**Integration Group for the Safety Case (IGSC) Symposium 2024**  
*MOVING TOWARDS THE CONSTRUCTION OF A SAFE DGR – GETTING REAL*

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| **Abstract Number: 3** | **Poster P7.1.5** |
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| **Abstract Title:** An Alternative Conceptual Model for Radiolysis Effects on Chemical Conditions in Salt Repositories  U.S. Department of Energy, Carlsbad Field Office, Carlsbad New Mexico 88220, USA  [andy.ward@cbfo.doe.gov](mailto:andy.ward@cbfo.doe.gov) | |
| **Abstract (300-500 words):**  An accurate actinide source term is a critical input to performance assessment (PA) calculations of direct brine releases from a disturbed repository and the actinide containment safety case but remains highly uncertain. Much of the uncertainty in actinide solubility is partly due to multiple simplifying assumptions. One such assumption is that radiolysis will not affect the chemical conditions of the repository. During the first compliance certification application (CCA), an isotope-specific Curie comparison of the inventories for spent nuclear fuel (SNF) and transuranic (TRU) waste inventory led to the conclusion that radiolysis causing oxidative corrosion was a minor concern in SNF storage and would therefore be a minor concern at the U.S. Department of Energy Waste Isolation Pilot plant (WIPP). The larger inventory of plutonium expected to be disposed of at the WIPP presents a challenge to this assumption. A reanalysis of the features events and processes (FEPs) resulted in radiolysis being screened into PA calculations, but only as a source of hydrogen gas (H2). The objectives of this study are to evaluate the assumption that radiolysis will not affect chemical conditions, nor the actinide source term, and to assess any contribution to the actinide containment safety case.  In this study, the Geant4-DNA extension of the Geant4 general-purpose Monte Carlo simulation toolkit is used to simulate water radiolysis and the subsequent chemistry under repository conditions. The time-dependent and linear energy transfer (LET)-dependent primary yields of radical anions and molecular species are quantified and the effects of scavenger species are assessed. Results show that scavenger species can affect the amount of H2 gas generated and suggest an overestimation in current PA calculations. The primary water radiolysis intermediates may cause the degradation of organic complexing agents, challenging the assumption of organic chelating agents that persist for the entire regulatory period and increase actinide solubility. Simulations also show the radiolytic oxidation of soluble ferrous ions (Fe2+), resulting from the anoxic corrosion of zero-valent iron (Fe0) in waste canisters, to the relatively insoluble ferric (Fe3+) hydroxides, which may have implications for actinide oxidation states and solubility.  Track structure simulation codes accurately reproduce the stochastic nature of interactions between ionizing radiation and matter, allowing the quantitative evaluation of radiolysis and the subsequent chemistry in the presence of scavengers. Simulation results challenge long-held assumptions about chemical conditions in deep geological repositories for transuranic waste. | |