Abstract for IMAMPC – oral communication on 4 July 2013

Applications of theoretical chemistry tools to nuclear safety issues

L. Cantrel [1,2], F. Louis [2,3] and V. Vallet [4]

(1) Institut de Radioprotection et de Sûreté Nucléaire, PSN-RES, SAG, Centre de Cadarache - BP 3, 13115 Saint Paul lez Durance, France, (*) laurent.cantrel@irsn.fr

(2) Laboratoire commun IRSN-CNRS-Lille1: "Cinétique Chimique, Combustion, Réactivité" (C3R), Centre de Cadarache, BP3, 13115 Saint Paul Lez Durance, Cedex, France

(3) Physico Chimie des Processus de Combustion et de l'Atmosphère (PC2A) UMR 8522 CNRS/Lille 1, Université Lille 1 Sciences et Technologies, Cité scientifique, Bât C11/C5, 59655 Villeneuve d'Ascq Cedex, France

(4) Laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM) UMR 8523 CNRS/Lille 1, Université Lille 1 Sciences et Technologies, Cité scientifique, Bât P5, 59655 Villeneuve d'Ascq Cedex, France

The IRSN (Institut de Radioproctection et de Sûreté Nucléaire) is a French institute in charge of research and expertise on nuclear safety and radioprotection. Fukushima situations reinforced the need to develop capabilities of predicting evolution and consequences of all possible accidental situations whatever are their postulated probability of occurrence. Of particular importance are the situations that can lead to the release of radionuclides produced by the fission of the nuclear fuel to the environment and thus to possible radiological consequences. Predicting the evolution of the chemical speciation and isotopic inventory of all radionuclides during the accident progress is essential not only to prepare the accidental and post-accidental situation management but also to define new devices to mitigate the environmental releases.

During the last decades, IRSN implemented among with French and foreign partners experimental research programs to develop the knowledge on radionuclides chemistry. But radionuclides that can mostly contribute to radiological consequences (iodine, ruthenium …) are extremely reactive and conditions of an accident in a nuclear installation can hardly reproduced experimentally to derive directly from pure empirical models that can be used to simulate radionuclides behaviour in such a broad range of severe accidental conditions. So a few years ago, IRSN decided to complement experimental approaches with theoretical chemistry one either to complete/interpret results of some experimental programmes and thus increase the value of their results or to get piece of information useful to decline/check some potential nuclear safety issues and bring data not available in literature and hardly reachable experimentally. To illustrate implementation of this mixed experimental/theoretical strategy quite new in the nuclear safety context, three examples will be presented:

- The behaviour of fission products in degraded fuel ;
- The chemistry of iodine in the reactor coolant system ;
- The chemistry of Plutonium in the fuel reprocessing cycle in case of accidental fires.

All these researches are led in close collaboration with some academic laboratories to associate all the specific skills needed to cover all the involved phenomena.