DEVELOPMENT AND IMPROVEMENT OF NUMERICAL METHODS AND TOOLS FOR MODELLING COUPLED PROCESSES

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Abstract should be written in 700-800 words and with 11 font size, Times New Roman, justified, single line spacing. It should not exceed 2 pages including tables and figures.

Understanding of multi-physical Thermo-Hydro-Mechanical-Chemical coupled processes (THMC) occurring in radioactive waste disposal is a major and permanent issue to support optimization of design and safety case abstraction . Numerical simulations are necessary to make predictive multiphysical analyses for time periods and space scales larger than experiments can cover [1, 2]. These numerical simulations require integrating, in a consistent framework, an increasing scientific knowledge acquired for each of the individual components of a system for radioactive waste disposal. This implies to consider couplings of different and non-linear processes from a wide range of materials with different properties as a function of time and space in ever-larger systems. The development of cutting-edge and efficient numerical methods is thus necessary, in the scope of having useful, powerful and relevant numerical tools for assessments. It is also necessary to manage the uncertainties associated to the input data feeding the models and the representation of the processes, to assess the range of variability of the results and to identify the main parameters and processes driving the behavior of the systems of interest. Managing uncertainties in these complex systems require the improvement and the development of innovative, appropriate and efficient numerical methods. To tackle the above-mentioned challenges a R&D work package entitled "DONUT : Development and improvement of numerical methods and tools for modelling coupled processes" has been launched about 4 years ago within the EURAD join programming initiative. Organized around four technical tasks the objectives of DONUT are the: (i) development of relevant, performant & cutting-edge numerical methods that can easily be implemented in existing or new tools, in order to carry out highperformance computing to study of highly coupled processes in large systems (reactive transport, 2phase flow & THM modelling in porous and fractured media), (ii) development of numerical scale transition schemes for coupled processes (meso to macro scale, or pore to Darcy scale) supporting the study of specific multi-scale couplings e.g. chemo-mechanics, (iii) development of innovating numerical methods to carry out uncertainty and sensitivity analyses, (iv) the realization of benchmark exercises, on representative test cases, to test the efficiency of developed methods (robustness,

accuracy, time computational) on relevant tools. The achievement of DONUT will be illustrated through relevant examples (e.g.[3-6]) . and will be discussed

References

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- 3. Kolditz, O., et al., *Digitalisation for nuclear waste management: predisposal and disposal.* Environmental Earth Sciences, 2023. **82**(1): p. 42.
- 4. Sochala, P., et al., *Uncertainty propagation in pore water chemical composition calculation using surrogate models*. Scientific reports, 2022. **12**(1): p. 15077.
- 5. Soulaine, C., et al., *porousMedia4Foam: Multi-scale open-source platform for hydrogeochemical simulations with OpenFOAM*®. Environmental Modelling & Software, 2021. **145**: p. 105199.
- 6. Prasianakis, N.I., et al., *Neural network based process coupling and parameter upscaling in reactive transport simulations*. Geochimica et Cosmochimica Acta, 2020. **291**: p. 126-143.