

Comparison of photochemical models UAM-V and AIRQUAL in Lyon area by PSA, Renault and Total Fina Elf

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1 Introduction

French oil companies and cars manufacturers have put their strength together in order to make regional air quality modelling. A common project, which will be presented at the conference, dealt with the simulation of a pollution episode that occurred over Lyon, a city of France.

The city of Lyon was selected because it was one of the 11 cities for which air quality evolution in 2010 had to be modelled within the program Auto Oil 2 of the European Commission. This programme, as well as its predecessor Auto Oil 1, was set up under the framework of European regulatory purposes on air quality. A large part of it was devoted to the study of urban impact assessment by using 3D Eulerian air quality models describing the transport and dispersion of chemically reactive pollutants for ten regional domains containing the 11 cities. Lyon had already been studied during Auto Oil 1, and was the only French city of the 2 programmes.

Trying to study Lyon air quality sensitivity to NO_x and COV emissions, in parallel to Auto Oil 2, the French Oil companies and car manufacturers, have selected a domain of 200 km over 200 km centred on Lyon, over which they have applied modelling tools. Simulations were driven over a period of 3 days (June 26th - 28th, 1995) that included an extreme photochemical pollution episode by ozone on the last two days. The year 1995 was chosen because it was the reference year for Auto Oil 2.

1.1 Modelling tools

The French oil companies and car manufacturers started their work by using the modelling chain distributed by the US company SAI (ICF Consulting). This chain includes the meteorological model SAIMM, the transport-dispersion model UAM-V, and the chemical reactions scheme Carbon Bound IV [1]. This modelling system is well known throughout scientific and regulatory community.

On the other hand, the French modelling system AZUR, developed by EDF (French Electric Company), IFP (French Petroleum Institute) and LISA (Laboratory of Atmospheric Sciences, University) was about to be adopted by AIRPARIF, the Parisian Air Quality Survey Association, as a modelling tool. The AZUR chain includes the meteorological model MINERVE, the 3D Eulerian transport-dispersion model AIRQUAL, and the chemical scheme MoCA 2.1 [2].

UAM-V and AIRQUAL are both transport-dispersion 3D Eulerian models, equivalent in complexity, and can be used for the same kind of applications. In a way, they are direct competitors. A program presented by us, the French oil companies and car manufacturers, in collaboration with IFP and ARIA Technologies, under the auspices of the FSH (« Fond de Soutien aux hydrocarbures ») dealt with a comparison of UAM-V/CB-IV and AIRQUAL/MoCA 2.1 models over Lyon regional domain under same meteorological and emission data. The meteorological fields for the two dispersion models were prepared with the same model MINERVE. Our modelling chain is resumed in Figure 1.

This study started with the constitution of a new emission inventory for the domain. This inventory takes into account all data we could gather. The geographical distribution of emissions according to the source type is not done as a function of the population density. Hence, this point may be different from the European Commission inventory. For this emission inventory we focused on detailed road transport emissions.

The two models have been compared by the way of sensitivity experiments to emissions and boundary conditions.

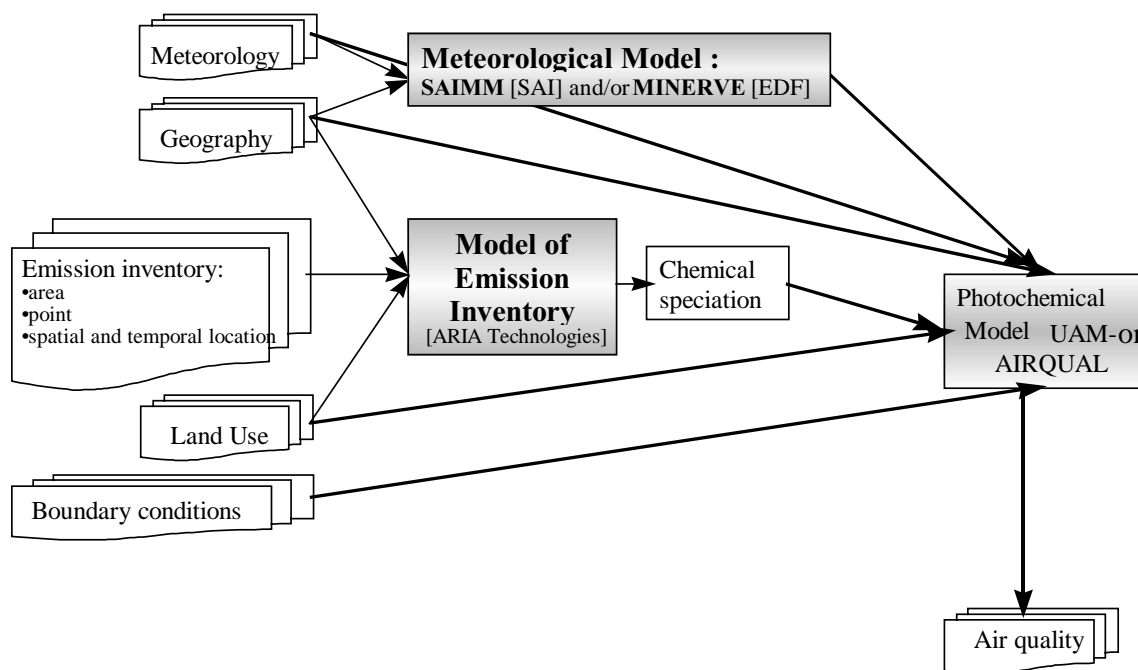


Figure 1 Air Quality Modelling Chain used during this study.

1.2 Emissions inventory

In a preliminary step we decided to update the emission inventory because the one we had before showed missing data, distribution according to population density only, tuning factors, etc. We also wanted to increase the precision of traffic scenarios.

The data and the distribution methods (time and space) that have been used are showed in table 1.

Generally, in order to establish these updated emission data, we have used a top-down methodology. That means that we have taken annual values of NO_x, VOC and CO emissions, which were given for administrative districts only, and by using space and time functions, we have obtained hourly and gridded data.

Table 1 Data used to update emissions inventory for Lyon region.

Emission Sources	Type of data	Reference
<u>Low level emissions (except traffic)</u>	<ul style="list-style-type: none"> Annual emissions by district (regional programmes for Air Quality, PRQA 94 for Rhône-Alpes, Auvergne, Bourgogne, Franche-Comté) VOC speciation by SNAP profile Spatial distribution, Time distribution. 	<ul style="list-style-type: none"> CITEPA CITEPA, GENEMIS CITEPA our work, + DRIRE, CITEPA, AIRPARIF
<u>Traffic emissions City of Lyon</u>	<ul style="list-style-type: none"> Output of a traffic model over LYON (a 50 km square over Lyon) Emission factors Car pool Spatial distribution Time distribution VOC speciation by SNAP profile 	<ul style="list-style-type: none"> CETE COPERT 2 CITEPA road web from traffic model CETE CETE CITEPA, GENEMIS
<u>Traffic emissions Outside Lyon</u>	<ul style="list-style-type: none"> same as low level emissions except for time distribution taken as above 	<ul style="list-style-type: none"> same as low level emissions except for time distribution taken as above from CETE
<u>Elevated point sources</u>	<ul style="list-style-type: none"> Annual emissions by district (regional programmes for Air Quality, PRQA 94 for Rhône-Alpes, Auvergne, Bourgogne, Franche-Comté) DRIRE 95 data for Rhône-Alpes, Physical data (\emptyset, height, gas speed, Temperature), VOC speciation by US EPA profile, Position : centre of grid cells containing address Time distribution. 	<ul style="list-style-type: none"> CITEPA DRIRE directly from industries, DRIRE US EPA cartes bleues IGN (conversion address into UTM) our work, + DRIRE, CITEPA, AIRPARIF

An exception was for traffic emissions. Officials could make available traffic data for main roads of our domain centre (Lyon and suburbs), on which emission factors, which were functions of vehicle speed, car pool, and statistics, could be applied. This higher level of detail for traffic emissions in one of the main improvements : traffic is no more proportional to population density which is a wrong criteria for freeways. That methodology enables us to make more precise traffic scenarios.

But note that compared to Auto Oil 2 emissions data, we obtain, on an annual basis, emissions which are higher from a factor 2.5 for NO_x and VOC in the central 100 km x 100 km domain (we had Auto Oil 2 data averaged over this 100x100 km² domain, only). These discrepancies appear to be in the estimations of traffic emissions. From our side, we are in accordance with official CITEPA data of traffic emissions for the Lyon and suburbs domain.

1.3 Base cases comparison

The above emission inventory has been used together with meteorological data (obtained with ARIA's model MINERVE) to run base cases with AIRQUAL and UAM-V. In addition to these common data bases, the two 3D Eulerian models were used with same horizontal resolution, and same vertical levels, at least for lower levels since AIRQUAL has more vertical levels.

The chemical codes of the two models are based on very different assumptions for chemical reactions reduction. We will not recall them here and will only give references to these. A description of Carbon Bond IV in UAM-V can be found in [1] and MoCA in AIRQUAL is described in [2].

The two base cases show discrepancies for ozone distribution on the middle day (June, 27th). Since CO concentrations distributions simulated by the two models are not so different, we concluded that the discrepancies are not mainly due to a different treatment of dynamics but to the chemical schemes.

The base cases simulations could be compared to few measurements time series obtained from air quality survey stations. Some difficulties are met with these comparisons. First, we compare data which have different meanings in term of space scale: measurements are representative of an undetermined volume around the emplacement of the captor, while simulation results are averaged over 16 km² in horizontal and 50 metres in vertical. Secondly, the place where larger discrepancies between AIRQUAL and UAM-V occurred were not documented by air quality survey stations.

With this in mind, we could only conclude to gross conclusions. No model could simulate the fact that according to the place the ozone maximum could be on the 27th or 28th of June. No model was better than the other one on all points. We had not enough element to conclude on the best candidate.

1.4 Sensitivity experiments

In addition to the base cases, we wanted to estimate the models sensitivities in response to input data uncertainties, and to know the level of significance of these sensitivities. To that aim, we have run 8 sensitivity simulations as part of a design of experiments. This has been done in parallel for AIRQUAL and UAM-V for the same 3 days as previously (meteorological data unchanged).

The design of experiments involved variations of biogenic VOC emissions (500% variation around base case emission inventory), low level VOC emissions (50% variation), VOC emitted by traffic (50% variation), NO_x emitted by traffic (30% variation), NO_x from elevated point sources (30% variation), and boundary conditions (variable or constant values). The above intervals correspond to uncertainties bars commonly admitted for emission inventories.

We have looked at criteria like NO_x and O₃ concentrations averaged over a day, distance of ozone maximum to Lyon city centre, differences between measurements and simulated data for each site of air quality survey.

NO_x and O₃ concentrations simulated by AIRQUAL and UAM-V are significantly sensitive to NO_x emitted by traffic and to COV emitted by traffic. The main difference is that on a large scale UAM-V does not seem to be significantly sensitive to variation of other parameters while AIRQUAL is sensitive to all of them but with a large variability according to the day (i.e. according to meteorology) without knowing where the truth is. These differences may be due among other causes to the chemical schemes or to a different ratio for the split of NO_x emissions between NO and NO₂.

As for the place of ozone maximum, it is closer to Lyon in AIRQUAL than in UAM-V. But, the distance between Lyon city centre and the ozone maximum is more sensitive to the experiment in AIRQUAL than in UAM-V and seems to be controlled by the ratio "VOC emissions/NO_x emissions" (NO_x or VOC emissions mean in average over the whole domain).

Curves for individual sensitivity experiments show that the ratio "VOC emissions/NO_x emissions" can control the time of ozone peaks occurrence but can not compensate all discrepancies between models and measurements.

1.5 *General conclusions*

The main conclusions of our study are the following:

A complete emission inventory for Lyon city and surroundings have been made by French Oil companies and car manufacturers with the help of IFP and ARIA Technologies.

In addition to the comparison between UAM-V and AIRQUAL with the same meteorological data, a base case and a design of experiments have been realised with UAM-V using SAIMM meteorological fields: in that case, results, differences to measurements, space distribution and sensitivity are strongly different to those put in evidence with the use of MINERVE meteorological data. There are improvements of some criteria but also damages of others. This is a confirmation of the fact that model sensitivity is very dependent on the quality of meteorology simulation.

The comparison between the two models could not tell which one is the best. There are not enough air quality survey sites in the area to permit a real validation of the models.

A tuning of emission data can modify some peaks but can not improve all aspects.

In this design of experiments we have shown that AIRQUAL is sensitive to a larger variety of parameters than UAM-V which focuses more on vehicles emissions.

Finally, should we do again the design of experiments, we may choose to study also sensitivity to the ratio "VOC emissions/NO_x emissions".

References

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