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# **REGIONAL APPLICATION OF THE** UAM IV PHOTOCHEMICAL OXIDANTS FORMATION 3-D MODE Nollet V., Caplain I., Déchaux J.C. and Hanoune B.

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## **Domain and data base**

As far as the formation of tropospheric photochemical oxidants is concerned, modeling is a tool that can not be ignored to help to understand the high complexity of this problem. In this paper we present a regional application of a 3-D eulerian model, the Urban Airshed Model (UAM). We have chosen a surface area about fifteen thousand square kilometers comprising the industrial zones and the conurbation areas in the Nord Pas de Calais region and the northwest part of Belgium (Figure 1).



Boundary conditions from Kent (UK), Belgium and french county Picardie are taken into account. Basic parameters of the inventory are a four square kilometer grid with a high level of database quality.

Figure 2 shows the structure of the inventory and Figure 3 the spatialisation procedure.



## The Urban Airshed model – UAM IV

The Urban Airshed Model (UAM) (Reynolds et al., 1979) is an Eulerian air quality model, usually applied to 8- to 72-hour smog episodes. The structure of the model can be presented as a 3-D grid covering the domain (*Figure 4*).

**UST** 



NAF - SNAP (a SNAP activity can be linked with several NAF codes)

(142 standardized files) containing specific sources, emission factors & energy consumptions. - 1 EXCEL file per actualization procedures.

Figure 2. Structure of the emission inventory.



**Figure 3.** Spatialization of the emission inventory.

## **Photolysis frequencies calculation**

The photolysis frequencies can be expressed as an integration of the product of the molecular absorption coefficient, the quantum yield and the solar actinic flux, spherically integrated radiance, at the altitude of measurement :



### Figure 4 : UAM IV Structure

The model calculates the concentrations of both inert and chemically reactive pollutants by simulating the physical and chemical processes in the atmosphere that affect pollutant concentrations : advection, turbulent diffusion, dry deposition, emissions and chemical reactions. Each of them is represented by a mathematical term of the atmospheric diffusion equation wich is solved by the UAM :



with:

: mean concentration of species i ♦ T : temperature U,v,w : horizontal and vertical wind speed components  $\mathbf{V}_{\mathbf{H}}, \mathbf{K}_{\mathbf{V}}$ : horizontal and vertical turbulent diffusion coefficients  $\mathbf{b}$   $\mathbf{R}_{i}$ : net rate of production of pollutant i by chemical reactions S<sub>i</sub>: emission rate of pollutant i  $L_i$ : net rate of removal of pollutant i by surface uptake processes

Such an air quality eulerian model demands numerous input data all over the domain concerned. They are divided into four categories : the meteorological data, the emissions, the initial and boundary conditions and the chemical parameters. Those data are presented in the table 1.

## $J_{S} = \int_{\lambda}^{\lambda_{2}} \sigma(\lambda, T) \cdot \phi(\lambda, T) \cdot F(\lambda) \cdot d\lambda$

Actinic flux should either be measured by actinic UV spectroradiometry or determined by theoretical calculations using a radiative transfer code. It also can be calculated by the way of an irradiance (surface integrated radiance) conversion method, as in this work.

The spectral irradiance was measured directly on may 1998 by cosine weighting detectors in the 300-450 nm wavelength range. A shadower was used to measure the diffuse part of the irradiance. Aerosol optical depth was also measured in order to convert these irradiance measurements into actinic fluxes.

The calculated actinic flux is convoluted with molecular absorption coefficients and the quantum yields values from the litterature.

For example the NO<sub>2</sub> photolysis frequencies calculated from irradiance measurements are compared on figure 5 with theoretical estimates of photolytic rate constants usually used in relevant photochemical smog models.

**Figure 5** : NO<sub>2</sub> photolysis frequencies for the May 13th 1998. Comparison between theoretical estimates of photolytic rate constants (Kenneth L. et al., 1980 and Jeffries H.E. et al., 1987) and calculated with our measurements

Meteorological data	Emissions data	Initial and boundary conditions	Chemical parameter s
Ground temperature	Stationnary sources	Surface type	Chemical mechanism
Vertical gradient of temperature	Mobile sources	Initial concentration s	Kinetic data
Mixing height		Concentratio ns at lateral boundaries	
Wind field		Concentratio ns at the top of the domain	
Atmospheric pressure			
Water concentration			
Solar radiation			

## **Chemical mechanisms**

An optimization of the chemical module and a study of sensitivity were carried out in order to introduce a better representation of the speciation of volatile organic compounds.

We used the version UAM/FCM (Flexible Chemical Mechanism) model.

Two mechanisms were used, the UAM default mechanism (Carbon Bond IV) and a more explicit one (SAPRC99).

## **Results and discussion**

During the period May 12 to 15th 1998, exceptional meteorological conditions for this time of year resulted into high ozone concentrations as measured by the regional french monitoring networks, namely AREMALM, AREMARTOIS, AREMASSE and the belgium network CELINE. Several critical exceedances to national standards were observed. The modeling domain we chose for the study is presented in figure 6. It includes : the main primary pollutants sources in the Nord-Pas de Calais region, i.e. : the Lille urban area, the urban and industrial Dunkerque area, most of the monitoring stations of the four networks of the region quoted before, and a few stations of the belgium CELINE monitoring network. The location of those stations is given in figure 7.



#### **Carbon Bond IV** mechanism

#### Mechanism condensed in families of structural

reactivity. A given molecule may be distributed in several families according to the type of bond (CC or CO) constituting it.

3 explicit species : ETH, FORM, ISOP

Structural families (5 species)

PAR (alkane), OLE (C=C), ALD2 (CHO) TOL (toluene and monosubstituted aromatics) XYL (xylene and disubstituted aromatics)

**35** species B6 reactions of which **11** photolytics

SAPRC99 mechanism

Specified mechanism represented by molecular families classified according to their reactivity with the OH radical.

• 18 explicit species : HCHO, ACET, MeOH...

Molecular families (17 species)

OLE (alkene), KET (ketone), ALK (alkane), ALD1 (aldehyde), BALD (benzaldehyde and other aromatic aldehydes)...

**71** species 186 reactions of which **27** photolytics



Figure 8 : Comparison of the measured and calculated ozone concentrations using two different mechanisms – Inland station

Figure 9 : Comparison of the measured and calculated ozone concentrations using two different mechanisms – Coastal station

Figure 6 : Modeling domain



We found that the model gives a satisfactory agreement concerning the formation of tropospheric ozone as far as inland monitoring stations used for comparing field measures and model calculated data are concerned (figure 8). However we have to take special care about the limit conditions. Therefore an extension of the modeling domain to a larger area is necessary in the future, in order to globally decrease the model sensitivity to the limit conditions. It is clear that this will involve a better partnership with our british and belgian neighboring teams.

It turned out that the modeling achievement was far less satisfactory as far as the coastal monitoring stations are concerned (figure 9). It is clear we have a lack of input data in this field concerning the sea breeze effect and the heterogeneous part of chemistry.

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