Air Quality Forecasting

Vincent-Henri.Peuch@meteo.fr
The two faces of Air Pollution

“London” Smog: primary pollution (sulfur dioxide, aerosols, soot, …)

“Los Angeles” Smog: secondary pollution (ozone and photochemical oxidants)

Concentrations of SO2 and « smoke » as well as the death rate during the 1952 smog episode [from Wilkins, 1954]

Variations of NO, NO2 and total oxidant in Pasadena, California, on 23/07/1973 [from Finlayson-Pitts and Pitts, 1977]
“Air quality is a trans-boundary, multi-pollutant/multi-effect environmental problem. Although significant and well directed efforts over more than two decades have led to a reduction in emissions, air pollution in Europe continues to pose risks and have adverse effects on human health, plants and on natural and man-made environments”


Three talks on AQ forecasts:
- introduction, overview and the Prév’Air system
- the RIU / Univ Köln system (H. Elbernh)
- the CMC system (R. Ménard)
Historical evolution of PM pollution (smoke) in Paris as measured by AIRPARIF. Mass is decreasing, but particules number seems to be growing (in the ultrafine mode, which has health impacts).

With increasing knowledge on environmental and health impacts of PM pollution, air quality thresholds become stricter in Europe. Data from [Puteaud, JRC report EUR 20411 EN, 2003].
Ozone background levels have been multiplied by 5 over the last century in Europe [Marenco et al., JGR 1995]. Background values are a key factor in strong regional/continental photochemical events.

**O₃ Pollution**

Current Legislation leads to a 1 to 4 ppb ozone increase in Europe between 2000 and 2020 (22 global models), [Dentener et al., GRL, 2005]. Though precursors are decreasing in Europe and North America, increases in Asia (India, China) appear to maintain and enhance high background ozone at the hemispherical scale.
Uses for RAQ forecasts & models

- Prevent exposure to AQ pollution events
- Regulatory purposes (episodic or long-term measures,...)
- Generate concentration estimates in places without monitors
- Estimate public health impacts from air pollution policies, though extremely high-resolution fields (~100m) are needed
- Explore scenarios, such as climate change, emissions changes
- ...

(From L. G. Anderson)
RAQ model components

- Atmospheric composition, clouds and radiation
- Transport and chemical boundary conditions
- Turbulent and convective mixing
- Met. forcings
- Wet deposition
- Homogeneous and heterogeneous chemistry
- Aerosol processes
- Natural and anthropic emissions
- Dry deposition
- Data assimilation
• Often, RAQ models are CTMs: i.e., they need external meteorological forcings at adapted resolutions (in general: at least every 3h, ~5km).

• The type and number of met. variables needed depend much on the RAQ model. Two extreme strategies are used in the international community, but all possibilities exist in between:
  • minimal set of variables (pressure, temperature, horizontal winds, humidity). This allows flexibility but implies that the RAQ model include many physical parameterizations (turbulent diffusion, convection, cloudiness, rain,…) with room for inconsistencies between the RAQ model and the meteorological model, that provides the forcings. Also, finer resolutions in the RAQ model than in the forcings can be used (describe finer emissions sources,…).
  • used « all » available met. Variables (mass fluxes, vertical velocities, 3D cloud fractions, liquid/solid water content…). This avoids the above shortcomings, but the configuration of the CTM often becomes very specific to its forcing met. model.

• With increasing CPU power available, RAQ models with on-line chemistry are also developing: emissions and « chemical » parameterizations are added in a meteorological model. The main advantage in the RAQ context is to avoid interpolations as much as possible: most often, feedbacks of chemical distributions on dynamics are neglected (no fundamental difference then with the CTM configurations). Still very challenging to use in forecast mode due to CPU costs.
Grids for the RAQ models

• Two competing constraints:
  • the modelling domain must be large enough (continental, hemispheric or global) to reduce the need for external chemical boundary conditions and their impact on the regional simulations
  • the resolution must be fine enough as surface heterogeneities are strong and ozone and PM chemistry are non-linear. Also, surface AQ observations used for model evaluation have generally limited spatial representativity. However, the resolution of the available emissions inventory is a limitation.

• Multi-domain RAQ models generalize in order to address both constraints. Coupling one-ways or two-ways (feed-back of the higher resolution domains on coarser ones).

• A large variety of grids are actually used, like for meteorological models. Similarly, a large variety of advection schemes are used. Popular methods include: PPM, Moments (« Prather ») method, semi-lagrangian methods (mixing ratio or flux forms)… Trade-off: mass and gradients conservation versus CPU/Mem requirements and dependency when increasing the number of tracers (mixing ratios, size bins, moments,…).

• The cost of advective transport is generally small (10%?) in RAQ models compared to integration of stiff ODE chemical systems. For this reason probably, models are generally using grids than spectral decomposition.
MOCAGE (Météo-France) : up to four levels of two-ways nested domain. Here : 4°, 0.5°, 0.1° (Prév’Air configuration)

FAQS (T. Russel, Georgia Tech Univ.) based on Model-3 : structured grids.
ESCOMPTE modelling exercise (18 configurations): forcings make a difference.
Menut et al. (LISA)
• PBL representation in the RAQ model is crucial specially for stable cases. Yet, parameterizations in the CTM are often crude: Kz type.
• There has been quite intense research on transport and mixing in the PBL (LES, chemistry versus mixing regimes,…). However, results have still to be transferred to the RAQ community.
• Plume-In-Grid approaches.
• Urban heat island effects.
Emissions

• Like for global modelling, natural and anthropic emissions is a crucial input to AQ modelling. At high resolution (~1 km or less), a bottom-up approach is needed (assimilation and inverse modelling?). Many efforts at the level of large cities, regions and countries are on-going in Europe (often for modelling and forecast needs), but often with varying methodologies.
• Emissions prepared for the EMEP model (EMEP center at met.no) is a reference but resolution is only 50km. The GENEMIS project (lead by Univ. Stuttgart) has finished with EUROTRAC-2, but some efforts are maintained. Some other groups have specialized also in the field: RIVM,…
• However, there is still a need for freely available « homogeneous » high temporal and spatial resolution emissions in Europe today. RAQ modelling teams across Europe often develop their own emissions inventory using specific regional inventories and « more or less » sophisticated down-scaling methods of EMEP or GENEMIS data.
• In addition:
  • specific PM emissions inventories are still rare; they are often based on CO emissions and BC/CO ratios.
  • many emissions sources depend upon the meteorology and land-use; for the sake of consistency, they should be parameterized in the model (rather than using inventories).
  • speciation of VOC in the emissions and in the chemical scheme of the RAQ model is a major problem
Anthropic emissions in France 2003, by compounds and activity types (CITEPA, see www.citepa.org).

EMEP model (50km x 50km) NOx emissions for 1999, in tons per grid-cell (www.emep.int).
The Paris area example:
Space and time evolution of emissions and primary pollutant concentrations.
Formation of radicals

Ozone PBL and tropospheric chemistry

HNO₃ + OH → NO₂ + HO₂

NO₂ + NO → O₃ + NO

O₃ + HO₂ → RO₂ + NO₂

RO₂ + VOC → HO₂ + RO

Deposition
Ozone isopleth diagrams

Though obtained in 0D configurations, such diagrams are very useful to characterize chemical schemes (the actual set of compounds and reaction taken into account).

The same ozone level can be reached in totally different chemical regimes!
Ozone plumes simulation

- State-of-the-art RAQ chemical schemes consider 60-80 species or group of species. Differences come primarily from the method used to account for VOCs. Popular schemes are: RACM/RADM, CB4, SAPRC,…

CHIMERE simulation 17/07/99 16 UTC (R. Vautard, IPSL)
OH and chemical regimes (ESCOMPTE)
Use a MOCAGE 6-days simulation and compute a zonal climatology (1°, 3h) for all compounds. Disable two-ways nesting. Compare the climatological BC run (CLIM) with the reference run (CTRL) over the fine resolution domain.
Vertical exchanges of ozone
A cooperative system for large scale air quality forecasting and mapping over Western Europe and France; developed in 2003 upon an initiative of the French Ministry of Ecology.

Operational purposes: in France, since 2004, public information related to pollution episodes (threshold exceedances) can be driven by forecasts (not only observations).

<table>
<thead>
<tr>
<th>INERIS</th>
<th>Public organization under the supervision of the Ministry of Ecology</th>
<th>Builds up and hosts the prev'air system AQ expertise for the Ministry</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADEME</td>
<td>National Agency of Environment</td>
<td>Builds up and hosts the NRT database AQ expertise for the Ministry</td>
</tr>
<tr>
<td>CNRS</td>
<td>National Research Centre</td>
<td>Model development: CHIMERE</td>
</tr>
<tr>
<td>Météo France</td>
<td>National Meteorological service</td>
<td>Model development: MOCAGE + meteorological forecasts</td>
</tr>
</tbody>
</table>
• **3D CTMs:** 
  – **CHIMERE** (CNRS-INERIS) 
  – **MOCAGE** (Météo-France) 

• Meteorological forecasts:
  – **AVN / NCEP** global data (+ **MM5** for higher resolution forecasts) 
  – **ARPEGE, ALADIN** 

• Emissions inventory based upon EMEP (downscaling to ~10km resolution over France)

• NRT observations data from local AQ monitoring organizations (AASQA) ; bilateral cooperation with other countries
• Daily peak and averaged concentration maps for: D+0, D+1 and D+2
• Forecasts available D+0 (early morning)
• Pollutants: O₃, NO₂ (France and Europe) and particulate matter (Europe)
• NRT Observations (hourly O₃, NO₂, PM2.5 and PM10)
• Analyses of surface obs for the previous and the current day
Example of forecasts
Surface ozone
MOCAGE 0.1° (ALADIN)

- Rural
- Intermediate
- Urban
AIRMARAIX (summer 2002)

17/06 to 21/07 2002
Saturday 03/09/2005

Legend: Ozone (µg/m³) Surface obs du 20050903 MAX model: echu0

Legend: dioxyde d'azote (µg/m³) Surface obs du 20050903 MAX model: echu0

Legend: Ozone (µg/m³) Surface obs du 20050903 MAX model: echu2

Legend: dioxyde d'azote (µg/m³) Surface obs du 20050903 MAX model: echu2

Marseilles (D)

Marseilles (D+2)
Saturday 03/09/2005

Paris (D)

Lyon-Grenoble (D)
Montge en Goële (J)
Moure-Nègre (J+1)
Puy de Dome (J+1)
### Skill-score evaluation

#### Ozone Peak Scores

<table>
<thead>
<tr>
<th>Averaged Observation (μg/m³)</th>
<th>Date</th>
<th>Rural stations</th>
<th>Suburban Stations</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>J - 1</td>
<td>105.9 (Nbr Obs: 5295)</td>
<td>102.4 (Nbr Obs: 11596)</td>
</tr>
<tr>
<td></td>
<td>J + 0</td>
<td>106.0 (Nbr Obs: 5251)</td>
<td>102.5 (Nbr Obs: 11503)</td>
</tr>
<tr>
<td></td>
<td>J + 1</td>
<td>106.2 (Nbr Obs: 5207)</td>
<td>102.7 (Nbr Obs: 11408)</td>
</tr>
<tr>
<td></td>
<td>J + 2</td>
<td>106.3 (Nbr Obs: 5162)</td>
<td>102.8 (Nbr Obs: 11319)</td>
</tr>
<tr>
<td><strong>Averaged Prediction (μg/m³)</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J - 1</td>
<td>104.6</td>
<td></td>
<td>104.5</td>
</tr>
<tr>
<td>J + 0</td>
<td>103.9</td>
<td></td>
<td>103.9</td>
</tr>
<tr>
<td>J + 1</td>
<td>103.3</td>
<td></td>
<td>103.1</td>
</tr>
<tr>
<td>J + 2</td>
<td>103.0</td>
<td></td>
<td>103.0</td>
</tr>
<tr>
<td><strong>Normalised Bias (%)</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J - 1</td>
<td>1.8</td>
<td></td>
<td>4.9</td>
</tr>
<tr>
<td>J + 0</td>
<td>1.2</td>
<td></td>
<td>4.3</td>
</tr>
<tr>
<td>J + 1</td>
<td>0.7</td>
<td></td>
<td>3.7</td>
</tr>
<tr>
<td>J + 2</td>
<td>0.7</td>
<td></td>
<td>3.7</td>
</tr>
<tr>
<td><strong>NMSE (%)</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J - 1</td>
<td>18.1</td>
<td></td>
<td>17.9</td>
</tr>
<tr>
<td>J + 0</td>
<td>18.9</td>
<td></td>
<td>18.4</td>
</tr>
<tr>
<td>J + 1</td>
<td>19.4</td>
<td></td>
<td>19.3</td>
</tr>
<tr>
<td>J + 2</td>
<td>20.3</td>
<td></td>
<td>20.3</td>
</tr>
<tr>
<td><strong>Correlation</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J - 1</td>
<td>0.82</td>
<td></td>
<td>0.83</td>
</tr>
<tr>
<td>J + 0</td>
<td>0.79</td>
<td></td>
<td>0.81</td>
</tr>
<tr>
<td>J + 1</td>
<td>0.77</td>
<td></td>
<td>0.80</td>
</tr>
<tr>
<td>J + 2</td>
<td>0.73</td>
<td></td>
<td>0.75</td>
</tr>
<tr>
<td><strong>E20% (%)</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J - 1</td>
<td>83</td>
<td></td>
<td>83</td>
</tr>
<tr>
<td>J + 0</td>
<td>81</td>
<td></td>
<td>82</td>
</tr>
<tr>
<td>J + 1</td>
<td>80</td>
<td></td>
<td>80</td>
</tr>
<tr>
<td>J + 2</td>
<td>77</td>
<td></td>
<td>78</td>
</tr>
</tbody>
</table>

May-September 2004 for the CHIMERE model
Statistical post-treatment of deterministic forecasts

- Multi-component linear regression with predictor selection
- Coefficients are specific to each site / hour of the day
- Used in an operational context

Result: [O3], then HU et T, then Tx, FF and FF(0h), then DT and day-type.

Potential predictors considered:
- MOCAGE forecast: [O3]
- ARPEGE/ALADIN forecast:
  - T, humidity, wind velocity
  - Tmax, (Tmax-Tmin)
  - FF(0h)
- day type: week or week-end

Relative frequency of selection of the day type versus hour of the day.
Hybrid determinitic and statistical forecasts allows scores over 90% in determining the ozone AQ index (10 levels in France) with an error of less than 1.
(Example here: summer 2004; Fontainebleau AIRPARIF site is in Ile-de-France)
June-August 2003 heat-wave

Number of days with $T_{\text{max}} > 35^\circ$

Number of days with $T_{\text{max}} > 40^\circ$
Jours avec pic dépassant 120 microgrammes.m⁻³
(mai à septembre 2003)

Jours avec pic dépassant 150 microgrammes.m⁻³
(mai à septembre 2003)

Jours avec pic dépassant 180 microgrammes.m⁻³
(mai à septembre 2003)

Jours avec pic dépassant 240 microgrammes.m⁻³
(mai à septembre 2003)

- Observations
- Mocage + AS (J)
- Mocage + AS (J+1)
- Mocage + AS (J+2)
- Mocage + AS (J+3)

Nombre total de jours
Some conclusions

• RAQ modelling and forecasting is a fast developing field. There are many more models than in meteorology. However, progress are often dependent upon progress in meteorological modelling (PBL, clouds, rain,...). Current PCs or clusters of PCs can be used for the forecasts.
• Off-line (CTM) approaches are more frequent than on-line coupled approaches, specially for forecasts. However, this is evolving with increasing CPU power at hand.
• Efforts have to be joined to obtain high-resolution emissions over Europe, specially for particles but also for ozone precursors. Assimilation (or inverse modelling) is an interesting path (see presentation by H. Elberb).
• Some centers in Europe perform today operational forecasts up to 3 or 4 days. Many more centers can do it during periods of time (campaigns,…).
• Access to NRT observations is very important for forecasts evaluation and NRT expertise by human AQ forecasters. Currently, few models include assimilation of surface data in their operational suite. However, most can do it in « research » mode. Skill-score indicators have still to be agreed upon. Work with national/regional AQ and environment agencies is mandatory.
• The importance of chemical boundary conditions is more and more recognized and many centers are developing hemispheric or global domains within their RAQ systems.

The GEMS project will benefit to all these points!
Physique et chimie de l'atmosphère

Belin

[1] (to appear, october 2005) and references therein