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A coupled thermo-mechanical and neutron diffusion numerical model for irradiated concrete

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Abstract: Neutron irradiation plays an important role in nuclear-induced degradation for concrete shielding materials, specifically in determining the radiation induced volume expansion (RIVE) phenomenon driving its failure. When analyzing at the structural level the effects of nuclear radiation on concrete, a non-uniformed distribution of neutron radiation must be considered. This can be done via particle transport calculations preventive to the thermo-mechanic study, or by solving numerically the coupled set of governing equations of the problem. In this work the second approach is pursued in the theoretical framework of the Finite Element Method (FEM). The proposed formulation not only considers an accurate neutron transport model based on the two-group theory, but also it includes the effects induced by thermal neutrons to the temperature field. The formulation lends itself to include RIVE and the other relevant radiation induced effects on the mechanical field. The governing equations are presented and discussed, and some results obtained by using the general 3D numerical formulation proposed herein are compared to results from literature obtained via analytical methods addressing simplified 1D problems.

Introduction

The biological shielding walls undergo a coupling effect of irradiation and temperature rise during the operation of nuclear power plants (NPPs). Both, neutron and gamma radiation produce internal heating from absorption of radiation energy. Additionally, at high fluence levels, they affect the microstructure and induce changes in certain mechanical properties of concrete (e.g., compressive strength, tensile strength, modulus of elasticity) [1]. Since neutron radiation can deteriorate the mechanical properties of concrete materials, it is critical to obtain accurate neutron radiation levels in concrete structures during their service life. Often, this problem is addressed via analytical simplified 1D studies [2].

For more complex geometries, however, the Finite Element Method (FEM) is generally accepted as an effective approach for solving coupled transient problems, also when porous multiphase materials are involved [3-5]. Based on FEM, some diffusion-deformation and diffusion-reaction-deformation coupling models are proposed in literature [6, 7]. As far as the authors know, a FEM thermo-mechanical-neutron diffusion coupled model for irradiated concrete has not yet been presented.

The thermo-mechanical-neutron diffusion coupled model proposed herein combines an elastic mechanical constitutive model with the two-group neutron-transport theory, and thermal diffusion.

This model can be used to quantify a realistic radiation flux, and temperature field on the domain of interest, by considering both, the fast neutron and thermal neutron fractions. In fact, both temperature and the neutron flux account for relevant state variables to predict damage and durability of biological shields in the NPPs and nuclear facilities, in general.

Mathematical Model

The governing equations of the multi-physics problem affecting irradiated concrete are outlined in this section. A general three-dimensional body is considered, that occupies a domain $B \in \mathbb{R}^3$ and is bounded by the surface S. Vector $\boldsymbol{X}$ is used for representing the position of an arbitrary material point of the body in a Cartesian coordinate system, that is $\boldsymbol{X} = [x, y, z]^T$.

Mechanical Model. The constitutive model for concrete is defined based on the small strain theory. Thermal effects and radiation-induced effects, are assimilated to an additional mechanical contribution in the definition of the total strain, according to an additive decomposition of the same strain (in the following, ∇ stands for the Nabla operator and indicates the gradient operator, while ∇^{T} indicates the divergence). Let S_{t} and S_{u} be complementary sub-surfaces of the boundary S of the body B, then the mechanical boundary conditions complete the set of equations governing the mechanical field. According to them, the surface loads $\bar{\mathbf{t}}$ are specified on S_{t}, characterized by normal outward vector $\mathbf{n}$ to the surface, and the displacement $\bar{\mathbf{u}}$ is specified on S_{u} (t denotes time). Hence,

$$\begin{cases} \mathbf{L}^{\mathrm{T}}\boldsymbol{\sigma} + \boldsymbol{b} = \mathbf{0} \\ \boldsymbol{\sigma} = \mathbf{D}\boldsymbol{\varepsilon}_e = \mathbf{D}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_T - \boldsymbol{\varepsilon}^{RIVE}) = \mathbf{D}\,\mathbf{L}(\boldsymbol{u} - \boldsymbol{u}_T - \boldsymbol{u}^{RIVE}) \\ \boldsymbol{\varepsilon}_T = \mathbf{I}\alpha(T - T_0) \\ \boldsymbol{\varepsilon}^{RIVE} = \mathbf{I}\kappa\varepsilon_{max}\frac{e^{\delta\Phi}-1}{\varepsilon_{max}+\kappa e^{\delta\Phi}} \\ \boldsymbol{\sigma}\,\mathbf{n} = \bar{\mathbf{t}}(\boldsymbol{X}, t) \quad \text{on } S_{\mathrm{t}} \\ \mathbf{u} = \bar{\mathbf{u}}(\boldsymbol{X}, t) \quad \text{on } S_{\mathrm{u}} \end{cases} \tag{1}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress; $\boldsymbol{b}$ is the body force per unit volume; $\boldsymbol{u}$ is the total displacement; $\mathbf{L}$ is the differential operator such that $\boldsymbol{\varepsilon} = \mathbf{L}\,\mathbf{u}$; $\boldsymbol{u_T}$ is the displacement component due to temperature, and $\boldsymbol{u}^{RIVE}$ is the component due to radiation; $\boldsymbol{\varepsilon}$ is the total strain vector; $\boldsymbol{\varepsilon_e}$ is the purely mechanical strain vector; $\boldsymbol{\varepsilon}_T$ is the strain induced by temperature, and $\boldsymbol{\varepsilon}^{RIVE}$ the one induced by radiation, i.e. RIVE; $\mathbf{D}$ is the elastic constitutive matrix; α is the thermal expansion coefficient (assumed isotropic). This model accounts for an estimate of RIVE in function of the neutron fluence Φ [n/cm^2] in line with the sigmoidal growth model proposed in [8], where $\mathbf{I} = [1\ 1\ 1\ 0\ 0\ 0]^T$ is the identity vector, and ε_{max}, κ, and δ are material parameters calibrated over irradiated concrete specimen of different aggregate nature.

Multi-group Neutron Diffusion Problem. Neutrons are either scattered in, attenuated or stopped by the absorbing medium during their transport processes. In this work the two-speed neutron diffusion model proposed in [9-11] is considered. This model is more realistic with respect to the one-speed diffusion model in relation to the fact that neutrons have a wide range of energy spectrum, in reality, ranging from 10MeV down to 0.01MeV. The two-group model assumes that the secondary neutrons from scattering reaction occurring within a specific kinetic group (fast group) represent a neutron source in the diffusion process of the group of lower kinetic energy (thermal group). The governing equation for the two-group theory for the so-called fast and thermal neutrons are

Fast group: $$\frac{1}{v_1}\frac{\partial \phi_1(\mathbf{X},t)}{\partial t} - \nabla^{\mathrm{T}}(\boldsymbol{D_1}(\mathbf{X},t)\nabla\phi_1(\mathbf{X},t)) + \Sigma_{R1}\phi_1(\mathbf{X},t) = 0 \tag{2}$$

Thermal group: $$\frac{1}{v_2}\frac{\partial \phi_2(\boldsymbol{X},t)}{\partial t} - \nabla^{\mathrm{T}}(\boldsymbol{D_2}(\mathbf{X},t)\nabla\phi_2(\mathbf{X},t)) + \Sigma_{a2}\phi_2(\boldsymbol{X},t) = \Sigma_{s12}\phi_1(\boldsymbol{X},t) \tag{3}$$

where subscripts $i = 1, 2$ stand for the fast and the thermal group, respectively. In Eq. (2) and Eq. (3) ϕ_i is the scalar neutron flux [n/(cm^2·s)]; v_i is the neutron speed; $\boldsymbol{D_i}$ is the neutron diffusion coefficient matrix; Σ_a is the macroscopic absorption cross section; Σ_R is the macroscopic removal cross section; Σ_{S12} is the macroscopic fast to thermal group-transfer cross section.

Let $S_{\phi 1}, S_{\phi 2}$ be complementary sub-surfaces of the boundary S of the body B, then the problem is completed by proper Dirichlet conditions of the kind

$$\phi_1 = \overline{\phi_1}\,(\boldsymbol{X}, t) \qquad \text{on } S_{\phi 1} \tag{4}$$

$$\phi_2 = \overline{\phi_2}\,(\boldsymbol{X}, t) \qquad \text{on } S_{\phi 2.} \tag{5}$$

Heat Conduction Problem. The temperature at which the shielding concrete is working during normal operations, along with the gamma radiation heating, can cause non-uniform thermal strains in concrete, at the scale of its constituents, so driving deterioration [12]. On the other hand, the neutron radiation also generates heat during the transport and attenuation processes, which could alter the thermal field in the wall. The classical heat conduction equation is

$$\rho c_p \frac{\partial T(\boldsymbol{X},t)}{\partial t} = \nabla^{\mathrm{T}}\big(\mathbf{k}\nabla T(\boldsymbol{X}, t)\big) + Q(\boldsymbol{X}, t) \tag{6}$$

where c_p is the specific heat capacity; ρ is the mass density; T is temperature; $\mathbf{k}$ is the thermal conductivity matrix; Q is the volumetric heat source.

Let S_1, S_2, S_3 be complementary sub-surfaces of the boundary S of the body B. Then, proper boundary conditions to the problem include a specified temperature on S_1, a specified heat flux on S_2, and specified convection boundary conditions on S_3

$$T = \bar{T}(\boldsymbol{X}, t) \qquad \text{on } S_1 \tag{7}$$

$$-\big(\mathbf{k}\nabla T(\boldsymbol{X}, t)\big)\,\mathbf{n} = \bar{q}\,(\boldsymbol{X}, t) \qquad \text{on } S_2 \tag{8}$$

$$-\big(\mathbf{k}\nabla T(\boldsymbol{X}, t)\big)\,\mathbf{n} = h(T(\boldsymbol{X}, t) - T_e) \qquad \text{on } S_3 \tag{9}$$

where $\bar{T}$ is the prescribed temperature; $\bar{q}$ is the prescribed heat flux; h is the heat transfer coefficient; T_e is the environment temperature; and T is the unknown temperature at the boundary.

Based on the two-group neutron diffusion model, heat generated either by absorption or scattering of neutrons is in good approximation due to the thermal neutron fraction. This is true as long as one accepts that heat due to scattering is negligible, if compared to heat generated by the capture of thermal neutrons. The neutron radiation induced heating rate by absorption can be estimated as [2]

$$Q(\boldsymbol{X}, t) = 1.6 \times 10^{-13}\, \Sigma_c \mathcal{E}_b \phi_2(\boldsymbol{X}, t) \tag{10}$$

where Σ_c is the macroscopic neutron capture cross section, and $\mathcal{E}_b$ is the binding energy for the capture process.

Weak formulation

The global coupled system of governing equations yields

$$\begin{cases} \mathbf{L}^{\mathrm{T}}\boldsymbol{\sigma} + \boldsymbol{b} = \mathbf{0} \\ \rho c_p \frac{\partial T(\boldsymbol{X},t)}{\partial t} = \nabla^{\mathrm{T}}\left(\mathbf{k}\nabla T(\boldsymbol{X},t)\right) + 1.6 \times 10^{-13}\Sigma_c \mathcal{E}_b \phi_2(\boldsymbol{X},t) \\ \frac{1}{v_1}\frac{\partial \phi_1(\boldsymbol{X},t)}{\partial t} - \nabla^{\mathrm{T}}\left(\boldsymbol{D_1}(\mathbf{X},t)\nabla\phi_1(\mathbf{X},t)\right) + \Sigma_{R1}\phi_1(\boldsymbol{X},t) = 0 \\ \frac{1}{v_2}\frac{\partial \phi_2(\boldsymbol{X},t)}{\partial t} - \nabla^{\mathrm{T}}\left(\boldsymbol{D_2}(\mathbf{X},t)\nabla\phi_2(\mathbf{X},t)\right) + \Sigma_{a2}\phi_2(\boldsymbol{X},t) = \Sigma_{s12}\phi_1(\boldsymbol{X},t). \end{cases} \tag{11}$$

A numerical solution to the boundary value problem is sought in agreement with the weighted residual method, that minimizes the residual of the differential problem over the domain B and the boundary S. In line with the FEM approach the body B can be discretized into finite elements $B_e | B = \cup B_e$, and the approximate solution for the state variables $\boldsymbol{u}$, T, ϕ_1, and ϕ_2 within each element are sought as linear combination of the shape functions $\mathbf{N}$ defined at the nodes of the element, and the solution at the same nodes.

By applying the Galerkin variational approach. The coupled problem illustrated herein reduces, therefore, to the following system

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \mathbf{M}_T & 0 & 0 \\ 0 & 0 & \mathbf{M}_{\phi_1} & 0 \\ 0 & 0 & 0 & \mathbf{M}_{\phi_2} \end{bmatrix} \begin{bmatrix} \dot{\boldsymbol{u}} \\ \dot{\boldsymbol{T}} \\ \dot{\boldsymbol{\phi}}_1 \\ \dot{\boldsymbol{\phi}}_2 \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{\boldsymbol{uu}} & 0 & 0 & 0 \\ 0 & \mathbf{K}_T & 0 & \mathbf{K}_{T\phi_2} \\ 0 & 0 & \mathbf{K}_{\phi_1} & 0 \\ 0 & 0 & \mathbf{K}_{\phi_1\phi_2} & \mathbf{K}_{\phi_2} \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{T} \\ \boldsymbol{\phi}_1 \\ \boldsymbol{\phi}_2 \end{bmatrix} = \begin{bmatrix} \boldsymbol{f}_{\boldsymbol{u}} \\ \boldsymbol{f}_T \\ \boldsymbol{f}_{\phi_1} \\ \boldsymbol{f}_{\phi_2} \end{bmatrix} \tag{12}$$

where $\boldsymbol{u}$, $\boldsymbol{T}$, $\boldsymbol{\phi}_1$, and $\boldsymbol{\phi}_2$ are the vectors of the nodal values of the state variables.
The coupled system can be solved by using a finite difference scheme in time, and the Newton–Raphson scheme.

Numerical Results

A slice of biological shield is considered in the numerical analysis of dimensions 100×100×80 cm. The temperature at the inner surface is set at 65°C, with an outer temperature of 20°C. Thermal convection boundary condition is imposed on the outer surface, by considering a heat transfer coefficient with air, while thermal symmetrical boundary conditions are imposed on the upper, down and lateral surfaces. On the inner surface a uniform constant value of 3.2×10^{10} n/(cm^2 s) for the fast neutron flux, and 4×10^{10} n/(cm^2 s) for the thermal neutron flux is assumed. The flux is directed outwards and involves the 80 cm thickness of the wall. The time of analysis is 1 year; the time step used in the analysis is 1×10^{-6} s. The concrete properties used in the analyses are listed in Table 1.

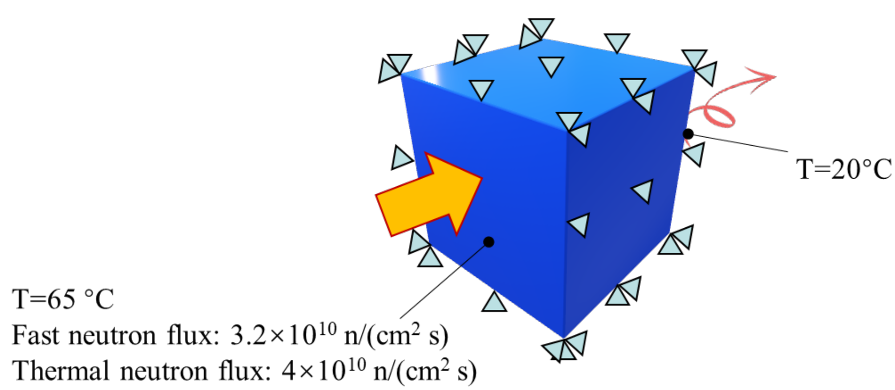

Figure 1: Studied portion of biological shielding wall with boundary conditions.

Table 1: Parameters used in the numerical example (thermal, and neutron diffusion parameters are taken from reference [2]).

E [MPa]	ν	α [°C^{-1}]	k [W/(cm·°K)]	ρ [kg/cm^3]	c_ρ [J/(kg·°K)]	h [W/(cm^2·°K)]
30000	0.2	$1\cdot10^{-5}$	8.7×10^{-3}	2.3×10^{-3}	650	0.0025

D_1 [cm]	D_2 [cm]	Σ_{R1} [cm^{-1}]	Σ_{s12} [cm^{-1}]	Σ_{a2} [cm^{-1}]	v_1 [cm/s]	v_2 [cm/s]	Σ_c [cm^{-1}]	$\mathcal{E}_b$ [MeV]
1.14	0.484	0.085	0.08	0.0094	4.37×10^8	2.2×10^5	0.0094	5.5

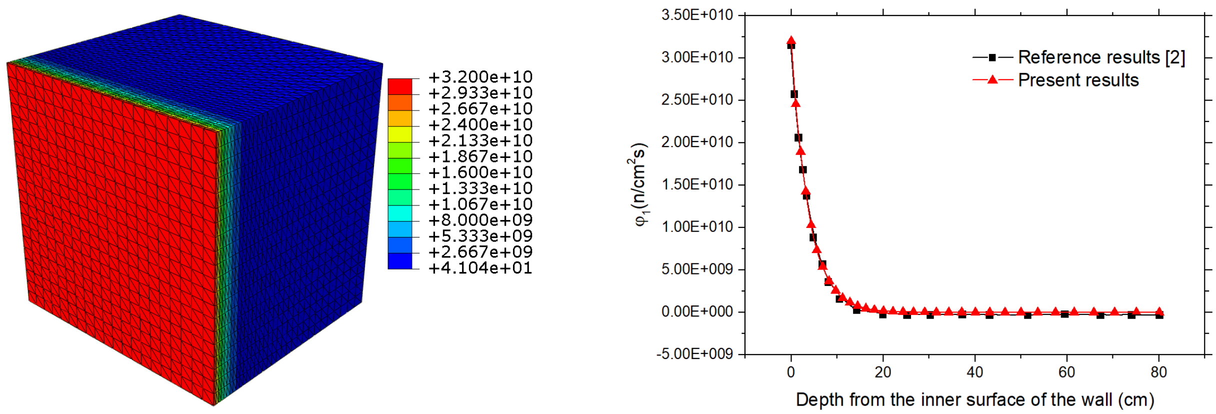

Figure 2: (a) Fast neutron flux field in the model; (b) fast neutron flux along the thickness of the wall.

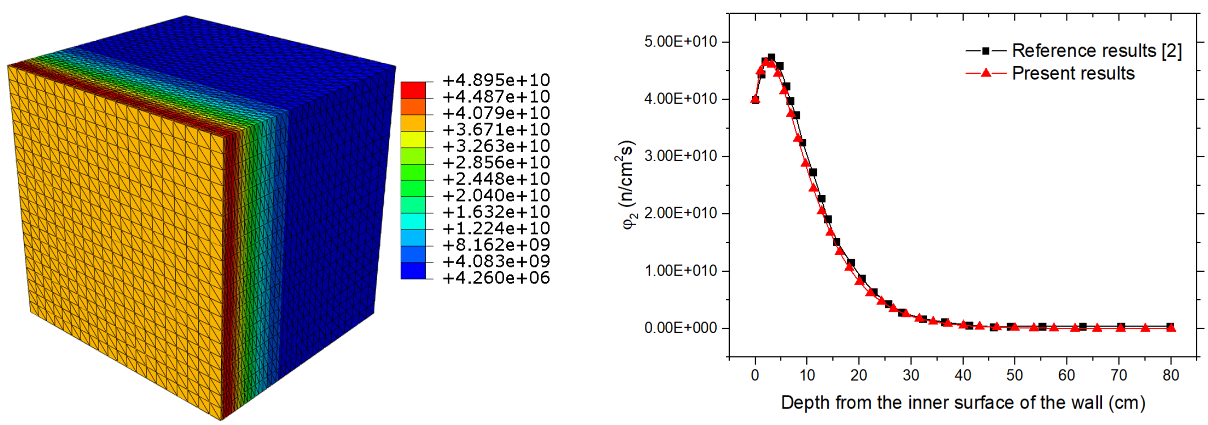

Figure 3: (a) Thermal neutron flux field in the model; (b) Thermal neutron flux along the thickness of the wall;

In Fig. 3 (b) a peculiar behavior of the thermal neutron flux at steady-state close to the hot surface is envisaged, showing a slight increase in this region, and a subsequent decrease in space, which indicates the attenuation of fast neutrons in the wall. On the other hand, the fast neutron flux (Fig. 2) shows a monotonic behavior, as expected.

Summary

Neutron radiation can deteriorate the mechanical properties of concrete materials at long term, therefore it is critical to obtain accurate neutron radiation levels in concrete structures during their service life.

A thermo-mechanical-neutron diffusion coupled formulation is proposed in this paper, which combines the mechanical constitutive model with the two-group neutron-transport theory, and the thermal diffusion theory. Some preliminary results are shown, that demonstrate the capability of the model to catch the main coupling mechanisms associated to the three problems, and, specifically the influence of the two kinetic groups of neutron fluxes to each other in the attenuation/absorption process within the shielding wall, as well as the local temperature increase due to neutron absorption.

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