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Air quality modelling: Bridging national and continental scales

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Abstract: The development of effective environmental policies is needed in order to meet regulatory standards and international legislation and agreements, both at national and supra-national level. The design, assessment and comparison of control strategies require the support of multi-scale integrated assessment modelling (IAM) systems. For instance, the development of ozone control strategies requires the understanding of the temporal and spatial multi-scale nonlinear processes governing tropospheric ozone levels and its complicated relationships with other atmospheric issues such as aerosols or acidification. IAM implies that science is being applied in the context of social and economic forces at work in society, so it has to be useful to generate both explanations and policy options. Regional (e.g. European) policies must rely on common, supra-national integrated assessment systems that necessarily imply a series of assumptions and simplifications that make them unsuitable for finer scales. More detailed and specific national systems are required to depict important phenomena that are out of reach of low-resolution models used at continental level. This is a challenging issue from the air quality modelling point of view, since model design, underlying hypotheses and input data must be consistent across the different systems and scales.

This paper describes the methodology followed in the development of the air quality IAM system for the Iberian Peninsula (SIMCA) to deal with these multi-scale issues.

Air quality simulation in SIMCA relies on the WRF-SMOKE-CMAQ system. The Weather Research and Forecasting (WRF) modelling system is used to develop the meteorological fields needed to reproduce the fate of air pollutant in the atmosphere. The model is initialized from global reanalysis and runs over a 48 km x 48 km spatial resolution European domain which provides boundary conditions for the national modelling domain with a spatial resolution of 3 km x 3 km. Meteorological outputs are then processed with the Meteorology-Chemistry Interface Processor (MCIP) which consistently interpolates and derives the variables required by the Community Multiscale Air Quality (CMAQ) system. This process involves data adaptation to a different staggered grid and potentially a different vertical-coordinate system. Likewise, the CMAQ system is run over the two nested domains using inputs from WRF and the Sparse Matrix Operator Kernel Emissions (SMOKE). This software provides an efficient and very flexible platform for emission processing. Although different formats and datasets are used for the emission inventories and projections feed to SMOKE, all of them (national inventory, EMEP inventory and Spain's Emission Projections, SEP) are based on official, consistent estimates, which, in turn, are used as inputs for European-scale integrated assessment modelling studies such as those carried out for the development of the European Air Quality Thematic Strategy on Air Quality. However, emission processing is adapted to the specific requirements and data availability of the different domains. This approach allows both, the incorporation of the best information available at different scales and the implementation of standards used in international modelling exercises (e.g. Eurodelta) and models such as RAINS/GAINS-EMEP. On the other hand, CMAQ outputs are perfectly suited for the inputs requirements of the air pollution effects modules of the national IAM system.

Keywords: *Air quality, multiscale modelling, integrated assessment modelling*

1. INTRODUCTION

Air pollution levels result from extremely complex interactions among meteorology, emissions, pollutant chemistry and dynamics in the atmosphere. A clear example of the difficulty of understanding ambient concentration levels can be found in ground-level ozone. Urban and regional O_3 levels are determined by emission of ozone precursors, multiple chemical reactions, physical transport and diffusion and deposition phenomena. The ozone dynamics involve processes extending over multiple spatial and temporal scales and complicated relationships with other atmospheric issues such as aerosols or acidification. This constitutes a very challenging issue both from the legal and scientific and technical point of view.

For instance, any emission reduction plan intended to improve air quality levels over a particular region must be based on the understanding of these relationships and must rely on a suitable modelling system. Therefore, the mathematical tool used to simulate the fate of the pollutants in the atmosphere must be able to cope with multiple spatial scales consistently. Depending on the theoretical basis and scale of application, different modelling systems may lead to different policy recommendations. In the scope of Integrated Assessment Modelling (IAM), it also implies that modelling tools should be able to accommodate different hypotheses and standards in accordance with other econometric, optimization and engineering models, usually intended for very particular purposes and domains. In the European context, this means that any national IAM system must include the most reliable and robust science and also the capacity to use information consistent with supra-national IAM activities (e.g. the inputs used in the IAM exercises under the UN-ECE Convention on Long-range Transboundary Air Pollution -CLRTAP- and the Clean Air For Europe –CAFE- program for EU countries). The methodological basis for the air quality IAM system for the Iberian Peninsula (SIMCA) was developed keeping these constraints in mind. The methods and criteria to achieve an effective linkage between continental, national and even regional or local scales are briefly discussed in this contribution.

2. THE SIMCA PROJECT

2.1. Overview

The IAM system for the Iberian Peninsula, schematized in Figure 1**,** is intended to assist the policy makers in the assessment and comparison of environmental policies and control strategies. The suitability of a given scenario, reflecting a particular emission abatement plan or strategy, is evaluated through the comparison of the results with emission thresholds established by Directives (National Emission Ceilings –NEC-) and Protocols (Kyoto) and pollution levels with current or, usually, future legal standards.

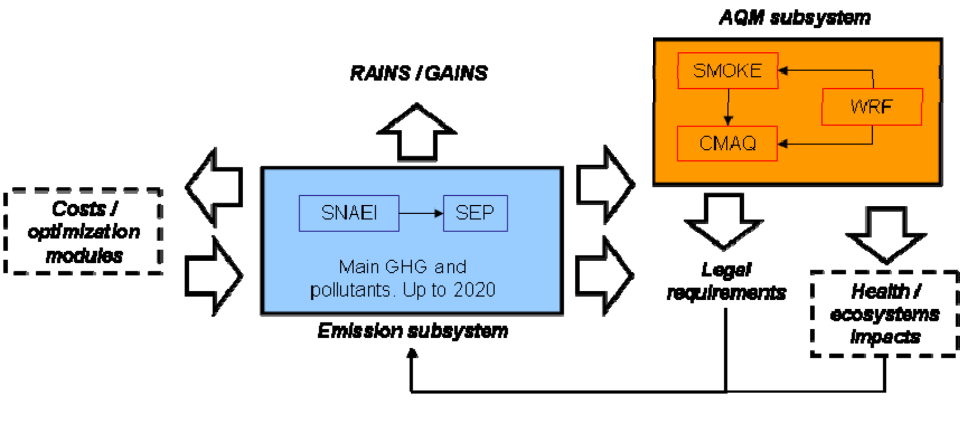

Figure 1. Basic flowchart of the SIMCA IAM system.

Consequently, the system consists of two major components, the emission subsystem and the air quality modelling (AQM) subsystem, described in the following sections. Regardless of legal requirements, it should be considered that emission abatement options may imply significant economic and societal costs, so the minimization of the cost/benefit ratio in the abatement solution is important. Costs and efficiencies of a series of technical measures are being evaluated in Spain. However, the implementation of the optimization module requires the substitution of the actual air quality modelling system (extremely expensive computationally) by some sort of statistical approximation which convenience is still under discussion.

SIMCA is also conceived as a necessary complement of the European-scale IAM systems, namely the Greenhouse Gas and Air Pollution Interactions and Synergies (GAINS)-EMEP Unified model system. Due to scale issues, such continental systems are unable to deliver spatially resolved results suitable for national or regional policies and are restricted to Europe-wide common features, being national particularities out of reach (Borge et al., 2006). At the same time, the national system is useful for model intercomparison, therefore providing a reference that may support the interpretation or discussion of the European results. Because of this, but mainly because of the intrinsic multiscale nature of air pollution processes, the AQM subsystem relays on a nested-domain strategy. In the following section the main criteria and methodological issues considered to keep the consistency between scales are shown. The discussion is divided in accordance with the three individual models involved in the simulation of air pollution (Figure 1).

3. BRIDGING SCALES IN THE AIR QUALITY MODELLING SUBSYSTEM

The AQM subsystem relies on the Community Multiscale Air Quality (CMAQ) model (Byun and Ching, 1999; Byun and Schere, 2006). Emissions are taken from an emission model based on the Sparse Matrix Operator Kernel Emissions (SMOKE) modelling system (UNC Carolina Environmental Program, 2005). The meteorological model selected to provide the meteorological fields required by the chemical-transport model (CTM) and the emission processing system is the Weather Research and Forecasting (WRF) modelling system (Skamarock and Klemp, 2008). This non-hydrostatic mesoscale model constitutes a state-of-the-art atmospheric simulation system based on the Fifth-Generation Penn State/NCAR Mesoscale Model (MM5) (Grell et al., 1994).

The modelling domains are shown in Figure 2. Although alternative configurations have been used in the SIMCA project (e.g. Borge et al, 2008b), currently, the modelling system is built over a mother domain with 48 km x 48 km resolution and a nested domain with 3 km x 3 km spatial resolution (solid rectangles in Figure 2). Depending on the particular study, other domains may be considered, for instance, a mother domain extended southward, covering the Sahara and Sahel deserts, which have been found to be important sources of natural PM_{10} affecting concentration levels in Spain (Borge et al., 2007).

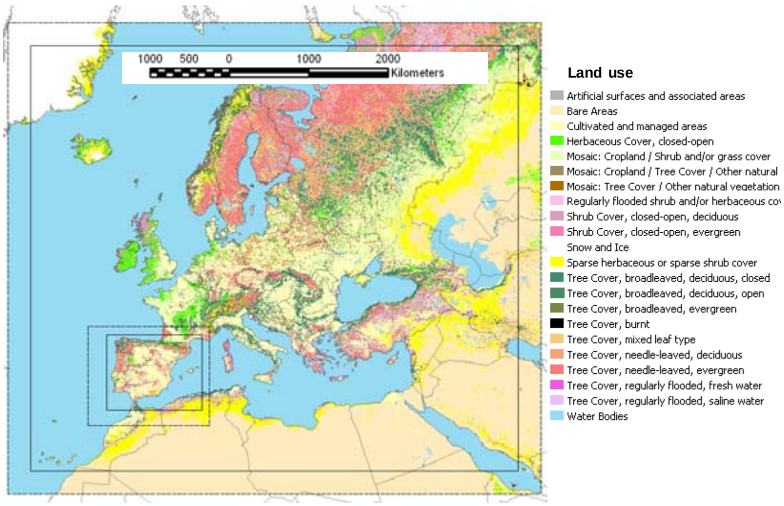

Figure 2. National and continental modelling domains.

Dashed rectangles in Figure 2 represent the modelling domains used for the WRF model. For this application, the mother domain covers an area of 6720 km x 5952 km in the x and y directions respectively. The nested domain is centred over the Iberian Peninsula and consists of 468 columns and 396 rows of 3 km x 3 km grid cells. The CMAQ and SMOKE domains (solid line in Figure 2) are slightly smaller (12 rows or columns) to avoid border effects. All the models are built over the same geographical projection system (Lambert Conformal with parameters α=20ºN, β=60ºN and γ=3ºW) and consider the same representation of the Earth (a perfect sphere with radius 6,370,997 m). The vertical structure of the modelling domain is also identical for all the models (30 layers corresponding to sigma levels of 1.000, 0.999, 0.997, 0.995 0.992, 0.987, 0.980, 0.970, 0.950, 0.910, 0.860, 0.800, 0.750, 0.700, 0.650, 0.600, 0.550, 0.500, 0.450, 0.400, 0.350, 0.300, 0.250, 0.200, 0.150, 0.100, 0.075, 0.050, 0.025, 0.010 and 0.000).

3.1. WRF-ARW/MCIP

As any other atmospheric mesoscale model, the Weather Research and Forecasting (WRF) model (Advanced Research WRF or Eulerian mass version, ARW) is based on the fundamental conservation equations (momentum, thermodynamics, etc.) which are resolved in accordance to the grid resolution. Since the model is based on the primitive physic equations (e.g. nonhydrostatic Euler equations for compressible fluids), it may be run in a wide range of spatial and temporal resolutions. In addition to the physics core, a series of sub-grid scale schemes and parameterizations are available. The effective linkage of meteorological drivers is achieved by applying a consistent representation of the dynamics along with the most appropriate parameterizations. For instance, cumulus parameterizations are intended to represent vertical fluxes due to unresolved updrafts and downdrafts and compensating motion outside the clouds. The Kain-Fritsch scheme

(Kain, 2004) is applied at 48 km x 48 km resolution, while no cumulus parameterization is needed in the innermost domain since those fluxes can be resolved explicitly at grid sizes of approximately 5-10 km (Skamarock et al., 2005). Other configuration options must be optimally set up in accordance to the grid resolution. Newtonian relaxation or nudging constitutes an important example (at least for policy-oriented, annual runs). Grid nudging should be applied to coarse domains with a spatial resolution similar to the atmospheric reanalysis used to initialize the model (e.g. 48 km). Oppositely, observational nudging towards individual meteorological stations should be also included for an optimal performance with fine resolutions such as 3 km (Borge et al., 2008b).

The coupling of a meteorological and chemical-transport model is not a trivial issue. The CMAQ Meterology-Chemistry Interface Processor (MCIP) is applied for the adaptation of WRF outputs. Because most meteorological models are not built for air quality modelling purposes, MCIP deals with issues related to data format translation, diagnostic estimations of parameters not provided, extraction of data for appropriate window domains, and reconstruction of meteorological data on different grid and layer structures. WRF-ARW and CMAQ both utilize the Arakawa C-grid and conformal map projections to represent the horizontal grid and coordinates, requiring no special interpolation between the two. MCIP, however, is capable to accommodate meteorological fields from the Arakawa-B grid used by MM5 (formerly used in SIMCA). MCIP may be also used to modify the vertical structure. Collapsing layers near the model lid, while preserving the original configuration in the boundary layer region, may lead to substantial savings in the CPU time needed to run the CTM, although it may interfere with the stability of the numerical solver.

To support the multiscale generalized coordinate implementation of the CMAQ CTM, MCIP provides appropriate dynamic meteorological parameters to allow mass-consistent air quality computations. Even if the mass conservation equation for air is solved in the meteorological model, this is a key issue, since some non-physical terms are added to the solutions from the nudging process. Besides assuring mass continuity, MCIP is useful to process land use information included in the WRF outputs. The coupler consistently adapts this information to the formats of the CTM and generates some additional information needed by the AQM such as dry deposition velocities for the chemical species being modelled.

3.2. SMOKE

Emissions constitute a key input to AQMs since they are one of the main sources of uncertainty (Russell and Dennis, 2000). This issue is also relevant for the analysis of the alternatives to improve air quality in a given region in future years as a result of the implementation of pollutant emissions abatement and from the integrated assessment modelling point of view (Reis et al., 2005). As for the implications for multi-scale studies, emissions constitute one the most challenging aspect. Emission-related inputs must be as detailed and specific as possible for the different domains involved in the simulation, and simultaneously they must be consistent across the scales.

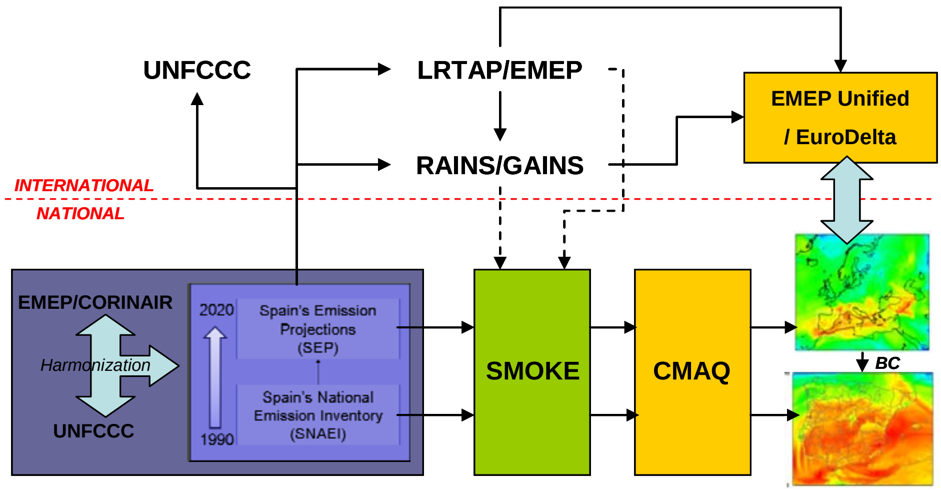

Figure 3. Emission-related information flow and linkage with national/international AQ modelling

In the SIMCA framework, Spain's emission estimates are taken from the National Atmospheric Emission Inventory (SNAEI) and the Spain's Emission Projections (SEP) for future years. Emission projections are essential when simulating plans and programs or policy options. Emissions from SEP are based on the Consistent Emission Projection (CEP) system (Lumbreras et al., 2008a, Lumbreras et al., 2008b). This projection model follows as closely as possible all the computation methods and information sources used in the elaboration of the SNAEI. Around 280 emission activities are currently being projected up to 2020. In addition, emission projections are consistent with supra-national standards and are compatible with the international reporting requirements (Kyoto Protocol, NEC Directive, Geneva Convention, etc.) and are currently used as national official estimates. In the case of AQ pollutants, this implies that the same emissions used to feed the AQM at national level are also the future estimates submitted to the LRTAP Convention. These emissions projections are, in turn, used by EMEP to elaborate the emission inventories used in European-scale AQ modelling exercises (Vestreng, 2003). As illustrated in Figure 3, such emissions are used to feed the CMAQ model to drive EU-scale modelling inside SIMCA. This approach allows both, to provide boundary conditions for the Iberian Peninsula domain and a contrast to the outputs from international modelling exercises such as those of the CAFE program or the EuroDelta project (van Loon et al., 2007).

The emission processing system, SMOKE, is used to incorporate all the information regarding emission estimates and any other information useful to perform the chemical speciation and temporal and spatial allocation of emissions (Borge et al., 2008a). Beside the consistency of the emission estimates, the flexibility of the emission model is essential to achieve coherent results. Emissions can be processed in SMOKE with a wide range of detail, from specific temporal and chemical profiles for individual point sources, to averaged processing patterns for aggregated SNAP-group level emissions used in the European domain. This feature allows, for instance, incorporating all the information from the SNAEI in the nested domain and simultaneously, accommodating ancillary information used at international level, such as temporal or spatial profiles generated in the EuroDelta project. SMOKE allows the incorporation of pre-gridded inventories as well. However, such inventories (e.g. 50 km x 50 km EMEP inventory) may be based on a different geographic projection system, and a mass-conservative interpolation scheme should be applied to keep consistency (see Borge et al., 2008a for details).

Differences in the processing method arise principally from the information availability. The vertical allocation of the emissions from point sources is an interesting example. It is assumed that area source emissions are released into the lower vertical layer of the 3D modelling domain. Emissions from point sources, however, have an important initial buoyancy and momentum which must be properly represented. SMOKE can take advantage from WRF meteorology to compute hourly plume rise for all point sources. The plume rise is expressed in terms of layer fractions for each source taking into account plume buoyancy and momentum as well as mixing depth and atmospheric stability conditions (Houyoux, 1998). This approach, however, requires detailed information about the precise location and emission conditions (physical height, flow, temperature and vertical velocity) of every individual stack. Such information is not available in the SIMCA mother domain (Figure 2) and a simplified method of emission layer assignment is used instead. All emissions are processed as area sources in the mother domain to be allocated according to EU-wide assumptions (Thunis et al., 2008) later on.

Figure 4 shows the correspondence of the vertical structure of the model (hydrostatic representation of the σ-levels for an average terrain height) in the first kilometre. From this correspondence and the splitting rations used in EMEP, the same vertical emission distribution can be considered in CMAQ.

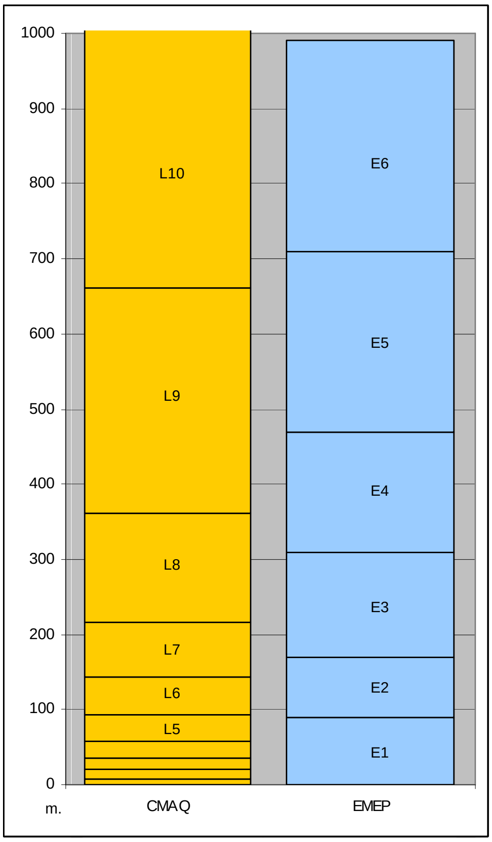

Figure 4. Comparison of the vertical structure of the SMOKE/CMAQ model and the EMEP model

When it is not possible to use the same source of information for the emissions being used in the different domains, it is important to assure that, at least, the estimation relies on similar approaches. This is the case for biogenic emissions in the European domain, which are not included in the EMEP inventory. Emissions of isoprene (Figure 5), monoterpenes and other biogenic volatile organic compounds are taken from the Global Emission Inventory Activity (GEIA), which is based on the algorithms proposed by Guenther et al., 1996, consistently with the EMEP/CORINAIR methodology used to compute biogenic VOCs emissions in the SNAEI and SEP.

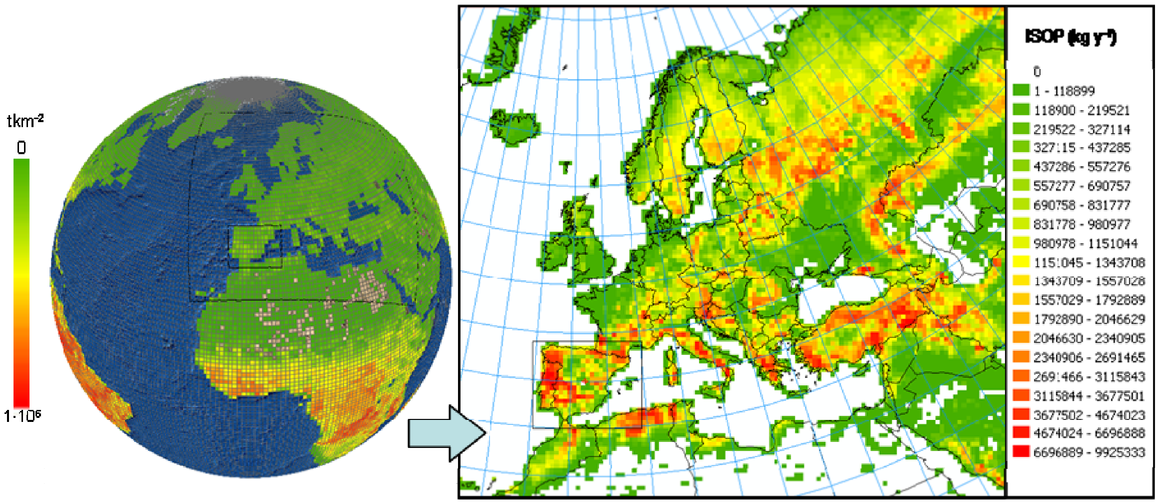

Figure 5. Isoprene emissions from GEIA (left) and interpolation (land use-driven) to SIMCA-EU domain

3.3. CMAQ

The design of the Community Multiscale Air Quality modelling system is based on the one-atmosphere paradigm, i.e. it considers that the influence of interactions at different dynamic scales and among multi-pollutants cannot be ignored (Byun and Ching, 1999). In order to accomplish the goals of the multi-scale system, a series of features are implemented in CMAQ:

- Scalable dynamics and thermodynamics: use of fully compressible form of governing equations and a generalized coordinate system
- Cell-based mass conservation (vs. total domain mass conservation). Use of proper variable states, such as density and entropy, instead of pressure and temperature and representation of governing equations in conservation form instead of advection form (including diffusion)
- Modular coding structure and versatile data handling method. Inclusion of a wide range of representation of scale-dependent processes (e.g. clouds or horizontal diffusivity)
- Robust nesting technique and a plume-in-grid approach to handle small scale air quality problems and subgrid scale plume dispersion and chemical reactions, respectively.

4. CONCLUSIONS

The basic methodology followed in the SIMCA project to cope with multi-scale air quality modelling and its implications for Integrated Assessment Modelling are briefly discussed in this paper. Air quality is essentially a multi-scale, multi-pollutant problem, and the IAM systems applied to evaluate abatement measures and drive policy options should be able to deliver suitable answers across the scales. From the modelling point of view, the achievement of this goal should be based in a nested-domain approach. Moreover, a consistent approximation to air quality at different scales relies on two basic issues.

- The representation of the atmospheric processes must be done through state-of-the science, comprehensive and flexible models, such as WRF-CMAQ, including the most up-to-date dynamics, parameterizations and numerics
- The input information must be as accurate as possible and consistent across the scales. In the scope of air quality IAM, emissions are particularly important. Emission-related information provided to the different domains should be based on the same computation methodology and ideally be consistent with national official estimates used for reporting purposes.

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