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DIRECT CALIBRATION OF PHASE-FIELD MODELS FOR COHESIVE FRACTURE AND TRANSPORT

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Abstract. The paper describes a simple identification procedure that can be used to construct a function relating the increased diffusivity or permeability to the current mechanical state of the material, based on an experimentally determined relation between the excess flux along the crack and the crack opening. The underlying mechanical model belongs to the class of phase-field formulations (or variational damage models) for quasibrittle materials, but the procedure would be applicable to other types of regularized failure models as well.

1 INTRODUCTION

Phase-field models, which can also be considered as a special class of variationally formulated gradient damage models, have become increasingly popular because of their versatility and efficiency. Nowadays, they undoubtedly represent the most widely used approach to modeling of brittle, quasibrittle [1] and ductile failure. In their original form, they were developed within a simple variational framework, later extended to more general formulations that can be adjusted to capture the specific features of materials with multiple dissipation mechanisms, including internal friction [2].

Gradient damage models of the phase-field type are based on incremental minimization of an energy functional that usually contains four terms—the stored elastic energy (dependent on strain and damage), the dissipated energy (dependent on damage), the higher-order regularizing energy (dependent on the gradient of a damage-related variable called the phase field), and the energy of external loads. Specific properties of a model of this kind are determined by the choice of two fundamental functions, one of which defines the relation between the damage variable and the phase field, while the other links the dissipation density to the damage (or to the phase field). At early stages of development, these functions were selected more or less by trial and error, and the primary objective was to control a single property—the fracture energy. This was sufficient for successful simulation of brittle fracture, but not appropriate for materials in which a large inelastic fracture zone develops and their behavior is characterized as quasibrittle. Later, the basic two functions were adjusted in order to cover a wider class of materials. Typically, one of these functions is prescribed by a relatively simple formula, and the other is endowed with a number of adjustable parameters that can be used to control the resulting properties.

Once a mechanical model that can describe cracking becomes available, it is tempting to use it in coupled problems that also involve transport phenomena. A simple approach can be based on linking the mechanical damage (or the related phase-field variable) to the modified transport properties of the material. In this way, the effect of cracking on the transport of pore fluids or chemical species can be incorporated.

In this work, we propose a novel method for direct identification of the dependence of excess diffusivity or permeability on the mechanical state of damage. The objective is to reproduce the prescribed (e.g., experimentally determined) dependence of the extra flux along the crack on the crack opening. It turns out that the identification can be done incrementally, in the sense that, in each step of the mechanical simulation, the description of the function to be identified is extended by a short interval, based on one simple equation.

2 BASIC EQUATIONS

For the present purpose, it is sufficient to consider models that exploit an energy functional in the form

$$\begin{aligned}\mathcal{E}(\mathbf{u},\phi) = \\ = \tfrac{1}{2}\int_\Omega (1-\omega(\phi))\nabla_s\mathbf{u} : \mathbf{D}_e : \nabla_s\mathbf{u}\,\mathrm{d}\mathbf{x} + \\ + \tfrac{1}{2}\int_\Omega g_{f0}\ell_0^2\|\nabla\phi\|^2\,\mathrm{d}\mathbf{x} + \\ + \int_\Omega D(\omega(\phi))\,\mathrm{d}\mathbf{x} - \int_\Omega \bar{\mathbf{b}}\cdot\mathbf{u}\,\mathrm{d}\mathbf{x}\end{aligned} \tag{1}$$

where $\mathbf{u}$ is the displacement field, ϕ is the phase field, ω is the damage variable in the traditional sense, $\mathbf{D}_e$ is the elastic stiffness tensor, g_{f0} is a parameter with the dimension of energy per unit volume, ℓ_0^2 is the internal length parameter, D is the dissipation function and $\bar{\mathbf{b}}$ is the body force vector. As usual, Ω denotes the spatial domain that represents the solid body analyzed.

Fully general formulations might incorporate additional refinements, e.g., a split of the elastic energy density into parts attributed to tension and compression, with the reduction factor $1-\omega$ applied only on the first part. However, for the present purpose, the format presented in (1) is sufficient.

Incremental minimization of functional $\mathcal{E}$ combined with the damage irreversibility condition leads to the equilibrium equations and to a damage evolution law that contains the Laplacean of the phase-field variable. This higher-order term acts as a localization limiter. In the one-dimensional setting, the equilibrium equation reads

$$((1-\omega(\phi))Eu')' + \bar{b} = 0 \tag{2}$$

and the damage evolution conditions can be written as

$$\begin{aligned}\omega_\phi(\phi)\tfrac{1}{2}Eu'^2 + g_{f0}\ell_0^2\phi'' - D_\phi(\phi) &\le 0 \quad (3)\\ \dot{\phi} &\ge 0 \quad (4)\\ \left(\omega_\phi(\phi)\tfrac{1}{2}Eu'^2 + g_{f0}\ell_0^2\phi'' - D_\phi(\phi)\right)\dot{\phi} &= 0 \quad (5)\end{aligned}$$

Here, E is the elastic modulus, primes correspond to spatial derivatives, and subscript ϕ indicates differentiation with respect to the phase-field variable, i.e., $\omega_\phi \equiv \mathrm{d}\omega/\mathrm{d}\phi$ etc.

In the absence of body forces, the equilibrium equation (2) makes it possible to express the strain as

$$\varepsilon = u' = \frac{\sigma}{E(1-\omega)} \tag{6}$$

where σ is the stress, uniformly distributed in space. In the active part of the process zone, characterized by $\dot{\phi} > 0$, condition (3) must be satisfied as an equality, and elimination of strain based on (6) leads to a second-order differential equation

$$\frac{\sigma^2\omega_\phi(\phi)}{2E(1-\omega(\phi))^2} + g_{f0}\ell_0^2\phi'' - D_\phi(\phi) = 0 \tag{7}$$

in which the only unknown function is the phase field, ϕ, while the stress σ is constant.

Numerically, equation (7) can be handled by the finite difference method. The stress level σ can be considered as a variable that parameterizes the damage process. At the onset of damage, the phase field has a zero value everywhere, the gradient term vanishes and equation (7) is satisfied if the stress level is set to $\sigma = f_t \equiv \sqrt{2ED_\phi(0)/\omega_\phi(0)} = \sqrt{2ED_\omega(0)}$.

In a typical numerical increment number k, the value of the phase field in the center of the process zone is increased to a chosen level $\phi^{(k)}_{max}$, and the stress is iteratively adjusted. Equation (7) is replaced by central differences, and the phase-field values at numerical grid points x_i are successively evaluated in an explicit manner, based on initial conditions $\phi(0) = \phi^{(k)}_{max}$ and $\phi'(0) = 0$. The stress level is adjusted until the obtained solution satisfies condition $\phi'^{(k)}(L_d^{(k)}/2) = \phi'^{(k)}(L_d^{(k-1)}/2)$ where $L_d^{(k)}$ is the active size of the process zone after step k, defined by $\phi^{(k)}(L_d^{(k)}/2) = \phi^{(k)}(L_d^{(k-1)}/2)$. In other words, at the first point where the phase-field variable at the end of the step has the same value as at the beginning of the step, the slope of the phase-field profile at the end of the step must also be the same as at the beginning of the step.

3 SPECIFIC PHASE-FIELD MODEL

As an example, consider the class of phase-field cohesive zone models proposed (within the framework of variational damage formulations) by Jirásek and Zeman [3]. In the present notation, it is described by functions

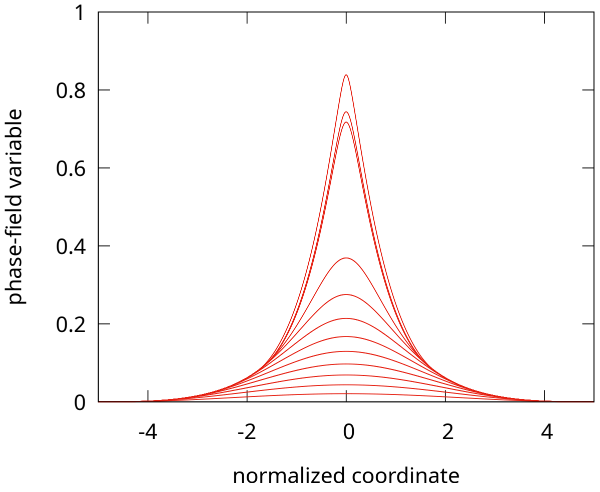
$$\begin{aligned} D_\omega(\omega) &= \tfrac{1}{2}Eg^{*2}(\omega) \qquad (8)\\ \omega(\phi) &= 1-(1-\phi)^{1/(1-p)} \qquad (9) \end{aligned}$$

where function g^* is defined implicitly by the equation

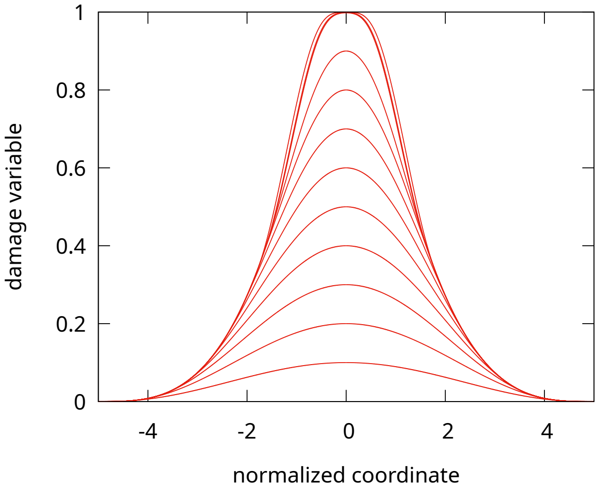
$$(1-\omega)g^*(\omega)\exp\left(\frac{g^*(\omega)-\varepsilon_0}{\varepsilon_f}\right) = \varepsilon_0 \qquad (10)$$

The dissipated energy density is defined here in terms of its derivative with respect to the damage variable, D_ω, and relations (8) and (10) are chosen such that the local response of the model (in the absence of localization) would correspond to exponential softening. Parameter $\varepsilon_0 = f_t/E$ specifies the limit elastic strain and ε_f controls the ductility. Function g^* that solves (10) is the inverse of function g that evaluates damage from strain.

(a) evolution of phase-field profile



(b) evolution of damage profile



(c) equivalent cohesive diagram

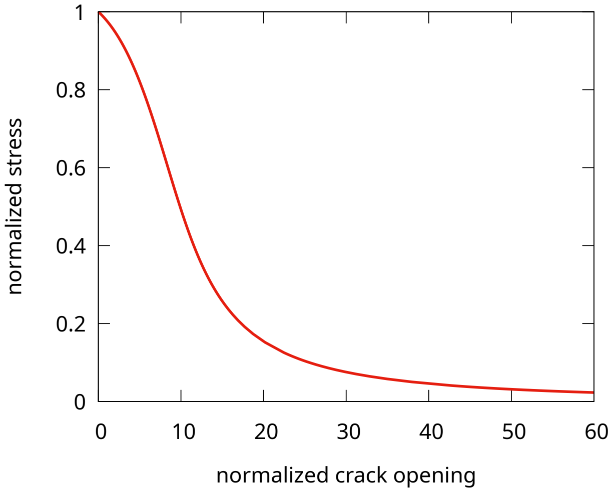


Figure 1: Localization characteristics of the regularized damage model.

Note that the specific form of expression (9) leads to $\omega(0) = 0$ and $\omega(1) = 1$. Parameter p is typically between 0.5 and 1, and the choice of $p = 0.8$ leads to a reasonable shape of the equivalent cohesive diagram.

The numerically computed localization characteristics of the model are presented in Fig. 1. Parts (a) and (b) show the evolution of the localized phase-field profile and of the corresponding damage profile. The equivalent cohesive diagram is plotted in Fig. 1c. It has a long tail, characteristic of quasibrittle materials. The equivalent crack opening w is evaluated by integrating the inelastic strain across the process zone, which can be written as

$$w = \int_{-L_d/2}^{L_d/2} \omega\varepsilon \,\mathrm{d}x = \frac{\sigma}{E}\int_{-L_d/2}^{L_d/2} \frac{\omega}{1-\omega}\,\mathrm{d}x \tag{11}$$

where L_d has to be understood as the maximum size of the process zone.

4 EFFECT OF DAMAGE ON TRANSPORT PROPERTIES

Transport of water or diffusion of chemical species through the pore space of concrete and similar porous materials is usually described by a parabolic partial differential equation in the general form

$$C\,\frac{\partial c}{\partial t} = \frac{\partial}{\partial \mathbf{x}} \cdot \left(K\frac{\partial c}{\partial \mathbf{x}}\right) \tag{12}$$

where c is the primary unknown field (e.g., concentration, water content, relative humidity, or pressure), C is the capacity and K is the diffusivity, permeability or conductivity, depending on the specific nature of the problem. In the simplest case, C and K are constant, and the transport problem is then linear. Often, the transport properties are affected by the current state, expressed by the value of c, which leads to a nonlinear problem. In addition, these properties can vary due to irreversible mechanical changes such as cracking. This calls for a coupled formulation that captures the simultaneous evolution of mechanical fields and of the field that characterizes the transport problem.

The increased diffusivity or permeability caused by cracking can be conveniently described by a model in which K depends on the damage or on the related phase-field variable. Our objective is to develop a framework for a systematic calibration of such models. Let us start by looking at a simple class of formulations proposed by Wu and De Lorenzis [4], with the increase of K considered as a power function with exponent m. The original source was dealing with an anisotropic diffusivity tensor, but since we are interested here in transport along the crack, it is sufficient to consider a simple scalar relation

$$K(\phi) = K_0 + \Delta K\,\phi^m \tag{13}$$

When the information on the evolution of the phase-field profile is available, it is possible to evaluate, for any stage of the degradation process, the resulting excess flux along the crack. The effect on transport properties can be characterized by the proportionality factor between this flux and the gradient along the crack, obtained by integrating the excess local diffusivity across the width of the process zone. Therefore, one can reuse the results of the one-dimensional simulation of the localization process and, by simple post-processing, evaluate the “excess crack diffusivity”

$$K_{cr} = \int_{-L_d/2}^{L_d/2} \left(K(\phi(x)) - K_0\right)\,\mathrm{d}x \tag{14}$$

Note that the physical dimension of K_{cr} is the physical dimension of K multiplied by length. For instance, if K is the diffusivity in m^2/s, then K_{cr} is expressed in m^3/s.

For the mechanical model presented in the previous section, the dependence of the excess crack diffusivity on the opening of the equivalent cohesive crack w (i.e., on the quantity that characterizes the current state of mechanical degradation) is plotted in Fig. 2. Exponent m ranges here between 1 and 7. Since the results scale with the final diffusivity increase ΔK, the curves are presented in a normalized format, with the actual K_{cr} divided by the value obtained at the ultimate crack opening. It is clearly seen that low values of exponent m, such as 1 or 2, lead to a fast initial increase of the crack diffusivity, followed by saturation. On the other hand, higher values of m, such as 4 or 7, suppress the early increase and delay the effects of cracking on diffusivity, which seems to be closer to experimental observations.

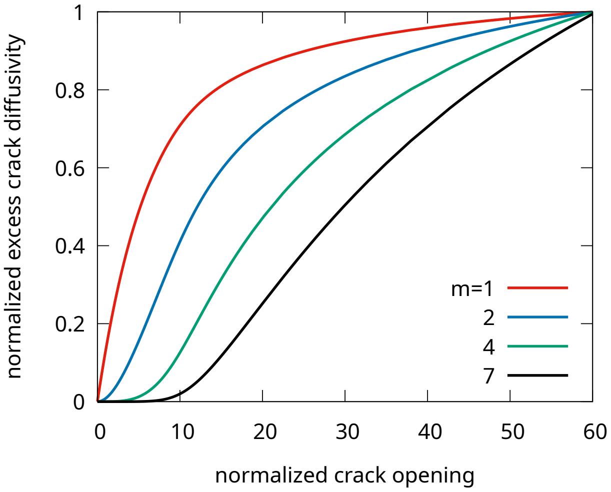


Figure 2: Normalized excess crack diffusivity evaluated using the power law (13) with various values of exponent m.

The performance of the model for increased diffusivity depends not only on the assumed local relation between the phase-field variable and the excess diffusivity, but also on the underlying mechanical model, which determines the shapes of the phase-field profiles and the evolution of the active process zone size. It is therefore difficult to arrive at universally valid conclusions and reliable general rules for the choice of function $K(\phi)$. Instead of using a fixed form of this function, it is preferable to deduce it directly from the experimental data. This can be achieved by modifying the post-processing algorithm. The dependence of K on ϕ can be constructed incrementally and described by a table of values with linear interpolation in between.

In a typical incremental step number k, the maximum value of the phase-field variable in the center of the process zone increases from $\phi_{max}^{(k-1)}$ to $\phi_{max}^{(k)}$, where $k = 1, 2, 3, \ldots$, and $\phi_{max}^{(0)} = 0$. The values of K that correspond to phase-field values up to $\phi_{max}^{(k-1)}$ have already been identified in the previous steps. Suppose that the dependence in the range between $\phi_{max}^{(k-1)}$ and $\phi_{max}^{(k)}$ is approximated by the linear function

$$K^{(k)}(\phi) = K_0 + \Delta K^{(k-1)} + a^{(k)}\left(\phi - \phi_{max}^{(k-1)}\right) \tag{15}$$

in which $\Delta K^{(k-1)} = K(\phi_{max}^{(k-1)}) - K_0$ is already known while the slope $a^{(k)}$ is yet to be determined. It is now possible to numerically approximate the integral in (14) by

$$\begin{aligned} K_{cr} = {} & \Delta x \sum_{i\in\mathcal{I}\setminus\mathcal{I}_k} \left(K(\phi(x_i)) - K_0\right) + \\ & + \Delta x \sum_{i\in\mathcal{I}_k} \left(\Delta K^{(k-1)} + a^{(k)}\left(\phi_i^{(k)} - \phi_{max}^{(k-1)}\right)\right) \end{aligned} \tag{16}$$

where Δx is the grid spacing used in spatial discretization, x_i are the coordinates of the grid points, $\phi_i^{(k)}$ are the values of the phase-field variable at these points at the end of step number k, $\mathcal{I}$ is the set of all subscripts i that correspond to these points, and $\mathcal{I}_k$ is the set of those subscripts i for which $\phi_i^{(k)} > \phi_{max}^{(k-1)}$. The expression in (16) can be written as

$$K_{cr} = K_{cr0}^{(k)} + P^{(k)} a^{(k)} \tag{17}$$

where

$$\begin{aligned} K_{cr0}^{(k)} &= \Delta x \sum_{i\in\mathcal{I}\setminus\mathcal{I}_k} \left(K(\phi(x_i)) - K_0\right) + \\ & \quad + \Delta x \sum_{i\in\mathcal{I}_k} \Delta K^{(k-1)} \end{aligned} \tag{18}$$

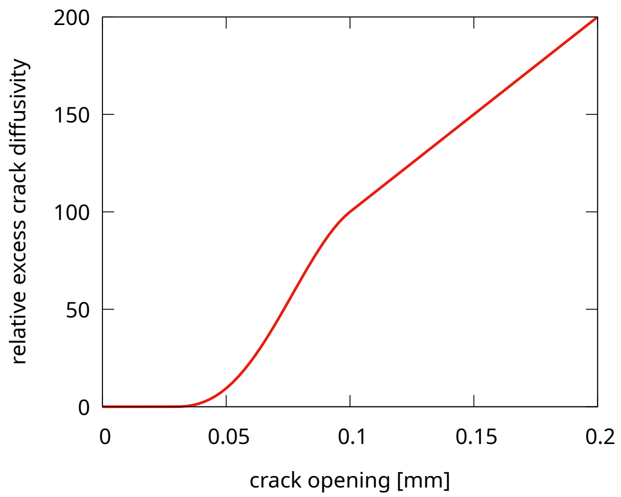
$$P^{(k)} = \Delta x \sum_{i\in\mathcal{I}_k} \left(\phi_i^{(k)} - \phi_{max}^{(k-1)}\right) \tag{19}$$

are constants that can be calculated. In addition, we can obtain the crack opening $w^{(k)}$ by numerical evaluation of the integral in (11). By setting $K_{cr} = K_{cr,exp}(w^{(k)})$ = the target value of crack diffusivity at crack opening $w^{(k)}$ evaluated from experiments, we can determine

$$a^{(k)} = \frac{K_{cr,exp}(w^{(k)}) - K_{cr0}^{(k)}}{P^{(k)}} \tag{20}$$

This means that the optimal function $K(\phi)$ is now known up to $\phi_{max}^{(k)}$, and we can proceed to the next step until the whole range is covered.

(a) empirical formula for excess crack diffusivity



(b) identified function $K(\phi) - K_0$

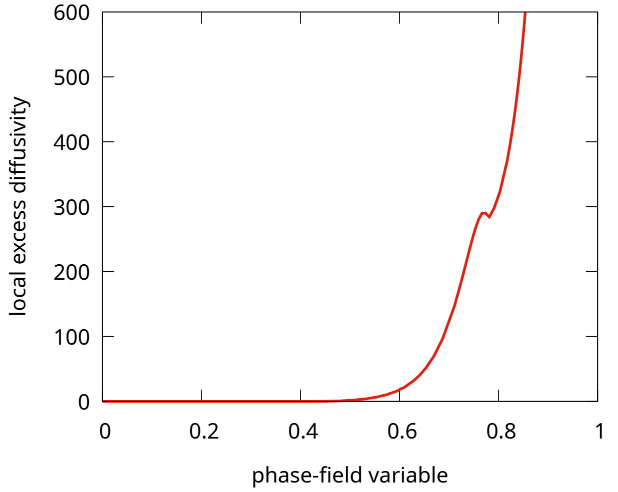


Figure 3: Identification of the dependence of diffusivity on the phase field which can reproduce experimental data.

The described identification procedure has been applied to the analytical formula proposed by Zhang et al. [5] for approximation of experimental data on diffusivity of chloride ions in concrete. Fig. 3a shows the prescribed dependence of the excess crack diffusivity on the crack opening, which has been exactly reproduced by the present approach with the numerically constructed function $K(\phi)$ depicted in Fig. 3b. The small irregularity (lack of monotonicity) in the region of ϕ slightly below 0.8 is related to the sudden change of curvature of the assumed experimental diagram at w slightly below 0.1 mm, and it can be eliminated if a small deviation from the assumed diagram is permitted.

5 CONCLUSION

We have described and tested a procedure for identification of the optimal form of function $K(\phi)$ that permits simulations of the effect of cracking on enhanced transport of fluids or chemical species along the process zone using a phase-field model for quasibrittle materials. Feasibility of the proposed approach has been demonstrated. A more detailed comparative study will be published in a follow-up journal paper, and applications to multi-dimensional simulations will be presented at the conference.

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