Air Quality Models: operational experience and challenges

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The Two Fundamental Scientific Questions of LBA Are:

- How does Amazonia currently function as a regional entity?
- How will changes in land use and climate affect the biological, chemical and physical functions of Amazonia, including the sustainability of development in the region and the influence of Amazonia on global climate?

The vast size of Amazonia and its position in the humid equatorial tropics give the region a potential for influencing global energy, water, carbon and trace gas budgets which we cannot afford to neglect in the search for understanding of how climate may change in the future.
Research Strategy

LBA integrates multi-disciplinary studies from the earth, life and human sciences, which meet not only their specific objectives but also contribute to the common LBA goals. By linking these individual, focused efforts the LBA approach ensures the transfer of experience, ideas and data across disciplinary boundaries.

LBA research will be scientifically organized into six themes:
- Physical Climate
- Carbon Storage and Exchange
- Biogeochemistry
- Atmospheric Chemistry
- Land Surface Hydrology and Water Chemistry
- Land Use and Land Cover Change

The Large Scale Biosphere-Atmosphere Experiment in Amazonia
• Fire is an important component of the carbon dynamics in the Amazon;
  • Biomass burning is also important for the Savannah dynamics in Central Brazil (a biome denominated Cerrado)
  • Sugar cane burning - SE Brazil

• LBA research product => operational product
  • Academic community <=> operational sector
    • Real time monitoring and prediction of air quality due to biomass burning (and urban sources)
Thanks to: Saulo Freitas, Karla Longo, Edmilson Freitas, Eder Vendrasco, Demerval Moreira, Maria Assunção F. da Silva Dias....
Deforestation in the Amazon
Plate 1. Examples of smoke from biomass burning in Brazil during SCAR-B. (a) A small cerrado fire north of Brasilia. (b) Lines of fire in cerrado northwest of Cuiabá. (c) Regional haze dominated by smoke over Cuiabá. (d) Cumulus clouds produced by fires near Marabá. Note the banded smoke layers. Photos by Peter V. Hobbs.
An example of the impact of biomass burning - pyro-clouds. Rondonia – September 2002
Ji-Paraná haze layer (SW Amazon)

21 SEP 2002
GOES-8 ABBA
FIRE PRODUCT

1745Z
19 SEP 2002

Fire summary for previous 3 hours
NOTE: Fire locators are not indicative of fire size
Aerosol concentration in Amazônia

Aerosol Concentrations in Amazonia changes from very low values of 5-12 µg/m³ to very high 500 µg/m³ in areas affected by biomass burning.

Contribution from Paulo Artaxo
High concentration of CO in Rondonia during the dry season.

Data from Luciana V. Gatti, IPEN

Contribution from Paulo Artaxo.
O$_3$ time series - pasture site in Rondonia
dry season 1999
INPE – AVHRR
FIRE PRODUCT

~2030 Z
19 SEP 2002

5085 hot spots

http://www.cplec.inpe.br/products/queimadas/
• How about the modeling strategy of the biomass burning component of the LBA program?
  • Aerosols
  • Gases
Modeling the Earth Atmosphere System

\[
\begin{align*}
\frac{\partial X_a}{\partial t} + L_a X_a &= N_a (X_a, X_o, X_v, X_c, X_s) + F_a (X_a, X_o, X_v, X_c, X_s) \\
\frac{\partial X_o}{\partial t} + L_o X_o &= N_o (X_a, X_o, X_v, X_c, X_s) + F_o (X_a, X_o, X_v, X_c, X_s) \\
\frac{\partial X_s}{\partial t} + L_s X_s &= N_s (X_a, X_o, X_v, X_c, X_s) + F_s (X_a, X_o, X_v, X_c, X_s) \\
\frac{\partial X_v}{\partial t} + L_v X_v &= N_v (X_a, X_o, X_v, X_c, X_s) + F_v (X_a, X_o, X_v, X_c, X_s) \\
\frac{\partial X_c}{\partial t} + L_c X_c &= N_c (X_a, X_o, X_v, X_c, X_s) + F_c (X_a, X_o, X_v, X_c, X_s)
\end{align*}
\]

- **atmosphere**
- **ocean+hydrology**
- **soil**
- **vegetation**
- **chemical species**

\[X_a = \{u, v, w, T, q_v, q_i, q_r, q_i, \ldots\}\]
\[X_o = \{u, v, w, T, s_v, \ldots\}\]
\[X_s = \{T^s, w^s, N^i, \ldots\}\]
\[X_v = \{\text{lai}^i, \text{sig}^i, \text{root}^i, \text{stom}^i, \text{VOC}^i, C^i, N_i, \ldots\}\]
\[X_c = \{CO_2, CH_4, O_3, NO_X, VOC's, SO_2, \ldots\}\]
Real Time Transport Monitoring of CO and PM2.5 using BRAMS (Brazilian Developments in RAMS)

GOES-8 ABBA Fire Product → Concentration of the previous day → CPTEC Global Model Analysis/Forecasts

Emission Model → CO and PM2.5 Source Emission → Tracer initial condition → Atmospheric initial and boundary conditions

RAMS ISAN module

RAMS model with in-line tracer transport

Products (48 h):
- a) Atmospheric fields
- b) CO and PM2.5 concentration

http://www.cptec.inpe.br

Product based on PhD thesis - Saulo Freitas and Karla Longo - USP
CATT-BRAMS 2

New version of the biomass burning aerosol model:
1. Calibration of emission model with SMOCC/RACCI 2002 data.
2. New condensate (ice and liquid water) interaction with short and long wave radiation (based on CARMA) - coupled with cloud microphysics and convective parameterization (meso-NH and ECMWF).
3. Plume rise mechanism for biomass burning emission.
4. GRELL parameterization for convective clouds with training (weights dependent on the closure assumption and geographically dependent); Max CAP dependent on TKE/LAND.
5. Shallow cumulus parameterization based on GRELL with ECMWF entrainment and Kain-Fritsch closure.
6. New NDVI (MODIS) data and adjustments of surface parameterizations based on LBA and other field experiments.
7. New global soil moisture analysis (now operational at CPTEC).
8. New forecasting cycle: 24 hr for assimilation of aerosol sources + 48 hr forecast, 2 grids (30°e 150 km, 40 vertical levels).
9. African emissions based on recent estimates (GFEDv2, dec2005), as well as anthropic emissions (RETRO, global at 0.5° resolution).
10. Data assimilation component in progress (remote sensing data).
Source Emission Parameterization

- Mass of the tracer emitted:

\[ M[\eta] = \alpha_{\text{veg}} \cdot \beta_{\text{veg}} \cdot E_{f,\text{veg}}^{[\eta]} \cdot a_{\text{fire}}, \]

- \( \alpha, \beta, E_f \): D. Ward et al., 1992, Ferek et al., 1995.
- \( a_{\text{fire}} \), position: GOES-8 ABBA Fire Product.
- \( \eta \): IGBP (v 2.0) 1 km resolution.
- \( \eta \): CO\(_2\), CO, PM2.5, CH\(_4\).

Freitas et al. 2005
Emission Rate Parameterization

ABBA Fire Pixels at 1145, 1445, 1745, 2045 UTC

- Surface Emission Rate:

\[ \bar{\Theta}[\eta](t, \varphi, \tau) = \frac{\rho(\tau)}{\rho_0 \Delta \zeta} M[\eta], \]

(Freitas, 1999)

Prins et al., 1996

Diurnal Cycle of the Burning

1500 LT

August

September 1995

Freitas et al. 2005
1D Plume raise cloud model: run at every grid point where biomass burning is detected

Freitas et al. 2005
GOES ABBA Source Emission for CO
kg/(m²s) - 19SEP2002

Freitas et al. 2005
The in-line model transport follows the Eulerian approach:

\[
\frac{\partial s}{\partial t} = \frac{\partial s}{\partial t}_{\text{adv}} + \frac{\partial s}{\partial t}_{\text{PBL turb}} + \frac{\partial s}{\partial t}_{\text{deep conv}} + W_{PM2.5} + R + Q,
\]

where:
- \textit{adv} grid-scale advection,
- \textit{PBL turb} sub-grid transport in the PBL,
- \textit{deep conv} sub-grid transport associated to deep convection,
- \textit{W} convective wet removal for PM2.5,
- \textit{R} sink term associated with generic process of removal e/ou transformation of tracers,
- \textit{Q} source emission associated to the biomass burning process.

Freitas et al. 2005
Parameterized Convective Transport

- Based on a new mass flux cumulus scheme (Grell, 1993; Grell and Devenyi 2002).
- Transport term:

\[
\frac{\partial s}{\partial t}_{\text{conv}} = m_b \frac{\partial}{\partial u} (s_u - \bar{s}) + m_d \frac{\partial}{\partial d} (s_d - \bar{s}) + \frac{\partial}{\partial z} s
\]

- Updraft detrainment
- Downdraft detrainment
- Environment subsidence
- Wet removal for PM2.5 based on Berge (1993) accounts for washout and rainout.

Freitas et al. 2005
Convective Transport of CO
24-25 Sep 2002

(a) GOES-8 Estimated Precipitation (mm) – 4 km resolution
12Z24–12Z25SEP2002

(b) Convective (GRELL) + Resolved Precipitation
Precipitation (mm) – 40 km resolution
12Z24–12Z25SEP2002

Freitas et al. 2005

GOES Precipitation
4 km resolution

Conv + Resolved Precipitation
40 km resolution

mm
Convective Transport of CO
21Z 24 Sep 2002

Vertical section at lat 10S
Freitas et al. 2005

vertical level 11.5 km

CO (ppb)
Plume of CO (ppb)
1100 m sigma-z
00Z 27 Aug 2002
40 km grid resolution

200 km grid resolution
South America and Africa

Freitas et al. 2005
Plume of PM2.5
00Z 27 Aug 2002
(column integrated - mg/m$^2$)

40 km grid resolution

200 km grid resolution
South America and Africa

Freitas et al. 2005
Comparison between MODIS Aerosol Optical Thickness - AOT 0.47 um and PM2.5 column integrated.

Work is under way to introduce AOT calculations in RAMS.
Low Troposphere and Long Distance Transport of PM2.5 and CO

Andes

Low Level Jets

Freitas et al. 2005
Low Troposphere and Long Distance Transport of PM2.5 and CO - Andes Low Level Jets

720mbar
NW - Flow  (several local sources)
MODIS aerosol + local sources - 15 km resolution
Solar radiation – 16Z19sep2002

without

and with the aerosol effect
Surface temperature - 16Z19Sep2002

without

and with the aerosol effect
Comparison between AERONET AOT 0.44 um and PM2.5 column integrated.
• Current research:
  • *Role of biomass burning aerosols in the cloud microphysical processes*
Warm clouds

Rainfall accumulation

Aerosol Concentration
Scheme of aerosol effects on precipitation

Accumulated rain

Maritime & moderate (wet) continental clouds (like GATE and PRESTORM)

Dry unstable situation (like Texas clouds)

Aerosol concentration

Khain & Rosenfeld, 2003
Conclusion

• Aerosol effect on microphysics in the transition season in the Amazon provides a good test for new developments

• Preliminary results indicate that aerosol and radiation effects combined change horizontal distribution of precipitation in a regional sense.
Reduction on the Convective precipitation (mm)

\[ \Delta P = (P - P_{\text{aer}}) \]

Longo et al. 2004

Radiative effect only
Vendrasco et al. 2008 conclusions on the radiative effect of biomass burning:

In the mean, the biomass burning radiative forcing tends to decrease the precipitation: thermodynamical effect dominates.

However, very large concentrations of aerosols may lead to an increase in the precipitation due to the dynamical forcing associated to the horizontal pressure gradients.

Thermodynamical versus dynamical forcing →

decrease or increase:

Dynamical forcing is similar to a local breeze effect caused by the smoke plumes
Next step in the academic $\leftrightarrow$ operational interaction:

• inclusion of photochemistry (Ozone...?)
Initial objective:

• Development of a simple model to simulate O3 photochemistry in the urban environment in an operational environment (high level of skill and efficiency);

Initial solution: meteorological model + off line photochemical model

• Problems:
  • Mass conservation
  • Consistency with the meteorological fields: some met. processes occur at very fast timescales – need frequent output – time consuming and memory intensive
  • Lack of possible feedbacks

Final solution:

bring simple photochemistry to RAMS (mesoscale model) – i.e., add photochemistry to tracer component (which includes consistent transport and turbulence model + radiation from the meteorological model.)
Application: Transport of pollutants by the sea-breeze - validation São Paulo case.

• Dispersion model in RAMS (based on the work of Dr. Saulo Freitas)
  – Variable sources (with respect to time);
  – Sinks;
  – Diurnal cycle of emissions is in agreement with anthropogenic sources in TEB;
  – Total emissions:
    • 8.1 g/day/m² type urban 1;
    • 2.67 g/day/m² type urban 2.
CO - Comparison with observations

Santo André

R = 0.794

R = 0.80747

Ibirapuera

R = 0.743

Santo Amaro

R = 0.752
A simple photochemical module in RAMS for operational forecast

- 15 main reactions related with ozone formation
- semi-implicit numerical integration
Main reactions

A) Inorganic

R1) $2\text{NO} + \text{O}_2 = 2\text{NO}_2$
R2) $\text{NO}_2 + h\nu = \text{NO} + \text{O}(^3\text{P})$
R3) $\text{O}(^3\text{P}) + \text{O}_2 + \text{M} = \text{O}_3 + \text{M}$  (M= air)
R4) $\text{O}_3 + \text{NO} = \text{NO}_2 + \text{O}_2$
R5) $\text{O}_3 + \text{NO}_2 = \text{O}_2 + \text{NO}_3$
R6) $\text{O}_3 + h\nu = \text{O}(^1\text{D}) + \text{O}_2$
R7) $\text{O}(^1\text{D}) + \text{H}_2\text{O} = 2\text{HO}$
R8) $\text{HO} + \text{CO} = \text{HO}_2 + \text{CO}_2$
R9) $\text{HO}_2 + \text{NO} = \text{HO} + \text{NO}_2$
R10) $\text{HO}_2 + \text{O}_3 = \text{HO} + 2\text{O}_2$

R1 = $k_1 [\text{NO}]^2 [\text{O}_2]_0$
R2 = $j_2 [\text{NO}_2]$
R3 = $k_3[\text{O}_2]_0[\text{M}]_0[\text{O}(^3\text{P})]$
R4 = $k_4 [\text{NO}][\text{O}_3]$
R5 = $k_5 [\text{NO}_2][\text{O}_3]$
R6 = $j_6 [\text{O}_3]$
R7 = $k_7 [\text{H}_2\text{O}][\text{O}(^1\text{D})]$
R8 = $k_8 [\text{CO}][\text{HO}]$
R9 = $k_9 [\text{NO}][\text{HO}_2]$
R10 = $k_{10} [\text{HO}_2][\text{O}_3]$

B) Organic  (RH – VOC’s )

R11) $\text{RH} + \text{HO} = \text{H}_2\text{O} + \text{RO}_2$
R12) $\text{RO}_2 + \text{NO} = \text{NO}_2 + \text{RCHO} + \text{HO}_2$
R13) $\text{RCHO} + \text{HO} = \text{RCO-O}_2 + \text{H}_2\text{O}$
R14) $\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$
R15) $\text{HO}_2 + \text{RO}_2 = \text{ROOH} + \text{O}_2$

R11 = $k_{11} [\text{RH}][\text{HO}].$
R12 = $k_{12} [\text{RO}_2.][\text{NO}]$
R13 = $k_{13} [\text{RCHO}][\text{HO}]$
R14 = $k_{14} [\text{HO}_2][\text{HO}_2]$
R15 = $k_{15} [\text{HO}_2][\text{RO}_2]$
Emission module

• Base: Information provided by São Paulo’s Environmental Agency (CETESB)
  – Necessity of adjustments in some emissions
  – NO, NO$_2$, CO, VOC, SO$_2$
  – Considers vehicular and industrial emissions
Operational forecast at IAG/USP

- 2 grids (16 and 4 km of horizontal resolution)
- 72 hours of simulation (02 - 05 Aug 99), twice a day - In. Condition of chemical components and aerosols provided by previous forecast - continuous process.
- Initialization: CPTEC/COLA AGCM + observations.
- Time step for chemical reactions 0.5 seconds.
- Different emissions for the two urban types (100% for type 1 and 30% for type 2)
- Boundary conditions provided by CPTEC air quality model
Results (from second grid – 4 km)

Nocturnal max. not well captured in off line models....
Measurements with the INPE Bandeirantes aircraft from 11 to 13 August 1999.

CO
O₃
CCN
Poluição de São Paulo - Vôo de 13/08/99
Concentração de O3

![Graph showing O3 mixing ratio (ppb) over time with various locations and altitudes listed.]

- São M. Paulista: 1.842 m
- Cubatão: 1.645 m
- São M. Paulista: 4.276 m
- Marginal: 2.3500 m
- Perfil: 4.440 m
- Serra do Mar: 1.315 m
- Santos: 1.842 m

Hora do dia: 12:00, 13:00, 14:00, 15:00, 16:00, 17:00, 18:01

O3 mixing ratio (ppb):
- 0
- 5
- 10
- 15
- 20
- 25
- 30
- 35
- 40

NO2:
-.Symbol line for NO2.

O3:
-.Symbol line for O3.

Perfil:
-Perfil Santos 1.842 m
-Perfil São Paulo 4440 m

Cpc:
-13000
-23500
Sugar Cane Burning
(Vendrasco at al. 2006)

- Source model.

<table>
<thead>
<tr>
<th>Constituente</th>
<th>Taxa de emissão [g s$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO</td>
<td>8.200E-01</td>
</tr>
<tr>
<td>NO$_2$</td>
<td>1.600E-01</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>4.797E-01</td>
</tr>
<tr>
<td>CO</td>
<td>1.155E+01</td>
</tr>
<tr>
<td>COV</td>
<td>5.500E-01</td>
</tr>
</tbody>
</table>

EMBRAPA, 1999.
Time of sugar cane burning time - O3

08-14Z

14-20Z

18-23Z
Time of sugar cane burning time - O3

08-14Z

14-20Z

18-23Z
Time of sugar cane burning time - O3

08-14Z

14-20Z

18-23Z
Impact of timing of sugar cane burning in O3 concentration in Sao Paulo
What is going on now:

• Improve VOC’s - more complexity in the chemical component (INPE/CPTEC, IAG/USP);

• Data assimilation during forecast cycle of chemical constituents (remote and direct measurements) - CPTEC

• Conversion to health indicator (INPE/CPTEC, IAG/USP)

• Introduce cloud microphysical effect of aerosols (a PhD thesis was recently completed J. Martins.);

• Field validation: interaction with CETESB (local EPA), LBA program;

• Implementation in other metropolitan areas (RJ - LNCC - Manaus - SIPAM);

• Smaller scales!!! - coupling with fire model? (field data available);
Conclusions:

• Significant progress in modelling of the aerosol emission and transport and inline photochemistry: JGR, Environmental Fluid Mechanics, Revista do Instituto de Estudos Avançados, RBMet, Atmos. Environment

• Involvement of students: began with Saulo Freitas, Karla Longo, Edmilson Freitas, Robinson Negron, J. Martins, PhD programs. New students; 6

• Validation: remote sensing, operational air quality data (CETESB), field campaigns (LBA) and in coming LPB program (Plata Basin).

• Multidisciplinary - vegetation, aerosol and photochemistry, radiative processes...

• Application: operational products already available

• www.cptec.inpe.br - www.master.iag.usp.br
Aerosol and dynamic vegetation

Without aerosols, LAI continuously decreases during transition.

Experiment reflects role of diffuse radiation in C dynamics during transition from dry to wet season in Rondonia.