Global sensitivity analysis to identify archetypes for the impact assessment of chemicals

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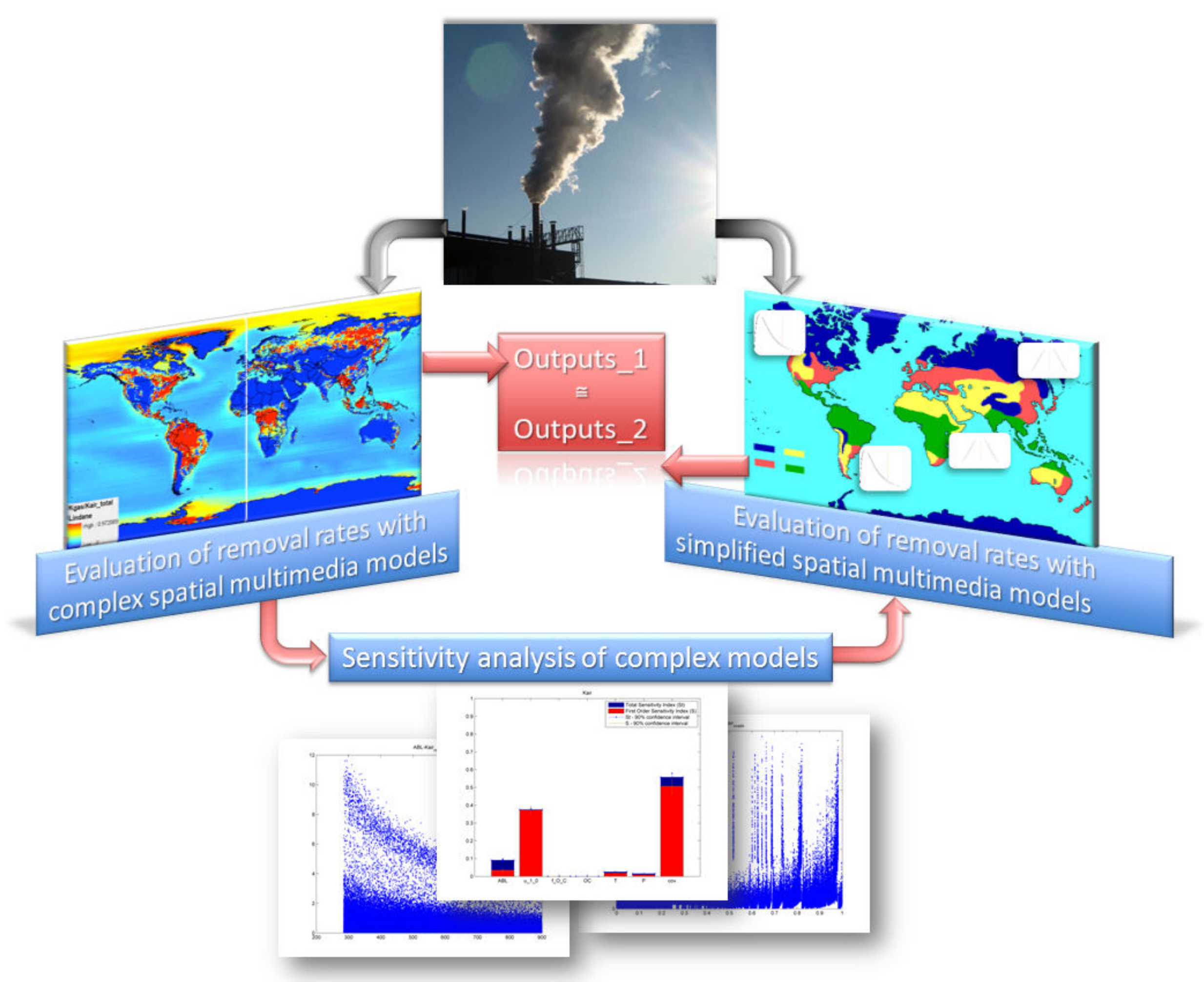
Emission of chemicals is increasing over years and the related impacts are greatly influenced by spatial differentiation. Chemicals are usually emitted locally but, due to persistence and physical chemicals properties, may exert global impact. Variability of environmental parameters may affect the fate and the exposure up to orders of magnitude of difference (Sala et al 2011). Accounting for spatial differentiation of chemical impacts requires the use of multimedia models, at various levels of complexity (from simple box model to computational intense and high spatial resolution model).



Methodology

Sensitivity analysis techniques have been applied to MAPPE Global (**Multimedia assessment of pollutant pathways in the environment** – Pistocchi et al 2011) to identify key parameters and support the development of emissions' archetypes (Ciuffo et al 2012). MAPPE is an advanced, multimedia, spatially resolved (1×1^0) model allowing evaluation of chemicals removal rates from air, water and soil.

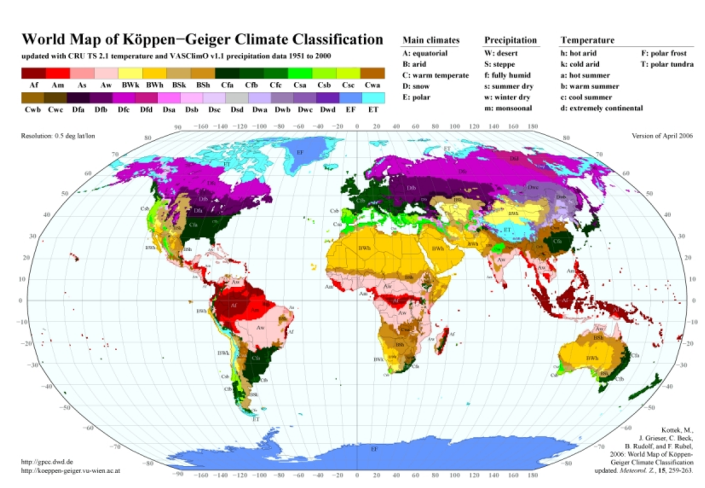
Using a **Monte Carlo framework**, we applied **variance-based sensitivity analysis techniques** to find out those environmental parameters explaining the highest share of the variability (namely the variance) in the model outputs. In particular, 5 analyses were carried out: an overall analysis for all the chemicals included in the model and four chemical-specific analyses in which we restricted the attention to a chemical pertaining to a specific class (a hydrophilic, a volatile, a hydrophobic, and a multimedia chemical were selected), thus, with peculiar characteristics.

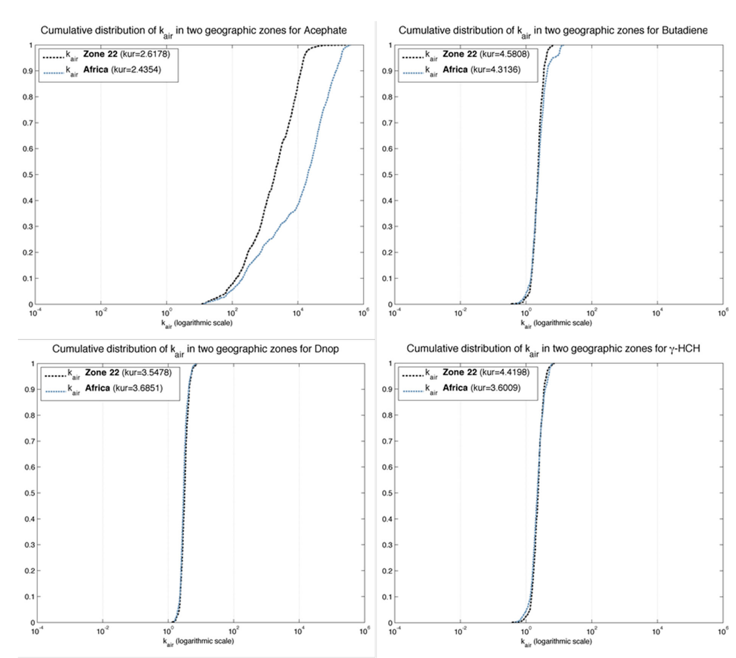
Results suggest the possibility of basing **emission archetypes on climatic zones** rather than on geo-political characteristics (e.g. continents, countries). This hypothesis is tested by evaluating and comparing the **distributions of the air removal rate within different climatic zones** (considering the Koppen-Geiger Climate Classification) **and within different continents**. The wider these distributions are, the higher the uncertainty introduced by the archetype is expected to be.

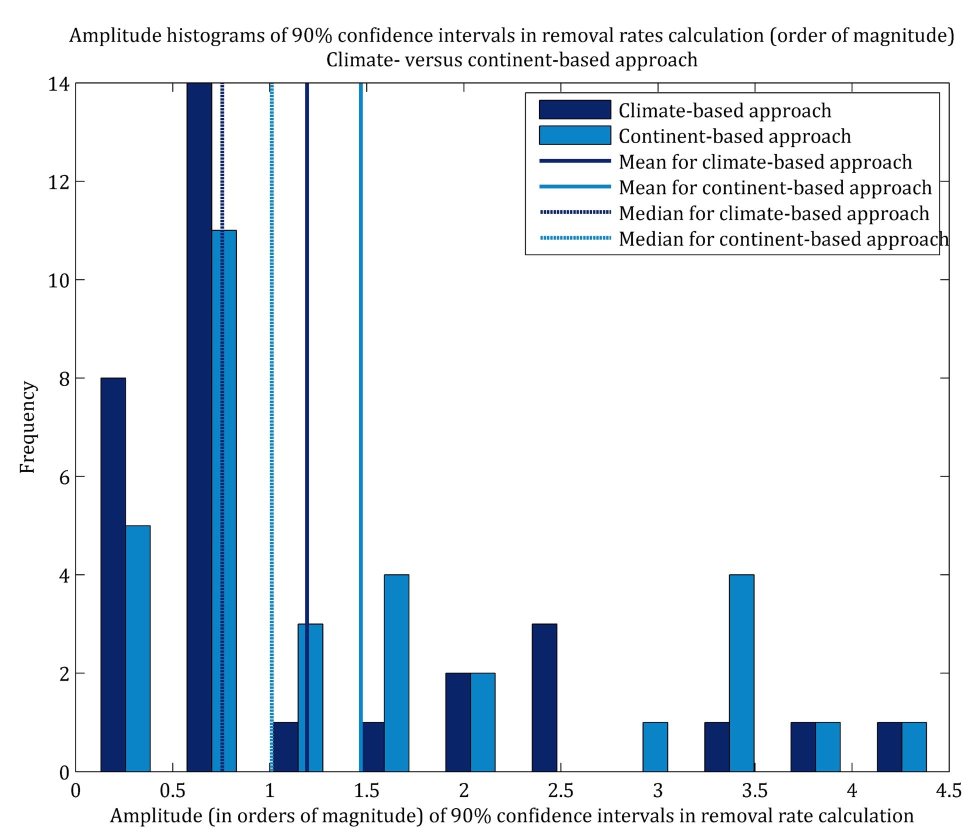
Air Compartment		
Chemical category	Key parameters for archetypes Absolute terms	Key parameters for archetypes Orders of magnitude
Overall	Chemical, P, ABL	Chemical, P, U_{10}
Hydrophilic	P, ABL	P, ABL
Lipophilic	U_{10}, P, ABL, OC, Cov	U_{10}, P, ABL, OC, Cov
High volatility	Cov, U_{10}, ABL	U_{10}, Cov, ABL
Multimedia	U_{10}, Cov, ABL, (T)	U_{10}, Cov, ABL, P, (T)

Input parameters

ABL	Atmospheric Boundary Level
U_{10}	Wind speed at 10 m
OC	Organic Carbon in air
T	Temperature
P	Precipitation
Cov	Coverage/land use (forest, impervious surface etc)
Chemical	Specific chemical







Results and discussion

Results open up several issues:

1) It is necessary to evolve the concept of spatial differentiation from the traditional approach based on scale/resolution (cell, country, and basin) to more "scenario-oriented" approaches. In this light, according to the results achieved, archetypes should be developed in order to be:
   - Compartment-specific
   - Chemical-specific
   - Target-specific
2) For chemicals characterized by low spatial-variability, the introduction of archetypes only bring an increased computational burden that is not justified by a real increase in the reliability of modeling activities. For this reason, first of all, it is necessary to identify the families of chemicals with sufficient variability to justify the effort of designing suitable archetypes. Then, these archetypes should be built taking into consideration the peculiarities of each chemical (or each group of them). A global sensitivity analysis might represent a suitable tool for this purpose. Preliminary results have shown that the hypothesis of basing environmental archetypes on climatic zones deserves further consideration.

The implications of climate archetypes' implementation are worth highlighting. First of all, archetypes may result in a significant reduction of the workload compared to the use of more complex spatially resolved models. Secondly, in the case of screening applications, archetypes may easily support the identification of hotspots of potential impact related to chemical fate. Finally, archetypes may be included in commercial LCA software, and identified through geographical coordinates so that practitioners could automatically perform calculations.

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