Modelling iodine interactions with atmospheric aerosols

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Following a severe nuclear reactor accident, radionuclides like caesium and iodine can be released into the atmosphere. Modelling tools should be able to predict the source term (Katata *et al.*, 2015) as well as dispersion. These data are used to predict radiological consequences and possible counter-measurements as population evacuation if needed.

During the Fukushima accident, significant differences between iodine activity measurements and predictions have been observed while a good agreement was obtained for caesium. This difference may result from the iodine chemical reactivity in the atmosphere not considered in the current dispersion crisis tools. Indeed, parameters like deposition velocity and the dose-effect factor depend on iodine chemical speciation and its physical form (gas, particle, liquid, solid). Therefore, the iodine chemical network in the atmosphere has to include heterogeneous reactions.

In a first step, an atmospheric iodine gas-phase mechanism was developed (Trincal, 2015) which contain 246 elementary reactions resulting from a critical review of the literature and was implemented into both 0D and 3D models. The simulations highlighted the important reactivity of iodine with atmospheric pollutants (NOx, O_3), which can lead to formation of iodine aerosols via the formation of iodine oxides or high-molecular weight organic iodine compounds.

In a second step, the modelling is extended in order to include an aerosol phase to take into account possible gas/particles interactions. A bibliographic review has been performed based on the available experimental and theoretical data about iodine-containing species reactions and interactions with the particles. For each potential reaction, data are analysed and selected by the following order of criteria : NIST and IUPAC recommendations, experimental data, theoretical data, and then estimations.

The gaseous phase mechanism has been completed with the heterogeneous reactions and a 0D study has been conduct to evaluate the iodine species speciation under various atmospheric conditions (temperature, photolysis, gas, and aerosols concentration ...).

In a near future, this work will be encapsulated in chemical transport models (Chimere and Polair3D in our case) to carry out simulations in more relevant conditions.

The last part will consist in simulating the Fukushima iodine atmospheric chemical transport.

This work takes part in the common laboratory C^3R IRSN/CNRS/Lille1.

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Trincal J., Modeling of the behaviour of iodine in the atmosphere, **2015**, Ph-D France, University Lille 1.