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# Interactions between sodium fire aerosols and fission products - a theoretical chemistry and experimental approach

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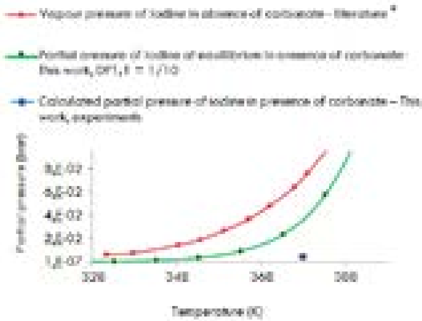
Within the framework of generation IV nuclear reactor safety assessment, the objective of this research work is to investigate the radiological and chemical source term in case of a core disruptive accident in case of a sodium-cooled fast nuclear reactor. This work investigates the interactions between sodium aerosols, formed after primary system sodium ejection in the containment, and gaseous iodine. Understanding the complex behaviour of surface reaction requires detailed knowledge of both macroscopic and microscopic processes that take place. To link these processes, we followed a combined theoretical and experimental approach. Firstly, methods to theoretically understand the thermodynamics of the heterogeneous reaction between sodium carbonate aerosols and fission products: I2, NaI and HI are proposed. *Ab initio*, density functional theory (DFT) calculations using Vienna *ab initio* simulation package are carried out. Secondly, interactions between (I2) g and $Na_2CO_3$ were investigated experimentally. (I2) g was generated by heating permeation tubes containing (I2)s, and, passing it through a reaction chamber containing $Na_2CO_3$ sorbent. The concentration of unreacted iodine was then measured at the exit of reaction chamber. DFT calculations show that for defect-free surfaces of ϒ- $Na_2CO_3$ phase, the (001) facet is the most stable. This ideal surface reacts very strongly with HI and NaI, at T<300°C, a low partial pressure of these species ($10^{-7}$ bar) is sufficient for achieving a surface coverage greater than 50%. However, I2 (g) would react weakly with this surface: to have a surface coverage of 10%, a high partial pressure of iodine is required ($10^{-2}$ bar). Experimental investigations suggest a stronger reactivity of iodine with exposed $Na_2CO_3$ sorbent, at T<100°C; a partial pressure limited to $10^{-6}$ bar is sufficient to obtain 10% surface coverage. Both theoretical and experimental approaches indicate very low gas phase capture of I2 (g) by $Na_2CO_3$. In summary, we aim to combine computational and experimental studies to increase our understanding of complex surface adsorption phenomena.



## Biography

Ankita Jadon is a young Nuclear Safety Researcher focused on challenges that sodium cooled reactor technology still offers. Her research lies primarily in the field of sodium fire aerosols produced in a severe accident. After completing her Master studies specializing in Nuclear Engineering at Ecole des Mines de Nantes, France, she started her professional career as Researcher at the French National Institute for Nuclear Safety (IRSN). In the laboratory, where she is a Doctoral Researcher, she is simulating and modeling interactions between sodium fire aerosols with iodine species in case of a severe accident in an SFR for a computer code which would be used to simulate severe accidents.

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