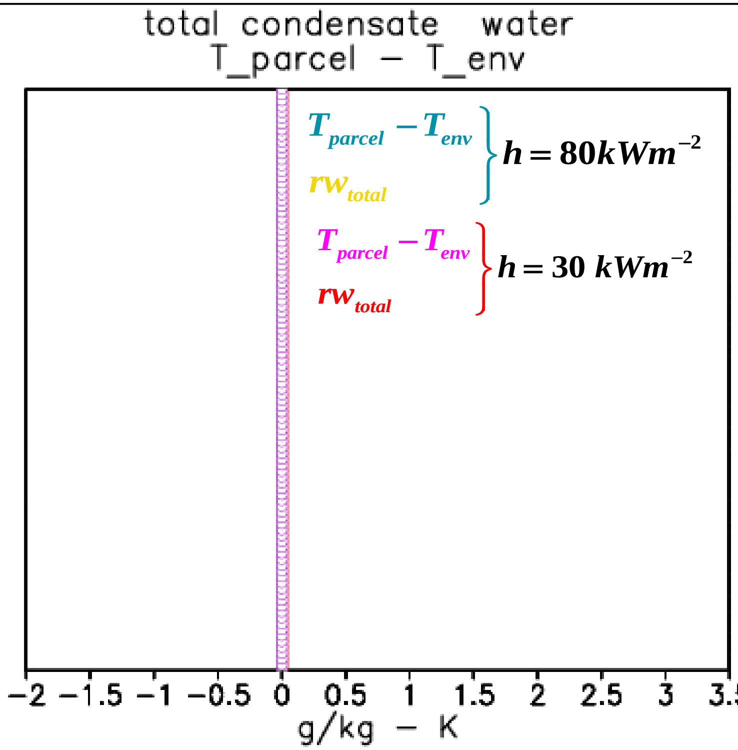
Biome: Forest

Time duration: 50 mn

Fire size: 20 ha

Heat flux: 80 kWm^{-2} / 30 kWm^{-2}





Freitas et al., ACP 2007

Including emission in the model

Biomass burning and wildfires:

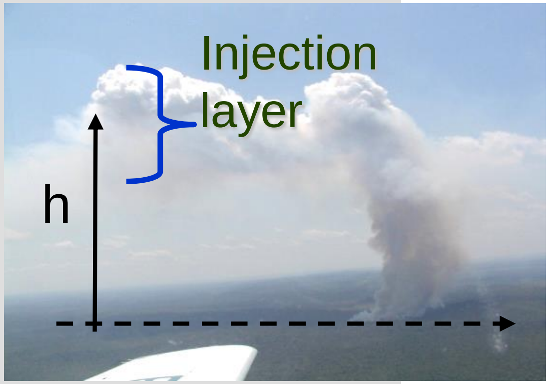
- Smoldering : mostly surface emission.
- Flaming: mostly direct injection in the PBL, free troposphere or stratosphere.

Plume rise model

total emission flux: F_η being λ the smoldering fraction

smoldering term : $$E_\eta = \frac{\lambda F_\eta}{\rho_{air} \Delta z_{\text{first phys. model layer}}}$$

flaming term : $$E_\eta = \frac{(1-\lambda) F_\eta}{\rho_{air} \Delta z_{\text{injection layer}}}$$

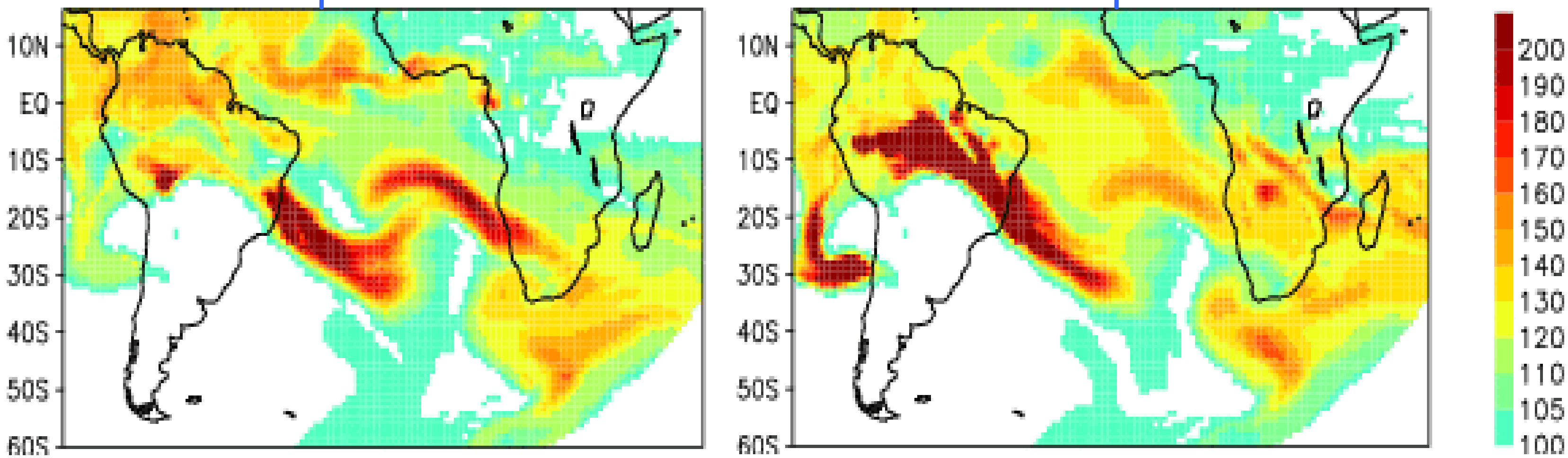


CATT-BRAMS comparison with AIRS 500 hPa CO

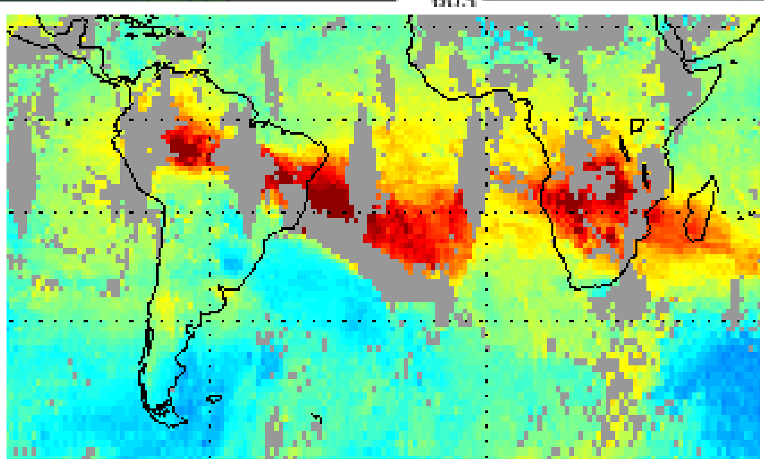
Model CO (ppbv) at ~5.8 km

without plume rise

with plume rise

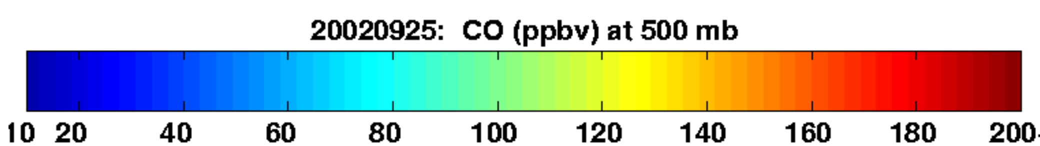


25 SEP 2002



CO (ppbv) from

AIRS at 500 hPa



In-line 1D pyro-cloud to estimate the injection layer

- Advantages:
  - Physical based formulation
  - Uses the actual atmospheric stability (hourly, diurnal, seasonal variability)
  - Includes the ambient wind interaction with the smoke plume (dilution, momentum exchange, bent-over)
  - Account for the cloud microphysics additional buoyancy (increase the final height)
- Disadvantages or requirements
  - Needs fire size***
  - Needs heat flux from fire***

*** some groups (INPE, King's College, e.g.) are working on getting remote sensing data to supply these information.

We did not talk about

- Dry and wet deposition
- Aerosols sedimentation
- Aerosols microphysics
- Chemical reactions (kinetic, photolysis)
- Volcanic, sea salt, dust emissions

- More lectures about these processes at
http://meioambiente.cptec.inpe.br/

Evaluating Aerosols Impacts on Numerical Weather Prediction: a WGNE/WMO initiative

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With inputs from: Mauricio Zarzur, Arlindo Silva, Angela Benedetti, Georg Grell, Oriol Jorba, Morad Mokhtari, Samuel Remy and WGNE Members Participants

Working Group on Numerical Experimentation (WGNE)
https://www.wmo.int/pages/about/sec/rescrosscut/resdept_wgne.html

Goals of the Exercise

- This project aims to improve our understanding about the following questions:

- How important are aerosols for predicting the physical system (NWP, seasonal, climate) as distinct from predicting the aerosols themselves?

- How important is atmospheric model quality for air quality forecasting?

- What are the current capabilities of NWP models to simulate aerosol impacts on weather prediction?

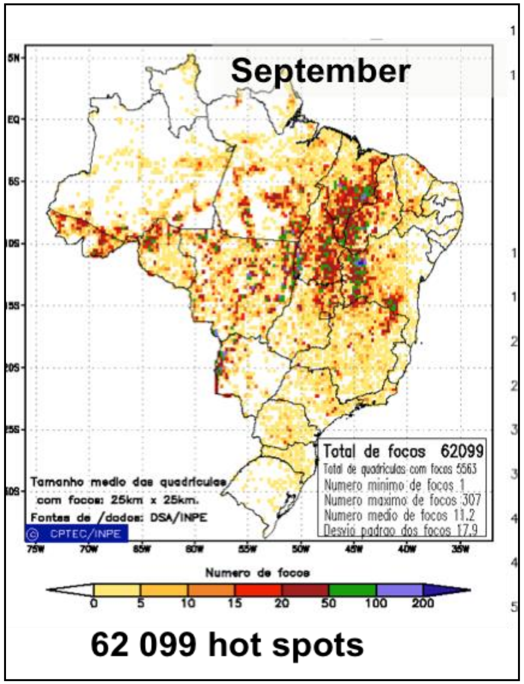
Protocol: Experiments

Experiment	Direct Effect	Indirect Effect	No aerosol Interaction
1	X		
2		X	
3	X	X	
4			X

Case Studies

1) Dust over Egypt: 4/2012

2) Urban Pollution in China: 1/2013



3) Smoke in Brazil: 9/2012

Participants (8 centers)

Participants	Case 1	Case 2	Case 3	Type of model	Complexity level	People Involved
CPTEC/Brazil			X	R	aerosol direct effect only	Saulo Freitas,Karla Longo, Mauricio Zarzur,
JMA/Japan	X	X	X	G	ind, dir, ind+dir, no-aer	Taichu Tanaka, Chiasi Muroi
ECMWF/Europe	X	X	X	G	(aerosol direct effect only	Angela Benedetti, Samuel Remy, Jean-Noel Thepaut
Météo-France/Met. Serv. Algeria	X			R	aerosol direct effect only	Morad Mokhtari, Bouyssel Francois
ESRL/NOAA/USA		X	X	R	aerosol direct and indirect effect	Georg Grell
NASA/Goddard/USA	X	X	X	G	direct effect only	Arlindo da Silva
NCEP/USA	X	X	X	G	direct effect only	Sarah Lu, Yu-Tai Hou, S.Moorthi, and F. Yang
Barcelona Super. Ctr. Spain	X			R	aerosol direct effect only	Oriol Jorba Casellas

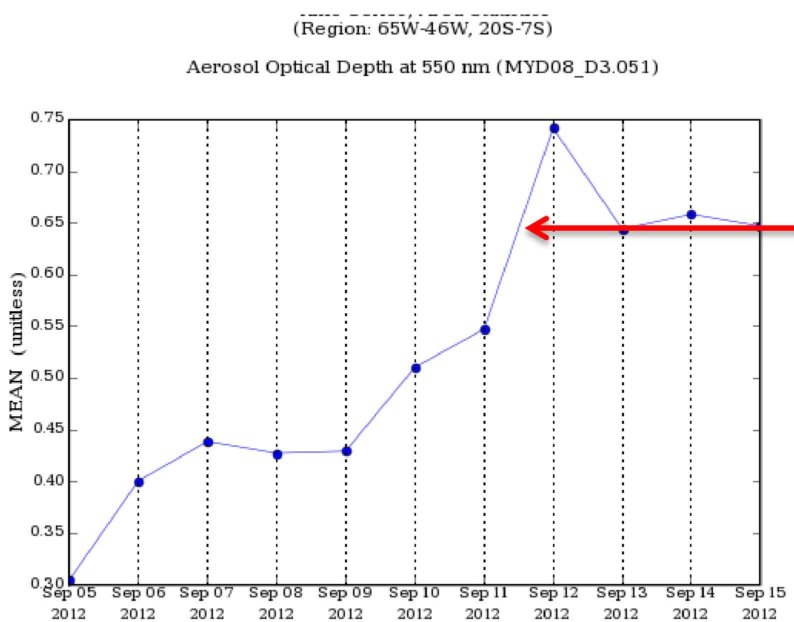
Case 3- Persistent Smoke in Brazil - SEP 2012

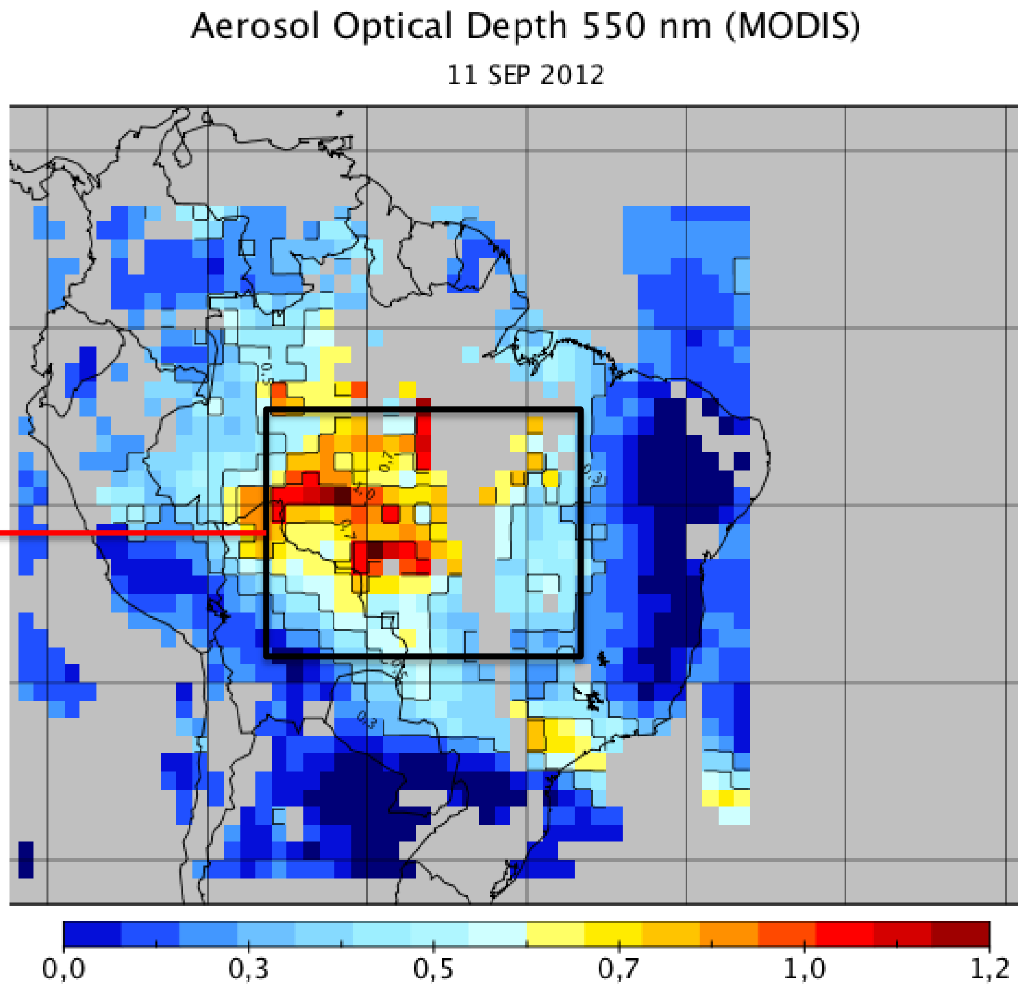
Forecasts

- September 5-15, 2012
- From 0 or 12 UTC
- 10 day forecasts

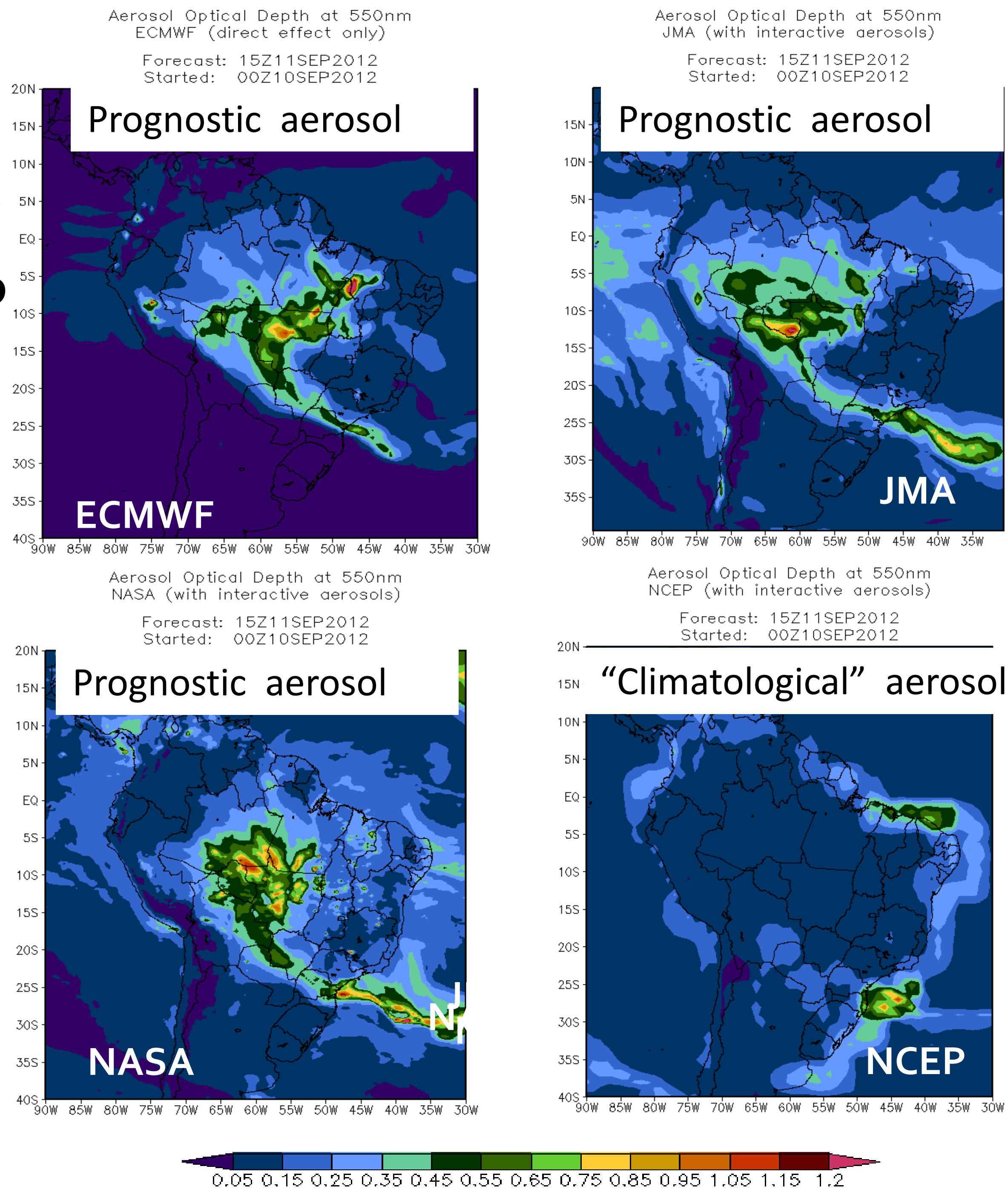
Model configuration: same as for NWP

Direct & Indirect effects





AOD at 550 nm
Fct.: 15UTC11SEP
Init.: 00UTC10SEP



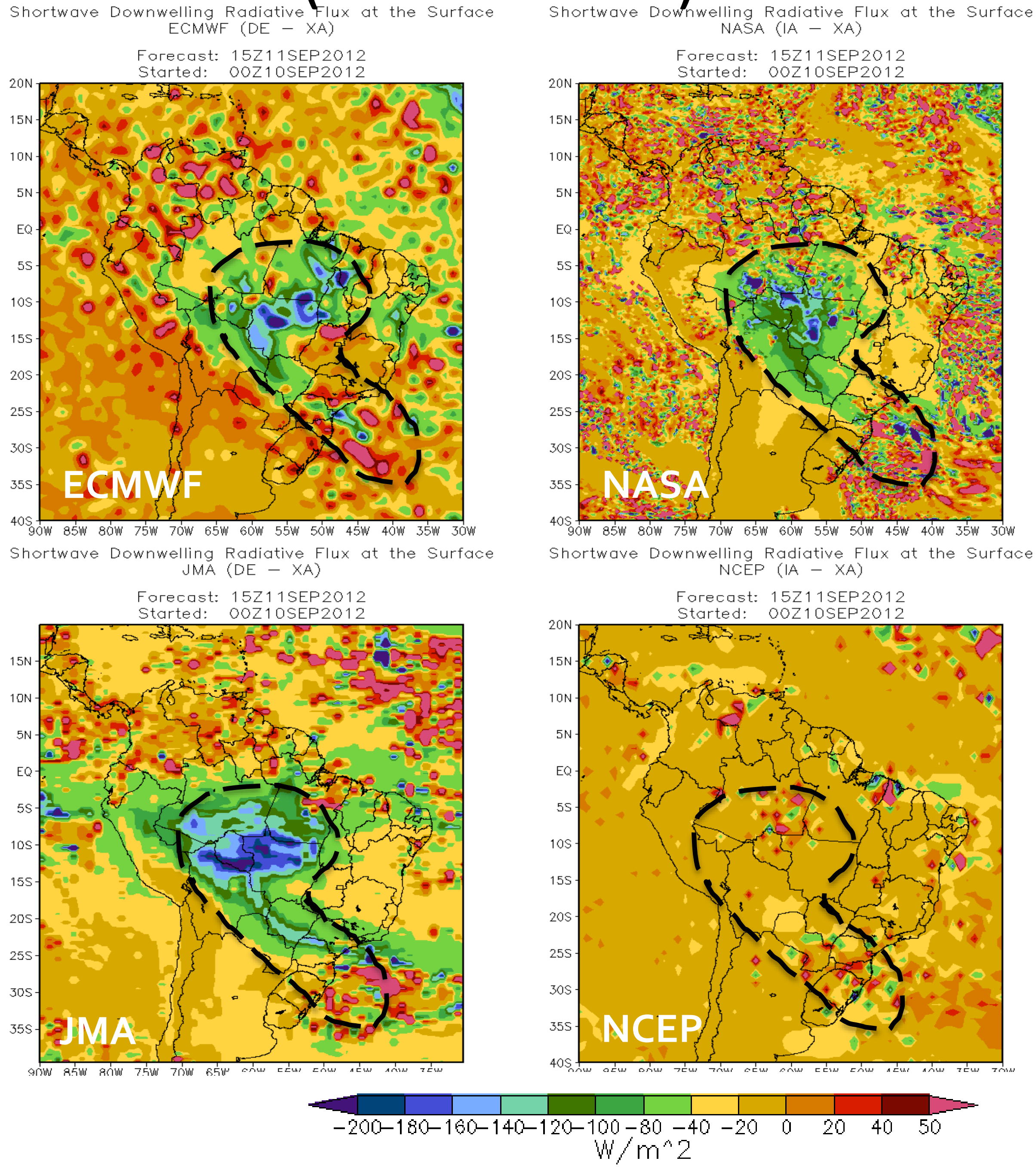
- **Similar prognostic aerosol distribution and AOD field.**
- **Climatological aerosol provides a completely unrealistic AOD field.**

SW Radiative Flux (AER-NOAER)

FCT.: 15UTC11SEP

Init.: 00UTC10SEP

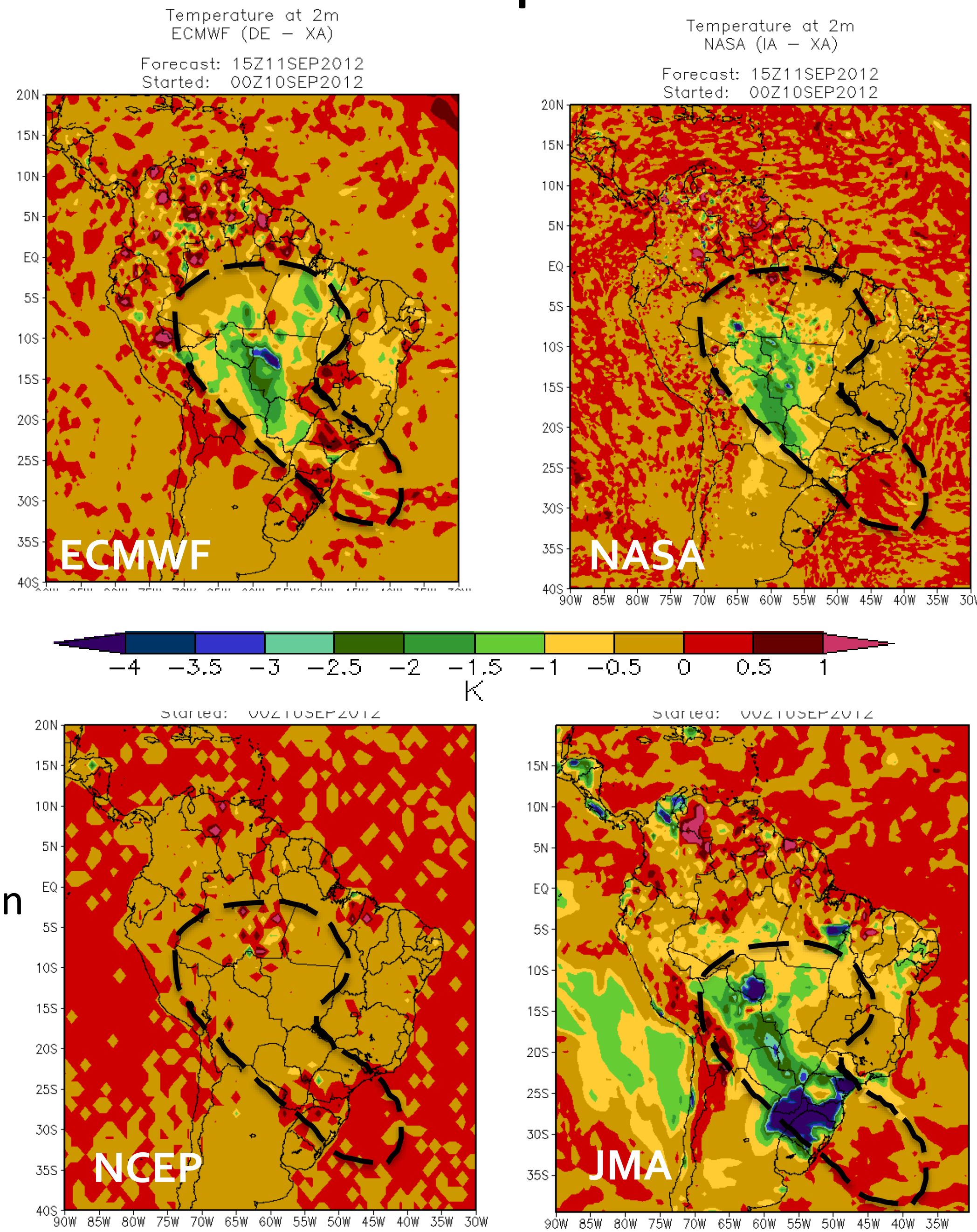
- Direct effect can produce a reduction of up to ~ 200 W/m^2 when applying prognostic aerosols.
- The use of climatological aerosols implies on much lower impact.



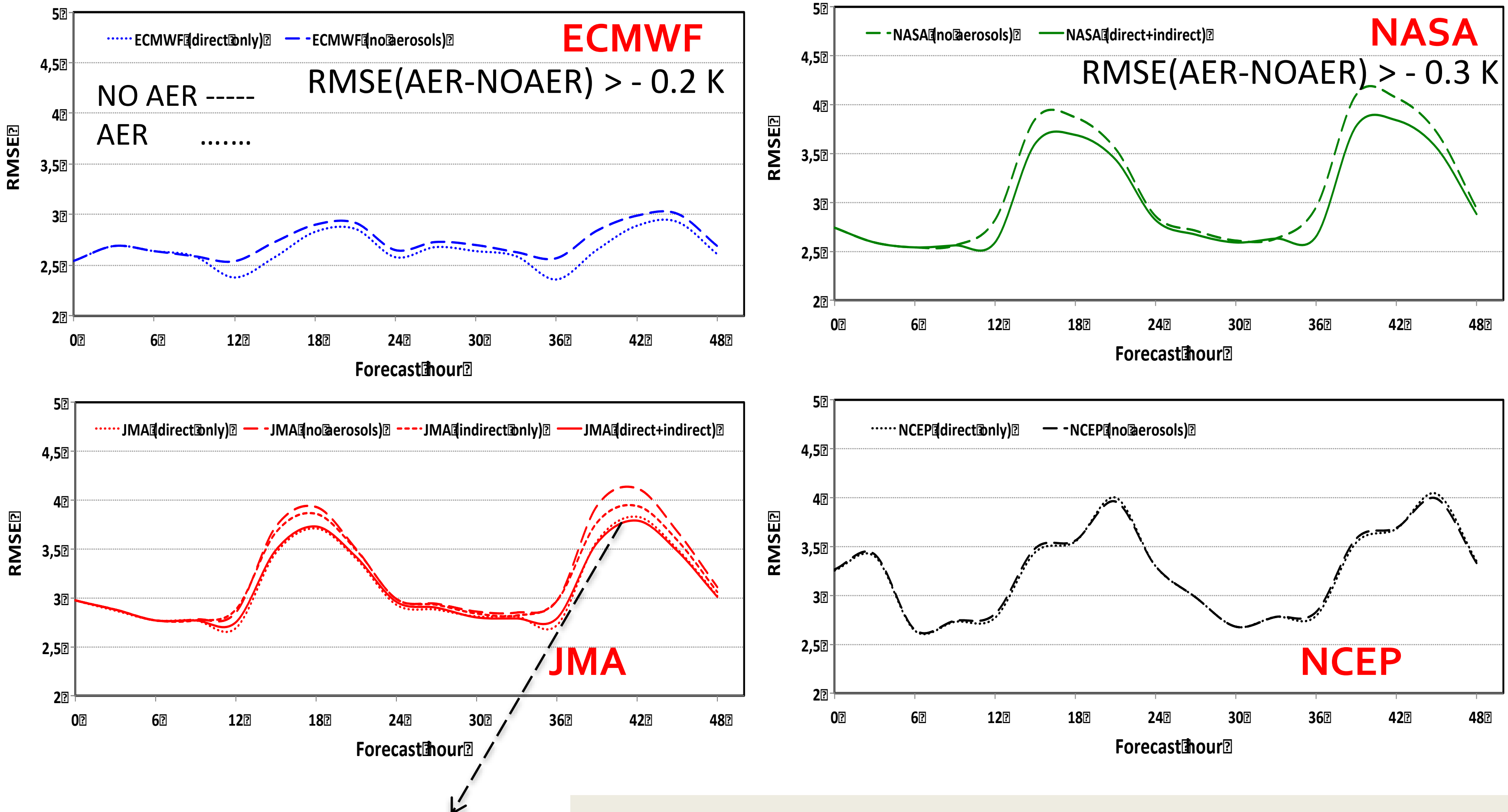
AER-NOAER : 2m Temperature

FCT.: 15UTC11SEP
Init.: 00UTC10SEP

- Direct effect can produce cooling of up to ~ 3.5 K when using prognostic aerosols
- Indirect effect can even produce larger reduction on T2m
- Use of climatological data implies in negligible impact.



RMSE: 2-m Temperature

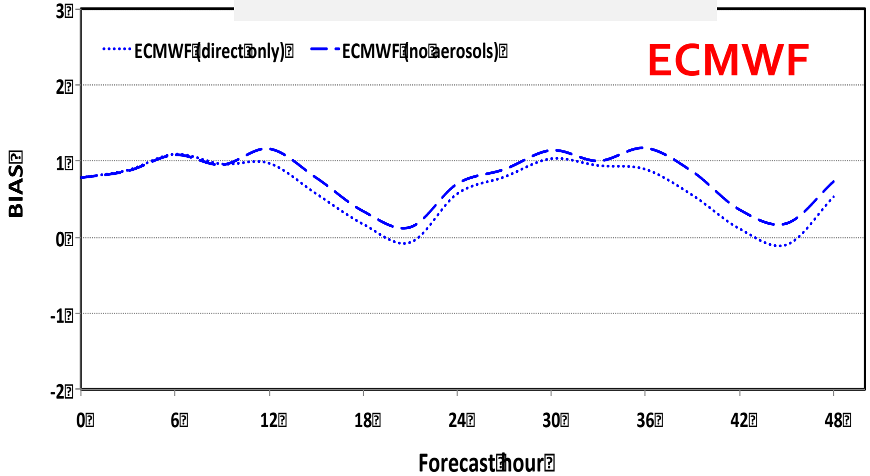


4.12 – no interaction
3.94 – indirect only
3.83 – direct only
3.79 – IND + DIR

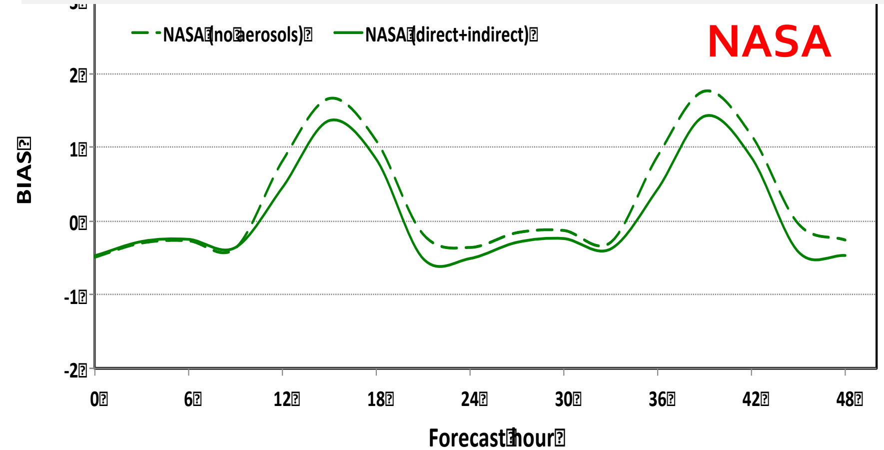
- ECMWF, NASA, JMA: Consistent and significative RMSE reduction
- NCEP : negligible change
- JMA : RMSE reduction increases with the aerosol treatment complexity

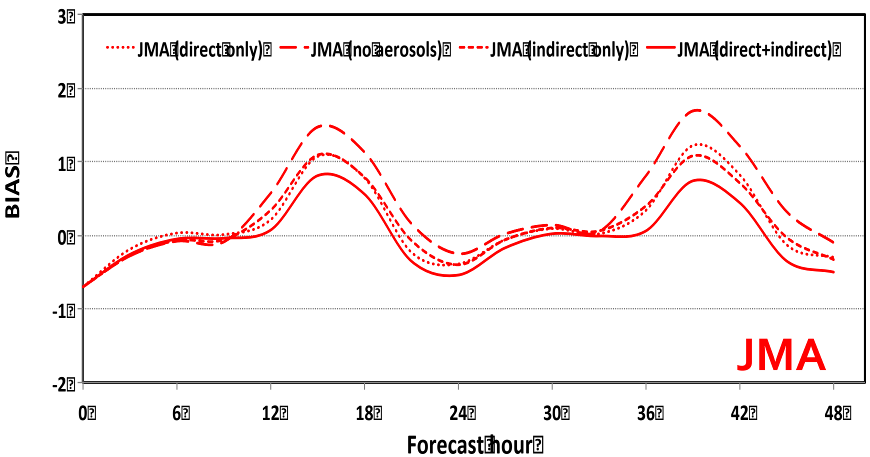
BIAS: 2m Temperature

Consistent bias reduction



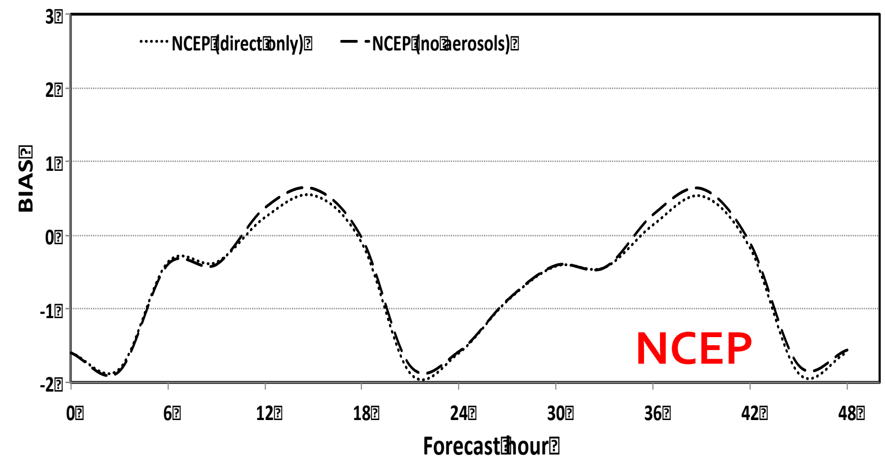
Bias decreases during the day, but increases* at night





Consistent bias reduction with increasing aerosol treatment complexity during the day, with a slight increase* during the night.

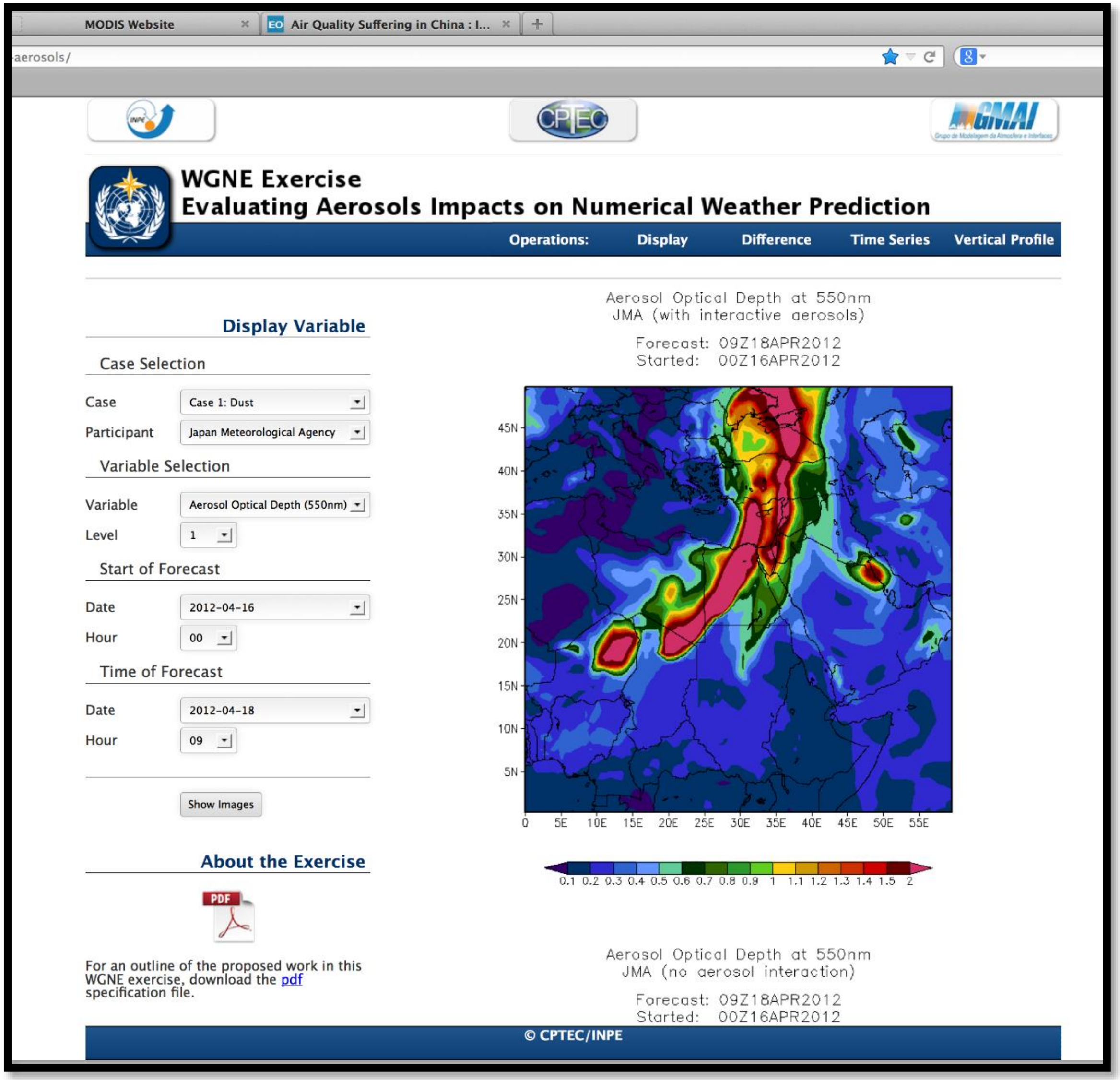
(*) Absolute value



Slight decrease of bias during 12-18 UTC

Analyzing the data with GrADS Online

Webpage hosted by CPTEC/Brazil for data analyzing and visualization
http://meioambiente.cptec.inpe.br/wgne-aerosols/



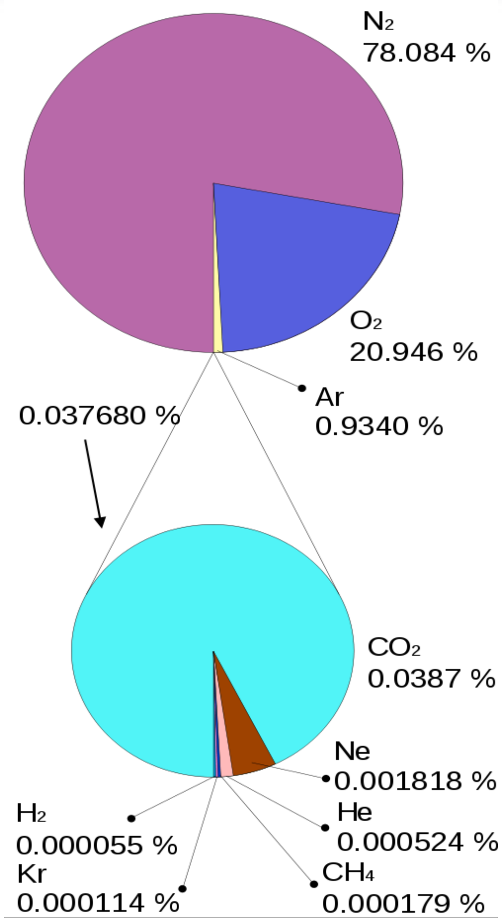
Developed by M. Zarzur

Thanks for your attention!
Questions ?

Background slides

Composition of dry atmosphere

Gas	Volume
Nitrogen (N_2)	780,840 ppmv (78.084%)
Oxygen (O_2)	209,460 ppmv (20.946%)
Argon (Ar)	9,340 ppmv (0.9340%)
Carbon dioxide (CO_2)	387 ppmv (0.0387%)
Neon (Ne)	18.18 ppmv (0.001818%)
Helium (He)	5.24 ppmv (0.000524%)
Methane (CH_4)	1.79 ppmv (0.000179%)
Krypton (Kr)	1.14 ppmv (0.000114%)
Hydrogen (H_2)	0.55 ppmv (0.000055%)
Nitrous oxide (N_2O)	0.3 ppmv (0.00003%)
Xenon (Xe)	0.09 ppmv ($9x10^{-6}$%)
Ozone (O_3)	0.0 to 0.07 ppmv (0% to $7x10^{-6}$%)
Nitrogen dioxide (NO_2)	0.02 ppmv ($2x10^{-6}$%)
Iodine (I)	0.01 ppmv ($1x10^{-6}$%)
Carbon monoxide (CO)	0.1 ppmv
Ammonia (NH_3)	trace
Not included in above dry atmosphere:	
Water vapor (H_2O)	~0.40% over full atmosphere, typically 1%-4% at surface



Composition of Earth's atmosphere as at Dec. 1987. The lower pie represents the trace gases which together compose 0.038% of the atmosphere. Values normalized for illustration.

Source: http://en.wikipedia.org/wiki/Atmosphere_of_Earth

Mass continuity equation:

Mathematically describes the dynamical and chemical processes that determine the distribution of chemical species.

Flux form: $\dfrac{\partial \rho_{[\eta]}}{\partial t} + \underbrace{\nabla \cdot (\rho_{[\eta]} \vec{v})} = Q_{[\eta]}$

transport — sources / sinks / chemical forcing

Advective form: $\dfrac{\partial s_{[\eta]}}{\partial t} + \overbrace{\vec{v} \cdot \nabla s_{[\eta]}} = \dfrac{Q_{[\eta]}}{\rho_a}$ **or** $\dfrac{ds_{[\eta]}}{dt} = \dfrac{Q_{[\eta]}}{\rho_a}$

where,

$\rho_{[\eta]}$ is the mass (or number) density of species η

ρ_a is the air mass (or number) density

$s_{[\eta]} = \dfrac{\rho_{[\eta]}}{\rho_a}$ is the mass (or volume) mixing ratio

$Q_{[\eta]}$ is the source (E) / sink (R) and / or chemical production / loss (P - L) rate of species η

$\vec{v}$ is the wind velocity vector

One important propertie: if $Q_\eta = 0 \Rightarrow$ no forcing

$\dfrac{ds_\eta}{dt} = 0 \Rightarrow s_\eta = cte \therefore$ following the air parcel (the Lagrangian point of view)

The Reynolds decomposition and averaging applied to the mass continuity equation of air: <u>the flux form</u> (1)

To solve numerically the mass continuity equation, it is convenient to perform the following decomposition:

$$\phi = \bar{\phi} + \phi''$$

where
$$\begin{cases} \bar{\phi} \text{ is the average of } \phi \text{ given by:} \\ \bar{\phi} = \dfrac{1}{\Delta t \Delta x \Delta y \Delta z} \displaystyle\int_t^{t+\Delta t} \int_x^{x+\Delta x} \int_y^{y+\Delta y} \int_z^{z+\Delta z} \phi \, dz\, dy\, dx\, dt, \\ \phi'' \text{ is the sub-grid scale perturbation,} \\ \Delta t \text{ is time interval of the average (or model timestep),} \\ \Delta x, \Delta y, \Delta z \text{ are the space interval of the average} \\ \text{(or model grid intervals).} \end{cases}$$

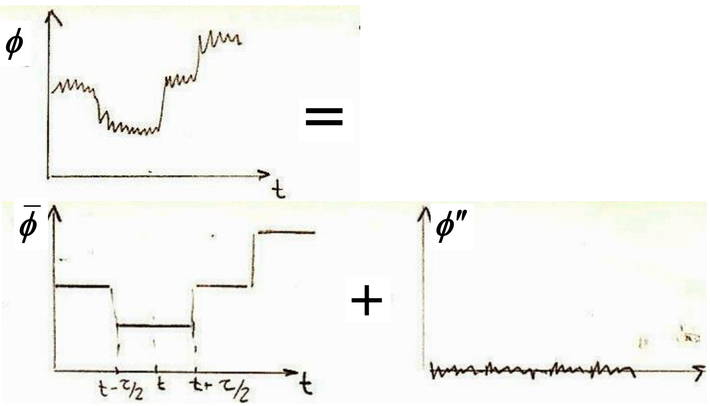
Some properties of the Reynolds average:

$$\begin{cases} \overline{\phi''} = 0 \\ \overline{\bar{\varphi}\phi''} = 0 \\ \overline{\varphi\phi} = \bar{\varphi}.\bar{\phi} + \overline{\phi''\varphi''}, \text{ and } \overline{\phi''\varphi''} \text{ is not necessarily zero.} \\ \overline{\dfrac{\partial \phi}{\partial \chi}} = \dfrac{\partial \bar{\phi}}{\partial \chi}, \text{ for } \chi \equiv x, y, z, t \end{cases}$$

From the air mass cont. equation: $\dfrac{\partial \rho}{\partial t} = -\dfrac{\partial (\rho u_i)}{\partial x_i}$

Applying the Reynolds decomposition: $\begin{cases} \rho = \bar{\rho} + \rho'' \\ u_i = \bar{u}_i + u_i'' \end{cases}$

$$\Rightarrow \frac{\partial(\bar{\rho} + \rho'')}{\partial t} = -\frac{\partial(\bar{\rho} + \rho'')(\bar{u}_i + u_i'')}{\partial x_i}$$



The Reynolds decomposition applied to the mass continuity equation of air: the flux form (2)

Performing the Reynolds average on the last equation:

$$\frac{\partial \overline{\bar{\rho}}}{\partial t} + \frac{\partial \overline{\rho''}}{\partial t} = -\frac{\partial \overline{\bar{\rho}\bar{u}_i}}{\partial x_i} - \frac{\partial \overline{\rho'' u_i''}}{\partial x_i} - \frac{\partial \overline{\rho'' \bar{u}_i}}{\partial x_i} - \frac{\partial \overline{\bar{\rho} u_i''}}{\partial x_i}$$

and, because $\overline{\phi''} \equiv 0$,

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \overline{\rho''}}{\partial t} = -\frac{\partial \bar{\rho}\bar{u}_i}{\partial x_i} - \frac{\partial \left(\overline{\rho'' u_i''}\right)}{\partial x_i} - \frac{\partial \overline{\rho''}\bar{u}_i}{\partial x_i} - \frac{\partial \bar{\rho}\overline{u''_i}}{\partial x_i}$$

Mass continuity eq. for air after Reynolds decomposition:

$$\therefore \underbrace{\frac{\partial \bar{\rho}}{\partial t}}_{\text{local tendency}} = -\underbrace{\frac{\partial \bar{\rho}\bar{u}_i}{\partial x_i}}_{\text{transport by the mean wind (advection)}} - \underbrace{\frac{\partial \overline{\rho'' u_i''}}{\partial x_i}}_{\text{sub-grid scale transport by the unresolved flows (diffusion, convection, etc.)}}$$

a) Deep continuity approximation: $\frac{\partial \rho_0 u_i}{\partial x_i} = 0$

Let $\bar{\rho} = \rho_0 + \rho' \Rightarrow \frac{\partial(\bar{\rho} - \rho')u_i}{\partial x_i} = 0$

Applying the Reynolds average: $\overline{\frac{\partial(\bar{\rho} - \rho')u_i}{\partial x_i}} = \frac{\partial\overline{(\bar{\rho} - \rho')u_i}}{\partial x_i} = 0$

$$\therefore \quad \frac{\partial \rho_0 u_i}{\partial x_i} \approx \frac{\partial \bar{\rho}\bar{u}_i}{\partial x_i} = 0$$

b) Shallow continuity approximation: $\frac{\partial u_i}{\partial x_i} = 0$

$$\therefore \quad \frac{\partial \bar{u}_i}{\partial x_i} = 0$$

For a tracer η:

$$\underbrace{\frac{\partial \bar{\rho}_\eta}{\partial t}}_{\text{local tendency}} = -\underbrace{\frac{\partial \bar{\rho}_\eta \bar{u}_i}{\partial x_i}}_{\text{transport by the mean wind (advection)}} - \underbrace{\frac{\partial \overline{\rho_\eta'' u_i''}}{\partial x_i}}_{\text{sub-grid scale transport by the unresolved flows (diffusion, convection. etc)}} + \underbrace{\bar{Q}_\eta}_{\text{the forcing (sources, sinks, deposition, chemistry)}}$$

The Reynolds decomposition applied to the mass continuity equation: the advective form

The mass continuity equation for air :

$$\frac{\partial\bar{\rho}}{\partial t}=-\frac{\partial\bar{\rho}\bar{u}_i}{\partial x_i}-\frac{\partial\overline{\rho'' u_i''}}{\partial x_i}\qquad(1)$$

The mass continuity equation for a tracer η :

$$\frac{\partial\bar{\rho}_\eta}{\partial t}=-\frac{\partial\bar{\rho}_\eta\bar{u}_i}{\partial x_i}-\frac{\partial\overline{\rho_\eta'' u_i''}}{\partial x_i}+\overline{Q_\eta}\qquad(2)$$

Recall the mass mixing ratio definition: $s_\eta=\frac{\rho_\eta}{\rho}$

$$\bar{\rho}_\eta=\overline{s_\eta\rho}=\overline{(\bar{s}_\eta+s_\eta'')(\bar{\rho}+\rho'')}=\overline{\bar{\rho}\left(1+\frac{\rho''}{\bar{\rho}}\right)(\bar{s}_\eta+s_\eta'')}\qquad(3)$$

$$\therefore\bar{\rho}_\eta\approx\bar{\rho}\bar{s}_\eta$$

$$\Rightarrow\frac{\partial\bar{\rho}\bar{s}_\eta}{\partial t}=-\frac{\partial\bar{\rho}\bar{s}_\eta\bar{u}_i}{\partial x_i}-\frac{\partial\overline{\rho_\eta'' u_i''}}{\partial x_i}+\overline{Q_\eta}$$

$$or\quad\bar{\rho}\left(\frac{\partial\bar{s}_\eta}{\partial t}+\bar{u}_i\frac{\partial\bar{s}_\eta}{\partial x_i}\right)=-\bar{s}_\eta\left(\frac{\partial\bar{\rho}}{\partial t}+\frac{\partial\bar{\rho}\bar{u}_i}{\partial x_i}\right)-\frac{\partial\overline{\rho_\eta'' u_i''}}{\partial x_i}+\overline{Q_\eta}\qquad(4)$$

How to determine $\frac{\partial\overline{\rho_\eta'' u_i''}}{\partial x_i}=?$

$$\rho_\eta''=\rho_\eta-\bar{\rho}_\eta=\rho s_\eta-\bar{\rho}\bar{s}_\eta=(\bar{\rho}+\rho'')(\bar{s}_\eta+s_\eta'')-\bar{\rho}\bar{s}_\eta$$

$$\rho_\eta''=\cancel{\bar{\rho}\bar{s}_\eta}+\rho''\bar{s}_\eta+\rho'' s_\eta''+\bar{\rho}s_\eta''-\cancel{\bar{\rho}\bar{s}_\eta}$$

$$\therefore\rho_\eta''=\rho''\bar{s}_\eta+\bar{\rho}\left(1+\frac{\rho''}{\bar{\rho}}\right)s_\eta''\cong\rho''\bar{s}_\eta+\bar{\rho}s_\eta''$$

Hence : $\rho_\eta'' u_i''=(\rho''\bar{s}_\eta+\bar{\rho}s_\eta'')u_i''$

and $\overline{\rho_\eta'' u_i''}=\overline{(\rho''\bar{s}_\eta+\bar{\rho}s_\eta'')u_i''}=\bar{s}_\eta\overline{\rho'' u_i''}+\bar{\rho}\overline{s_\eta'' u_i''}\qquad(5)$

Using (5) $\Rightarrow$ (4) $\therefore$

$$\bar{\rho}\left(\frac{\partial\bar{s}_\eta}{\partial t}+\bar{u}_i\frac{\partial\bar{s}_\eta}{\partial x_i}\right)=-\bar{s}_\eta\left(\frac{\partial\bar{\rho}}{\partial t}+\frac{\partial\bar{\rho}\bar{u}_i}{\partial x_i}\right)-\frac{\partial(\bar{s}_\eta\overline{\rho'' u_i''})}{\partial x_i}-\frac{\partial(\bar{\rho}\overline{s_\eta'' u_i''})}{\partial x_i}+\overline{Q_\eta}\qquad(6)$$

However, $\frac{\partial(\bar{s}_\eta\overline{\rho'' u_i''})}{\partial x_i}=\bar{s}_\eta\frac{\partial\overline{\rho'' u_i''}}{\partial x_i}+\overline{\rho'' u_i''}\frac{\partial\bar{s}_\eta}{\partial x_i}$

Hence, from (6)

$$\bar{\rho}\left(\frac{\partial\bar{s}_\eta}{\partial t}+(\bar{u}_i+\frac{\overline{\rho'' u_i''}}{\bar{\rho}})\frac{\partial\bar{s}_\eta}{\partial x_i}+\frac{1}{\bar{\rho}}\frac{\partial(\bar{\rho}\overline{s_\eta'' u_i''})}{\partial x_i}\right)=$$

$$-\bar{s}_\eta\underbrace{\left(\frac{\partial\bar{\rho}}{\partial t}+\frac{\partial\bar{\rho}\bar{u}_i}{\partial x_i}+\frac{\partial\overline{\rho'' u_i''}}{\partial x_i}\right)}_{=0\ \text{(see eq. (1))}}+\overline{Q_\eta}\qquad(7)$$

We further assume that $\left|\frac{\overline{\rho'' u_i''}}{\bar{\rho}}\right|\ll|\bar{u}_i|$.

$$\therefore\boxed{\frac{\partial\bar{s}_\eta}{\partial t}+\bar{u}_i\frac{\partial\bar{s}_\eta}{\partial x_i}+\frac{1}{\bar{\rho}}\frac{\partial(\bar{\rho}\overline{s_\eta'' u_i''})}{\partial x_i}=\frac{\overline{Q_\eta}}{\bar{\rho}}}$$

In terms of the basic state reference density ρ_0

$\bar{\rho}=\rho_0+\rho'=\rho_0(1+\rho'/\rho_0)\approx\rho_0$, since $(|\alpha'|/\alpha_0\ll1)\Rightarrow$

$$\therefore\boxed{\frac{\partial\bar{s}_\eta}{\partial t}+\bar{u}_i\frac{\partial\bar{s}_\eta}{\partial x_i}+\frac{1}{\rho_0}\frac{\partial(\rho_0\overline{s_\eta'' u_i''})}{\partial x_i}=\frac{\overline{Q_\eta}}{\rho_0}}$$

Numerical solution of the mass continuity equation: using splitting operator

$$\left(\frac{\partial s}{\partial t}\right) = \left(\frac{\partial s}{\partial t}\right)_{adv} + \left(\frac{\partial s}{\partial t}\right)_{\substack{turb\\CLP}} + \left(\frac{\partial s}{\partial t}\right)_{conv} + \ldots + \left(\frac{\partial s}{\partial t}\right)_{chem}$$

- Current computational resources do not allow numerical solution of the continuity equation with all terms simultaneously (the transport term couples the 3 space dimensions with N species = Nx Ny Nz Nspecies ~ 10^4 – 10^5 equations)

- The splitting operator methodology is commonly used to solve each process independently and then couple the various changes resulting from the separate partial calculations (Yanenko 1971, Seinfeld and Pandis 1998, Lanser and Verwer 1998).

- The final solution can be achieved by the parallel or sequential (direct, symmetrical, weighted) techniques.

$$\begin{cases} \left(\frac{\partial \bar{s}}{\partial t}\right)_{adv} = -\sum_i \bar{u}_i \frac{\partial \bar{s}}{\partial x_i} \\ \left(\frac{\partial \bar{s}}{\partial t}\right)_{\substack{turb\\CLP}} = -\frac{1}{\rho_0} \sum_i \frac{\partial \rho_0 \left(\overline{u_i' s'}\right)_{turb}}{\partial x_i} \\ \left(\frac{\partial \bar{s}}{\partial t}\right)_{conv} = -\frac{1}{\rho_0} \sum_i \frac{\partial \rho_0 \left(\overline{u_i' s'}\right)_{conv}}{\partial x_i} \\ \ldots \\ \left(\frac{\partial \bar{s}}{\partial t}\right)_{emissions} = E \\ \left(\frac{\partial \bar{s}}{\partial t}\right)_{chem} = P - L \end{cases}$$

Parallel Splitting Operator

Parallel splitting (as used in RAMS/BRAMS):

Each partial and simpler problem is solved from the same initial condition at the beginning of the timestep:

$$\frac{\partial \bar{s}}{\partial t} = A + D + C + E + R + PL$$

$$\bar{s}(t+\Delta t) = \bar{s}(t) + \frac{\partial \bar{s}}{\partial t}\Delta t = \bar{s}(t) + (A + D + C + E + R + PL)\Delta t$$

$$\left\{ \begin{array}{l} \frac{\partial \bar{s}^A}{\partial t} + A = 0 \\ \frac{\partial \bar{s}^D}{\partial t} + D = 0 \\ \dots \\ \frac{\partial \bar{s}^{PL}}{\partial t} + PL = 0 \end{array} \right|_{\bar{s}(t)} \Bigg\rangle \left\{ \begin{array}{l} \Delta s^A : \frac{\text{change due}}{\text{adv. only}} \\ \Delta s^D : \frac{\text{change due}}{\text{diff. only}} \\ \dots \\ \Delta s^{PL} : \frac{\text{change due}}{\text{chem. only}} \end{array} \right. \Bigg\rangle$$

The solution is the sum of the changes on concentration due each operator:

$$\bar{s}(t+\Delta t) = \bar{s}(t) + \Delta s^A + \Delta s^D + \dots + \Delta s^{PL}$$

Serial or Sequential Splitting Operator

Serial splitting:

Each partial and simpler problem is solved using as initial condition the solution just updated from the application of the previous partial operator.

$$\frac{\partial \bar{s}}{\partial t} = A + D + C + E + R + PL$$

$$\left.\frac{\partial \bar{s}^A}{\partial t} + A = 0\right|_{\bar{s}(t)} \rightarrow \Delta s^A : \frac{\text{change}}{\text{due adv.}} \rightarrow \bar{s}^A(t+\Delta t) = \bar{s}(t) + \Delta s^A \rightarrow$$

$$\rightarrow \left.\frac{\partial \bar{s}^D}{\partial t} + D = 0\right|_{\bar{s}^A(t+\Delta t)} \rightarrow \Delta s^{A+D} : \frac{\text{change due diff.}}{\text{after applied adv.}} \rightarrow \bar{s}^{A+D}(t+\Delta t) = \bar{s}^A(t+\Delta t) + \Delta s^{A+D} \rightarrow$$

$$\rightarrow \ldots \rightarrow \left.\frac{\partial \bar{s}^{PL}}{\partial t} + PL = 0\right|_{\bar{s}^{A+D+C+E+R}(t+\Delta t)} \rightarrow \Delta s^{A+D+C+E+R+PL} : \frac{\text{change due chem. after}}{\text{applied all others processes}} \rightarrow$$

$$\rightarrow \bar{s}^{A+D+C+E+R+PL}(t+\Delta t) = \bar{s}^{A+D+C+E+R}(t+\Delta t) + \Delta s^{A+D+C+E+R+PL}$$

The solution is the concentration after the last operato had been apllied

$$\bar{s}(t+\Delta t) \equiv \bar{s}^{A+D+C+E+R+PL}(t+\Delta t) = PL[R[E[C[D[A(\bar{s}(t))]]]]]$$

in this case the order in which the operators are applied is important.

Sub-grid scale transport processes

$$\frac{\partial \bar{f}}{\partial t} + \underbrace{\bar{u}\frac{\partial \bar{f}}{\partial x} + \bar{v}\frac{\partial \bar{f}}{\partial y} + \bar{w}\frac{\partial \bar{f}}{\partial z}}_{\text{transport of scalar by the mean wind or grid-scale advection term}} = \underbrace{- \frac{1}{r_0}\left(\frac{\partial r_0 \overline{u'f'}}{\partial x} + \frac{\partial r_0 \overline{v'f'}}{\partial y} + \frac{\partial r_0 \overline{w'f'}}{\partial z}\right)}_{\text{sub-grid transport by the un-resolved flow (turbulence, cumulus convection, e.g.)}} + \overline{Q_f}$$

$$\left(\frac{\partial \bar{f}}{\partial t}\right)_{\text{convective transport}} = - \frac{1}{r_0}\left(\frac{\partial r_0 \overline{u'f'}}{\partial x} + \frac{\partial r_0 \overline{v'f'}}{\partial y} + \frac{\partial r_0 \overline{w'f'}}{\partial z}\right)$$

$$\left(\frac{\partial \bar{f}}{\partial t}\right)_{\text{convective transport}} \approx - \frac{1}{r_0}\frac{\partial r_0 \overline{w'f'}}{\partial z}$$

sub-grid scale transport associated with the cumulus convection

$\overline{w'f'}$ is the eddy convective flux

How to estimate ?

Let ϕ a scalar. Start from the traditional Reynolds decomposition:

$\phi = \overline{\phi} + \phi'$ with $\overline{\phi'} = 0$

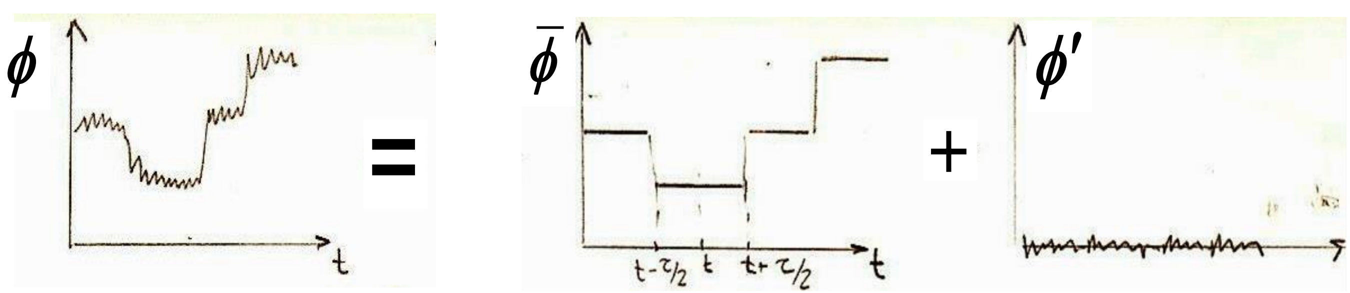
Hence:

$$\overline{w\phi} = \overline{(\overline{w} + w')(\overline{\phi} + \phi')}$$

or

$$\overline{w\phi} = \overline{\overline{w}\,\overline{\phi}} + \underbrace{\overline{\overline{w}\phi'}}_{=0} + \underbrace{\overline{w'\overline{\phi}}}_{=0} + \overline{w'\phi'}$$

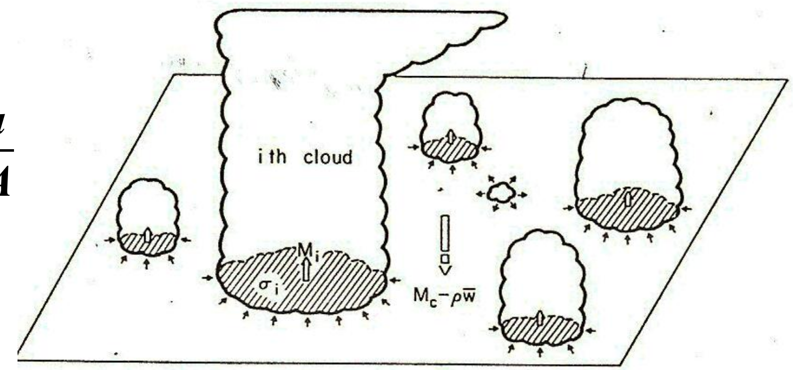
$$\therefore \quad \overline{w\phi} = \overline{w}\,\overline{\phi} + \overline{w'\phi'} \Rightarrow \boxed{\overline{w'\phi'} = \overline{w\phi} - \overline{w}\,\overline{\phi}}$$



Define the grid box area (A) and the cumulus area (a).

The fractional coverage with cumulus elements: $\sigma = \dfrac{a}{A}$

Define area average: $\bar{\phi} = \sigma \bar{\phi}^c + (1-\sigma)\bar{\phi}^e$



total area A, $\bar{\phi}^e$

cumulus area a, $\bar{\phi}^c$

From area average definition, one can write:

$$\overline{w\phi} = \underbrace{\sigma\, \overline{w\phi}^{c}}_{\text{Average over cumulus elements}} + \underbrace{(1-\sigma)\,\overline{w\phi}^{e}}_{\text{Average over environment}}$$

and

$$\bar{w}\bar{\phi} = \left[\sigma \bar{w}^c + (1-\sigma)\bar{w}^e\right]\left[\sigma\bar{\phi}^c + (1-\sigma)\bar{\phi}^e\right]$$

Use Reynolds averaging again for cumulus elements and environment separately:

$$\overline{w\phi}^{c} = \bar{w}^c\bar{\phi}^c + \underbrace{\overline{w''\phi''}^{c}}_{=0}$$

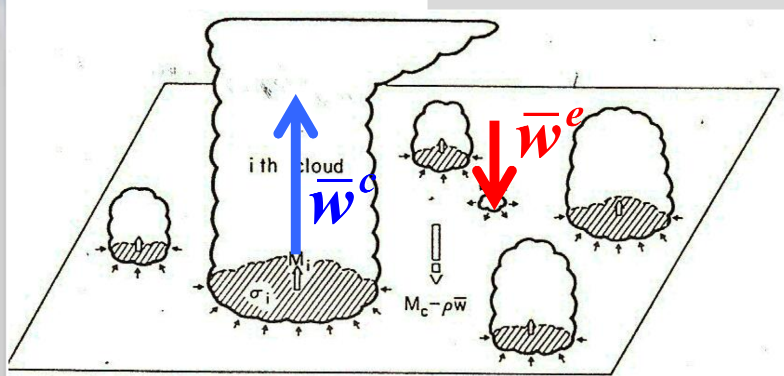
$$\overline{w\phi}^{e} = \bar{w}^e\bar{\phi}^e + \overbrace{\overline{w''\phi''}^{e}}^{=0}$$

neglect sub-plume correlations

with some algebra:

$$\overline{w'\phi'} = \overline{w\phi} - \overline{w}\,\overline{\phi} = \sigma\left(1-\sigma\right)(\overline{w}^{c} - \overline{w}^{e})(\overline{\phi}^{c} - \overline{\phi}^{e})$$

$\overline{w'\phi'}$ **:** the vertical eddy transport of ϕ per unit horizontal area and air density.



total area A, $\overline{\phi}^{e}$

cumulus area a, $\overline{\phi}^{c}$

$$\sigma = \frac{a}{A}$$

The Vertical Eddy Transport: the approximation of small area covered by cumulus

Vertical eddy transport:

$$\overline{w'\phi'} = \overline{w\phi} - \bar{w}\bar{\phi} = \sigma\left(1-\sigma\right)(\bar{w}^c - \bar{w}^e)(\bar{\phi}^c - \bar{\phi}^e)$$

Assume the small area approximation:

$$\sigma << 1 \Rightarrow (1-\sigma) \approx 1; \quad \bar{w}^c >> \bar{w}^e$$

We also assume that : $\bar{\phi}^e \approx \bar{\phi}$

$\Rightarrow$ the environmental mean is aprrox. by the model mean.

$$\therefore \overline{w'\phi'} = \sigma \bar{w}^{c*}(\bar{\phi}^c - \bar{\phi})$$

Define convective mass flux : $m_c = \bar{\rho}_{air}\sigma\bar{w}^{c*}$

$$\therefore \overline{w'\phi'} = \frac{m_c(\bar{\phi}^c - \bar{\phi})}{\bar{\rho}_{air}}$$

$\rightarrow$ aproximation used by the most conven-tional mass-flux based parameterizations

Sub–grid scale convective transport parameterization:

$$\left(\frac{\partial\bar{\phi}}{\partial t}\right)_{conv} = -\frac{1}{\bar{\rho}_{air}}\frac{\partial\left(\bar{\rho}_{air}\overline{w'\phi'}\right)}{\partial z} = -\frac{1}{\bar{\rho}_{air}}\frac{\partial\left[m_c(\bar{\phi}^c - \bar{\phi})\right]}{\partial z}$$

The Formulation for the Vertical Eddy Transport: not assuming the small area approximation

The general expression for the vertical eddy transport is:

$$\overline{w'\phi'} = \overline{w\phi} - \bar{w}\bar{\phi} = \sigma(1-\sigma)(\bar{w}^c - \bar{w}^e)(\bar{\phi}^c - \bar{\phi}^e)$$

As expected $\overline{w'\phi'} = 0$ for $\begin{cases} \sigma = 0, & \text{no clouds.} \\ \sigma = 1, & \text{clouds occupy the entire grid,} \\ & \text{=> the transport is explicitly resolved.} \end{cases}$

Eliminating the environmental quantities (they are not well defined when $\sigma \sim 1$), the eddy transport can be expressed as

$$\overline{w'\phi'} = \overline{w\phi} - \bar{w}\bar{\phi} = \frac{\sigma}{(1-\sigma)}(\bar{w}^c - \bar{w})(\bar{\phi}^c - \bar{\phi})$$

where σ and $\bar{w}^c$ must be determined. It is required that the parameterization must converge to an explicit simulation of cloud processes as $\sigma \to 1$:

$$\left.\begin{aligned} &\Rightarrow \lim_{\sigma\to 1} \bar{w}^c = \bar{w} \\ &\Rightarrow \lim_{\sigma\to 1} \bar{\phi}^c = \bar{\phi} \end{aligned}\right\} \quad \begin{aligned} &(\bar{w}^c - \bar{w}) \sim (1-\sigma) \text{ or higher} \\ &(\bar{\phi}^c - \bar{\phi}) \sim (1-\sigma) \text{ or higher} \end{aligned}$$

$\therefore (\bar{w}^c - \bar{w})(\bar{\phi}^c - \bar{\phi}) \sim (1-\sigma)^2$ or higher when $\sigma \to 1$.

The Arakawa et al. (2011) choice is:

$$(\bar{w}^c - \bar{w})(\bar{\phi}^c - \bar{\phi}) = (1-\sigma)^2\left[(\bar{w}^c - \bar{w})(\bar{\phi}^c - \bar{\phi})\right]^*$$

where * denotes a limiting form expected when $\sigma \ll 1$. Using this choice:

$$\boxed{\overline{w\phi} - \bar{w}\bar{\phi} = \sigma(1-\sigma)\left[(\bar{w}^c - \bar{w})(\bar{\phi}^c - \bar{\phi})\right]^*}$$

where σ and $\left[(\bar{w}^c - \bar{w})(\bar{\phi}^c - \bar{\phi})\right]^*$ must be determined to close the unified parameterization.

V E T

The closure of conventional cumulus parameterization can determine the eddy transport for a full adjustment to a quasi-equilibrium state, given by:

$$\left(\overline{w\phi}-\bar{w}\bar{\phi}\right)_{adj}$$

$$=> \left(\overline{w\phi}-\bar{w}\bar{\phi}\right)_{adj}=\frac{\sigma}{(1-\sigma)}\left[(\bar{w}^{c}-\bar{w})(\bar{\phi}^{c}-\bar{\phi})\right]^{*}$$

$\therefore$

$$\overline{w\phi}-\bar{w}\bar{\phi}=(1-\sigma)^{2}\left(\overline{w\phi}-\bar{w}\bar{\phi}\right)_{adj}$$ $\Rightarrow$ this is the vertical eddy transport that includes the scale dependence trough σ

where σ and $\left(\overline{w\phi}-\bar{w}\bar{\phi}\right)_{adj}$ must be determined to close the unified parameterization.

The term $\left(\overline{w\phi}-\bar{w}\bar{\phi}\right)_{adj}$ can be calculated from a conventional cumulus parameterization.

In GF, there are 4 closures (G, KF, MC and omega) and the ensemble.

Also, in GF scheme , σ is calculated by the entrainment (ε) rate and the grid-cell area:

$\varepsilon=\frac{b}{R}$, where R is the radius of the convective plumes (up and downdraft), $b=0.2$

$$\therefore \sigma=\frac{2\pi R^{2}}{\Delta x\Delta y}=\frac{2\pi b^{2}}{\Delta x\ \Delta y\ \varepsilon^{2}}$$

The mass flux approach: Extension to an ensemble of clouds with up/downdrafts

$$\left(\frac{\partial \bar{s}}{\partial t}\right)_{conv} = -\frac{1}{\rho_0}\frac{\partial(\rho_0 \overline{w's'})}{\partial z}$$

Ensemble of clouds with up/downdrafts

$$\overline{w's'} = \int_{\lambda} \left[s_u - \tilde{s}\right]\eta_u(\lambda,z)m_u(\lambda,z_{b,u})d\lambda - \int_{\lambda} \left[s_d - \tilde{s}\right]\eta_d(\lambda,z)m_d(\lambda,z_{b,d})d\lambda$$

- u,d : updraft / downdraft flows
- m,η : mass flux where the flows originate / normalized mass flux profile
- $s_{u/d}$: in cloud value of the scalar
- $\tilde{s}$: enviroment value of the scalar
- $\bar{s}$: the model value
- $\int_{\lambda}$: represents the integral over all clouds present in the model grid box

2D spectral model:
Deep and shallow (non-precipitating) cumulus

1) Case of deep / precipitating convection:

$$\overline{w's'}(z) = \underbrace{\eta_u\left[s_u - \tilde{s}\right]m_u(z_b)}_{updraft} - \underbrace{\eta_d\left[s_d - \tilde{s}\right]m_d(z_d)}_{downdraft}$$

where $\eta_{u,d} = \dfrac{m_{u,d}(z)}{m_u(z_{b,d})}$,the normalized mass flux.

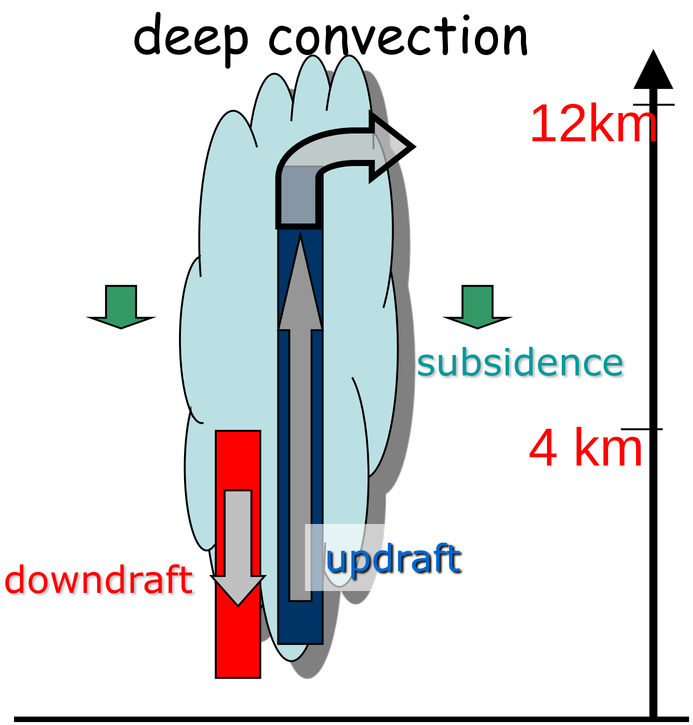
Defining $\varepsilon = \dfrac{m_u(z_b)}{m_d(z_d)}$

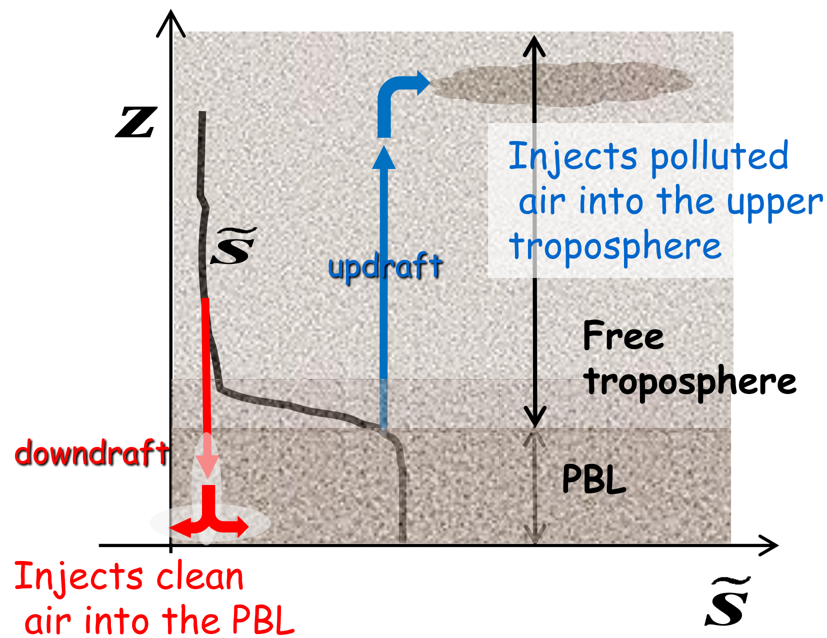
and from the mass conservation :

$m_u = m_d + \widetilde{M}$,

the un-resolved flux can be described as:

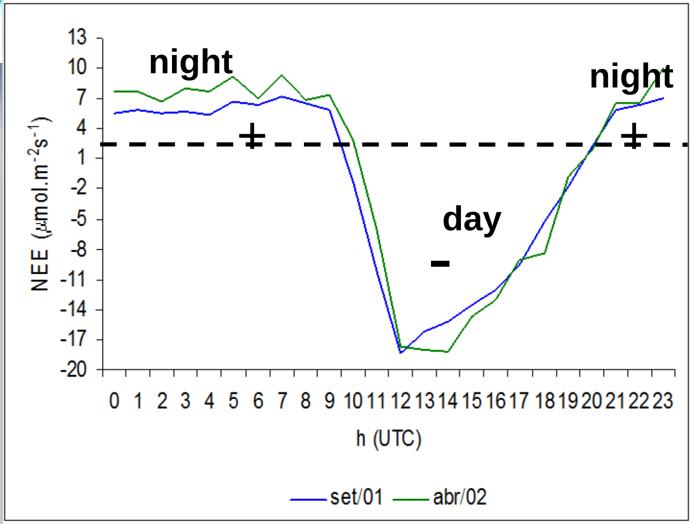
$$\frac{\overline{w's'}}{m_u(z_b)} = \eta_u s_u - \varepsilon \eta_d s_d - \tilde{\eta}\tilde{s}$$

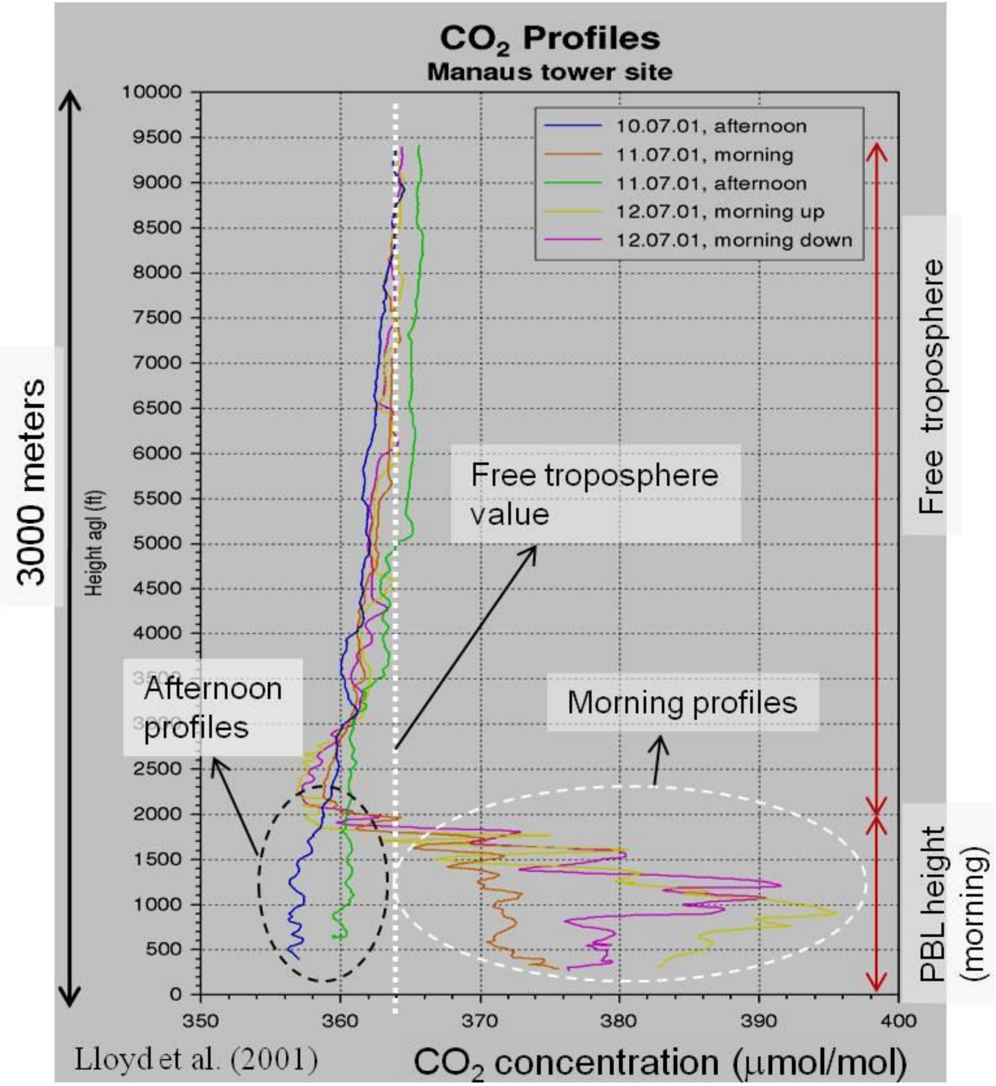




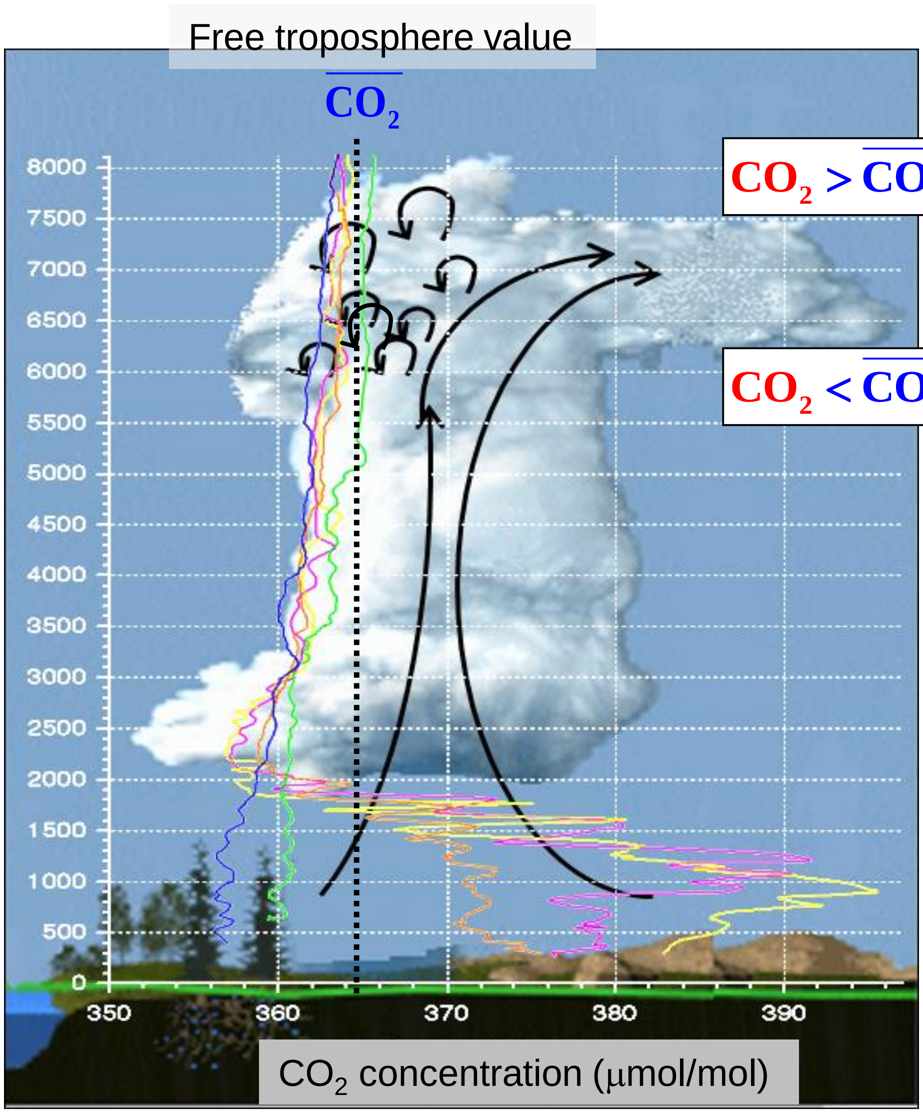
The CO_2 profile: diurnal variation and the rectifier effect

CO_2 surface flux on Amazon





The CO_2 profile: diurnal variation and the rectifier effect

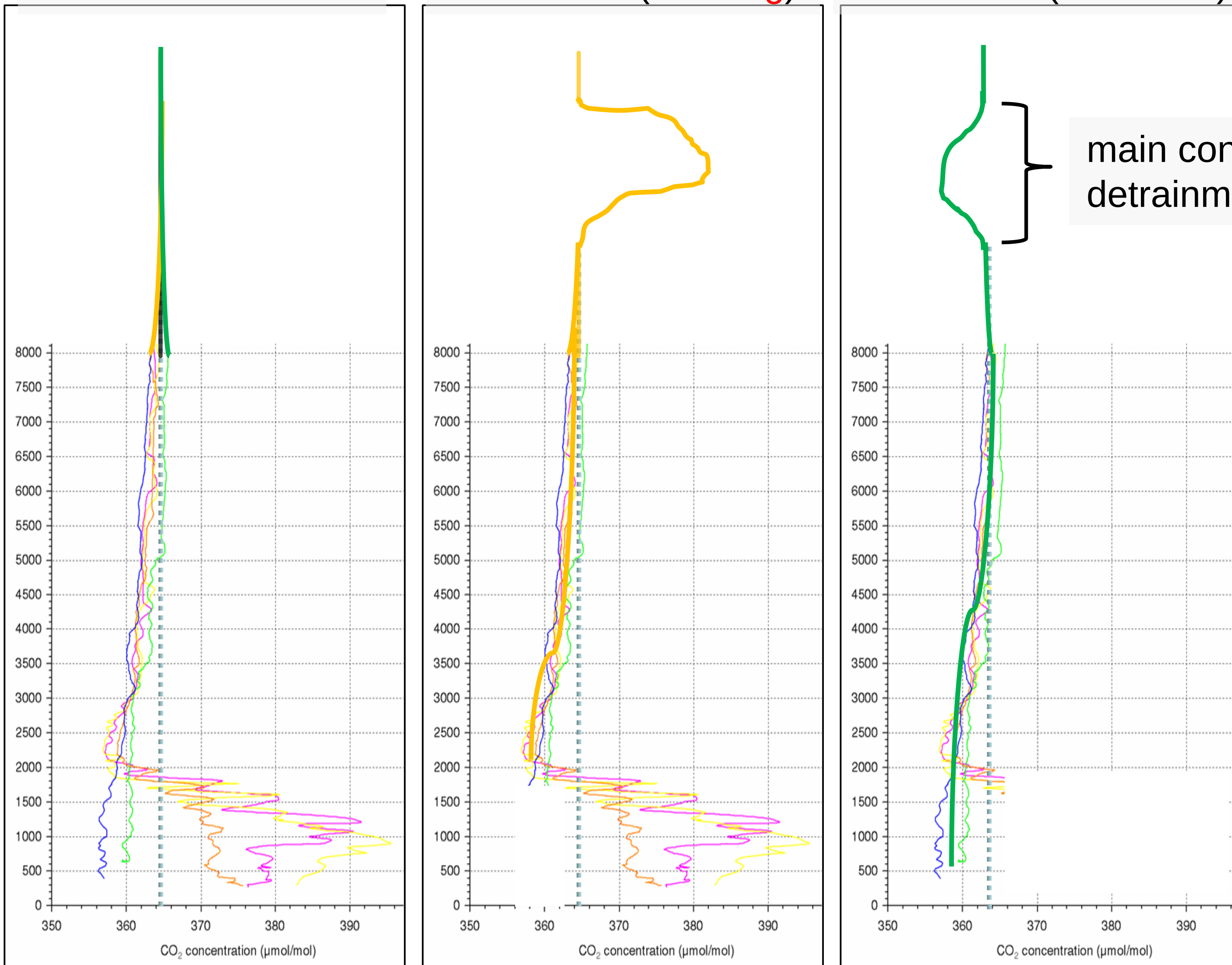


$CO_2 > \overline{CO_2}$ Morning => CO_2 enriched detrainment air mass.

$CO_2 < \overline{CO_2}$ Afternoon => CO_2 depleted detrainment air mass.

The CO_2 profile: diurnal variation and the rectifier effect

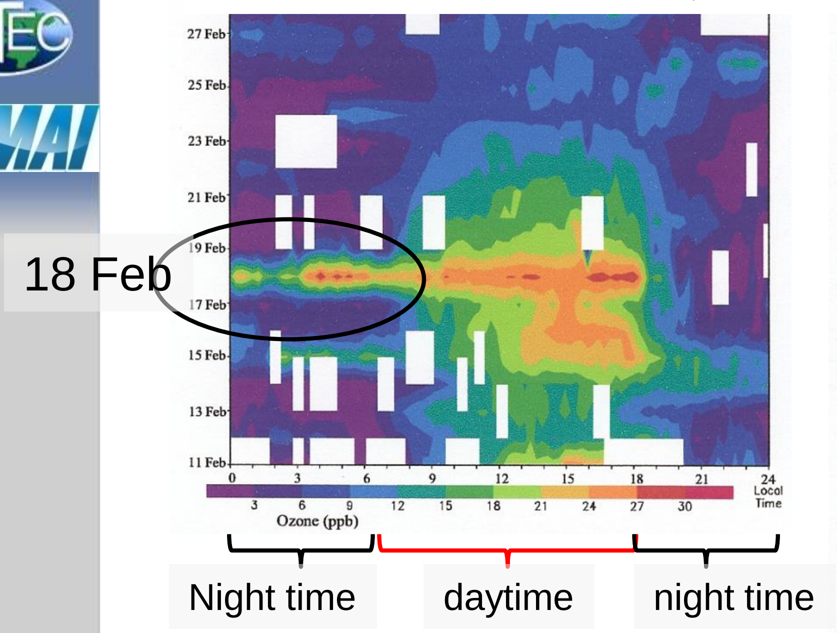
CO_2 profile before convection	CO_2 profile after convection (morning)	CO_2 profile after convection (afternoon)



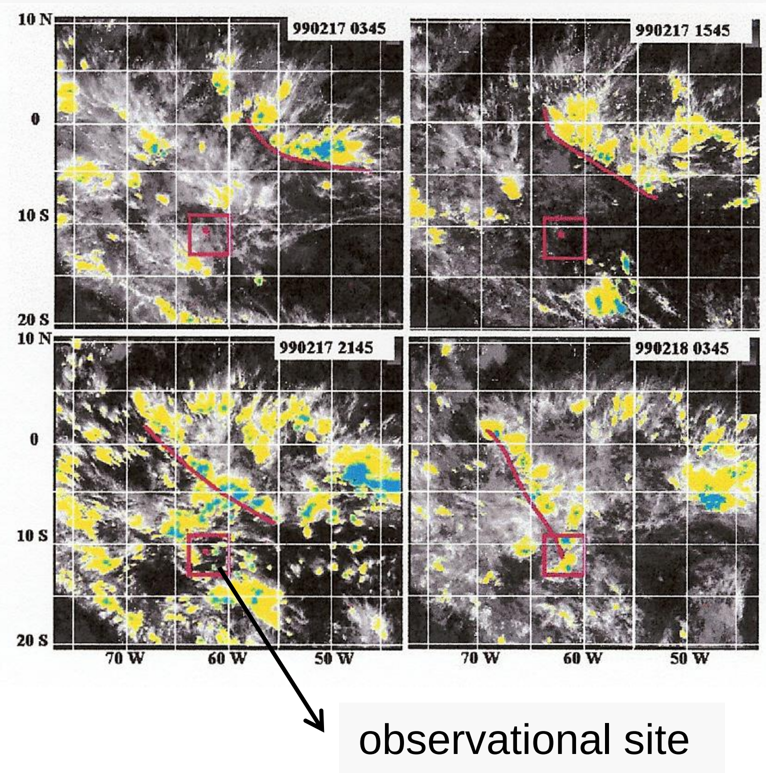
main convective detrainment layer

Transport of ozone to the surface by convective downdrafts at night (Betts et al., 2002)

Surface Ozone mixing ratio (ppb) on Rondonia site : Feb 11-28, 1999



Sequence of pictures, showing the passage of squall-line from de coast to Rondonia From 0345 UTC Feb 17 to 0345 UTC 18 Feb



Static control: the mass conservation equation

$$\mu - \delta = \frac{1}{m(z)} \frac{\partial m(z)}{\partial z}$$

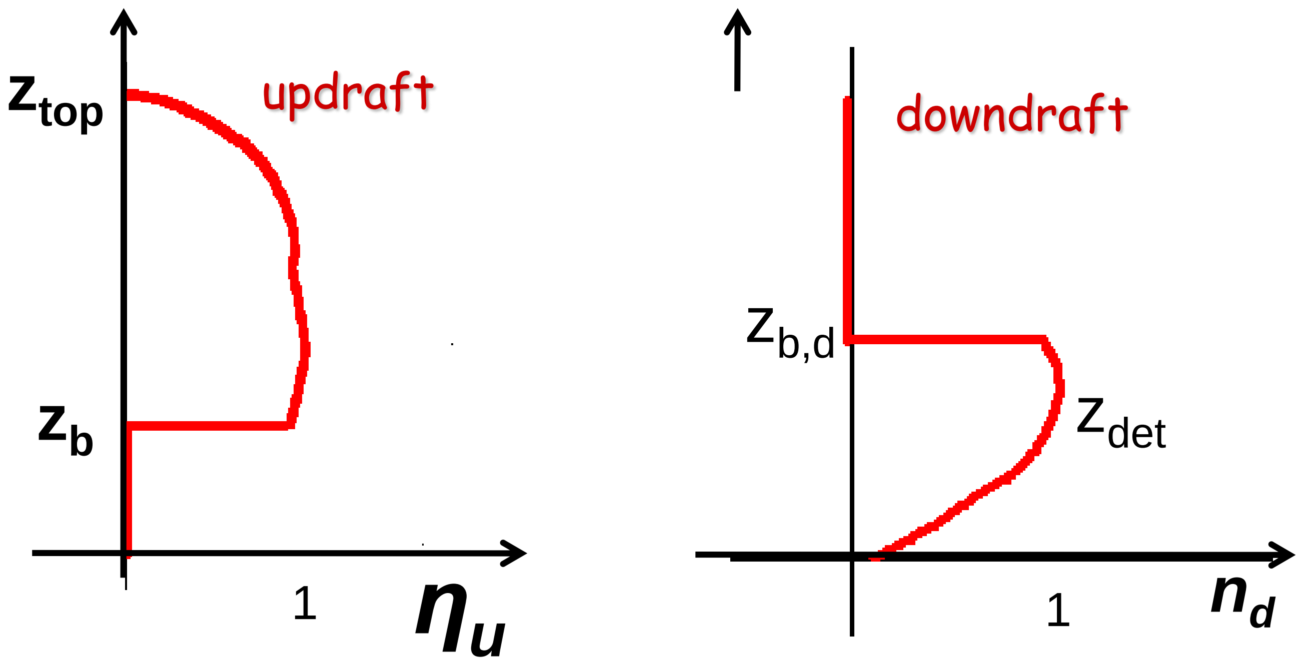
$$\mu - \delta = \frac{1}{\eta(z)} \frac{\partial \eta(z)}{\partial z}$$

$m(z) = m(z_b)\eta(z)$

$m(z_b)$: cloud base mass flux

$\eta(z)$: normalized mass flux

μ / δ : entrainment/detrainment mass rates



Mass Conservation Equation: an example of the vertical variation

entrainment up / downdraft:

$$\mu_{u,d} = \frac{0.2}{R}, \quad \text{R = raio da nuvem (12 km)}$$

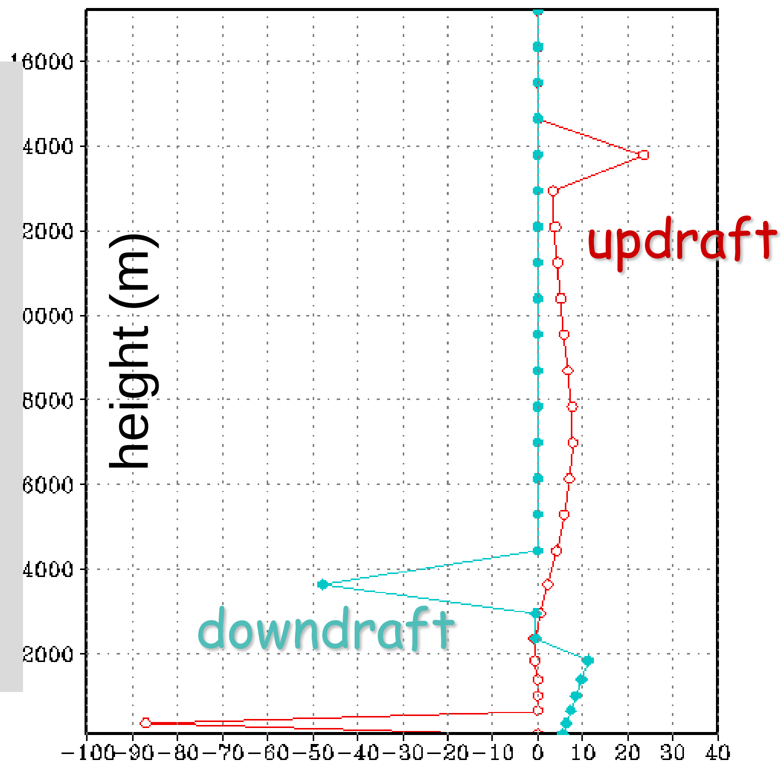
detrainment updraft:

$$\delta_u(k) = \begin{cases} 0.3\mu_u \\ \delta_u(k-1) + \dfrac{0.5\mu_u}{\Delta k_{stable}} \end{cases}$$

detrainment downdraft:

$$\delta_d(k) = \begin{cases} 0, k > k_{\det} \\ \mu_d + \left\{ 1 - \dfrac{a\left[z(k) - z_1\right] + (1-a)(z_{\det} - z_1)}{a\left[z(k+1) - z_1\right] + (1-a)(z_{\det} - z_1)} \right\} \dfrac{1}{\Delta z}, k \le k_{\det} \end{cases}$$

a=1-p (percentual de massa desentranhada na superfície)



$\delta - \mu$

(detrainment - entrainment)

Conservation equation for a scalar: provides the scalar inside cloud

$$\frac{\partial m_u \alpha_u}{\partial z} = \left(\frac{\partial m_u}{\partial z}\right)_e \tilde{\alpha} - \left(\frac{\partial m_u}{\partial z}\right)_d \alpha_u + S_u$$

where
- $m_u \mu_u, \delta_u = \frac{1}{m_u}\left(\frac{\partial m_u}{\partial z}\right)_{e,d}$: entraiment / detrainment mass rate
- $\tilde{\alpha}$: environment value
- α_u : in cloud (updraft) value
- S_u : sources / sinks

$$\frac{\partial m_u \alpha_u}{\partial z} = m_u \mu_u \tilde{\alpha} - m_u \delta_u \alpha_u + S_u$$

$$m_u \frac{\partial \alpha_u}{\partial z} + \alpha_u \frac{\partial m_u}{\partial z} = \mu_u \tilde{\alpha} - \delta_u \alpha_u + S_u$$

From the mass conservation: $\frac{\partial m_u}{\partial z} = m_u \mu_u - m_u \delta_u \Rightarrow$

$$\frac{\partial \alpha_u}{\partial z} + \alpha_u(\mu_u - \delta_u) = \left(\mu_u \tilde{\alpha} - \delta_u \alpha_u + \frac{1}{m_u} S_u\right)$$

$$\frac{\partial \alpha_u}{\partial z} = -\alpha_u \mu_u + \alpha_u \delta_u + \mu_u \tilde{\alpha} - \delta_u \alpha_u + \frac{1}{m_u} S_u$$

$$\therefore \quad \boxed{\frac{\partial \alpha_u}{\partial z} = \mu_u(\tilde{\alpha} - \alpha_u) + \frac{1}{m_u} S_u}$$

For conserved quantities : $S_u = 0$

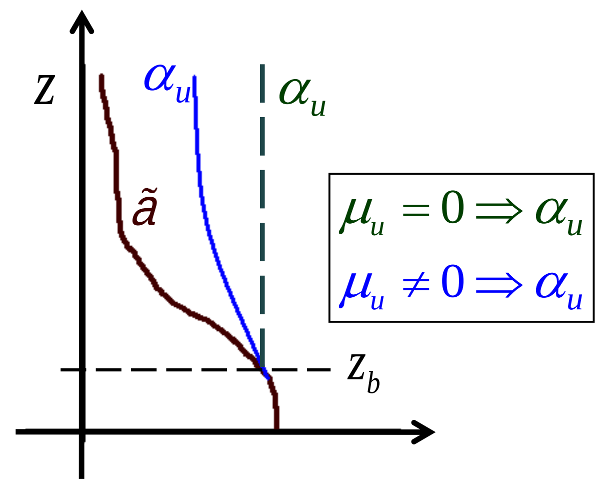
$$\Rightarrow \frac{\partial \alpha_u}{\partial z} = \mu_u(\tilde{\alpha} - \alpha_u)$$

From the boundary condition for α_u at cloud base :

$$\alpha_u(z_b) = \tilde{\alpha}(z_b)$$

And for especified $\mu_u = \mu_u(z)$ and $\tilde{\alpha}(z) \equiv \bar{\alpha}(z)$,

the equation can be integrated and α_u can be determined.



Parameterized Deep Convective Transport

From : $\frac{1}{m_u(z_b)}\left(\frac{\partial \overline{w's'}}{\partial z}\right)_{deep\ conv} = \frac{\partial}{\partial z}\left(\eta_u s_u - \varepsilon\eta_d s_d - \bar\eta\tilde s\right)$

we can write

$$\frac{\partial}{\partial z}\left(\eta_u s_u - \varepsilon\eta_d s_d - \bar\eta\tilde s\right) = \frac{\partial \eta_u s_u}{\partial z} - \varepsilon\frac{\partial \eta_d s_d}{\partial z} - \frac{\partial \bar\eta\tilde s}{\partial z}$$

However using the mass conservation equation:

$$\frac{\partial \eta_u s_u}{\partial z} = \eta_u\frac{\partial s_u}{\partial z} + s_u\frac{\partial \eta_u}{\partial z} = \eta_u\frac{\partial s_u}{\partial z} + s_u(\mu_u - \delta_u)\eta_u$$

and $\frac{\partial s_u}{\partial z} = \mu_u\left(\tilde s - s_u\right)$

$$\therefore \frac{\partial \eta_u s_u}{\partial z} = \eta_u\mu_u\left(\tilde s - s_u\right) + s_u(\mu_u - \delta_u)\eta_u$$

$$\Rightarrow \frac{\partial \eta_u s_u}{\partial z} = \eta_u\mu_u\tilde s - \cancel{\eta_u\mu_u s_u} + \cancel{s_u\mu_u\eta_u} - s_u\delta_u\eta_u$$

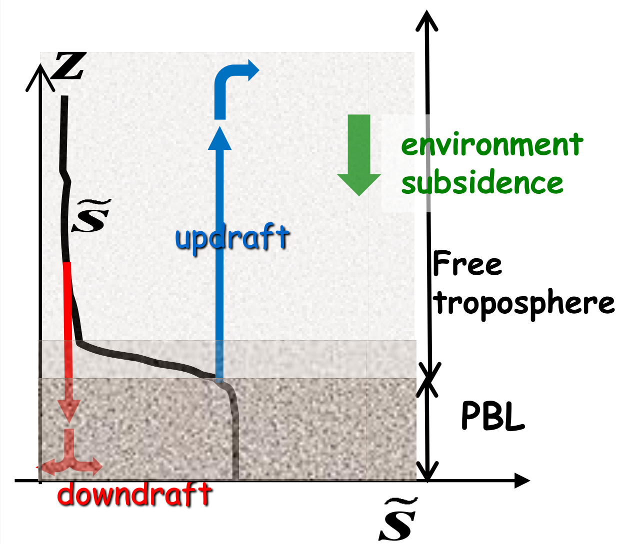
we also have :

$$\frac{\partial \bar\eta\tilde s}{\partial z} = \bar\eta\frac{\partial \tilde s}{\partial z} + \tilde s\frac{\partial \bar\eta}{\partial z}$$

but : $\frac{\partial \bar\eta}{\partial z} = \frac{\partial \eta_u}{\partial z} - \varepsilon\frac{\partial \eta_d}{\partial z} = \left(\mu_u - \delta_u\right)\eta_u - \varepsilon\left(\mu_d - \delta_d\right)\eta_d$

$$\therefore \frac{1}{m_u(z_b)}\left(\frac{\partial \overline{w's'}}{\partial z}\right)_{deep\ conv} = \cancel{\eta_u\mu_u\tilde s} - s_u\delta_u\eta_u - \varepsilon\left(\cancel{\eta_d\mu_d\tilde s} - s_d\delta_d\eta_d\right) - \bar\eta\frac{\partial \tilde s}{\partial z} - \left(\cancel{\mu_u} - \delta_u\right)\eta_u\tilde s + \varepsilon\left(\cancel{\mu_d} - \delta_d\right)\eta_d\tilde s$$

$$\frac{1}{m_u(z_b)}\left(\frac{\partial \overline{w's'}}{\partial z}\right)_{deep\ conv} = \underbrace{\left(\tilde s - s_u\right)\delta_u\eta_u}_{\text{updraft detrainment}} \underbrace{- \varepsilon\left(\tilde s - s_d\right)\delta_d\eta_d}_{\text{downdraft detrainment}} \underbrace{- \bar\eta\frac{\partial \tilde s}{\partial z}}_{\text{enviroment subsidence}}$$



Parameterized deep convective transport

$$\left(\frac{\partial \bar{s}}{\partial t}\right)_{\substack{deep\\conv}} = \frac{1}{\rho_0}\frac{\partial}{\partial z}\left(\rho_0 \overline{w's'}\right)$$

$$\left(\frac{\partial \bar{s}}{\partial t}\right)_{\substack{deep\\conv}} = \frac{m_u(z_b)}{\rho_0}\left[\delta_u \eta_u \left(s_u - \tilde{s}\right) + \delta_d \varepsilon \eta_d \left(s_d - \tilde{s}\right) + \tilde{\eta}\frac{\partial \tilde{s}}{\partial z}\right]$$

updraft detrainment — downdraft detrainment — environment subsidence

The closure problem

The static control and entrainment /detrainment assumptions determine the vertical structure of the tracer transport, however the determination of the overall magnitude of the transport requires the determination of the mass flux at cloud base : $m_u(z_b)$

We apply Grell's cumulus scheme that provides the mass flux using an ensemble version of closures (moist convergence, Arakawa&Schubert, Grell, stability (like Kain&Fritsch), Brown).

Parameterized Wet Convective Removal

Equilibrium between aqueous and gas phases (Henry's law)

$$\rho_{\substack{fase\\aquosa}} = k_H r_{lw} \rho_{\substack{fase\\gasosa}}$$

solubility:

$$k_H(T) = RTk_H^{\theta}\, e^{\left[-\frac{\Delta_{sol}H}{R}\left(\frac{1}{T}-\frac{1}{T^{\theta}}\right)\right]}, \quad \begin{cases} T^{\theta} = 298.15\text{K} \\ \Delta_{sol}H : \text{enthalpy change} \\ k_H^{\theta} : \text{ equilibrium constant at } T^{\theta} \end{cases}$$

wet removal tendency (sink term W):

$$\left(\frac{\partial \bar{s}}{\partial t}\right)_{\substack{wet\\removal}} = -\frac{k_H r_{lw} \hat{s}_{\substack{fase\\gasosa}}\ prec}{\Delta z} \quad \begin{cases} prec : \dfrac{\text{convective precip rate}}{\text{(from cumulus parameterization)}} \\ r_{lw} : \text{ cloud liquid water/ice mixing ratio (from CP)} \\ \hat{s}_{\substack{fase\\gasosa}} : \text{ in-cloud gas phase mixing ratio} \end{cases}$$

total mass deposited on surface:

$$m_{sfc} = \int_{sfc}^{\substack{cloud\\top}} \left(\frac{\partial \bar{s}}{\partial t}\right)_{\substack{wet\\removal}} \rho_{air}\, dz$$

Backup slides

How to include this sub-grid scale transport in large scale models?

- **Global mapping of maximum emission heights and resulting vertical profiles of wildfire emissions (Sofiev et al., 2013)**

2.1 Calculation of the top height of fire emission plumes

Calculation of characteristic injection profile is based on a recently suggested semi-empirical formula for the fire-plume top height (Sofiev et al., 2012). According to this methodology, the plume top H_p depends on the fire radiative power FRP, ABL height H_{abl}, and Brunt-Väisälä frequency in the free troposphere N_{FT}:

$$H_p = \alpha H_{abl} + \beta \left(\frac{FRP}{P_{f0}}\right)^{\gamma} \exp(-\delta N_{FT}^2 / N_0^2). \quad (1)$$

The values for coefficients α, β, γ, and δ, and normalising constants P_{f0} and N_0 are: $\alpha = 0.24$; $\beta = 170\,m$; $\gamma = 0.35$; $\delta = 0.6$, $P_{f0} = 10^6\,W$, and $N_0^2 = 2.5 \times 10^{-4}\,s^{-2}$. These coefficients have been obtained from calibration of the formula (1) using MISR fire plume observations. As dis-

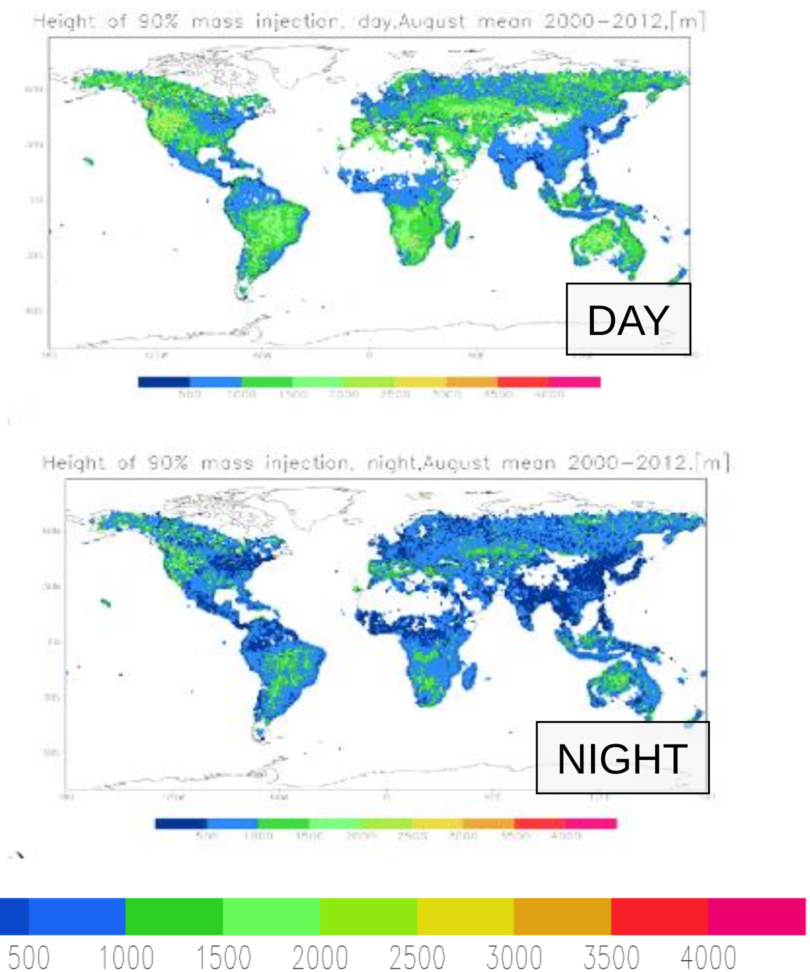
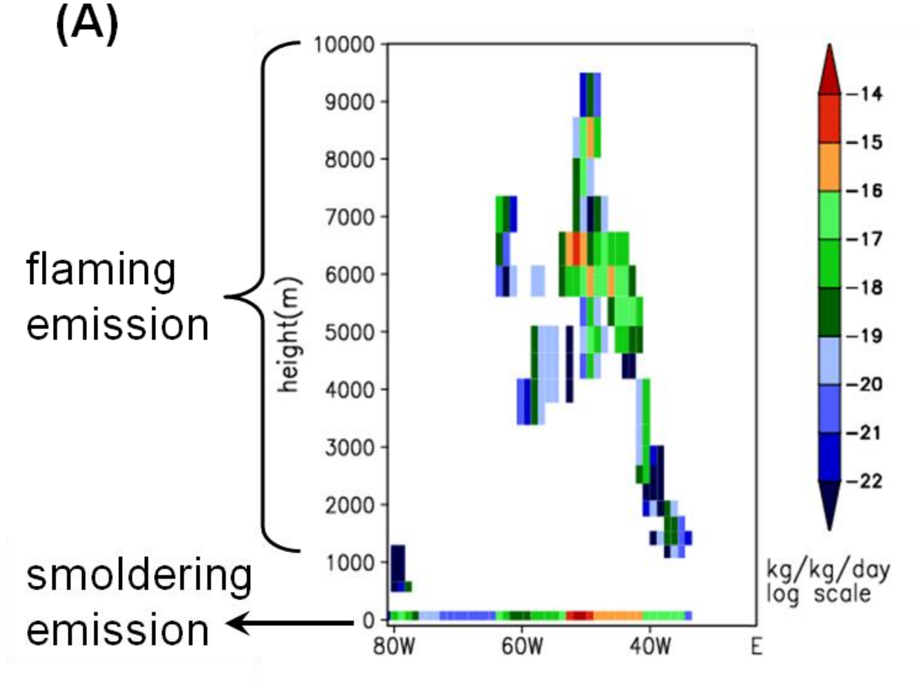


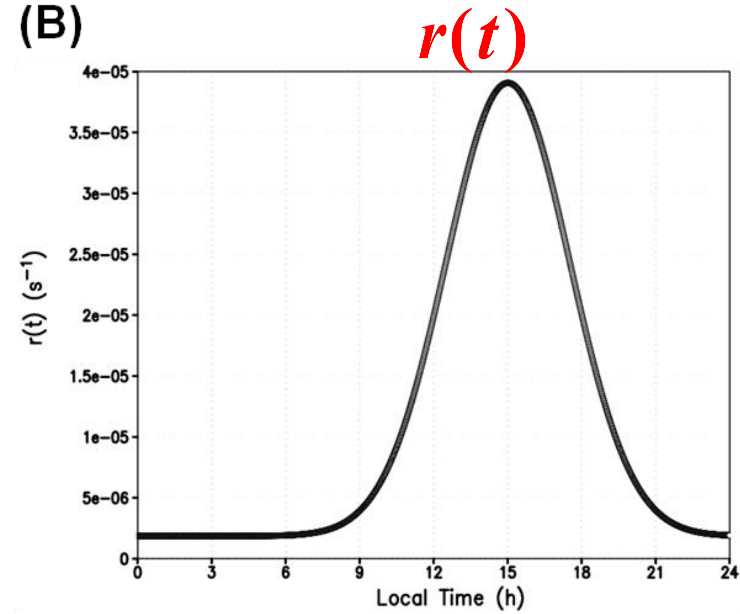
Fig. 4. Injection height for 90 % of mass for night (left) and day (right) for February (top) and August (bottom). Unit = [m].

Including emission in the model

3-D Emission Field:

Diurnal cycle of the burning:





3-D Instantaneous emission rate:

$$E_\eta(t) = r(t) E_\eta$$

Plume-rise of vegetation fires:
typical energy fluxes (kWm^{-2})

Biome type	Lower bound kWm^{-2}	Upper bound kWm^{-2}	Flaming consumption
Tropical forest	30.	80.	45%
Woody savanna - cerrado	4.4	23.	75%
Pasture - grassland cropland	3.3		97%

Refs: Carvalho et al, 1995-2001-2005 (com. pessoal);

Riggan et al, 2004;

Ward et al, 2002;

Ferguson et al, 1998;

Cochrane et al; 200X-com. pessoal;

Miranda et al, 1993.