Estimation of uncertainties in model-ready emissions inventories for air quality modeling applications

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Uncertainty in Emissions Inventories

- Real-world emissions result from processes that are generally difficult to measure and fully characterize. Anthropogenic and biogenic activities involve complex physical and chemical processes such as combustion, evaporation, resuspension, erosion, degassing, and others responsible for substantial emissions of harmful gaseous and particulate matter air pollutants.
- Emissions inventories (EI) use ***assumptions*** and ***approximations*** of the underlying processes to provide ***estimates*** on pollutants' mass contributions and emission characteristics during a given period for sources located in a geographic area. They are essential instruments for air quality management during the design and evaluation of emission control strategies, air quality forecasting, and evaluation of health and environmental impacts.

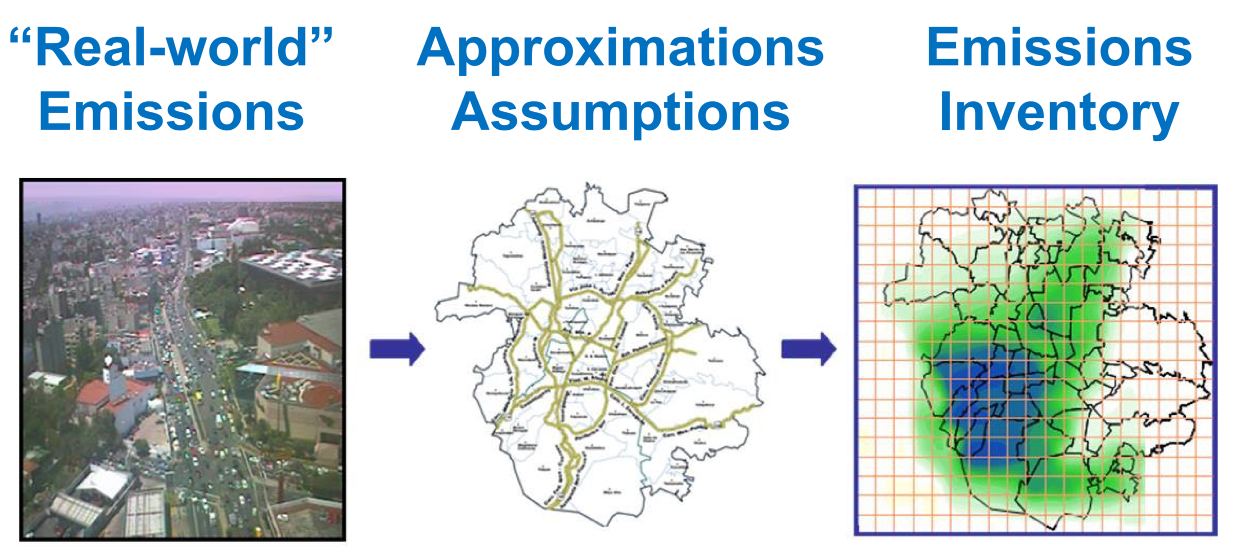


Figure 1. Emissions inventories are estimated by applying approximations and assumptions of the underlying physical and chemical processes in "real-world" emissions.

- Uncertainty in an EI represents the lack of knowledge of the "real-world" emission value[1]. A high-quality EI has small relative uncertainties and systematically neither over -nor underestimates the verifiable emissions. Thus, there is a strong need to better characterize uncertainties estimates in model-ready EIs used in air quality modeling applications.

Sources of Uncertainty

Bottom-up EIs use databases of emission factors (EF) and activity data (AD) to estimate emissions. EIs are further transformed into model-ready files for air quality models by aggregating emission rates by pollutant and source in a computational domain. The sources of uncertainty in the whole process are[2]:

- ***Structural Uncertainty***
  - **Understanding** of emission process.
  - **Choice** of emission models (simple vs complex).
  - **Simplification** of emission process (approximations).
- ***Parametric Uncertainty***
  - **Random sampling and measurement errors** of EF and AD.
  - **Representativeness** of input data of "real-world" conditions.
  - **Missing data.** A common challenge in EI preparation is lack of data.
  - **Surrogates (proxies)** are usually used to account for missing data.
  - **Calculation errors.**
- ***Disaggregation Uncertainty***
  - **Spatial** resolution.
  - **Spatial** distribution of proxies.
  - **Temporal** distributions of sources.
  - **Chemical** distributions of profiles.

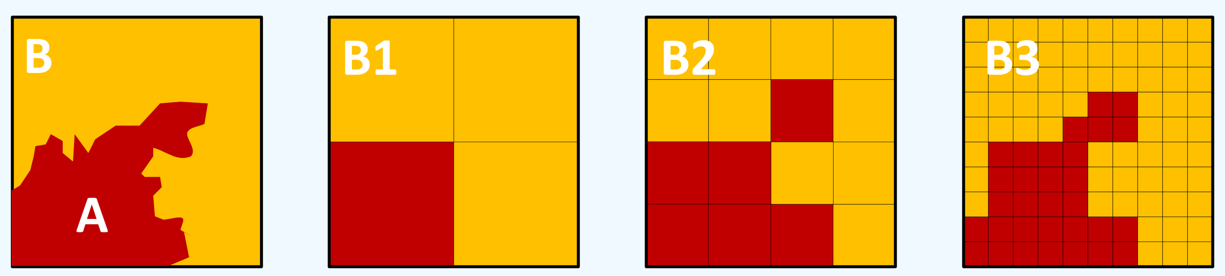


Figure 2. Uncertainties in the inputs are introduced in the spatial disaggregation of proxies (A) in the modeling domain (B) from low (B1) to high (B3) resolution.

Development of Model-Ready EIs

The development of model-ready EIs requires the combination of multiple activity data, emission factors, approximations and assumptions that are input to emission models[3,4]. The results are further spatially, temporally, and chemically distributed, and post-processed according to the air quality model formatting requirements. Uncertainties are introduced in each and all of these steps and propagate to the final model-ready EI output.

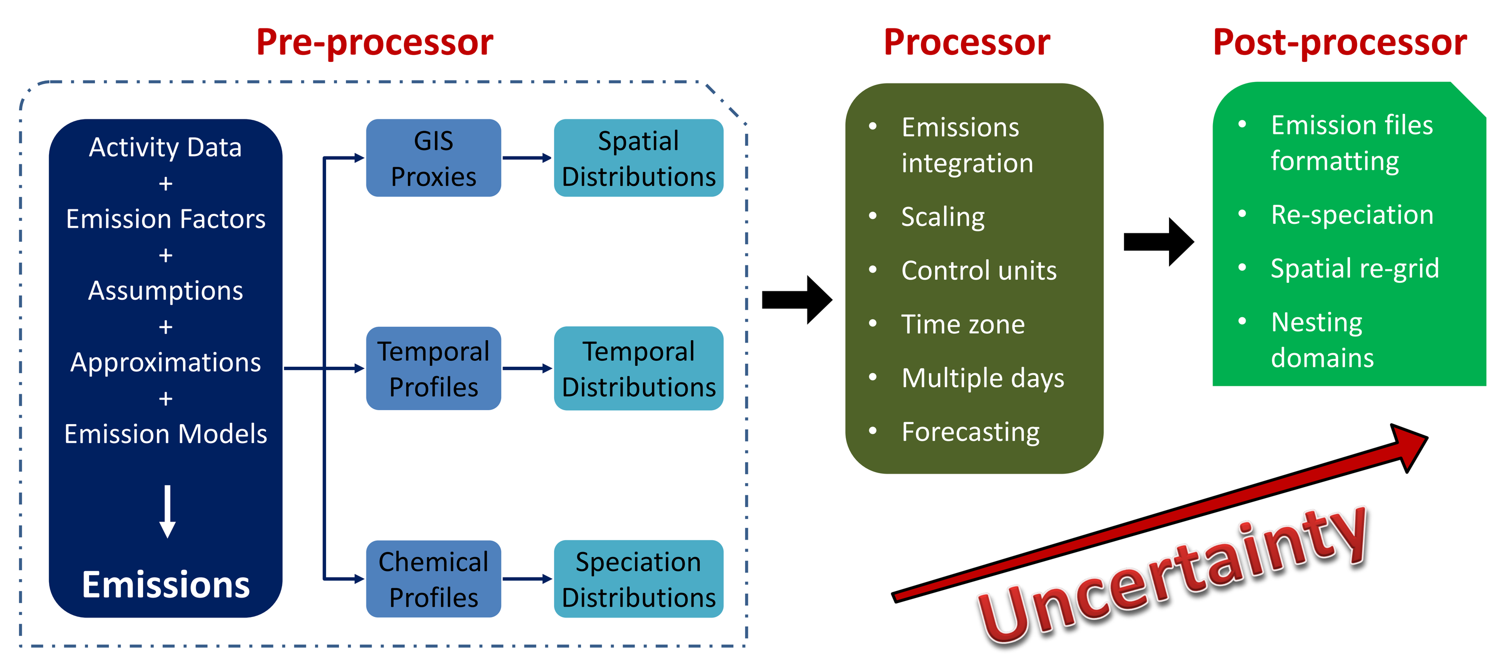


Figure 3. Model-ready EIs are constructed by pre-processing, processing, and post-processing steps with high-dimensionality input data. Each step contributing to the overall EI uncertainty.

The process is repeated for each source type (area, mobile, and point), subcategory (e.g., industrial combustion, gasoline vehicles, etc.), pollutant, and time step. Biogenic emissions are obtained with either on-line or off-line emission models and the emissions are aggregated.[5] The results are gridded emissions for each pollutant as a function of time. The process can be computationally- and time-demanding, and prone to high uncertainties.

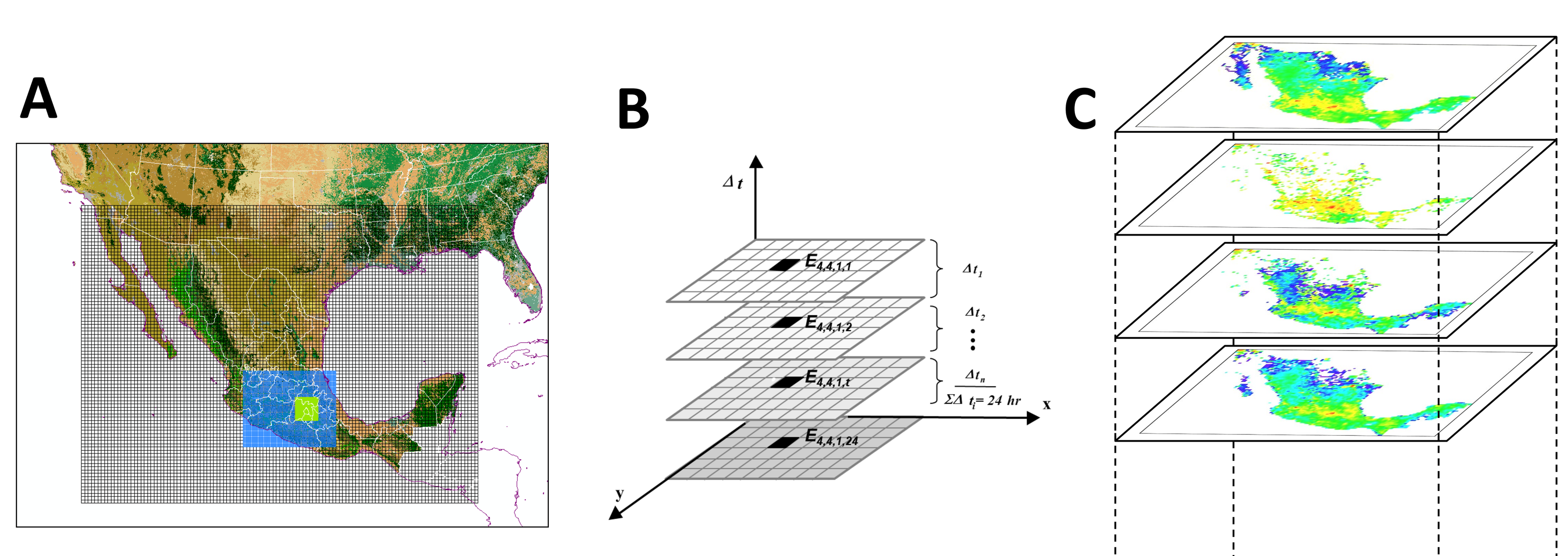
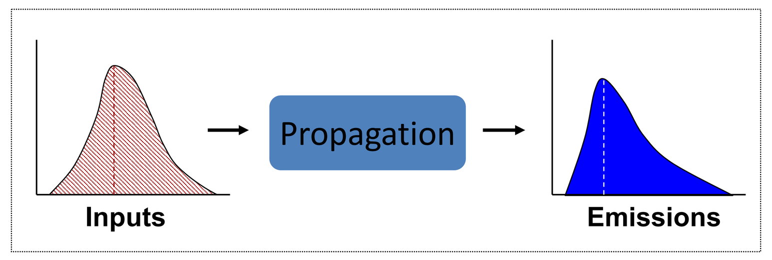


Figure 4. For each selected modeling domain (A), emissions data are gridded in space and distributed in time (B) for each pollutant (C).

Traditional treatments of Uncertainty



Other than qualitative methods that rely on scores and ratings of input/output data, traditional quantitative methods are based on either interval analysis or probabilistic uncertainty propagation techniques.

Probabilistic Methods

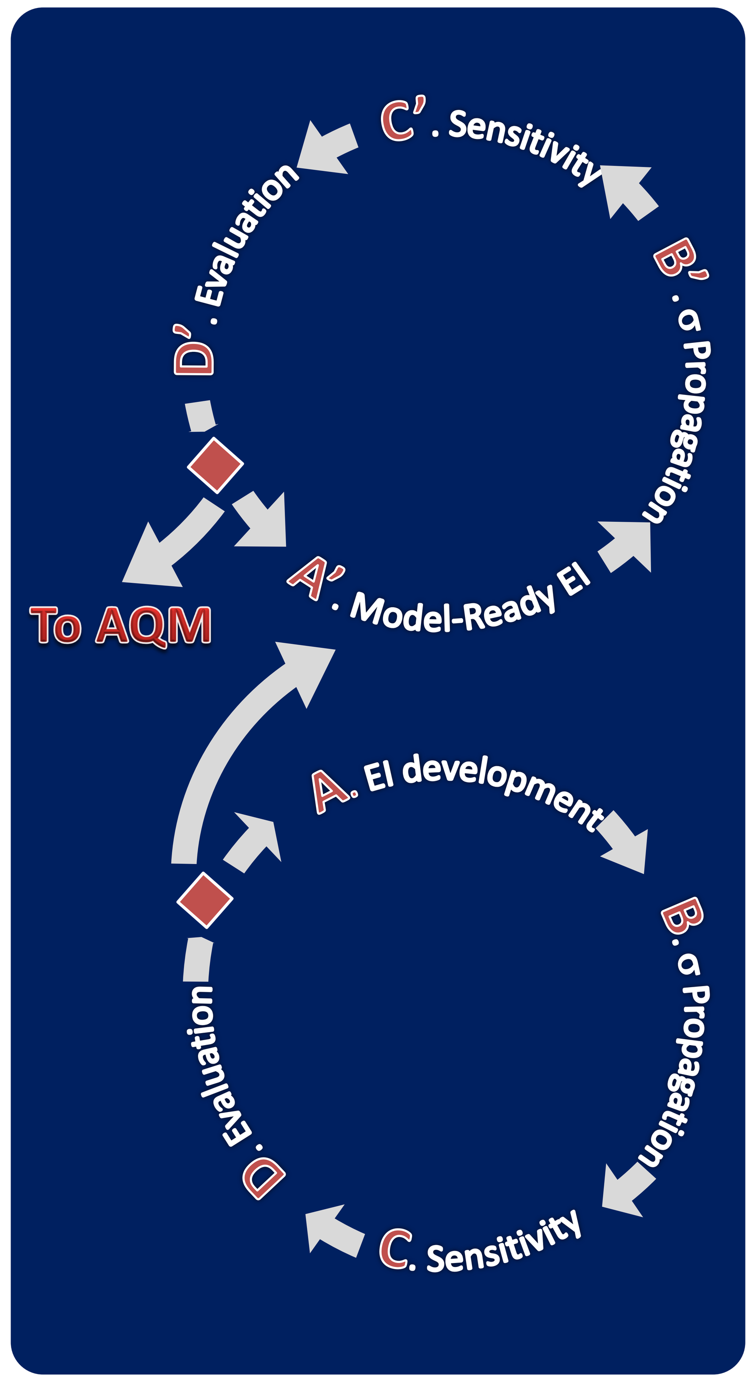
- **Analytical Calculations**: They are easy to implement and in some cases they can provide exact solutions. However, they have limited applicability as their accuracy and simplicity tends to diminish as the complexity of the assessment increases.
- **Numerical Methods**:
  - Monte Carlo and Bootstrap
  - Latin hypercube sampling
  - Bayesian statistics
  - Others (Fourier, quasi-Monte Carlo, etc.)

Sensitivity analysis can also be applied in combination with probabilistic methods to identify which inputs contribute the most to the overall uncertainty in the results.

Comprehensive treatment of Uncertainty

Traditional treatments of uncertainty are often applied to EIs to quantify ***parametric*** and ***structural*** uncertainties. However, they are less suitable for assessing ***disaggregation*** uncertainties in **model-ready** EIs for air quality modeling applications due to the high data dimensionality involved. The following guideline for treatment of uncertainties in model-ready EIs for air quality model applications is proposed.

Number of parameters	Description
$10^1 - 10^2$	Emission source categories
$1 - 10^2$	Chemical species
$10^2 - 10^4$	Number of grid cells
$10^1 - 10^2$	Number of time steps



- A. Development of EI with the use of AD, EF, assumptions, approximations and emission models.
- B. Parametric and structural uncertainties propagation using traditional probabilistic methods.
- C. Sensitivity analysis to identify larger uncertainty contributors.
- D. EI evaluation with emission measurements, observations, and top-down approaches.
- If the uncertainties in the EI are not adequately constrained, go back to A; otherwise go to A'.
- A'. Development of model-ready EI with spatial proxies, as well as temporal and chemical profiles.
- B'. Disaggregation uncertainties propagation with analytical methods.
- C'. Sensitivity analysis to identify larger uncertainty contributors.
- D'. Spatial, temporal and chemical evaluation with satellite data, ambient measurements.
- If uncertainties well constrained, it can be used for AQM applications, otherwise go back to A'.

Conclusions

The quantification of uncertainties must be an essential component of air quality modeling applications, as it describes the accuracy and qualifies the level of confidence in the emission fields. Uncertainty analysis applied with sensitivity analysis can also help identify inputs that contribute the most to the overall uncertainties. However, most modeling applications focus on traditional methods for assessing parametric uncertainties and less on structural and disaggregation uncertainties of model-ready EIs. An alternative approach for estimating desegregation uncertainties of complex systems with high data dimensionality can be applied by combining analytical and probabilistic methods. The central step in this approach is the emission evaluation using emission measurements, satellite data, ambient measurements, and top-down approaches.

References

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