EMICAT2000: DEVELOPMENT OF A HIGH SPATIAL RESOLUTION EMISSION MODEL FROM THE NORTHEASTERN IBERIAN PENINSULA USED WITHIN THE MODELS-3/CMAQ FRAMEWORK

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1.0 INTRODUCTION

Emission inventories files required by Models-3/CMAQ for applications in the United States are processed by tools such as MEPPS or SMOKE, integrating national or regional emission databases with results by emission models (e.g. MOBILE6, BEIS3). Application and exploitation of Models-3/CMAQ in other regions is conditioned to the applicability and potential adaptation of these emission tools; nevertheless, flexibility of the model allows the use of specific emission models developed with additional tools and according to the proper characteristics of the zone under study, which can be used as a more accurate alternative.

We developed the EMICAT2000 emission model for its implementation within Models-3/CMAQ applications in the northeastern Iberian Peninsula (Catalonia, Spain). This region has a complex topography, showing marked changes of relief, climate and vegetation, into a relative small territory. Air pollutants emissions are related with ozone (O_3) pollution episodes, mainly in summer-time. EMICAT2000 is a GIS emission model developed with high spatial ($1km^2$) and time (1h) resolutions, to provide emissions of the most important air pollutants for this complex region.

2.0 EMISSION SOURCES

EMICAT2000 was developed prioritizing O_3 precursors (NO_x, NMVOCs), and considering the most important emitter sources: on-road traffic, vegetation, and industries. The on-road traffic emission model includes the hot exhaust, cold exhaust and evaporative emissions, using a digital map of the all the highways and the most important roads and streets (daily average traffic > 3000).

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2.1 On-road traffic

EMICAT2000 uses the method and emission factors of the European model EMEP/CORINAIR – COPERTIII as basis, and includes monthly, daily and hourly traffic profiles; differencing the vehicle park composition between weekdays and weekends.

Three kinds of emissions were included: (1) *hot exhaust*, (2) *cold,* and (3) *evaporative emissions*. Hot exhaust emissions were estimated using equation (1):

$$E_r^{ihot}(k,d) = \sum_{j=1}^{n} Clf.Crd.DAT_{rj}(k).L_r(k).F_j^{ihot}(s_r) \quad (1)$$

where E_r^{ihot} *(k, d)* (g d^{-1}) is the hot exhaust emission of the pollutant *i* during one day in the road section *r* (urban, rural or highway type) allocated into the cell k^{th}, F_j^{ihot} (s_r) (g km^{-1}, it is an function of the speed s_r) is the emission factor of the pollutant *i* for the vehicle *j*, $L_r(k)$ (km) is the length of the road section *r*, $DAT_{rj}(k)$ (number of vehicles per day) is the daily average traffic of the vehicle *j*, *Clf* is the coefficient for daily traffic (weekday or weekend), *Crd* is the ratio between daily traffic for a specific month and DAT; and *n* (equal to 36) is the number of vehicles categories.

Full description of model, modeling hypothesis, and exploitation of results (weekday vs. weekend on-road traffic emissions) are described in Parra (2004).

2.2 Industries

We included hourly real records for some stacks, which were connected to the emission monitoring network of the Environmental Department of the Catalonia Government. Other industrial emissions were estimated using the basic emission model (activity level x emission factor); e.g., equation (2) represents the emission model used for power generation.

$$E_{ij}(k,h) = 1000000.F_{hj}F_{dj}F_{mj}.PG_j(k).EF_{ij} \quad (2)$$

where $E_{ij}(k, h)$ (g h^{-1}) is the hourly emission of the pollutant i due to the power generation of the central j, which is allocated in the k^{th} cell; F_{hj}, F_{dj} and F_{mj} are the hourly, daily and monthly generation fractions; $PG_j(k)$ is the annual power generation (GWh yr^{-1}) and EF_{ij} is the respective emission factor (g kWh^{-1}).

2.3 Vegetation

The emission model for vegetation (isoprene, monoterpenes and other NMVOCs) describes the particular emitter behavior of some Mediterranean species. Emission factors were defined according to land-use categories, as result of an exhaustive selection of emission factors of the most important vegetal species. A huge database of hourly records of superficial temperature and solar radiation was incorporated.

Isoprene emission model is described by equation (3):

$$E_{iso}(k,h) = EF_j^{iso}.ECF(T,P).FBD_j.A \quad (3)$$

where A is the area of each grid cell (1km^2), FBD_j is the foliar biomass density (g m^{-2}) of the j land-use category, $ECF(T,P)$ is the environmental correction factor (adimensional) owing to temperature and photosynthetically active radiation, EF_j^{iso} is the standard isoprene emission factor (µg g^{-1} h^{-1}) and $E_{iso}(k, h)$ is the hourly (g h^{-1}) isoprene emission.

Detailed explanation of model and results obtained from this source are described in Parra *et al.* (2004)

2.4 Other sources

Emissions by fossil fuel consumption and residential and commercial solvent use were also included.

2.5 Speciation

Emissions were speciated according to the categories of the lumped-structure Carbon Bond IV chemical mechanism (CBM-IV).

3.0 RESULTS

3.1 Annual emissions

Primary air pollutants reached 599 kt yr^{-1}, corresponding to 267 kt of CO (45%), 137 kt of NMVOCs (23%), 107 kt of NO_x (18%), 65 kt of SO_2 (11%) and 23 kt of TSP (4%). NMVOCs sources are more diverse, representing on-road traffic a 36%, 34% due to vegetation, 17% to industries and 13% to use of solvents. Regarding to NO_x, 58% were emitted by on-road traffic and 39% by industries. Last percentage includes 14% from power generation, 9% from cement production and 8% from oil refining.

Figure 1 shows the annual CO emission distribution. Higher values are mainly located on the Metropolitan Area of Barcelona and on the axis of highways following the coastline. Figure 2 shows the industrial sources included in EMICAT2000. Figure 3 depicts the annual biogenic NMVOCs emission, which is mainly produced by shrub lands, coniferous and deciduous forest. The sources included define the spatial and temporal configuration of emissions. The potential aggregation of other sources will have a minor contribution.

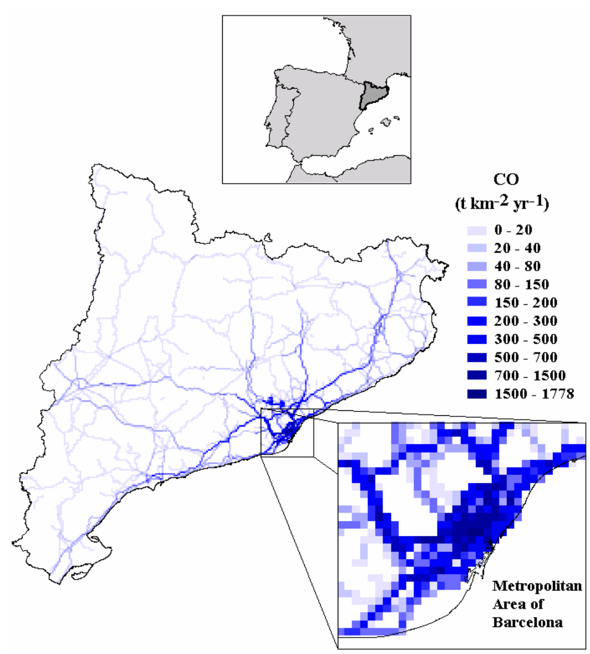

Fig. 1 Location of Catalonia and CO emission distribution due to on-road traffic during the year 2000.

3.2 Monthly emissions

Higher emissions of O_3 precursors take place in summertime (Figure 4). NO_x increase is mainly due to a higher traffic, especially by the influence of foreign tourism vehicles and vacation period.

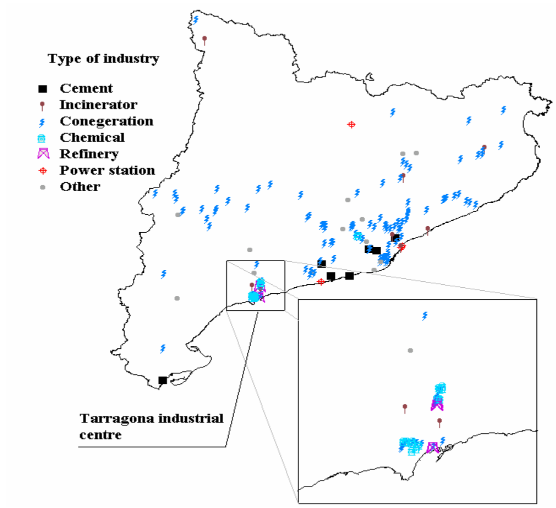

Fig. 2 Industrial sources included in EMICAT2000

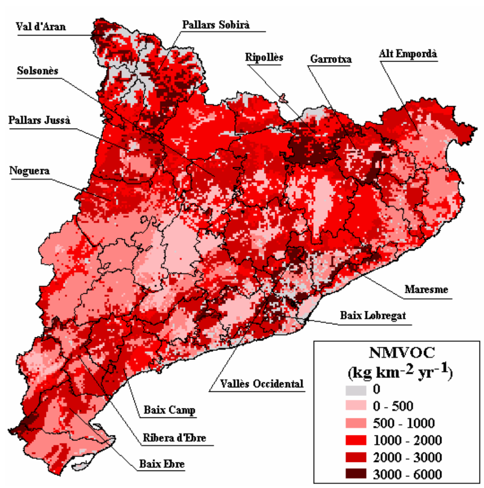

Fig. 3 Biogenic NMVOCs emission in the northeastern Iberian Peninsula during 2000. Main emitter sources are shrub lands, coniferous and deciduous forest

Increasing of NMVOCs is explained by the highest temperature and solar radiation, implying important vegetation and on-road traffic evaporative emissions. These are the causes that most of O_3 exceedances are present during summertime in the northeastern Iberian Peninsula. There is a great influence of the vegetation profile.

3.3 Hourly emissions

Figure 5 shows the speciated NMVOCs contribution by sectors during 14 August, 2000. PAR is the main lumped-species emitted (76%), although it is the least reactive.

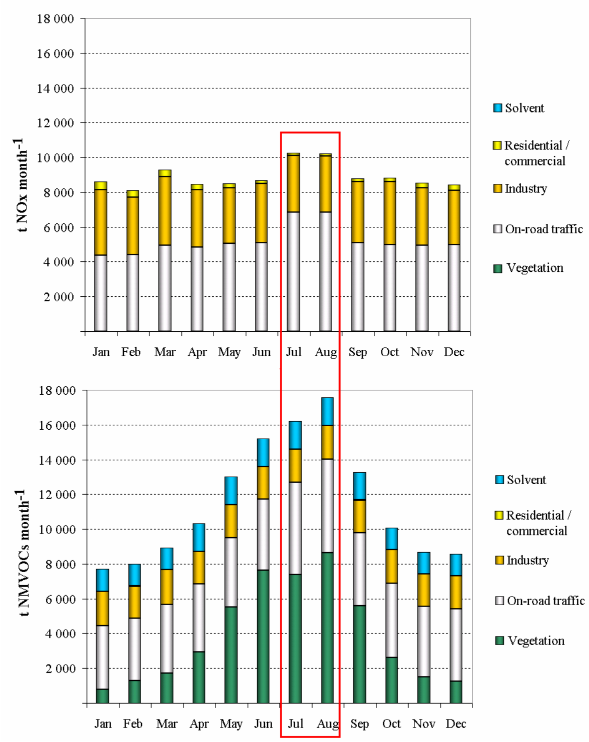

Fig. 4 Monthly emissions of NO_x and NMVOCs in the northeastern Iberian Peninsula during 2000.

65% of PAR is emitted by on-road traffic and 28% by vegetation. The ISOP species (highest rate constant) represents just about 1% of the NMVOCs speciated emissions. 64% and 28% were emitted by on-road traffic and vegetation, respectively. Composition of speciated emission is complex with comparative low emission of very reactive species against high emission of low reactive species.

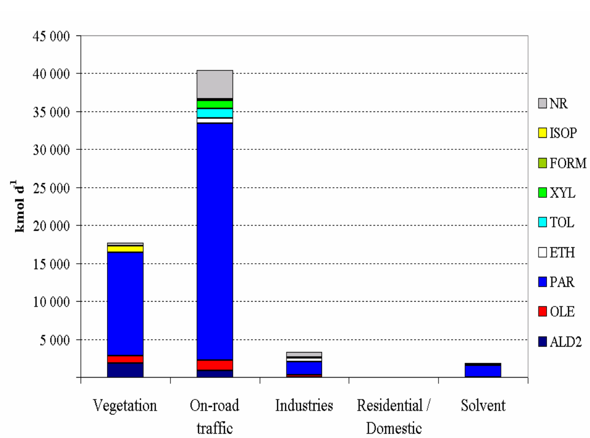

Fig. 5 Contribution of speciated NMVOCs in the northeastern Iberian Peninsula for 14 August 2000

4.0 INTEGRATION OF EMISSION FILES INTO MODELS-3/CMAQ

4.1 netCDF protocol

Text emission files are built in two sections: 1) the header, containing information about the configuration of the study domain, 2) the emission data organized according to the netCDF protocol. Figure 6 shows the arrangement of rows and columns on the XY plane. Indexes follow the relations: i+1 = ROW, j+1 = COL, k+1 = LAY; being ROW, COL, and LAY the number of rows, columns and layers, defining domain.

For each species, emission data are arranged by hours. Hourly data is built by layers, and layers data is arranged by rows. For its implementation into the Models-3/CMAQ framework, previous text file should be converted to binary format

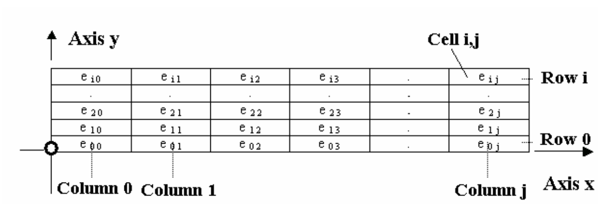

Fig. 6 Arrangement of rows and columns of the emission files reference system

4.2 Emission files with lower resolution

Selection of grid-cell size is important since the characteristics of species are assumed uniform in each grid cell and chemical species are represented by concentration. To provide emission data with coarser spatial resolution, EMICAT2000 integrates emissions with cells of 1, 2, 4 and 8 km. Figure 7 shows emission maps of hourly PAR species (12 LST) for 15 August 2000. Maps with 1 or 2 km cells depict the emission configuration in detail. The axis of the most important highways and roads are clearly defined and most of this species are emitted mainly from the Barcelona Metropolitan Area. Within a coarser spatial resolution, emission features get lost.

5.0 CONCLUSIONS

We developed the EMICAT2000 model, which provides emission inventories for the complex configuration of the northeastern Iberian Peninsula. This model provides directly the emission files required by Models-3/CMAQ. Successful results for photochemical modeling are currently obtained (Jiménez *et al.*, 2004). This approach could be considered for similar exploitation of Models-3/CMAQ in different regions worldwide.

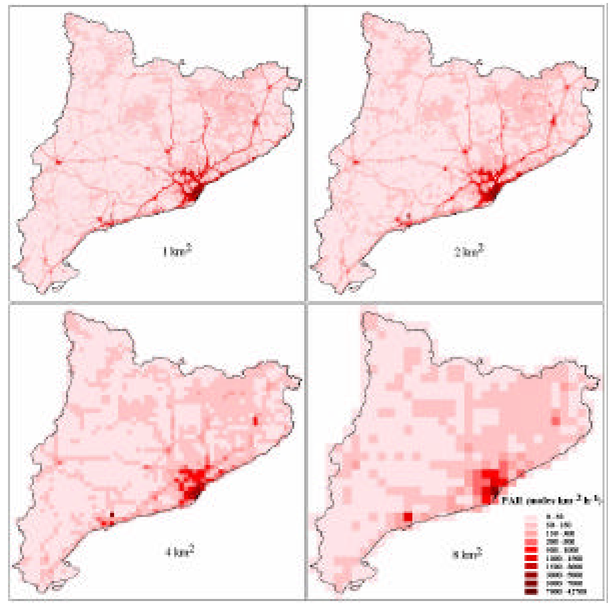

Fig. 7 PAR (paraffin bond) emissions (12 LST, 15 August 2000) in Catalonia with different spatial resolution

6.0 ACKNOWLEDGEMENTS

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7.0 REFERENCES

Parra, R., 2004. Development of the EMICAT2000 model for the estimation of air pollutants emissions in Catalonia and its use in photochemical dispersion models. Ph.D. Dissertation, Technical University of Catalonia (Spain).

Parra, R., S. Gassó and J.M. Baldasano, 2004. Estimating the biogenic emissions of non-methane volatile organic compounds from the North Western Mediterranean vegetation of Catalonia. *Sci. Total Environ.*, 329, 241-259.

Jiménez, P., O. Jorba, R. Parra and J.M. Baldasano, 2004. Evaluation of Models-3/CMAQ in very complex terrains: high-resolution application to the northeaster Iberian Peninsula. 3rd Annual CMAS Models-3 conference. October 18-20, Chapel Hill, NC.