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A mesoscale hydration-integrated burgers model for predicting early-age viscoelastic response of graphite containing cementitious materials

Nour Zeaiter[1], Julien Yvonnet[2], Benoit Bary[3], Gabriele La Valle[4]

[1] Université Paris-Saclay, CEA, Service de recherche en Corrosion et Comportement des Matériaux, 91191 Gif Sur Yvette, France. nour.zeaiter@cea.fr
[2] Univ Gustave Eiffel, MSME, CNRS UMR 8208, F-77454 Marne-la-Vallée, France, France. julien.yvonnet@univ-eiffel.fr
[3] Université Paris-Saclay, CEA, Service de recherche en Corrosion et Comportement des Matériaux, 91191 Gif Sur Yvette, France. benoit.bary@cea.fr
[4] Univ Gustave Eiffel, MSME, CNRS UMR 8208, F-77454 Marne-la-Vallée, France, France. gabriele.la-valle2@univ-eiffel.fr

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Abstract

Within the context of immobilizing long-lived, low-level nuclear waste (LL-LL) containing graphite from first-generation French reactors, this study investigates the early-age behavior of graphite-containing mortars, comparing matrices based on alkali-activated slag (AAS) and ordinary Portland cement (OPC) to assess their viscoelastic performance. The novelty of this work lies in the explicit integration of hydration effects into a mesoscale viscoelastic model, where the mortar matrix is described by a hydration-dependent linearized Burgers rheological law. This formulation allows capturing the continuous evolution of viscoelastic properties during early hydration, which is critical for evaluating early-age mechanical performance. A multi-scale modeling framework is developed to capture the progressive development of viscoelastic behavior of heterogeneous cementitious materials. At the mesoscale, numerical simulations are performed on a Representative Volume Element (RVE) comprising graphite inclusions modeled as isotropic elastic phases with constant mechanical properties. The evolving viscoelastic

behavior of the surrounding matrix allows the application of the superposition principle, and a series of numerical relaxation tests is conducted to extract the components of the effective relaxation tensor, parameterized by the hydration degree. These precomputed mesoscale properties are then transferred to the macroscopic scale: spline interpolation is used to construct a continuous representation of the effective relaxation tensor, which is subsequently employed in a convolution integral to describe the time-hydration-dependent stress-strain relationship. Finally, a 3D finite element simulation is performed on a quarter of the waste package, representing the composite geometry. The evolution of the hydration degree $\xi(x, t)$ is described using a standard thermochemical kinetics law, and the homogenized properties are continuously updated from the interpolated mesoscale dataset. This approach enables the treatment of arbitrary linear viscoelastic laws and diverse microstructural morphologies. The model is calibrated using experimental creep data from literature obtained at various loading times corresponding to different hydration states of the material. These datasets capture the progressive evolution of viscoelastic properties during early hydration, providing a consistent basis for validating the multi-scale predictions. The agreement between simulations and experiments confirms the robustness of the proposed framework. Overall, this multi-scale approach demonstrates that AAS mortars exhibit a more favorable early-age viscoelastic response than OPC, with reduced creep and a more pronounced evolution of properties during hydration. This provides a reliable tool for optimizing AAS-based mixtures for nuclear-waste immobilization applications, where early-age mechanical performance is critical.

Keywords:

Multi-scale modelling Computational homogenization Linear viscoelasticity Hydration Burgers models