

Simulating the Effects of Neutron Irradiation on Concrete with the MOSAIC Software



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In nuclear power plants, the concrete biological shield is used to contain neutron and gamma radiation emitted by the reactor. Depending on the design and operating condition, the inner surface of the concrete biological shield may be exposed to high fluences. Within the framework of aging management and subsequent license renewal of U.S. nuclear power plants, it becomes critical to understand the effects of irradiation on the concrete and other materials over extended periods of operation.

The primary degradation mechanism in irradiated concrete is radiation-induced volumetric expansion (RIVE). It is caused by the amorphization of certain mineral phases contained in concrete aggregates (e.g., sand, crushed rocks, gravels). These mineral phases expand during the amorphization process, while the cement paste that binds the aggregates together remains mostly unaffected by the irradiation. This causes the concrete to swell and opens micro-cracks due to differential strains between the different mineral phases and the cement paste. Experimentally, this is measured as an increase in dimension and a loss of mechanical properties, such as Young's modulus, and tensile or compressive strength.

The effects of neutron radiation vary significantly from one concrete to another resulting in unusually large scatter of experimental data on irradiated concrete. This is caused by the fact that different minerals have a different susceptibility to neutron irradiation. Generally, quartz and silicate-bearing minerals swell much more than limestone and carbonate-bearing minerals, while some vitreous minerals, such as opal, may even shrink instead of swell.

This indicates that radiation susceptibility of a given concrete depends on the mineral composition of the rocks used as aggregates, which is typically not reported at the time of construction. For this reason, the Materials Research Pathway is developing the Microstructure-Oriented Scientific Analysis of Irradiated Concrete (MOSAIC) software. MOSAIC is a tool to assess the susceptibility to neutron irradiation of concrete based on an analysis of an actual concrete specimen (e.g., a core from a concrete structure).

The first step in the analysis is determining the microstructure and mineral composition of the specimen. This requires two experimental characterization techniques: micro-X-ray fluorescence (XRF) and two-modulator generalized ellipsometry microscopy (2MGEM). Micro-XRF provides a map of the chemical composition across the specimen surface, while 2MGEM provides a map of the optical properties of the surface. Both techniques require the same simple specimen preparation and can thus be combined to identify the minerals present in the specimen. Notably, the optical information is used to distinguish between minerals that have the same chemical composition (such as quartz and opal) but different crystal structures (and thus, different irradiation susceptibility). By using appropriate thresholds on the chemical composition, the cement paste and porosity can also be identified in the specimen.

The second step in the analysis is to perform a numerical simulation on the microstructure obtained above. Since the data from the micro-XRF and 2MGEM is presented on regular grids, the Fast Fourier Transform (FFT) method is ideal to compute the mechanical

response of the material. The mechanical behavior of concrete under irradiation is controlled by the following three factors:

- The RIVE of the minerals present in the concrete. MOSAIC uses the Irradiated Minerals, Aggregates, and Concrete (IMAC) database, which contains a large collection of experimental results from the literature and uses these results to calibrate theoretical models for the RIVE of each mineral as a function of the neutron fluence and temperature.
- The brittle behavior of both the minerals and the cement paste. MOSAIC uses a sequential nonlinear solver to compute the spread of damage in the microstructure. The damage algorithm is nonlocal to limit spurious oscillations arising from the FFT calculations and reduce the sensitivity of the method to the spatial discretization.
- The viscoelastic behavior of the cement paste. This is critical to assess the long-term performance of irradiated concrete as creep can delay the onset of damage caused by irradiation. In MOSAIC, this is accounted for using a finite difference scheme, which is automatically combined with the sequential

nonlinear solver to resolve the coupled creep-damage-expansion problem.

The numerical specimen can be subject to various boundary conditions in terms of macroscopic strain or stress, temperature, and fluence, thus allowing for the simulation of either experimental conditions, or conditions representative of long-term operations, including mechanical restraints induced by the unirradiated section of the biological shield.

This two-step process is illustrated in Figure 1, in which the micro-XRF and 2MGEM maps are combined to identify the cement paste and minerals in a concrete specimen, after which an irradiation simulation is carried out under free mechanical boundary conditions (corresponding to an accelerated experiment in a test reactor).

With this tool, concrete specimens extracted from nuclear power plants could be analyzed to estimate their susceptibility to neutron irradiation in conditions that are representative of the long-term operations of the reactor.

Figure 1: MOSAIC flowchart. The micro-XRF and 2MGEM images of the same specimen (left) are analyzed to obtain the phase composition (middle), which is then used as an input for the nonlinear FFT solver that computes the strain, stress, and damage in the microstructure (right).

