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Toward the development of a three-step coupled modeling for the assessment of air leakage ratio through cracked reinforced concrete walls

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Abstract This study compares the performance of two models, the combined beam particle model, and the continuous damage model, in simulating crack patterns in concrete under split loading conditions. Results show that both models have good agreement with experimental results in terms of the force-displacement curve, while the combined beam particle model provides a more detailed and accurate description of crack patterns. However, the continuous damage model has a faster computational time. This study serves as a foundation for future developments of a three-step model based on weak coupling between Finite Element-Discrete Element-Computational Fluid Dynamics, used to estimate leakage rate during severe accident scenarios.

Key-words damage, cracking, discrete element method, flow leakage measurement.

I. INTRODUCTION

In case of severe accident conditions such as large break LOCA (Loss Of Coolant Accident), radioactive releases will go out of the RCS (Reactor Coolant System). Subsequently, the integrity of the second barrier is lost. This will cause a rise in (relative) pressure and temperature to 4.2 bars and around 150 °C. Such conditions induce cracking in the internal walls of the CCB (Concrete Containment Building), leading to leaks. The numerical assessment of such leaks heavily depends on the characterization of the fracture features, including crack geometry opening fluctuation, tortuosity, and roughness (Akhavan et al., 2012; Jourdain et al., 2014; Rastiello et al., 2016, 2015). In the synthesis of the second benchmark of VeRCORS¹ project, (Charpin et al., 2021) mentioned the complexity of the numerical assessment of the leak-tightness of a pre-stressed concrete containment wall. This is mainly due to physical complexity (including thermo-hydration, drying, creep, damage, pre-stressing, transfer properties, etc.), which affects the global air tightness of a concrete structure.

Numerous models within the continuum mechanics framework have been developed to investigate the cracking mechanisms and how they affect concrete deterioration. Discrete cracking models such as extended Finite Element Method (X-FEM) (Belytschko et al., 2003) and Embedded Finite Element

¹ VeRCORS (Vérification Réaliste du Confinement des Réacteurs) is a 1/3 scale mock-up of a 1300 MWe nuclear reactor Concrete Containment Building CCB.

Method (E-FEM) (Jourdain et al., 2014), continuous models such as Continuum damage models (Richard et al., 2015), and lattice models like in (D'Addetta et al., 2002) are the three primary methods used to simulate concrete cracking (Mier, 1984). Discrete methods are renowned for their ability to explicitly represent concrete cracking and its characteristics (initiation, length, opening, tortuosity). A discrete model called DEAP after "Discrete Element Analysis Program" resulting from the mechanics of rigid solids has been developed (Oliver-Leblond, 2019, 2015; Vassaux et al., 2016).

In the study conducted by (Matallah et al., 2010), a procedure known as [OUVFISS](#) was developed for the estimation of crack opening by post-processing a continuous damage model. This procedure was then applied in a subsequent study by (Matallah and La Borderie, 2016) to evaluate the flow rate based on modified permeability matrix using Poiseuille's law. While this method is relatively simple, it relies heavily on the accurate characterization of parameters which takes into account the effect of tortuosity and roughness of the crack, as highlighted by (Rastiello et al., 2014). Therefore, there is a need for an intermediate tool to effectively describe the crack parameters and used as an intermediate tool between the global mechanical simulation and complex CFD simulations. One can use a weak local/global coupling between the continuous damage model and the beam particle model (Oliver-Leblond, 2015; Oliver-Leblond et al., 2013) to reduce the computational time cost of the discrete simulations by only perform the discrete computation on highly damaged areas. This coupling will be applied to an experimental case study, COBRA project (French acronym of "Building confinement of the reactor in case of accident"), which is one of the perspectives of this paper.

Our goal within this study is to perform Brazilian mechanical 3D simulations for two models, the combined beam particle model (DEAP) and the continuous damage model (CONCYC) and validate the results with experimental studies found in the literature in terms of macroscopic behavior (force-displacement or force crack opening curve). After that, extract the explicit cracking patterns from DEAP which will be then used as an input for CFD simulations to evaluate air/air-steam leakage rate through concrete cracks. Finally, compare the two results, [OUVFISS](#) and DEAP, in terms of crack opening.

The outline of this paper is as follows: first, a brief description of COBRA project with the global methodology. The second part a brief description on the two models, damage (Richard et al., 2015; Vassaux, 2015) and DEAP. Finally, Illustration of the boundary conditions on the Brazilian splitting specimen for both models with the results of the simulations with a brief overall discussion and perspective.

II. Experimental description and global strategy

COBRA project

COBRA is a program designed to evaluate the ability of reinforced concrete enclosures in French 1300 MWe nuclear power plants to prevent the release of hazardous materials during severe accident conditions. The program includes both experimental tests on two reinforced concrete models and numerical simulations using finite element modeling, validated using data from the experimental tests. The models are based on the ANR (National Research Agency) ECOBA project

(French acronym of “Study of the Confinement of Reinforced Concrete Structures”) (Nahas et al., 2014) and represent a representative structural volume of a typical 1300 MWe PWR (Pressurized Water Reactor) containment vessel. The program aims to address the lack of a widely accepted method for predicting the rate of leakage from a pre-stressed concrete enclosure without a metal liner during an accident. The two models have similar geometry, see Figure 1, and consist of footings, a zone of interest, and gussets. They differ in that one was poured in a single casting, while the other was made in two castings to assess the influence of concreting resumptions. Six actuators, as shown in

Figure 2, are used to apply pressure and create cracks in the ZOI (Zone Of Interest). Data will be collected on leakage ratio, aerosol retention, displacement, temperature, and strain and temperature fields.

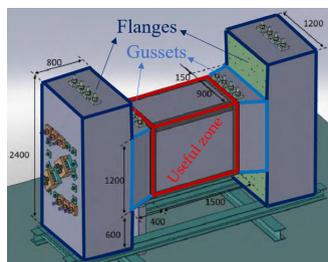


Figure 1 Geometry of COBRA models

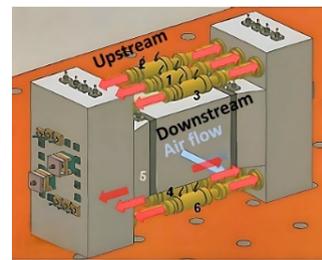


Figure 2 COBRA setup

Global strategy

The global strategy of this study involves several steps as illustrated in Figure 3. The first step is to use the CONCYC damage model (Richard et al., 2015; Vassaux, 2015) implemented in [Cast3M finite element](#) to conduct a simulation of an RSV containment structure using the COBRA program. This allows us to obtain the displacement field of the entire structure. In the second step, we use the displacement field at the boundary of the highly damaged zone as a boundary condition in DEAP simulation to obtain explicit crack patterns. Finally, we use these crack geometries in CFD simulation rather than the simplified method of using two parallel plates with a constant crack opening. The following paragraphs are a brief description for each model.

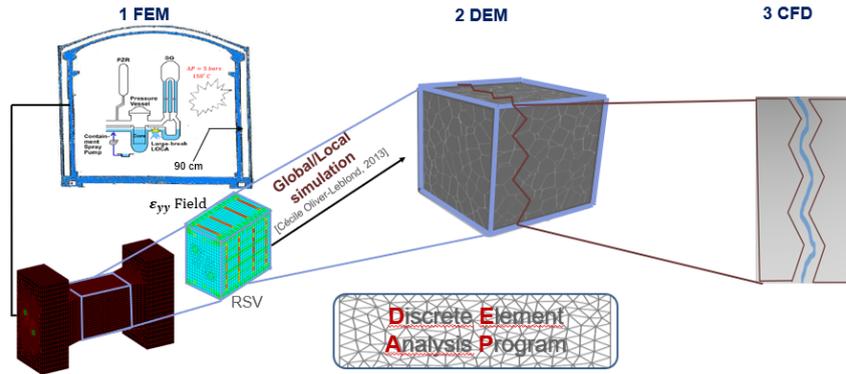


Figure 3 Global strategy

III. Continuum models

Continuous damage model CONCYC

The constitutive model developed by (Richard et al., 2015; Vassaux, 2015) describes the behavior of quasi-brittle materials under cyclic loading using isotropic continuum damage mechanics. It decomposes the effective stress of the volume element, $\underline{\underline{\sigma}}$, into two different tensors: the stress transmitted in the healthy matrix, $\underline{\underline{\sigma}}^m$, and the stress transmitted in all the cracks when they close considering both crack closure and hysteretic effects $\underline{\underline{\sigma}}^f$, see Equation (1).

$$\underline{\underline{\sigma}} = \underline{\underline{\sigma}}^m + \underline{\underline{\sigma}}^f = (1 - D)\mathbf{C} : \underline{\underline{\epsilon}} + \mathbf{C} : \left[\underline{\underline{\epsilon}}^f - \frac{\underline{\underline{\epsilon}}_{max}^f}{\alpha_0} \times \log \left(1 + \exp \left[-\frac{\alpha_0}{I_1(\underline{\underline{\epsilon}}_{max}^f)} I_1(\underline{\underline{\epsilon}}^f) \right] \right) \right] \quad (1)$$

Where D is the isotropic damage variable, $\underline{\underline{\epsilon}}$ the second-order total strain tensor, \mathbf{C} the fourth-order Hooke's tensor, $\underline{\underline{\epsilon}}^f$ homogenized contribution of crack openings to the total strain of the RSV, $\underline{\underline{\epsilon}}_{max}^f$ maximum crack strains, α_0 crack closure velocity and \mathbf{I}_1 refers to the direction normal to crack surface.

To improve the material's behavior under multiaxial stress, the author suggested two enhancements, different model for each enhancement, based on a reference evolution of D derived from Mazars' work (Mazars, 1984). The first enhancement modifies the softening behavior by affecting the free energy related to damage $\Psi^{m,D}$ considering that crack propagation in a volume of material is slowed when the material is confined, resulting in higher peak loads and more ductile behavior. Hence, the damage can be written as in Equation (2).

$$D = 1 - \frac{Y_0}{\bar{Y}} \exp \left[-\frac{B_0}{\kappa} (\bar{Y} - Y_0) \right] \quad (2)$$

where B_0 stands for a parameter controlling the softening behavior and the energy rate is denoted by $\bar{Y} = \frac{1}{2} E \epsilon_0 \epsilon^{eq}$ with the equivalent strain $\epsilon^{eq} = \sqrt{\langle \underline{\underline{\epsilon}} \rangle_+ : \langle \underline{\underline{\epsilon}} \rangle_+}$, and the elastic limit strain ϵ_0 . The elastic limit energy rate, $Y_0 = \frac{1}{2} E \epsilon_0^2$. variable κ is used to express the level of confinement.

The second enhancement affects the elastic surface of the material by modifying dissipation potential φ^m . The non-associated pseudo-potential of dissipation is formulated using the Mazars failure criterion and expressed in terms of thermodynamic variables, see Equation (3).

$$\varphi^m = \bar{Y} - (Y_0 + Z) \quad (3)$$

The thermodynamic force associated with z is denoted by Z , which increases the minimum threshold of for the elements to be considered as damaged elements. The modification allows for controlling the material's contraction level in the context of the dissipation potential, thus enhancing the model's accuracy and applicability, see Equation (4).

$$\bar{Y} = \frac{1}{2} E \epsilon_0 \epsilon^{eq} = \frac{1}{2} E \epsilon_0 \left(\sqrt{\langle \underline{\epsilon} \rangle_+ : \langle \underline{\epsilon} \rangle_+} + \frac{k_0}{K_c} \langle I_1(\mathbf{C} : \underline{\epsilon}) \rangle_- \right) \quad (4)$$

Fracture mechanics theory states that energy dissipated by cracking in a volume is dependent on crack surface. To account for this, $G_{F,0}$ must be constant. In simulations, energy dissipated by cracking depends on the fineness of the mesh used to discretize the medium. Two methods to solve this problem are the crack energy regularization method by (Hillerborg et al., 1976) and the nonlocal regularization method by (Pijaudier-Cabot and Bažant, 1987). For more information, see (Richard et al., 2015; Vassaux, 2015) on the reclosure of the crack and the hysteretic effects.

Combined Beam-Particle Model

In this model, concrete is simulated using polygonal rigid particles connected by brittle beams and frictional contact after beam failure. This model can reproduce failure patterns of compressive or tensile simulations (Vassaux et al., 2016). The mesh generation process is inspired by (Moukarzel and Herrmann, 1992), involving superimposing a grid on the specimen, randomly generating particle centroids within each cell, and performing Delaunay's triangulation and Voronoi's tessellation to control mesh heterogeneity as shown in Figure 4 and Figure 5.

The beam-particle model simulates cohesive forces using Euler-Bernoulli beams connecting particle centroids as shown in Figure 6 and described in Equation (5). These beams have four parameters to calculate cohesive forces and moments between particles: length and cross section are specific to each beam and determined by the mesh geometry, while modulus of Elasticity and inertia coefficient are the same for all beams. More information can be found in (Delaplace and Desmorat, 2007; Oliver-Leblond, 2019, 2015; Vassaux, 2015; Vassaux et al., 2016).

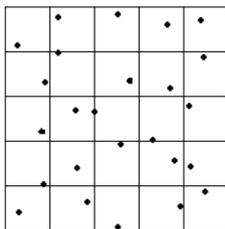


Figure 4 Random generation of the particle's nuclei

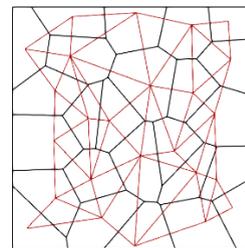


Figure 5 Generation of the beams (Delaunay's triangulation) and the particles (Voronoi Tessellation)

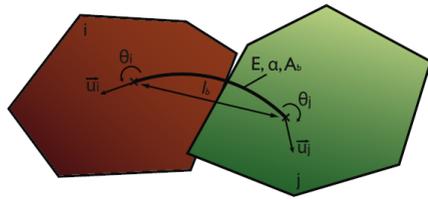


Figure 6 Two cohesively linked particles.

$$F_{coh,ij} = \begin{cases} F_{N,ij} = \frac{EA_{b,ij}}{l_{b,ij}}(\underline{u}_i - \underline{u}_j) \cdot \underline{n}_{b,ij} \\ F_{T,ij} = \frac{12EI_{b,ij}}{l_{b,ij}^3}(\underline{u}_i - \underline{u}_j) \cdot \underline{t}_{b,ij} - \frac{6EI_{b,ij}}{l_{b,ij}^2}(\theta_i - \theta_j) \\ M_{Z,ij} = \frac{6EI_{b,ij}}{l_{b,ij}^2}(\underline{u}_i - \underline{u}_j) \cdot \underline{t}_{b,ij} + \frac{4EI_{b,ij}}{l_{b,ij}}(\theta_i - \theta_j) \end{cases} \quad (5)$$

IV. Brazilian simulation

Boundary conditions

In order to develop a proof of concept for this approach, experiments found in the literature will be used as reference. Brazilian mechanical test have been conducted to obtain a localized macro-crack (Rastiello et al., 2018). This type of load is most likely to produce macro cracks in concrete, as it causes the specimen to experience maximum tensile stress. The boundary conditions shown in Figure 7 were adapted from those presented in (Rastiello et al., 2015) for the continuous CONCYC model in [CAST3M](#). The mesh size was chosen to be 2 mm based on the results of a sensitivity study on mesh size. The figure also illustrates the specimen tensile strength field generated from the turning band method (Mantoglou and Wilson, 1982) in order to take into account concrete heterogeneity.

The boundary conditions for DEAP model are different, as the specimen stability would be compromised if the blocked particles connecting beams were broken. Therefore, additional boundary conditions as shown in Figure 8 were applied to prevent rotation around the x-axis. Also, the material heterogeneity is considered in this approach.

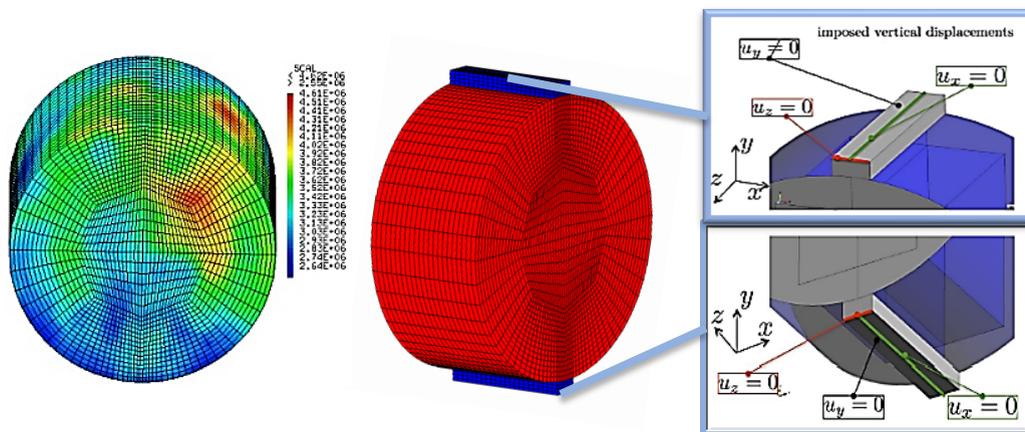


Figure 7 Boundary conditions for FEM with tensile strength random field (Rastiello et al., 2015)

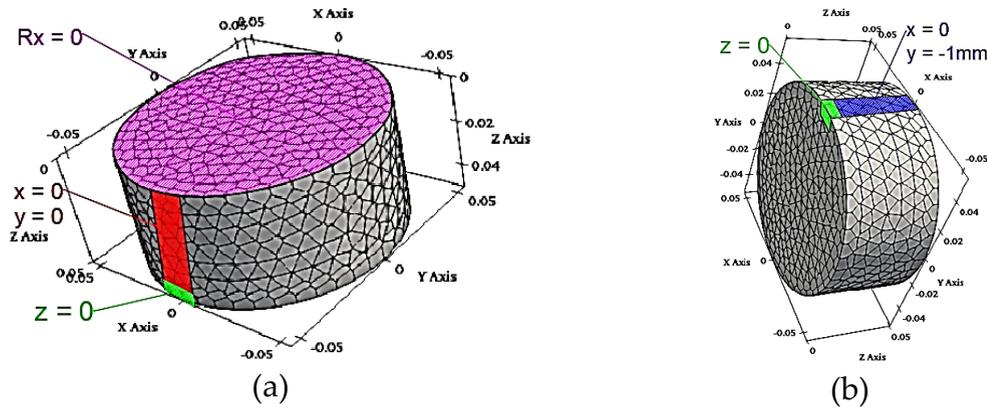


Figure 8. DEAP simulation dimensions and setup and boundary conditions

Results

The following section presents the results of the simulations described previously. These results were validated based on experimental data from (Rastiello et al., 2014) and the models were calibrated using these experimental results. Figure 9 illustrates the damage field distribution in (a) and the crack opening field obtained from the [OUVFISS](#) procedure implemented in [Cast3M](#) finite element software from the work of (Matallah et al., 2010) in (b). We can see that the material is highly damaged in the middle area, and we can observe an irregular crack surface, but we can't extract the crack information which is a limitation for [OUVFISS](#) procedure. Since we don't know how the crack is oriented and connected with other elements. All we know is the average crack opening per element. Regarding DEAP simulation. Figure 10 shows the displacement field in the x-axis direction (perpendicular to the loading) in (a) and the developed macro-crack geometry with 10 μm crack opening threshold (all cracks less than this value are neglected). It illustrates that the crack is not straight, and the crack opening is not homogeneous which as observed experimentally. The validation of both continuous and discrete models is shown in Figure 11, which presents a comparison between the models and experimental data in terms of force-displacement curve and crack mouth opening displacement (CMOD)-displacement curve. The CMOD is calculated by taking the average relative displacement between two points at the middle of the specimen on both faces. Additionally, the figure compares the crack opening estimated by the [OUVFISS](#) procedure (by taking the maximum value for the green curve and the summation of the values for the purple curve, also averaged for both faces). Also, it shows the crack opening for DEAP simulation estimated by the relative displacement between two cracked particles in black. The figure demonstrates the good agreement between the experimental results and the two models in terms of relative displacement and that the DEAP program's estimate of crack opening is more precise compared to that of [OUVFISS](#) and it is much closer to the relative displacement estimations.

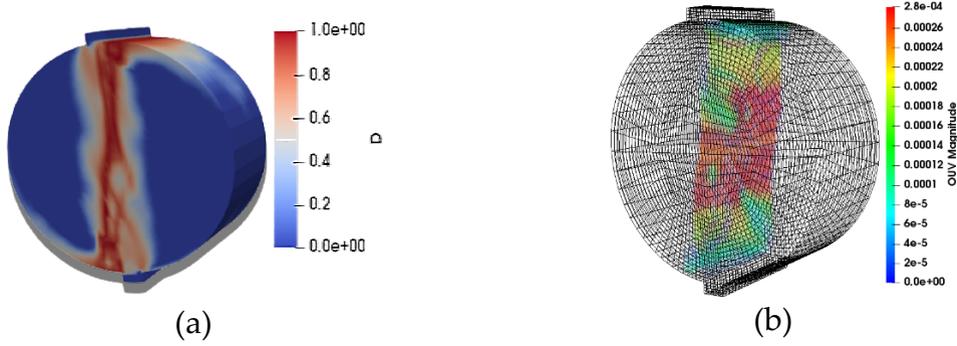


Figure 9. CAST3M simulation (a); Damage field (b) crack opening field

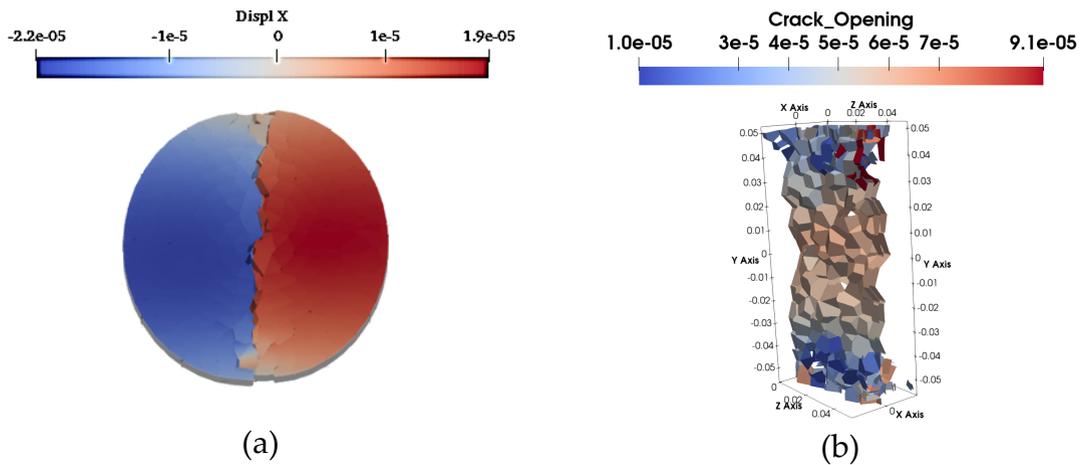


Figure 10. DEAP simulation (a); Displacement field (b) macro-crack with opening field

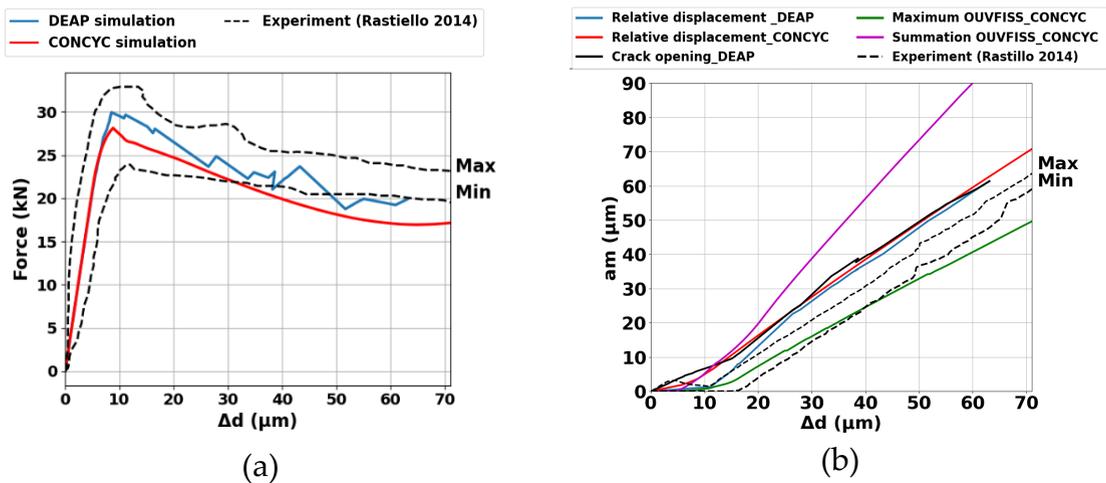


Figure 11. Validation of both models (a) Force vs change diameter (b) CMOD vs change diameter

Discussion and perspectives

In this study, we present the first step towards the development of a future work that aims to estimate air leakage rate during severe accident scenarios. The study focuses on comparing the performance of two models, DEAP and CONCYC, in simulating crack patterns in concrete under split loading conditions in concrete. The results of the simulation showed that both models were

able to accurately predict the global behavior and force-displacement curve of the concrete samples under split loading conditions. However, the DEAP model was found to be more precise in the description of crack patterns, specifically in terms of crack tortuosity and length, see Figure 10 (b), opening, see the blue curve in Figure 11 (b). Additionally, the results of this study showed that the DEAP model was more precise in estimating crack opening compared to [OUVFISS](#). This is because in DEAP simulation, the crack opening is calculated from the relative displacement of nodes while [OUVFISS](#) uses plastic opening. The initial abrupt change observed in the black curve is likely attributed to the fact that it depicts the crack opening estimated by DEAP in three dimensions, while the blue curve represents only the relative displacement along the x-axis.

Also, these comparisons do show that relative displacement is better than the built-in value of inelastic strains in the case of a continuous model.

Despite the DEAP model's precision, it is important to note that the [OUVFISS](#) procedure is well suited for simulating crack patterns in concrete at large scales because of its lower computational cost for comparable element size, see Table 1 .

Table 1 Computational costs comparison considering the same maximum displacement reached by DEAP (87 μm)

Model	Time (hours)	Average element size (mm)	CPU cores	CPU frequency (GHz)
CONCYC	2.20	2	12	2.1
DEAP	2.42	8	8	3.2

In addition, the result shows that there is a difference in the maximum displacement that the DEAP and CONCYC models were able to simulate. Specifically, it appears that the DEAP simulation stopped after around 60 μm , and no solution could be found beyond that point. In contrast, the CONCYC model was able to reach up to 325 μm until a solution could not be found. This difference in maximum displacement could be due to the existence of large quantity of cracks at the middle of the specimen which leads to make DEAP model reached a level of nonlinearity that it could not handle, and thus, the simulation failed. Also, the CONCYC model may have been able to handle this level of nonlinearity. A modification of the boundary condition for DEAP model could be done in order to go further in the simulation

Our conclusion is that DEAP model will be used for crack description as it provides a discontinuous description of crack patterns, giving us a more detailed understanding of the cracking process, which will be beneficial for future flow simulations. Meanwhile, the description of the crack is obtained for relatively low CMOD levels for DEAP simulation which is one of the observed disadvantages of the model. In contrast, the continuous presentation of the CONCYC model does not provide the same level of detail. Therefore, we conclude that DEAP is a more suitable choice for simulating crack patterns in concrete with possible future enhancements to reach higher levels of CMOD. Also, considering the mesh size with the size of the specimen, the transposition to the COBRA mock-up is expected to be significantly more computationally intensive. To tackle this challenge, a weak coupling between the two models will be developed.

This study has two main perspectives: the development of a MATLAB tool to extract crack geometry from DEAP simulations and the integration of DEAP and CONCYC models in large-scale

simulations. The MATLAB tool is currently under development and testing, it will enable the extraction of detailed crack geometry information from DEAP simulations, which is not currently possible with existing tools. The second objective is to take advantage of the strengths of both models in a large-scale simulation. The CONCYC model is well suited for simulating the global behavior of concrete structures, while the DEAP model is particularly good at simulating detailed crack patterns. By coupling the two models through a weak coupling approach, the simulation time can be reduced while still obtaining a detailed description of crack patterns. This is especially relevant for the COBRA project, which aims to simulate concrete behavior under severe accident scenarios.

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