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MOSAIC: An Effective FFT-based Numerical Method to Assess Aging Properties of Concrete

Christa E. Torrence¹, Alain B. Giorla², Yujie Li³, Elena Tajuelo Rodriguez², Jose D. Arregui Mena², Thomas M. Rosseel⁴ and Yann Le Pape^{5*}

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Abstract

As the nuclear fleet in the United States ages and subsequent license renewal applications grow, the prediction of concrete durability at extended operation becomes more important. To address this issue, a Fast-Fourier Transform (FFT) method is utilized to simulate aging-related degradation of concrete within the Microstructure Oriented Scientific Analysis of Irradiated Concrete (MOSAIC) software. MOSAIC utilizes compositional phase maps to simulate damage from radiation-induced volumetric expansion (RIVE), applied force, creep, and thermal expansion. This compositional detail allows each mineral in the microstructure to be assigned specific material properties, allowing the simulation to be as accurate and representative as possible. The principal goal of MOSAIC is to simulate the effects of nonlinear aging mechanisms occurring in nuclear concrete on the macroscopic mechanical properties, using only the aggregate microstructure compositional information as a starting point. Several realistic example simulations are shown to demonstrate the utility and uniqueness of the MOSAIC software.

1. Introduction

As the fleet of commercial nuclear light water reactors across the United States ages, interest in possible materials degradation associated with extended operation grows along with a focus on obtaining subsequent license renewals. Along with this growing interest, the Nuclear Regulatory Commission (NRC) is performing extensive safety and environmental impact reviews before granting a 20-year license renewal.

Concrete is the primary component in critical structures such as the containment building, the spent fuel handling building and the concrete biological shield (CBS) in light water reactor plants, hence any change in concrete's properties is of high importance to understand and to predict aging. Damage to safety-related concrete structures can lead to a plant shutdown, as occurred at the Crystal River power plant in Florida. Cracks formed through the containment building, with repair estimates exceeding 3 billion US dollars, which

led to a permanent closure of the plant (Duke Energy 2013). Multiple time-dependent and degradation mechanisms are at play as concrete ages, including creep, damage, radiation-induced expansion, internal and external chemical attacks such as freeze-thaw, alkali-silica reaction (ASR), and delayed ettringite formation (DEF) (Graves *et al.* 2014). Hardened concrete is a heterogeneous composite composed of coarse aggregates, sand and hydrated cementitious materials forming a complex porous network. Natural aggregates are collections of rock-forming minerals, primarily in a crystalline state. Hardened cement paste is mainly composed of poorly-crystallized calcium-silicate-hydrates (C-S-H), whose structure presents similarities to those of the natural minerals tobermorite and jennite (Taylor 1997). The composition of aggregates plays a significant role in concrete damage when subject to ASR and neutron irradiation due to mismatches in volumetric expansion rates of their mineral components.

While the construction data including the concrete composition and the 28-day compressive strength are generally accessible to the operator, aging concrete data is extremely limited for several reasons: 1. In-service concrete data on nuclear concrete is severely limited by practical and regulatory restrictions; 2. The building standards and codes applicable to nuclear constructions provide limited information about the effects of degradation on concrete properties (e.g., ACI Committee Report 349.3R: Evaluation and Repair of Existing Nuclear Safety-Related Concrete Structures); 3. In most cases, in-service monitoring is limited to visual inspection; and 4. Critical characterization documenting the mineralogy and microstructure of concrete constituents is scarcely available. Given that concrete is inherently a multiphase and multiscale assemblage of complex natural rocks

¹Ph.D Student, Texas A&M University, 400 Bizzell St. College Station, TX 77843, USA.

²R&D Associate Staff, Oak Ridge National Laboratory, 1 Bethel Valley Rd. Oak Ridge, TN 37830, USA.

³Post doctoral Research Associate, Oak Ridge National Laboratory, 1 Bethel Valley Rd. Oak Ridge, TN 37830, USA.

⁴Materials Research Lead, Light Water Sustainability Program, Oak Ridge National Laboratory, 1 Bethel Valley Rd. Oak Ridge, TN 37830, USA.

⁵Senior R&D Staff, Oak Ridge National Laboratory, 1 Bethel Valley Rd. Oak Ridge, TN 37830, USA.

*Corresponding author, E-mail: lepapeym@ornl.gov

and more or less well-crystallized hydrates forming a porous network that is unique for a given structure, the effects of aging mechanisms in concrete are difficult to characterize and predict with traditional experimental and numerical methods. Most of the applied methods rely on macroscopic observations and continuum models assuming homogeneity of the material. These challenges create a need to combine high-resolution characterization methods with advanced numerical methods to predict effectively the evolving properties subject to aging.

The CBS is of particular interest due to its critical role in a nuclear power plant (NPP). Besides the containment building, the CBS serves an important safety role as a primary line of defense in case of a failure in the nuclear reactor core. For this reason, it is important to deepen the understanding of the aging of concrete's properties, to understand the impact of irradiation on aging, and to have access to predictive technologies.

At the macroscale, a variety of software and code packages exist to simulate nuclear concrete under physical stress (Maruyama *et al.* 2016; Piotrowski *et al.* 2012) and/or chemical attack (Kari and Puttonen 2009). The concrete containment structure in NPPs has been studied extensively at full scale using FEM (Hora and Patzk 2007; Tamayo and Awruch 2016; Prinja *et al.* 2005; Lundqvist and Nilsson 2011; Huang *et al.* 2017). These works provide valuable information on loss of prestress, weak points, and long-term macroscale behavior. However, when looking at concrete damage, the macroscale models do not capture the local nuances that influence crack patterns. Du and colleagues (2012) performed a comparison of macroscale simulations, mesoscale simulations, and experimental data and found that the mesoscale simulations matched the experimental damage patterns more closely than the macroscale simulations.

Significant advances in meso-scale numerical simulation of concrete have been made in the past few decades, including lattice-based models (Kawai 1978; Bolander and Saito 1998; Suzuki *et al.* 2005; Nagai *et al.* 2005; Yamamoto *et al.* 2013), finite element models (Hafner *et al.* 2006; Pomaro *et al.* 2011; Xiong *et al.* 2020) and FFT (Moulinec and Suquet 1994, 1998a; Monchiet and Bonnet 2012; Lavergne *et al.* 2015a). Finite element analysis has proven successful in many structural and mesoscale level models, including those with realistic aggregate shapes. Maruyama and colleagues had success using a thermohydronechanical FEM model to calculate irradiation-induced damage, but did not include the effects of RIVE (Maruyama *et al.* 2012). A survey of the literature found numerous mesoscale concrete fracture models, (Ren *et al.* 2015; Briffaut *et al.* 2013; Du *et al.* 2012); however, the inclusion of RIVE was only reported in Giorla and Le Pape (2015). MOSAIC is a continuation of the research of Giorla *et al.* (2015).

This work aims to build an understanding of the rela-

tionships between aggregate mineralogy and aging degradation of concrete, meaning the scale of the work is on the order of millimeters. MOSAIC incorporates viscoelastic, damage, RIVE, shrinkage, and thermal expansion material properties into a single micromechanical simulation software. As MOSAIC is modeling on the scale of micrometers, difficulties with finite element model (FEM) can arise when meshing very fine and small morphologies because retaining the morphology of the minerals and aggregates is difficult to do with this approach. Similarly, lattice-based models generally assume that aggregates are made of homogeneous phases, incompatible with the compositional approach to modeling the aggregates. As such, Fast-Fourier Transform (FFT) is selected for this work due to its ability to retain morphological detail at a low memory cost.

2. Microstructure description

Hardened concrete is a heterogeneous composite composed of coarse aggregates, sand, and hydrated cementitious materials forming a complex porous network. Natural aggregates are rocks composed of various minerals, primarily in a crystalline state. Hardened cement paste is primarily composed of semi-crystalline C-S-H with an atomic structure similar to those of the natural minerals tobermorite and jennite (Taylor 1997). The composition of aggregates is important when modeling concrete damage due to differences in material properties between the composing minerals. As such, a strength of MOSAIC lies in its incorporation of detailed compositional data into the micromechanical analysis. Using a pixel-based approach, each pixel in the two-dimensional microstructure image is assigned to a mineral or a cementitious phase.

MOSAIC offers two routes to import microstructural and compositional information. The first and most detailed method is importing X-ray fluorescence (XRF) or Energy-dispersive X-ray spectroscopy (EDS) data in the form of processed counts and spectra or elemental images, such as presented in **Fig. 1**. Other characterization techniques such as scanning electron microscopy (SEM), Electron backscatter diffraction (EBSD), Raman spectroscopy and ellipsometry can be used to input data in the form of images or maps. The secondary and simplest route is to upload a single image. Material phases are assigned through thresholding based on grayscale, RGB color values, XRF processed counts, or EDS processed counts. Pre-processing of image data is available, including watershed segmentation, gradient computation, kernel dilation and erosion, and differing structuring elements.

As many of the minerals that compose the cement paste and aggregates contain many of the same elements in similar ratios and due to the uncertainties in the weight concentrations provided by elemental quantification techniques, the thresholding of these values can be challenging and often require combining several tech-

niques. Further information regarding the use of combining volume fraction of phases obtained by Rietveld refinement of X-ray diffraction (XRD) data and XRF

data in MOSAIC can be found in (Li *et al.* 2020). **Figure 2** shows varied concrete microstructures with detailed phase information reconstructed from XRF data

Fig. 1 Elemental intensity images from micro-XRF (a) Calcium, (b) Silicon, (c) Sulfur, (d) Potassium, (e) Manganese, (f) Iron. Grayscale value shows intensity, with white representing the highest intensity.

Fig. 2 Illustrations of MOSAIC phase maps. Top-left: Phase map of mortar computed from the XRF data in Fig. 1. Top-right: 92% quartz aggregate concrete (Le Pape *et al.* 2019); Bottom-left: Granite; Bottom-right: Sandstone (Li *et al.* 2020).

with 10-50 μm resolution. The thresholded image is classified into four phases: 1. Calcite (CaCO_3); 2. Ankerite [$\text{Ca}(\text{FeMgMn})(\text{CO}_3)_2$]; 3. Hardened cement paste and 4. Porosity.

2.1 Interface detection

The cement paste region immediately surrounding an aggregate is known as the interfacial transition zone (ITZ), a region of higher porosity than the bulk cement paste. The strength and stiffness of the ITZ is typically estimated to be approximately one-third of the bulk cement paste strength (Mindess *et al.* 2003). Unless the aggregates exhibit low tensile strength and toughness, fracture in normal strength concrete generally propagates through the ITZ regions, as they are the weakest points in the material. As such, it is important to include the ITZ in mechanical simulations accounting for damage or fracture. Furthermore, the boundaries between rock-forming mineral grains can also be identified, if desired.

An algorithm to detect the pixels that compose an ITZ or mineral-mineral interface is included in MOSAIC. This function works by assessing the material assignment of the pixels that surround the pixel in question. If neighboring pixels include both cement paste and mineral phases the pixel in question is identified as ITZ. If two or more mineral phases are identified as neighbors and no neighbors are of the cement paste phase, the pixel is classified as a mineral-mineral interface, as seen in **Fig. 3**. The width of the ITZ is correlated to the resolution of the m-XRF-based microstructural image. Hence, the ITZ size considered here varies between 15 and 50 μm depending on the image resolution. These dimensions are comparable to the width of physical ITZ reported in the literature (Ollivier *et al.* 1995; Scrivener *et al.* 2004; Grondin and Matallah 2014). Each type of interface detection is optional and

not required to run a complete mechanical simulation in MOSAIC.

- i. ITZ: Neighboring pixels include both cement paste and one or more minerals.
- ii. Mineral-Mineral Interface: Neighboring pixels include two or more different minerals and no neighbors are of the cement paste phase.

3. Concrete properties of interest

In NPPs, concrete undergoes a variety of degradation mechanisms including mechanical loading, creep in post-tensioned systems, internal volumetric expansions caused by physical (irradiation, freeze-thaw) or chemical degradation (alkali-silica reaction, delayed ettringite formation, embedded steel corrosion). These mechanisms cause the formation of microcracks or fractures in the material. Mismatch in the properties between neighboring minerals that comprise the aggregates and cement paste can cause localizations in the stress and strain fields, potentially inducing damage. MOSAIC utilizes the composition knowledge by assigning the appropriate constitutive properties to each pixel based on its phase assignment. Moreover, the irradiated minerals, aggregate and concrete (IMAC) database links to MOSAIC, providing detailed material parameters for the identified minerals (Le Pape *et al.* 2018). The principal objective of MOSAIC is to simulate the effects of nonlinear aging mechanisms occurring in nuclear environments on the macroscopic mechanical properties of specific concrete microstructures. These properties include strength, Young's modulus and dimensional change.

The modeling scale of MOSAIC's concrete microstructures is typically in the order of 10-50 μm , which is the scale of the constitutive crystals or hydrates forming the concrete constituents. Accurate modeling of these

Fig. 3 Microstructure (left) containing cement paste (gray) and minerals (blue, black, and green), with identified ITZ (red) and mineral/mineral interfaces (yellow) (right).

extremely heterogeneous microstructures therefore accounts simultaneously for the anisotropic elastic properties, creep and shrinkage, cracking/fracture and physically-induced deformations (eigenstrains).

3.1 Anisotropic elasticity

At the modeling scale (10-100 μm) of MOSAIC, the concrete constituents are aggregate-forming minerals, cement paste hydrates, mineral-mineral interfaces, and interfacial transition zones (ITZ) between the bulk of the cement paste and the aggregates. These constituents vary from crystalline, to poorly-crystallized hydrates (e.g., C-S-H) to vitreous form (e.g., obsidian). The ITZ is also generally characterized by a highly directional behavior. While concrete is macroscopically regarded as an isotropic material, MOSAIC explicitly accounts for anisotropy in the constituents' elastic stiffness tensors (Le Pape 2020). The IMAC database contains 43 minerals commonly found in concrete aggregates. Their elastic stiffness tensors correspond to more than approximately 100 references collected from the open literature and obtained using experimental means (e.g., resonant frequency) or first principle-based simulations. The orientation of the crystal is governed by its first Euler angle.

3.2 Creep

Creep is the phenomena of a material deforming slowly over time under constant load. This behavior is found primarily in C-S-H, which constitutes most of the volume in hardened cement paste. While the structure of C-S-H is still an active area of research, it is widely accepted that it is semi-crystalline and formed by layered sheets (Nonat 2004; Richardson and Groves 1992; Taylor 1986). It comprises central layers of Ca and O atoms with dreierketten silicate chains attached on top and bottom. These layers are stacked with water, and in some cases also Ca atoms, occupying the interlayer space (Garbev *et al.* 2008; Richardson and Groves 1992; Taylor 1986). There are several mechanisms that have been proposed to explain creep in C-S-H. The most common is the sliding of the aforementioned sheets with respect to each other under sustained stress (Ulm *et al.* 1999; Alizadeh *et al.* 2010; Tamtsia and Beaudoin 2000; Thomas 1937; Lynam 1934; Jennings 2004; Acker 2004; Vandamme and Ulm 2009a), but other mechanisms, such as dissolution under stress (Li *et al.* 2018; Moradian *et al.* 2018; Pignatelli *et al.* 2016) or a change of site of a particular bond between Ca ions bridging oxygen atoms in silicate groups due to stress or thermal activation (Gartner *et al.* 2017), have also been discussed in the literature. Additionally, creep and stress relaxation are not independent of one another and the combined viscoelastic response is termed 'creep-relaxation'. This causes time-dependent deformation of the material, leading to a relaxation of stress. This is important to consider, as creep-relaxation plays two separate but important roles in the lifespan of structural

components: (1) Loss of prestressing in post-tensioned containment buildings and (2) Micro-cracking control by relaxing the stresses caused by internal expansions developed by temperature gradients, alkali-silica reaction (ASR) or RIVE.

Although concrete creep exhibits both reversible and irreversible strain, creep is currently modeled in MOSAIC assuming viscoelasticity theory (Mindess *et al.* 2003). Creep compliance, $J(t)$ describes the evolution of the material's compliance while under load. Eq. (1) gives the relationship between strain (ε), creep compliance, and stress (σ), where t is the current age of the sample and t' is the age at loading.

$$\varepsilon(t) = \int_0^t J(t-t') \frac{\delta\sigma(t')}{\delta t'} dt \quad (1)$$

3.2.1 Linear viscoelasticity

Linear viscoelastic materials maintain a linear relationship between stress and strain at all points in time. Creep compliance can be characterized in a variety of ways; in this work, a Kelvin-Voigt chain is used to describe the creep of concrete. A selected number of Kelvin-Voigt elements are strung together, with an optional lone dashpot depicted in **Fig. 4** and in analytical form in Eq. (2) (Mindess *et al.* 2003).

$$\varepsilon(t) = \frac{\sigma(t)}{E_1} \cdot (1 - \exp^{-\frac{E_1 t}{\eta_1}}) + \frac{\sigma(t)}{E_2} \cdot (1 - \exp^{-\frac{E_2 t}{\eta_2}}) + \frac{\sigma(t)}{E_3} \cdot (1 - \exp^{-\frac{E_3 t}{\eta_3}}) \quad (2)$$

The generalized Maxwell-Kelvin model used in the linear viscoelastic approach calibrates a sufficient number of creep compliance constants associated with a series of characteristic times. For long-term extrapolation (e.g., over the lifespan of a structure using 1-3 years creep test), the predictive capabilities of the generalized Maxwell-Kelvin model decrease when time exceeds the highest characteristic time. Alternatively, concrete and other cementitious materials creep can be modeled by a logarithmic trend (Vandamme and Ulm 2009b; Masoero *et al.* 2013; Hilaire *et al.* 2014a). The logarithmic viscoelasticity model in MOSAIC differs from the linear viscoelasticity implementation by the treatment of the lone dashpot (Giorla *et al.* 2017). While optional to include in linear viscoelasticity, it is permanent in logarithmic viscoelasticity. The lone dashpot has a time-dependent viscosity and incorporates the age of the material at the time of loading, unlike the constant viscosity assigned in the linear viscoelastic regime. The time-dependent changes of this dashpot help represent the long-term asymptotic creep behavior of concrete, as well as non-recoverable creep strain.

Fig. 4 Two Kelvin-Voigt units with a lone dashpot.

3.3 Shrinkage

Shrinkage generally falls into two categories - autogenous and drying. Autogenous shrinkage is the result of the hydration of the cement paste, while drying shrinkage is the result of water loss from the concrete. The current version of MOSAIC does not account for time-dependent microstructures resulting from hydration. MOSAIC can, however, assess shrinkage as a function of the relative humidity and/or any other user-selected variable such as the water content, fluence, and/or temperature. The numerical relationship between shrinkage and the selected variable(s) is described by a numerical function defined by the user in the input file.

3.4 Radiation-induced volumetric expansion (RIVE)

Aggregates make up nearly 70% of concrete's volume. Naturally, changes that the aggregate components undergo will play a significant role in changing the properties of the macroscale concrete. A well-known example of this is the alkali-silica reaction (ASR) that results in the formation of an expansive gel, causing damage. Similarly, irradiation induces disordering in minerals, causing expansive amorphization (Le Pape 2015; Le Pape *et al.* 2019). Composition of aggregates varies with their type and source. Minerals that make up natural aggregates commonly include silicates of varied structures (quartz, feldspars, micas, pyroxenes etc.), carbonates (calcite, dolomite etc.) and metal oxides. These minerals have differing susceptibility to RIVE, meaning in the presence of irradiation, the mismatch in expansion can cause local concentrations in the stress and strain fields.

MOSAIC incorporates multiple RIVE models. The neutron irradiation-induced amorphization (gradual disordering of the crystalline structure) causes the expansion of rock-forming minerals. The amplitude and rate of expansion at the macroscopic scale vary with the atomic structure and are described by empirical laws as a function of fluence and irradiation temperature, to account for annealing effects. With increasing neutron fluence, the RIVE of silica-bearing minerals can be represented by a sigmoid (Zubov and Ivanov 1966) or approaching trends. Metal oxides and carbonate-bearing minerals are respectively modeled by exponential and "threshold" laws. See details in (Le Pape *et al.* 2018). These RIVE laws are directly accessed by MOSAIC when linked to the IMAC database.

3.5 Thermal expansion

Equation (3) defines the relationship between the change in length (ΔL) and the change in temperature (ΔT), determined by the coefficient of thermal expansion (α). Much like RIVE, the mismatch in magnitude of expansion can be a cause for concern and is of interest to predict. MOSAIC uses Eq. (3) to calculate the eigenstrain induced by temperatures higher than the user-defined reference temperature (Mindess *et al.*

2003).

$$\frac{\Delta L}{L} = \alpha \Delta T \quad (3)$$

3.6 Coupled creep damage

An isotropic damage governed by a unique scalar variable varying from 0 to 1 is implemented in MOSAIC although the 'algorithm could be extended to other forms of damage or irreversible phenomena including orthotropic damage or visco-plasticity' (Giorla *et al.* 2017). Damage is calculated by considering the stress-strain curve of the material to be the failure envelope. The stress strain curve can be used to represent brittle materials, pseudo-plastic materials, linear softening, or exponential softening (Giorla and Le Pape 2015; Giorla *et al.* 2017). The aggregates' RIVE causes the development of stresses in the cement paste. The stored mechanical energy eventually needs to be dissipated through cracking or viscous strains. These competitive mechanisms require a coupled damage-creep model. MOSAIC couples the calculation of the damage and creep by incorporating an instantaneous Young's modulus that accounts for the damage and magnitude of creep currently present in the material. The pseudo-plastic, linear softening, or exponential softening is also taken into account (Giorla *et al.* 2017).

The resolution of the nonlinear problem is based on a step-by-step sequence of linear systems using a procedure similar to that proposed by (Rots and Invernizzi 2004; Zhu and Yvonnet 2015) accounting for the time dimension (Giorla *et al.* 2017). The corresponding set of constitutive differential equations coupling the logarithmic creep and isotropic damage is as follows:

$$\begin{aligned} \sigma &= (1-d)C_e : [\varepsilon - \varepsilon_r - \varepsilon_c - \varepsilon^*] \\ \sigma &= (1-d)[C_r : \varepsilon_r + E_r : \dot{\varepsilon} - r] \\ \sigma &= (1-d) \left[1 + \frac{t}{\tau_c} \right] E_c : \dot{\varepsilon}_c \end{aligned} \quad (4)$$

where C_e is the elastic stiffness tensor of the phase; C_r and E_r are the hardened cement paste (hcp) stiffness and viscosity tensors of the Kelvin-Voigt module, respectively; E_c is the initial viscosity tensor of the dashpot; ε^* is the imposed deformation (i.e., shrinkage, RIVE, and thermal strains); and τ_c is the characteristic time of the logarithmic creep.

4. Numerical method

FFT is a numerical method that efficiently transforms a function of time into a function of frequency. This technique has many applications in electrical engineering, but in the 1990's it gained recognition as a method to compute homogenized properties of periodic heterogeneous microstructures (Moulinec and Suquet 1994, 1998a, 1998b). FFT solvers have successfully been im-

plemented in the modeling of linear elasticity, plasticity, viscoelasticity, and finite strains (Lavergne *et al.* 2015a; Moulinec and Suquet 1998b; Kabel *et al.* 2014).

Consider a two-dimensional domain of a periodic, heterogeneous material. Linear elasticity governs the material behavior, where C is the stiffness tensor, x is the spatial position, ε is the strain, and ε_{eigen} is the eigen-strain. The eigenstrains, such as thermal expansion strain, do not contribute to the overall stress in the domain. The relationship between these variables is given in Eq. (5).

$$\sigma(x) = C(x) : (\varepsilon(x) - \varepsilon_{eigen}(x)) \quad (5)$$

The FFT method uses a homogeneous reference material with constant stiffness C_0 . If a macroscopic strain E is applied to the material, the displacements will be periodic with the same pattern as the material property. Calculations of the fluctuation in the displacement field performed on the unit cell are used to determine the overall properties of the material. Stress fluctuations in the material are measured by the stress polarization field τ , given in Eq. (6).

$$\tau(x) = (C(x) - C_0) : (x) \quad (6)$$

Eq. (6) obeys Eq. (7), where Γ_0 is the reference material's fourth-order Green tensor and $*$ is the convolution product operator.

$$(x) = E - (\Gamma_0 * \tau)(x) \quad (7)$$

The convolution product is evaluated simply in Fourier space, where ξ represents frequency, and the hat symbol ($\hat{\cdot}$) represents a variable in Fourier space, simplifying the calculation of Eq. (7) into the piecewise function given in Eq. (8).

$$\hat{\varepsilon}(\xi) = \begin{cases} -\hat{\Gamma}_0(\xi) : \hat{\tau}(\xi) & (\xi \neq 0) \\ E & \xi = 0 \end{cases} \quad (8)$$

The Fourier transform of a real, integrable function is given in Eq. (9), where i is the square root of -1 and x represents the spatial position. MOSAIC utilizes the FFTW library to perform all Fourier transforms (Frigo and Johnson 2005).

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(x) e^{i\pi x \xi} dx \quad (9)$$

MOSAIC assumes the reference material is isotropic. The first Lamé parameter (λ_0), and the shear modulus (μ_0) of the reference material are used to calculate the Green operator in Fourier space ($\hat{\Gamma}_0$), first defined in Moulinec and Suquet 1998, shown in Eq. (10). Where ξ is zero, $\hat{\Gamma}_0$ is not defined, leading to the definition of $\hat{\varepsilon}(0) = E$.

$$\hat{\Gamma}_{0,ijkl} = \frac{1}{4\mu_0 \|\xi\|^2} (\delta_{ki} \xi_l \xi_j + \delta_{lj} \xi_k \xi_i + \delta_{li} \xi_k \xi_j + \delta_{kj} \xi_i \xi_l) - \frac{\lambda_0 + \mu_0}{\mu_0 (\lambda_0 + 2\mu_0)} \frac{\xi_i \xi_j \xi_k \xi_l}{\|\xi\|^4} \quad (10)$$

Two FFT algorithms are implemented in MOSAIC. The basic algorithm uses a fixed-point iterative procedure, while the accelerated algorithm is an extension of the basic algorithm with improved convergence properties.

4.1 Basic algorithm

This algorithm solves Eq. (7) with a fixed-point iterative procedure. The speed of this algorithm is the result of calculating the convolution product in Fourier space and the polarization field in real space (Moulinec and Suquet 1994; Moulinec and Silva 2014). In this algorithm, the reference material is defined as:

$$\mu_0 = \frac{\mu_{\max} + \mu_{\min}}{2}, \lambda_0 = \frac{\lambda_{\max} + \lambda_{\min}}{2} \quad (11)$$

To determine convergence, three types of error are calculated: error on the boundary condition (E_{bc}), equilibrium error (E_{eq}), and strain compatibility error (E_{comp}). Total error ε is calculated to be the maximum of the three normalized errors, shown in Eq. (12).

$$E = \max\left(\frac{E_{bc}}{E_{bc}^0}, \frac{E_{eq}}{E_{eq}^0}, \frac{E_{comp}}{E_{comp}^0}\right) \quad (12)$$

Boundary condition error is calculated in Eq. (13), where $\langle \cdot \rangle$ represents the spatial average.

$$E_{bc} = \frac{\|\langle \varepsilon^n(x) - E \rangle\|}{\|E\|} \quad (13)$$

Equilibrium error is calculated as the divergence of the stress field. This is calculated in Fourier space, as shown in Eq. (14).

Algorithm 1 Basic FFT scheme

Material properties $\mathbb{C}(\mathbf{x})$, $\epsilon_{imp}(\mathbf{x})$, and $\hat{\Gamma}_0(\xi)$ are provided

Initial strain field $\epsilon^0(\mathbf{x})$ is provided

$\hat{\epsilon}^0 = \mathbf{FFT}(\epsilon^0)$

while not converged do

for each $\mathbf{x}$ **do**

$\sigma^n(\mathbf{x}) = \mathbb{C}(\mathbf{x}) : (\epsilon^n(\mathbf{x}) - \epsilon_{imp}(\mathbf{x}))$

end for

$\hat{\sigma}^n = \mathbf{FFT}(\sigma^n)$

for each $\xi \neq 0$ **do**

$\hat{\epsilon}^{n+1}(\xi) = \hat{\epsilon}^n(\xi) - \hat{\Gamma}_0(\xi) : \hat{\sigma}^n(\xi)$

end for

$\hat{\epsilon}^{n+1}(0) = E^{n+1}$

$\epsilon^{n+1} = \mathbf{FFT}^{-1}(\hat{\epsilon}^{n+1})$

end while

Fig. 5 Basic FFT algorithm scheme.

$$E_{eq} = \frac{\sqrt{\sum_{\xi} \|\xi \cdot \hat{\sigma}^n(\xi)\|^2}}{\|\hat{\sigma}^n(0)\|} \quad (14)$$

The strain compatibility error is also calculated in Fourier space, given in Eq. (15).

$$E_{comp} = \max \left(\frac{\|2\xi_1\xi_2\hat{\epsilon}_{12}^n(\xi) - \xi_2\xi_2\hat{\epsilon}_{11}^n(\xi) - \xi_1\xi_1\hat{\epsilon}_{22}^n(\xi)\|}{\sqrt{\sum_{\xi} \hat{\epsilon}_{ij}^n(\xi) : conj(\hat{\epsilon}_{ij}^n(\xi))}} \right) \quad (15)$$

4.2 Accelerated algorithm

The accelerated algorithm is an improvement on the basic FFT scheme. It includes two parameters, α and β , each set to a default value of 2. These values can be changed by the user; several publications specify convergence for specific α and β values, summarized below:

- 1) Eyre and Milton (1999) show convergence for $\alpha = \beta = 2$
- 2) Moulinec and Silva (2014) show convergence for $0 < \alpha < 2$, $0 \leq \beta < 2$, $\lambda_0 > 0$, $\mu_0 > 0$
- 3) Michel *et al.* (2001) show convergence for $\alpha = \beta = 1$

$$\mu_0 = \sqrt{\mu_{\max} + \mu_{\min}}, \lambda_0 = \sqrt{\lambda_{\max} + \lambda_{\min}} \quad (16)$$

4.3 Damage algorithm

A damage variable, d , varying between 0 (no damage) and 1 (total damage) describes the level of irreversible damage. Failure criterion, C , is the minimum stress or strain level to be reached in order to initiate damage. C is a function of time, d , material parameters, and displacement. The failure envelope surface is described by

$C = 0$. Damage is calculated at the start of a time step and is assumed to be constant throughout the time step. Several equations are enforced to ensure irreversibility, given in Eq. (17).

$$C \cdot \dot{d} = 0, C \leq 0, \dot{d} \geq 0 \quad (17)$$

Quasi-brittle materials that do not exhibit hardening must obey the condition in Eq. (18).

$$\frac{\delta C}{\delta d} \leq 0 \quad (18)$$

The damage algorithm is described by the following steps.

- 1) Initialization: damage values are initialized as $d_0 = d_s$, time values as t_0 , and location values as x_0 . Damage is considered constant through the time step.
- 2) Resolution: t_i , $x_{s,i}$, and d_i are known and as a result, the displacements at the end of the time step (x_i).
- 3) Failure criteria: The displacements at the beginning and end of the time step are used to calculate the failure criteria at the end of the time step.
- 4) Damage: t_{i+1} is the first time when a location can reach failure. The damage is increased at t_{i+1} to $d_{i+1} + \delta d$. The magnitude of δd can be set to be larger or smaller, and the choice is a balance of precision and computing time. This is repeated until E is less than its failure surface at t_{i+1} . This defines d_{i+1} .
- 5) Iteration: Return to Step 2 with $x_{s,i+1}$ and d_{i+1} .
- 6) Exit: Convergence of the algorithm is determined to be when $C < 0$ in all pixels. This occurs after a finite number of iterations because of the fixed damage increment δd .

In order to reduce the effects of pixel-size effects, the strains and failure criterion can be smoothed to make the damage algorithm nonlocal. A kernel of radius r_{nl} is used to smooth the local strain field, using a quadratic kernel. The radius is considered a characteristic of the process fracture zone. This helps to replicate how damage occurs based on the local microstructure and nonlocal strains (Giorla *et al.* 2017). Additional details on the damage algorithm can be found in Giorla *et al.* (2017). However, when the complexity of the microstructure increases (e.g., **Fig. 2**), the fracture process occurs in very localized zones (see Section 7.3.) such as the so-called inter-particle interfaces (grain boundaries of aggregates) and the interfacial transition zones, before spreading within the cement pastes. In this case, the simulations are thus conducted using the local damage model.

As a pixel becomes damaged, MOSAIC reduces its stiffness proportionally. When the pixel has reached its maximum damage, the stiffness is reduced to a nonzero value, the same value assigned to porosity. The selection of the nonzero stiffness assigned to porosity and cracked pixels can be any value above zero. The lower the magnitude of this value, the longer the computational time to calculate the subsequent time steps, but the higher the

Algorithm 2 Accelerated FFT scheme

Parameters α and β are provided
 Material properties $\mathbb{C}(\mathbf{x})$, $\epsilon_{imp}(\mathbf{x})$, and $\hat{\Gamma}_0(\xi)$ are provided
 Initial strain field $\epsilon^0(\mathbf{x})$ is provided
while not converged do
 for each x do
 $\tau_{\alpha}^n(\mathbf{x}) = \mathbb{C}(\mathbf{x}) : \epsilon^n(\mathbf{x}) + (1 - \beta) \mathbb{C}_0 : \epsilon^n(\mathbf{x})$
 $\tau_{\beta}^n(\mathbf{x}) = \alpha \mathbb{C}(\mathbf{x}) : (\epsilon^n(\mathbf{x}) - \epsilon_{imp}(\mathbf{x})) - \beta \mathbb{C}_0 : \epsilon^n(\mathbf{x})$
 end for
 $\hat{\tau}_{\beta}^n = \text{FFT}(\tau_{\beta}^n)$
 for each $\xi \neq 0$ do
 $\hat{\epsilon}_{\beta}^{n+1}(\xi) = -\hat{\Gamma}_0(\xi) : \hat{\tau}_{\beta}^n(\xi)$
 end for
 $\hat{\epsilon}_{\beta}^{n+1}(0) = \beta \mathbf{E}^{n+1}$
 $\epsilon_{\beta}^{n+1} = \text{FFT}^{-1}(\hat{\epsilon}_{\beta}^{n+1})$
 for each x do
 $\epsilon^{n+1}(\mathbf{x}) = (\mathbb{C}(\mathbf{x}) + \mathbb{C}_0)^{-1} : (\tau_{\alpha}^n(\mathbf{x}) + \mathbb{C}_0 : \epsilon_{\beta}^{n+1}(\mathbf{x}))$
 $\sigma^{n+1}(\mathbf{x}) = \mathbb{C}(\mathbf{x}) : (\epsilon^{n+1}(\mathbf{x}) - \epsilon_{imp}(\mathbf{x}))$
 end for
end while

Fig. 6 Accelerated FFT algorithm scheme.

accuracy. A value of 1 GPa is generally chosen by the authors to balance computational time and accuracy.

5. Periodicity enforcement

As the mathematics behind the FFT solvers assume the microstructure is periodic, applying this technique to a non-periodic microstructure can result in discontinuities at the edges of the domain. This can lead to results that include erroneous cracking and over prediction of the stress or strain magnitude at the edges of the microstructure. In order to alleviate these issues, three optional tools are included in MOSAIC to manipulate a microstructure and enforce periodic boundary conditions. To be considered periodic, a microstructure's opposing edges must be identical. An example of periodicity of the edges and corners is shown in Fig. 7.

5.1 Border addition

The simplest method of enforcing the constraint that each edge be identical to the opposing edge is to add a border. This method adds a fixed-width border to each side of the microstructure. The width and material prop-

erties of the border are defined by the user. Border material is commonly assigned as matrix material or given homogenized properties of the entire microstructure. The latter can be used in self-consistent schemes. Addition of a border to the original microstructure is seen in Fig. 8.

5.2 Mirroring

Mirroring is used to create a new microstructure that is four times the size of the original. This is accomplished by mirroring the microstructure across two adjacent boundaries and again diagonally, as seen in Fig. 9.

5.3 Particle rearrangement

The final option to enforce periodicity is to extract the particles from the microstructure and place them into a new, empty microstructure. The placement into the new microstructure is done in a random, periodic manner. Overlap between the particles in the new microstructure is prohibited. Furthermore, a minimum distance between particles can be specified.

In order to retain the composition detail of the aggre-

Fig. 7 Periodic boundary conditions shown with a wall intersection (left) and a corner intersection (right).

Fig. 8 Original microstructure (left) with blue border added (right).

gates, MOSAIC identifies all of the connected mineral phases that compose an aggregate and locks them together. Thus, when aggregates are translated into the new microstructure, the connected mineral phases are moved together, retaining the composition detail.

Any aggregates that have contact with a boundary are discarded, as the entirety of the aggregate is not visible in the original microstructure. The original volume fraction of aggregates is retained in the new microstructure, therefore if aggregate(s) are discarded, the size of the new microstructure will be reduced to retain the desired

volume fraction. Before placement into the new microstructure, the aggregates are sorted by area. The placement process is described by **Fig. 10**, selecting aggregates in order from largest area to smallest area. A rearranged microstructure is given in an example in **Fig. 11**.

6. Software structure

MOSAIC is written in C++. The functions and algorithms described thus far are implemented in MOSAIC using a variety of classes:

Fig. 9 Original microstructure (left) mirrored (right).

Fig. 10 Methodology of creating a new microstructure from extracted aggregates.

Fig. 11 Original microstructure (left) rearranged with periodic boundary conditions, using only aggregates fully contained within the original image (right).

Table 1 Material properties for bilayer microstructure.

Material	Young's Modulus (GPa)	Poisson's Ratio
A	10	0.2
B	20	0.2

Table 2 Numerical results for applied uniaxial tensile stress to bilayer material.

Material	Stress XX (Pa)	Stress YY (Pa)	Strain XX	Strain YY
A	1.3E+06	-5.8E-11	6.4E-05	-1.6E-05
B	6.6E+05	2.05E-10	6.4E-05	-1.6E-05
Global	1.0E+06	7.28E-11	6.4E-05	-1.6E-05

Table 3 Numerical results for applied shear strain to bilayer material.

Material	Stress XX (Pa)	Stress YY (Pa)	Stress XY (Pa)	Strain XX	Strain YY	Strain XY
A	0	0	5.6E+06	0	0	6.6E-04
B	0	0	5.6E+06	0	0	1.3E-03
Global	0	0	5.6E+06	0	0	1.0E-03

- 1) Field objects store numerical values on a regular grid. Multi-dimensional grids are utilized to store data of arbitrary dimensions
- 2) Fields can store real or imaginary data
- 3) Operation classes contain functions that alter Field objects
- 4) Operations can receive multiple Fields as input but give a single Field output
- 5) Operations are performed either on the entire microstructure or on a single pixel.
- 6) IterativeSolver classes perform the numerical computations.
- 7) An IterativeSolver class contains a series of Operations that are used to perform individual calculations shown in the FFT algorithms
- 8) IterativeSolver houses the convergence criteria and monitors the number of iterations to prevent infinite iterations.

7. Numerical examples

7.1 Validation

Before performing a phase map simulation of concrete, a bilayer material consisting of two equal volume fraction phases, was simulated under imposed uniaxial stress and imposed shear strain.

The first simulation is the application of an applied 1 MPa uniaxial tensile stress in the X-direction with the material properties described in **Table 1**. It is expected that the strain will be uniform across the whole material and the stress will be uniform across each phase. This is confirmed by the results given in **Table 2**, where 'Stress XX' and 'Strain XX' are the principal stress and strain in the direction of the X-axis, respectively. Similarly, 'Stress YY' and 'Strain YY' represent the principal stress and strain in the direction of the Y-axis respectively, matching the stress and strain uniformity expectations.

Next, a shear strain of 0.001 is applied to the bilayer microstructure. Analytical results give uniform stress

across the whole material but differing strains by phase. Numerical results are seen in **Table 3**.

7.2 Applied stress

Moving to a more complex simulation scenario, the phase map in the top-left of **Fig. 2** is simulated for an imposed compressive stress and strain. The material properties for each mineral phase in the microstructure are given in **Table 4**. The FFT solvers do not allow for a stiffness of zero, a small elastic modulus of 1 GPa is assigned to the porosity phase. This value is arbitrary and user-defined. A lower value lends to higher precision in the calculations but a slower computational time.

Table 5 gives the numerical results, given in averages by phase. **Figure 13** shows the X-direction component of the strain and stress fields resulting from the applied uniaxial stress, where lighter values indicate a higher magnitude. It can be seen that both the stress and strain values are highest around the borders of pores. Within the mineral phases, the strains are greatest in the cement paste phase, while the stresses are highest in the calcite grains.

Fig. 12 Bilayer example microstructure, material A in gray and material B in green.

Table 4 Material properties for the phase map seen in Fig. 2.

Material	Young's Modulus (GPa)	Poisson's Ratio	Area Fraction	Coefficient of Thermal Expansion
Calcite	80	0.2	61.44%	0.0001
Ankerite	100	0.2	0.32%	0.0001
Cement paste	20	0.2	34.68%	0.00001
Porosity	1	0.2	3.55%	0.0

Table 5 Numerical results for applied uniaxial compressive stress to phase map in Fig. 2.

Material	Stress XX (Pa)	Stress YY (Pa)	Strain XX	Strain YY
Calcite	1.27E+06	-2.32E+04	-1.52E-05	3.54E-06
Ankerite	-1.21E+06	-1.77E+05	-1.12E-05	1.20E-06
Cement	-8.38E+05	1.56E+04	-4.04E-05	1.08E-05
Global	-1.0E+06	0.035	-3.19E-05	8.46E-05

Table 6 Stress and strain calculations from thermal expansion simulation.

Time (days)	Temperature (°C)	Strain XX	Strain YY	Strain XY	Stress XX (Pa)	Stress YY (Pa)	Stress XY (Pa)
1	21	7.38E-05	7.25E-05	-5.39E-07	1.12	1.19	0.013
3	23	0.00022	0.00022	-1.62E-06	-1.97	-2.09	-0.019
6	26	0.0044	0.0044	-3.24E-06	-1.98	-2.11	-0.018
10	30	0.00074	0.00073	-5.40E-06	-1.75	-1.87	0.021
15	35	0.0011	0.0010	-8.09E-06	1.88	2.01	0.02
21	41	0.0015	0.0015	-1.13E-05	-1.89	-2.03	-0.02

Table 7 Creep modulus (GPa) and viscosity characteristic time (days) values used to define the linear viscoelastic behavior of the cement paste phase.

E_1	η_1	E_2	η_2	E_3	η_3	E_4	η_4	E_5	η_5	E_6	η_6	η_7
90 GPa	1 days	80 GPa	10 days	75 GPa	25 days	60 GPa	100 days	40 GPa	250 days	75 GPa	500 days	1000 days

7.3 Thermal expansion

The phase map in **Fig. 2** was subjected to a simulation of twenty-one days of increasing temperature. Numerical results averaged over the whole domain in **Table 6** demonstrate that the magnitude of the stress remains negligible in the simulation of unconfined thermal expansion, as expected. In **Fig. 14** the strain in the X- and Y-directions is shown to be spatially distributed across the microstructure. As the mineral phases in the aggregates were assigned a thermal expansion coefficient one

order of magnitude higher than the cement paste, the mismatch in expansion can be seen in **Fig. 14**.

7.4 Creep

A constant, compressive uniaxial stress of 10 MPa was applied to the **Fig. 2** phase map. The material properties remain the same as found in **Table 4**, with the addition of a linear viscoelastic description added to the cement phase. The creep modulus and viscosity terms used in the linear viscoelastic creep model are given in **Table 7**,

Fig. 13 The X-direction component of the strain vector (left) and stress tensor (right). Lighter values indicate higher magnitude.

where the parameters are estimated values used to demonstrate the calculation of creep. The change in the relaxation modulus from simulating just over 2 years of creep of the phase map in **Fig. 2**, top-left, is shown in **Fig. 15**. The relaxation modulus, $E(t)$, is calculated from Eq. (1).

It can be seen in **Fig. 15** that concrete's relaxation modulus evolves over time whilst subjected to a constant load. Experimental data on concrete from (Baranikumar *et al.* 2019) is used for comparison to demonstrate the calculation of realistic creep behavior.

7.5 Irradiation-Induced expansion and damage

The effects of irradiation of concrete are complex (Le Pape 2020). Predictive models need to include irradiation induced aggregate-forming minerals expansion, creep and shrinkage of the cement paste, cracking in the cement paste, the interfacial transition zone and the aggregates. The mineral-mineral interfaces were not defined due to a lack of data regarding the properties of the interfaces. An illustration of such a simulation is presented in this section. The irradiation of the concrete presented in (Maruyama *et al.* 2017) and corresponding

to the phase map shown in the top-right corner of **Fig. 2** is simulated. The neutron fluence is gradually increased at constant flux to reach $0.967 \text{ n}\cdot\text{pm}^{-2}$ ($E > 10 \text{ keV}$) at 230 days. A value of 10 keV is chosen as that is the threshold linked to the IMAC database. The irradiation temperature of 66.7°C is assumed uniform in the specimen. The elastic tensors of the aggregate-forming crystalline minerals can be found in (Le Pape *et al.* 2020). The cement paste, ITZ and intra-aggregate interfaces are assumed isotropic with Young's moduli equal to 12 GPa, 4.5 GPa and 65 GPa. Their respective tensile strengths are 5 MPa in the cement paste and the ITZ and 20 MPa in the intra-aggregate interfaces.

Figure 16 summarizes the evolutions of RIVE and damage in concrete resulting from the RIVE in the aggregate-forming minerals over a 230-day period. In this simulation, the damage originates in the weaker ITZ region, before spreading out into the mineral-mineral interfaces and cement paste matrix. As the aggregates continue to expand into the cement paste, the damage continually builds until the entirety of the cement paste matrix is damaged, as seen in **Figs. 16** and **17**. Percent damage is defined as the percentage of the materials

Fig. 14 The X-direction component of the strain vector (left) and the Y-direction component (right) after thermal expansion. Lighter values indicate higher magnitude.

Fig. 15 Evolution of relaxation modulus from a MOSAIC creep simulation, plotted against experimental data.

assigned a damage material law that have cracked.

More precisely, damage to the microstructure is reproduced in **Fig. 17**, where red depicts damaged pixels. Linkage to the IMAC database provides a wealth of data

that allows MOSAIC to predict expansion and crack patterns through and around the aggregates without the knowledge of the aggregate source or overall properties.

While the literature on macroscopic and meso-scale

Fig. 16 Simulation of a prolonged irradiation experiment in accelerated condition of JEEP-II test reactor: The concrete RIVE obtained with MOSAIC is plotted in red while the accumulated damage is represented by the blue curve. The final RIVE resulting from the neutron fluence at the end of the experiment is close to 4%. The green marks correspond to the post-irradiation volumetric change obtained by (Maruyama *et al.* 2017). The red pixels in the microstructure maps indicate the location of damage at varied fluences.

Fig. 17 Damage, shown in red, at a) 0.9 days, b) 5.75 days, c) 36 days, and d) 230 days.

models of creep (Aydin *et al.* 2007; Shokoohfar and Rahai 2017; Benboudjema and Torrenti 2008; Lavergne *et al.* 2015b; Sellier *et al.* 2016; Hilaire *et al.* 2013, 2014b) and damage (Ren *et al.* 2015; Briffaut *et al.* 2013; Du *et al.* 2012; Cervenka *et al.* 2011; Zhang *et al.* 2012) in concrete is abundant, MOSAIC uses an original time adaptive scheme coupled with nonlocal damage calculation (Giorla *et al.* 2017). Its application to irradiation-induced damage simulation in MOSAIC is a continuation of the research of (Giorla *et al.* 2015, 2017) using code AMIE. Within the application of nuclear concrete, the impact of irradiation on concrete has gained attention in recent years. Different modeling strategies of irradiated concrete are available in the literature including analytical methods based on the homogenization theory of heterogeneous materials (Le Pape 2015; Jing and Xi 2017), lattice-based modeling using the rigid-body spring model (RBSM) (Nagai *et al.* 2005) and finite element analysis (FEA) (Pomaro *et al.* 2011; Salomoni *et al.* 2014; Xotta *et al.* 2015; Giorla and Le Pape; Giorla *et al.* 2017). Because the radiation induced expansion of concrete is governed by the aggregates' RIVE which vary immensely with the mineral composition, the approaches mentioned above require to either characterize or make assumption on the concrete-forming aggregate irradiated properties. The main advantage of FFT-based MOSAIC simulation is that the effects of the aggregates' mineralogy are explicitly accounted for.

7.6. Limitations of MOSAIC

Currently, MOSAIC simulates small size of concrete on the order of micrometers to millimeters. This scale is largely controlled by the resolution and sample size limitations of the XRD and XRF instrumentation. Mapping the detailed compositional data for larger areas is paramount to larger-scale MOSAIC simulations, although these resources are not available to the authors at the time of this paper.

Because MOSAIC assumes periodic boundary conditions, the loss of material stability due to cracks or localization results in strain softening, and thus the standard homogenization rules, e.g., periodic boundary conditions and volume average of stress, are not applicable for general fracture problems (Geers *et al.* 2010; Bazant 2010; Baek *et al.* 2020). The formation of strong localization bands in heterogeneous microstructures occurs mainly under external loading. The presented simulations correspond to loading scenarios such as internal swelling caused by irradiation. Hence, the development of damage is distributed through the microstructure. Then, damage gradually expands through the entire volume fraction of damageable elements. For these studied cases, damaged pixels are somewhat "uniformly" distributed within the microstructures. The standard homogenization rules are still considered acceptable. However, for strong localization problems, further developments need to be considered.

8. Conclusions and future work

A micromechanical analysis software named MOSAIC is developed and presented in this paper. MOSAIC is an efficient computational tool that simulates the mechanical behavior of a composite material under a variety of loading and environmental conditions. Designed with nuclear concrete in mind, the strength of MOSAIC is its ability to incorporate detailed compositional data and RIVE characteristics into a complete micromechanical simulation. Each mineral phase is assigned its constitutive properties for RIVE, thermal expansion, viscoelasticity, strength, and anisotropic stiffness. This capability highlights the uniqueness and strength of the MOSAIC software to generate time-dependent micromechanical behavior and damage of concrete from the compositional information alone. As the field of nuclear concrete lacks experimental data in many areas, MOSAIC helps to fill in the gaps by performing many virtual experiments on a single-phase map - expanding the amount of data that can be collected from each sample.

Depicted here as a two-dimensional analysis tool, MOSAIC is presently being expanded to perform simulations in a three-dimensional domain in order to simulate more complex loading conditions, concrete microstructure morphologies, and three-dimensional damage propagation. Description and demonstration of the 3D MOSAIC software will be presented in a future publication.

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