Geophysical Research Abstracts,
Vol. 11, EGU2009-7943-2, 2009
EGU General Assembly 2009

Implementation of an online chemical mechanism within a global-regional atmospheric model: design and initial steps

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Chemical processes in air quality modelling systems are usually treated independently from the meteorological models. This approach is computationally attractive since off-line chemical transport simulations only require a single meteorological dataset to produce many chemical simulations. However, this separation of chemistry and meteorology produces a loss of important information about atmospheric processes and does not allow for feedbacks between chemistry and meteorology. To take into account such processes current models are evolving to an online coupling of chemistry and meteorology to produce consistent chemical weather predictions.

The Earth Sciences Department of the Barcelona Supercomputing Center (BSC) develops the NMMB/BSC-DUST (Pérez et al., 2008), an online dust model within the global-regional NCEP/NMMB numerical weather prediction model (Janjic and Black, 2007) under development at National Centers for Environmental Prediction (NCEP). Current implementation is based on the well established regional dust model and forecast system DREAM (Nickovic et al., 2001). The most relevant characteristics of NMMB/BSC-DUST are its on-line coupling of the dust scheme with the meteorological driver, the wide range of applications from meso to global scales, and the inclusion of dust radiative effects allowing feedbacks between aerosols and meteorology. In order to complement such development, BSC works also in the implementation of a fully coupled online chemical mechanism within NMMB/BSC-DUST. The final objective is to develop a fully chemical weather prediction system able to resolve gas-aerosol-meteorology interactions from global to local scales.

In this contribution we will present the design of the chemistry coupling and the current progress of its implementation. Following the NCEP/NMMB approach, the chemistry part will be coupled through the Earth System Modeling Framework (ESMF) as a pluggable component. The chemical mechanism and chemistry solver is based on the Kinetic PreProcessor KPP (Sandu and Sander, 2006) package with the main purpose to maintain a wide flexibility when configuring the model. Such approach will allow using a simple general chemical mechanism for global applications or a more complex mechanism for regional to local applications at higher resolution.

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