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Numerical modelling of the quasi-brittle behavior of materials by considering microcracks effect

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1 INTRODUCTION

In the steelmaking industry, the inner lining of ladles is made of refractory ceramics, which are quasi-brittle materials constantly subjected to thermal shocks, due to filling and emptying of melted iron. The thermal shock resistance of these materials depends on their fracture toughness, which can be experimentally measured using the brittleness number, determined through the Wedge Splitting Test (WST).

Experimentally, it is observed that pre-existing microcracks have a significant impact on the mechanical behavior of quasi-brittle materials. The goal of this study is to investigate the sensitivity of the brittleness of the material with respect to pre-existing microcracks using numerical modelling.

The numerical method retained for this study is the Distinct Element Method (DEM), which has the ability to circumvent the limitations of more conventional continuum approaches in capturing microstructural effects required to simulate fracture propagation. Using DEM to model fracture mechanisms in a continuum media is a new approach in the ceramics community, still under active development (André 2019). Here, the general purpose DEM software *PFC3D* (Itasca 2018) is used. A pseudo-continuum media is modelled using the Flat-Joint contact model (Potyondy 2012). The local bond tensile strength is used as a local fracture criteria parameter. To control brittleness, a new approach based on a random Weibull distribution of this local criteria is proposed. The impact of this randomization procedure on the apparent brittleness of the material is assessed. First, Cyclic Direct Tensile Tests are performed on different virtual samples. Then, the numerical samples are subjected to WST, which is widely use in materials science communities to characterize fracture behavior of materials determine their brittleness number.

2 DESIGN AND ANALYSIS

2.1 *Numerical model of Direct Tensile Test*

The contact model used for this study is the Flat Joint Model (FJM), initially proposed by Potyondy (Potyondy 2012 & 2013). A cubic numerical sample of 10×10×10 cm was constructed and subjected to a direct tensile load until the tensile strength of the sample is reached and macroscopic failure occurs.

Table 1 shows the calibrated values of the local parameters and the corresponding material macro-properties of the sample. Stresses and strains are monitored during the simulation and used to calculate the Young's modulus and Poisson's ratio of the sample.

At this stage, the local fracture parameter, i.e., the local bond tensile strength, has a uniform value of 10 MPa. Subsequently, a cyclic test on this sample is simulated to assess the potential non-linear behavior of the modelled refractory. The sample was subjected to seven cycles of loading. However, the stress-strain curve of this simulation did not exhibit significant non-linear behavior. Hence, this perfectly brittle behavior does not correspond to a real behavior of refractories, which have non-linear behavior. This outcome advocates for the necessity to revise the model and introduce new assumptions able to capture the non-linear behavior of the material.

Table 1. Local parameters input values and the apparent values for the DEM models of this study.

Material properties	Value	Unit
Young's modulus	27.5	GPa
Poisson ratio	0.125	(-)
Tensile strength	10.5	MPa
Micro-mechanical and local parameters	Value	Unit
Effective modulus of bond (*E**)	*20*	GPa
Stiffness ratio of contact (*K**)	*4*	(-)
Tensile strength of contact (t)	*10*	MPa
Cohesion of bond (c)	*25*	MPa
Friction angle of bond (ϕ)	*0*	Degree

2.2 *Weibull Distribution and randomization process*

Experimentally, it was observed that maximum tensile strengths of samples of materials with defects are statistically following a non-linear curve. This curve can be fitted to a Weibull distribution.

In 1939 Waloddi Weibull introduced a new statistical distribution function (Weibull 1939) where the probability of failure of the material under a tensile load ($Pf(\sigma)$) is given as (Lei 1998):

$$P_f(\sigma) = 1 - \exp\left[-\left(\frac{\sigma}{\sigma_{u_0}}\right)^{m_0}\right] \tag{1}$$

Where σ is the tensile stress (MPa), m_0 is the Weibull modulus and σ_{u0} is a scaling parameter.

In the remainder of this study, the local bond tensile strength is randomized following a Weibull probability distribution, and the emergent non-linear behavior of the material at the macro-scale is assessed in the following sections.

3 RESULTS AND DISCUSSION

3.1 *Non-linear behavior and cyclic loading*

Figure 1 shows the stress-strain diagrams obtained under cyclic tension loading tests for:

a) A sample with the randomized values for the average local tensile strength of the bonds of 10 MPa, following a Weibull distribution (with a modulus $m_0 = 3$). The specimen was subjected to six cycles of tensile loadings.
b) A real cyclic loading of a quasi-brittle refractory.

During each cycle of tensile loading, the number of microcracks increase in the numerical model, which leads to an irreversible decrease of the apparent rigidity, which is related to the Young's modulus. The number of cracks is also shown in the diagram.

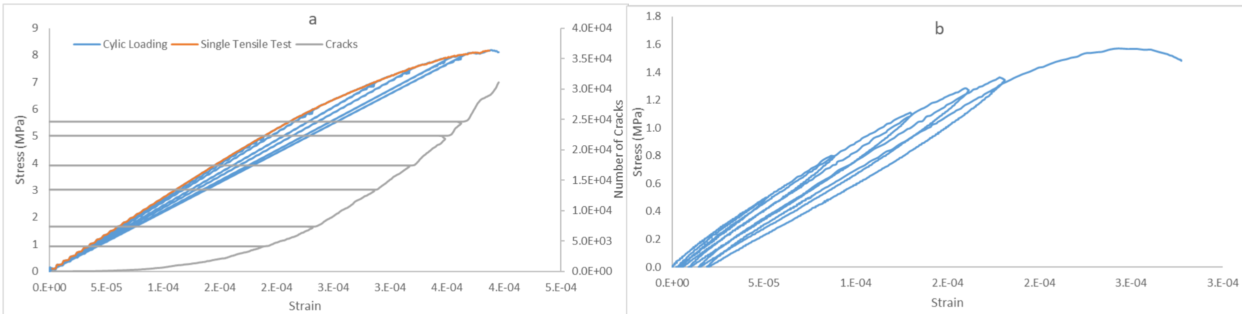

Figure 1. Stress-strain curves for cyclic tensile loading: (a), a randomized Weibull distributed sample for the local tensile strength, its cyclic tensile loading and its direct tensile test (the pushover). (b), A cyclic tensile loading for a real refractory ceramic (Kaczmarek 2019).

Unfortunately, there are no acoustic emission results available for sample b. Nevertheless, in the simulation, the evolution of the number of cracks is qualitatively consistent with typical acoustic emission responses of refractories subjected to cyclic loads.

Overall, the simulation result is showing an apparent plastic behavior on the stress-strain diagram, which is qualitatively following the non-linear behavior of a real typical refractories (sample b). As expected, the introduction of a Weibull distribution of the local tensile strength promotes diffuse damage during each cycle, and results in a non-linear behavior of the material at the macro-scale.

3.2 *Case Study: Wedge Splitting Test*

3.2.1 *Description of the test*

The principle of the WST is to open a notch by a wedge, in a displacement driven experiment, to produce a stable fracture propagation. Recent developments, in combination with Digital Image Correlation (DIC), enable to monitor crack branching (Dupré 2018) during the WST. In fact, in this test, the pre-existing microcracks and crack branching play a key role in evaluating the fracture energy of the material.

Numerically, a cubic sample of 10×10×10 cm with a pre-fabricated notch is constructed. Two rigid walls are used to push the inner sides of the notch outwards and produce a mode I fracture. The simulation is displacement driven, similar to the experiment.

Two virtual samples are constructed: one with a uniform value of 10 MPa for the local tensile strength and the other one using a Weibull distribution ($m_0 = 3$) of this parameter (See section 2.2). Figure 2 shows these two samples at the end of the simulations.

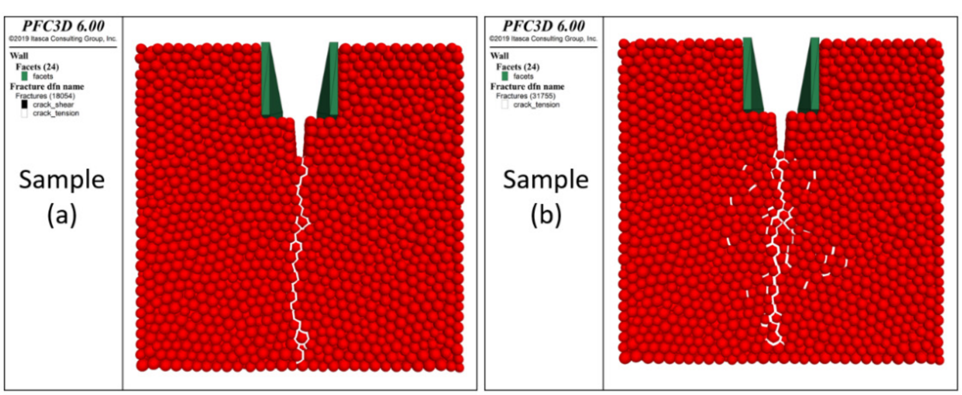

Figure 2. Comparison of the crack paths and crack branching in wedge splitting test for two samples: sample (a), uniform local tensile strength, sample (b) with a Weibull distribution of local tensile strength.

Sample (a) was broken with a single fracture, without any crack branching, which corresponds to the behavior of a highly brittle material. Sample (b) exhibits crack branching, which indicates a quasi-brittle behavior. This result confirms the conclusion of the previous section. Here, the material is dissipating more energy through the initiation of microcracks and crack branching, which results in a higher fracture energy for this sample.

3.2.2 *Brittleness Number*

A quantitative verification is considered for the WST results. For this purpose, the brittleness number is defined as: (Harmuth 1997):

$$B = \frac{f_t^2 . l}{G_f . E} \tag{2}$$

Where *ft, l, Gf, E* are the tensile strength, sample length, specific fracture energy and Young's modulus. The brittleness number is also defined as:

$$B \propto \frac{energy\ stored\ elastically\ at\ crack\ initiation}{fracture\ energy\ for\ total\ fracture} = \frac{W_{Elastic}}{W_{Fracture}} = \frac{f_t^2 . l}{2G_f . E}$$

Hence, to calculate the brittleness number in this numerical study, the force-displacement diagrams are plotted (Fig. 3). Then, by integrating the area under the force-displacement plots and calculating the elastic and fracture works, the brittleness number are calculated using Equation 2. In addition, figure 3 is showing the evolution of the number of cracks during the simulations. As expected, a higher number of cracks and earlier initiation of cracks occurred in the sample with the randomized values for the local tensile strength.

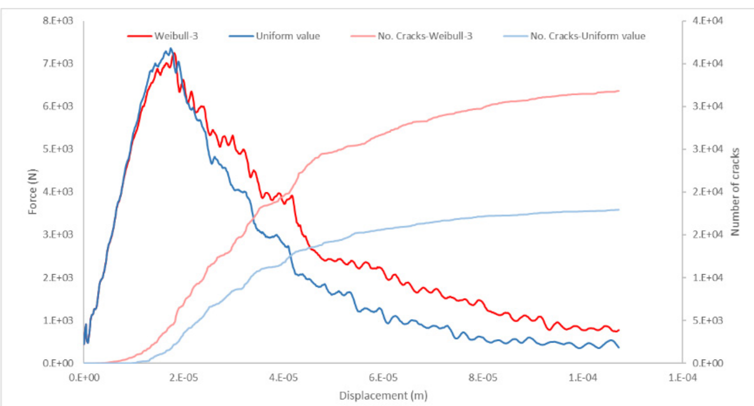

Figure 3. Comparison of the force displacement diagrams and number of microcracks for wedge splitting test for two samples.

The calculated brittleness number for the Weibull distributed sample is 0.38. Whereas, for the sample with a uniform value of the local tensile strength the brittleness number is 0.55. These results show that using Weibull distributions for local tensile strength influences the brittleness of the sample. Moreover, by using Weibull distributions, the post-peak area in the force-displacement is increasing, which is correlated to higher fracture energy. As a result, the brittleness number of the material is decreasing.

In addition, regarding the post-peak behavior and the different brittleness number, peaks remain approximately constant (less than 2% decrease). This observation may facilitate the calibration process of the brittleness of the material against experimental results. However, due to the mechanical and numerical modelling complexity of the wedge splitting test, this assertion requires further investigations.

4 CONCLUSIONS

Random local strength following the Weibull distributions in DEM models can be used to reproduce the quasi-brittle behavior of refractory ceramics. It can also be used to calibrate fracture energy and the brittleness number of the material.

This procedure may be used to promote a new numerical approach, helping to design and simulate optimal microstructures, accounting for pre-existing cracks, which reproduce at the macro-scale the non-linear behavior of the materials under cyclic loads.

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