

## Simulació numèrica mesoscalar de l'ozó troposfèric a Catalunya

Sara Ortega Jiménez

**ADVERTIMENT.** La consulta d'aquesta tesi queda condicionada a l'acceptació de les següents condicions d'ús: La difusió d'aquesta tesi per mitjà del servei TDX ([www.tesisenxarxa.net](http://www.tesisenxarxa.net)) ha estat autoritzada pels titulars dels drets de propietat intel·lectual únicament per a usos privats emmarcats en activitats d'investigació i docència. No s'autoritza la seva reproducció amb finalitats de lucre ni la seva difusió i posada a disposició des d'un lloc aliè al servei TDX. No s'autoritza la presentació del seu contingut en una finestra o marc aliè a TDX (framing). Aquesta reserva de drets afecta tant al resum de presentació de la tesi com als seus continguts. En la utilització o cita de parts de la tesi és obligat indicar el nom de la persona autora.

**ADVERTENCIA.** La consulta de esta tesis queda condicionada a la aceptación de las siguientes condiciones de uso: La difusión de esta tesis por medio del servicio TDR ([www.tesisenred.net](http://www.tesisenred.net)) ha sido autorizada por los titulares de los derechos de propiedad intelectual únicamente para usos privados enmarcados en actividades de investigación y docencia. No se autoriza su reproducción con finalidades de lucro ni su difusión y puesta a disposición desde un sitio ajeno al servicio TDR. No se autoriza la presentación de su contenido en una ventana o marco ajeno a TDR (framing). Esta reserva de derechos afecta tanto al resumen de presentación de la tesis como a sus contenidos. En la utilización o cita de partes de la tesis es obligado indicar el nombre de la persona autora.

**WARNING.** On having consulted this thesis you're accepting the following use conditions: Spreading this thesis by the TDX ([www.tesisenxarxa.net](http://www.tesisenxarxa.net)) service has been authorized by the titular of the intellectual property rights only for private uses placed in investigation and teaching activities. Reproduction with lucrative aims is not authorized neither its spreading and availability from a site foreign to the TDX service. Introducing its content in a window or frame foreign to the TDX service is not authorized (framing). This rights affect to the presentation summary of the thesis as well as to its contents. In the using or citation of parts of the thesis it's obliged to indicate the name of the author.

## 8. Bibliografia

- Baertsch-Ritter, N., Prevot, A.S.H., Dommen, J., Andreani-Aksoyoglu, S., Keller, J., 2003. Model study with UAM-V in the Milan area (I) during PIPAPO: simulations with changed emissions compared to ground and airborne measurements. *Atmospheric Environment*, 37, pp 4133-4147.
- Beneito, J. (2006). Desenvolupament, aplicació i validació d'un model numèric per al pronòstic de l'ozó troposfèric a Catalunya. Ph.D. Thesis, University of Barcelona, 178 pp.
- Beneito, J., Soler, M.R., Alarcón, M., 2007. A simple model system to forecast tropospheric ozone concentrations. *Física de la Tierra*, 19, pp 87-106. *Experimental and Modelling Micrometeorology*, Ed. Yagüe, Sanchez and Rees.
- Brulfert, G., Chollet, J. P., Jouve, B., Villard, H., 2005. Atmospheric emission inventory of the Maurienne valley for an atmospheric numerical model. *Science of the Total Environment*, 349, pp 232-248.
- Byun, D.W., Kim, S.T., Kim, S.B., 2007. Evaluation of air quality models for the simulations of a high ozone episode in the Houston metropolitan area. *Atmospheric Environment*, 41, pp 837-853.
- Cape, J.N., 2008. Surface ozone concentrations and ecosystem health: Past trends and a guide to future projections. *Science of the total environment*, 400, pp 257-269.
- Carnevale, C., Gabusi, V., Volta, M., 2006. POEM-PM: an emission modelling for secondary pollution control scenarios. *Environmental Modelling & Software*, 21, pp 320-329.
- Chang, J.S., Brost, R.A., Isakson, I.S.A., Madronic, S., Middleton, P., Stockwell, W. R., Walcek, C.J., 1987. A three-dimensional Eulerian acid deposition model: physical concepts and formulation. *Journal of Geophysical Research*, 92, pp 14681-14700.
- Colls, J., 1997. *Air Pollution. An introduction*. E & FN Spon., 341 pp.
- Costa, M., Baldasano, J.M., 1996. Development of a source emission model for atmospheric pollutant in the Barcelona Area. *Atmospheric Environment* 30, pp 309-318.
- Cressman, G.P., 1959. An operational objective analysis system. *Monthly Weather Review*, 87, 367-374.
- Doménech, X., 1995. *Química atmosférica. Origen i efectos de la contaminación*. Miraguano Ediciones, Madrid.
- Eder, B., Kang, D., Pleim, J., Yu, S., Otte, T., Pouliot, G., 2009. A performance evaluation of the National Air Quality Forecast Capability for the summer of 2007. *Atmospheric Environment*, 43, pp 2312-2320.
- EMEP/CORINAIR 2004 Emiss Inv Guidebook-3rd Edition September 2004 UPDATE <http://reports.eea.eu.int/EMEPCORINAIR4/en>
- Figueruelo, J.E., Dávila, M.M., 2004. *Química Física del Ambiente y de los Procesos Medioambientales*. Editorial Reverté, Barcelona. 591 pp.
- Forster, P., V. Ramaswamy, P. Artaxo, T. Berntsen, R. Betts, D.W. Fahey, J. Haywood, J. Lean, D.C. Lowe, G. Myhre, J. Nganga, R. Prinn, G. Raga, M. Schulz and R. Van Dorland, 2007: Changes in Atmospheric Constituents and in Radiative Forcing. In: *Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to*

the Fourth Assessment Report of the Intergovernmental Panel on Climate Change [Solomon, S., D. Qin, M. Manning, Z. Chen, M. Marquis, K.B. Averyt, M. Tignor and H.L. Miller (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA.

Gear, C.W., 1971. Numerical Initial Value Problems in O.D.E. Prentice Hall, Englewood Cliffs.

Gent, J.F., Triche, E.W., Holford, T.R., Belanger, K., Brachen, M.B., Beckett, W.S., Leaderer, B.P., 2003. Journal of the American Medical Association 290, 14, pp 1859-1867.

Gery, M.W., Whitten, G.Z., Killus, J.P., Dodge, M.C., 1989. A photochemical kinetics mechanism for urban and regional scale computer modelling. Journal of Geophysical Research, 94, D10, pp 12925-12956.

Grell, G.A., Dudhia, J., Huufler, D.r., 1994. A description of the fifth generation Penn State/NCAR Mesoscale Model (MM5). NCAR. Tech. Note. NCAR/TN-398+STR, 122 pp.

Grossi, P., Thunis, P., Martilli, A., Clappier, A., 2000. Effect of sea breeze on air pollution in the greater Athens area: part II: Analysis of different Emissions Scenarios. Journal of Applied Meteorology, 39, 4, pp 563-575.

Guderian, r., Tingey, D.T., Rabe, r., 1985. effects of photochemical oxidants on plants. Air Pollution by Photochemical Oxidants (edited by Guderian R.), pp 129-333. Springer, Berlin.

Guenther, A., Zimmerman, P., Wildermuth, M., 1994. Natural volatile organic compound emission rate estimates for U.S. woodland landscapes, Atmospheric Environment, 28, pp 1197-1210.

Hanna, S.R., Chang, J.C., Fernau, M.E., 1998. Monte Carlo estimates of uncertainties in predictions by a photochemical grid model (UAM-IV) due to uncertainties in input variables. Atmospheric Environment, 32, pp 3619-3628.

Hanna, S. R., Lu, Z., Frey, H.C., Wheeler, N., Vukovich, J., Arunachalam, S., Fernau, M., Hansen, D.A., 2001. Uncertainties in predicted ozone concentrations due to input uncertainties for the UAM-V photochemical grid model applied to the July 1995 OTAG domain. Atmospheric Environment, 35, pp 891-903.

Hertel, O., Berkowicz, R., Christensen, J., Hov, O., 1993. Test of two numerical schemes for use in atmospheric transport-chemistry models. Atmospheric Environment, 27, pp 2591-2611.

Hestvedt, E., Hov, O., Isaksen, I.S.A., 1978. Quasi steady state approximation in air pollution modelling. Comparison of two numerical schemes for oxidant prediction. International Journal of Chemical Kinetics, 10, pp 971-994.

Hewitt, C., Lucas, P., Wellburn, A., Fall, R., 1990. Chemistry of ozone damage to plants. Chemistry and Industry 15, pp 478-481.

Hobbs, P.V., 1995. Basic, physical chemistry for the atmospheric sciences. Cambridge University Press. 206 pp.

Jacob ,D.J., 2000. Heterogeneous chemistry and tropospheric ozone. Atmospheric Environment, 34, pp 2131-2159.

- Jimenez, P., Jorba, O., Parra, R., Baldasano, J.M., 2006. Evaluation of MM5-EMICAT2000-CMAQ performance and sensitivity in complex terrain: High resolution application to the northeastern Iberian Peninsula. *Atmospheric Environment*, 40, pp 5056-5072.
- Johnson, C., Heshaw, J., McInnes, G. 1992. Impact of aircraft and surface emissions of nitrogen oxides on tropospheric ozone and global warming. *Nature*, 355, pp 69-71. doi:10.1038/355069a0
- Krishnamurti, T.N., Bounoua, L., 1996. An introduction to numerical weather prediction techniques. CRC Press LLC, Florida, 293 pp.
- Mc Cree, K. J., 1972. Test of current definitions of photosynthetically active radiation against leaf photosynthesis data. *Agricultural Meteorology* 10, 442-453.
- Ortega, S. , Soler, M. R., Beneito, J. and Pino, D., 2004. Evaluation of two ozone air quality modelling systems. *Atmospheric Chemistry and Physics*, Vol. 4, pp 1389-1398, 25-8-2004. <http://www.copernicus.org/EGU/acp/>
- Ortega, S., Soler, M.R., Alarcón, M., Arasa, R., 2009a. MNEQA, an emissions model for photochemical simulation. *Atmospheric Environment*, pp 1-12. In press. doi: 10.1016/j.atmosenv.2009.04.046
- Ortega, S., Soler, M.R., Alarcón, M., Arasa, R., 2009b. The role of temperature in tropospheric ozone. *International Journal of the Environment and Pollution*. In press.
- Parra, R., 2004. Desarrollo del modelo EMICAT2000 para la estimación de emisiones de contaminantes del aire en Cataluña y su uso en modelos de dispersión fotoquímica. PhD Dissertation, Universitat Politècnica de Catalunya, 364 pp. <http://www.tds.cat/TDX-0803104-102139>
- Parra, R., Jiménez, P., Baldasano, J.M., 2006. Development of the high spatial resolution EMICAT2000 emission model for air pollutants from the north\_eastern Iberian Peninsula (Catalonia, Spain). *Environmental Pollution*, 140, pp 200-219.
- Russell, A.G., Dennis, R.L., 2000. NARSTO critical review of photochemical models and modeling. *Atmospheric Environment*, 34, pp 2283-2324.
- Seinfeld, J.H., Pandis, S.P., 1998. *Atmospheric chemistry and physics: from air pollution to climate change*. Wiley-Interscience publication, USA, 1326 pp.
- Shea, KM, Truckner, RT, Weber, RW and Peden, DB, 2008. Climate change and allergic disease. *Journal of allergy and clinical immunology*, 122, 3, pp 443-453.
- Silibello, c., Calori, G., Brusasca, g., Catenacci, G., Fnzi, G., 1998. Application of a photochemical grid model to Milan metropolitana area. *Atmospheric Environment*, 32, 11, pp 2025-2038.
- Theloke, J., Friedrich, R., 2007. Compilation of a database on the composition of anthropogenic VOC emissions for atmospheric modeling in Europe. *Atmospheric Environment* 41, 4184-4160.
- Thiébaux, H.J., Pedder, M.A., 1987. *Spatial objective analysis: with application in atmospheric science*. Academic Press, 299 pp.
- Trasande, L., Thurston, GD, 2005. The role of air pollution in asthma and other pediatric morbidities. *Journal of allergy and clinical immunology*, 115, 4, pp 689-699.

- Tuia, D., Ossés de Eicker, M., Zah, R., Osses, M., Zarate, E., Clappier A., 2007. Evaluation of a simplified top-down model for the spatial assessment of hot traffic emissions in mid-sized cities. *Atmospheric Environment* 41, pp 358-3671.
- Ure, A.M., Davidson, C.M., 1995. *Chemical speciation in the environment*. Blackie academic & professional. 408pp.
- Van Aardenne, J., 2001. Task force. ETC-ACC. *Emission Inventory Guidebook*. 7 november 2001.
- Vautard, R., Honore, C., Beekmann, M., Rouil, L., 2005. Simulation of ozone during the August 2003 heat wave and emission control scenarios. *Atmospheric Environment*, 39, pp 2957-2967.
- Vestreng, V., Rigler, e., Adams, M., Kindbom, K., Pacyna, J.M., Denier van der Gon, H., Reis, S., Travnikov, O. 2006. Inventory review 2006, Emission data reported to LRTAP and NEC Directive, Stage 1, 2, and 3 review and Evaluation of inventories of HM and POPs. EMEP/MMSC-W Technical Report 1/2006 ISSN 1504-6179. <http://www.emep.int>
- Yu, S., Eder, B., Dennis, R., Chu, S.H., Schwartz, S.E., 2006. New unbiased symmetric metrics for evaluation of air quality models. *Atmospheric Science Letters* 7, pp 26-35.
- Zhang, M., Uno, I., Zhant, R., Han, Z., Wang, Z., Pu, Y., 2006. Evaluation of the Models-3 Community Multi-scale Air Quality (CMAQ) modelling system with observations obtained during the TRACE-P experiment: comparison of ozone and its related species. *Atmospheric Environment*, 40, pp 4874-4882.
- Zhang, Y., Liu, P., Pun, B., Seigneur, C., 2006a. A comprehensive performance evaluation of MM5-CMAQ for the summer 1999 southern oxidants study episode-Part I: Evaluation protoclos, databases, and meteorological predictions. *Atmospheric Environment*, 40, pp 4825-4838.
- Zhang, Y., Liu, P., Queen, A., Misenis, C., Pun, B., Seigneur, C., Wu, S.Y., 2006b. A comprehensive performance evaluation of MM5-CMAQ for the summer 1999 southern oxidants study episode-Part II: gas and aerosol predictions. *Atmospheric Environment*, 40, pp 4839-4855.