

MIXED-MODE HIGHER-ORDER TERMS COEFFICIENTS ESTIMATED USING THE OVER-DETERMINISTIC METHOD

L. Šestáková^{*}

Abstract: The so-called 'over-deterministic' method (ODM) is applied on a mixed-mode configuration in order to determine higher-order terms coefficients of the Williams expansion approximating the stress and displacement fields in a cracked body. Results obtained agree very well to data found in literature (calculated by means of hybrid crack elements and boundary collocation method) and therefore further convergence studies are made in order to find some restrictions and recommendations corresponding to use of the ODM. Note, that more than five terms of the Williams expansions are considered and investigated in this contribution.

Keywords: Crack, Williams expansion, higher-order terms coefficients, FE analysis, overdeterministic method.

1. Introduction

It has been shown in recent years that conventional linear elastic fracture mechanics using a single controlling parameter, *i.e.* the stress intensity factor, for assessment of the initiaiton and propagation of a crack is not suitable in the case of quasi-brittle materials (such as ceramics or concrete). Therefore, not only the first (singular) term of the Williams series approximation of the crack tip asymptotic field (represented through the stress intensity factor), but also the other (higher-order) terms of the asymptotic field should be taken into account. It has been documented that the higher-order terms are of great relevance because they can predict the constraint of crack tip fields (Chao & Zhang, 1997; Berto & Lazzarin, 2010) and interpret the size/geometry/boundary effect, which both correspond to the extent of the zone around the crack tip with the nonlinear material behaviour, that is (in size) comparable to the typical structural dimensions (Karihaloo, 1999; Karihaloo et al., 2003; Veselý & Frantík, 2010).

The use of numerical techniques (such as finite element method) for higher-order terms determination is unavoidable for more complicated crack problems. The coefficients of the third and higher-order terms of the crack tip asymptotic field are very difficult to obtain. So far, there have been very few FE methods with the ability of calculating the coefficients of the higher-order terms, *e.g.* hybrid crack element method (HCE), boundary collocation method (BCM), etc. (Karihaloo & Xiao, 2001; Tong et al., 1997; Su & Fok, 2007; Xiao et al., 2004). However, all of these methods require special elements or complicated FE formulations. In this paper, the over-deterministic approach (ODM) based on the formulation of linear least-squares is introduced and tested on calculations of mixed-mode higher-order terms coefficients in Williams expansion (Williams, 1957). The main advantage of this method is that conventional finite elements (FE) can be used.

2. Problem description

Because only mode I configurations (three-point bend single edge notched beam and wedge splitting test) have been modelled in autor's previous work (Šestáková, 2011), a mixed-mode cracked specimen configuration has been chosen for testing of the ODM in this paper, see Fig. 1. Higher-order terms have been estimated on a plate with an angled edge-crack under uniaxial tension (AECT), whereas the crack angle was chosen as $\beta = 30^\circ$, see Fig. 1 and (Ayatollahi & Nejati, 2010) for detailed geometry.

^{*} Ing. Lucie Šestáková, Ph.D.: Institute of Structural Mechanics, Faculty of Civil Engineering, Brno University of Technology; Veveří 331/95; 60200, Brno; CZ, e-mail: sestakova.l@fce.vutbr.cz



Fig 1: *A plate with an angled edge-crack under uniaxial tension,* $\beta = 30^{\circ}$ *.*

Results determined by means of the ODM (using displacement fields obtained from conventional FE analysis) have been compared to data found in literature. Moreover, more than five first higherorder terms have been investigated and a study on the displacement field influence on the data convergence has been carried out.

2.1. Displacement field around the crack tip

Williams (1957) derived that the linear elastic stress field in a cracked plate subjected to an arbitrary in-plane load can be expressed in the so-called Williams series expansion. Because the ODM is based on the numerically calculated displacements field around the crack tip (due to its better accuracy in comparison to the stress field), it is necessary to introduce the relations for displacements u and v:

$$u = \sum_{n=0}^{\infty} \frac{r^{n/2}}{2\mu} a_n \left[\left(\kappa + \frac{n}{2} + (-1)^n \right) \cos \frac{n}{2} \theta - \frac{n}{2} \cos \left(\frac{n}{2} - 2 \right) \theta \right] + \sum_{n=0}^{\infty} \frac{r^{n/2}}{2\mu} b_n \left[\left(-\kappa - \frac{n}{2} + (-1)^n \right) \sin \frac{n}{2} \theta + \frac{n}{2} \sin \left(\frac{n}{2} - 2 \right) \theta \right]$$
(1)
$$v = \sum_{n=0}^{\infty} \frac{r^{n/2}}{2\mu} a_n \left[\left(\kappa - \frac{n}{2} - (-1)^n \right) \sin \frac{n}{2} \theta + \frac{n}{2} \sin \left(\frac{n}{2} - 2 \right) \theta \right] + \sum_{n=0}^{\infty} \frac{r^{n/2}}{2\mu} b_n \left[\left(\kappa - \frac{n}{2} + (-1)^n \right) \cos \frac{n}{2} \theta + \frac{n}{2} \cos \left(\frac{n}{2} - 2 \right) \theta \right]$$
(2)

In Eq. (1) and (2), *r* and θ correspond to the polar coordinates centred at the crack tip (considering the crack with traction-free faces lying on the negative *x*-axis), μ is the shear modulus ($\mu = E/2(1 + \nu)$) and $\kappa = (3 - \nu)/(1 + \nu)$ for plane stress or $\kappa = 3 - 4\nu$ for plane strain; *E* and *v* are Young's modulus and Poisson's ratio. First two terms coefficients in Eq. (1) and (2) are related to the well-known mode I stress intensity factor $K_{\rm I}$ ($a_1 = K_{\rm I}/\sqrt{2\pi}$) and to the in-plane *T*-stress ($a_2 = T/4$), respectively. Third and higher-order terms were in the past rather ignored and are not connected to any conventional fracture parameters.

2.2. Principle of the over-deterministic method (ODM)

It has been mentioned that there exist several methods for determination of the higher-order terms. The so-called over-deterministic method has been chosen for the analysis presented in this work. This method has a really big advantage – there is no need to use complicated crack elements, which ensures only minimal requirements on the FE software. The ODM is well explained for example in (Ayatollahi & Nejati, 2010) and for the sake of brevity only the basic strategy is described further.

Šestáková L.

_____ 1303

The ODM is based on the knowledge of the displacements field near the crack tip, see Eqs. (1) and (2). Important inputs for the method are therefore nodes displacements u and v obtained from numerical calculation for the particular geometry. Higher-order terms coefficients a_n and b_n are then calculated from a system of 2k equations, where k is the number of nodes selected around the crack tip. The number of higher-order terms can be chosen arbitrarily, but there are some restrictions: in order to obtain an over-determined set of equations, a relation between the number of nodes k and the number of the higher-order terms coefficients calculated should be satisfied:

$$2k > N + M + 2 \quad , \tag{3}$$

where N corresponds to the number of mode I terms, a_n , of the Williams series expansion and M to the number of mode II terms, b_n (see Eqs. (1) and (2)).

There are also other recommendations introduced in (Ayatollahi & Nejati, 2010) connected to the number of nodes selected for the calculations or their distance from the crack tip, etc.; convergence criteria are discussed in the referred paper as well. Some suggestions published in (Ayatollahi & Nejati, 2010) are taken into consideration during this study and further investigations in this field are made and discussed.

2.3. Numerical model

In order to obtain the displacement field near the crack tip, a numerical model corresponding to the geometric and loading configuration introduced in Fig. 1 was created. The dimensions of the specimens were taken from (Ayatollahi & Nejati, 2010): W = 1, h = 1, a = 0.6, $\beta = 30^{\circ}$ and the thickness was assumed to be unity and the units were self-consistent (therefore no units are presented). 8-node isoparametric elements (PLANE82) with plane stress conditions were used to model the cracked specimen. An FE mesh used for the whole analysis can be seen in Fig. 2, including corresponding boundary and loading conditions ($\sigma = 1$).



Fig. 2: FE mesh of the plate with an angled edge-crack under uniaxial tension (AECT) used for the analysis; displacements of the highlighted nodes were used for application of the ODM.

The crack singularity was modelled through the first row of elements that is made of the so-called crack elements with shifted mid-side nodes. Because the coefficients of the Williams expansion do not depend on material properties, arbitrary values can be considered for Young's modulus and Poisson's ratio; E = 1 and v = 0.25 in the study presented.

In the first step of the analysis, displacements u, v of the fifth ring nodes around the crack tip, see Fig. 2a, were used for determination of the higher-order terms coefficients $a_1...a_{10}$ and $b_1...b_{10}$ by means of the ODM. Then the study was extended to determination of the coefficients a_n and b_n up to order N = M = 20, and therefore more nodes had to be used for evaluation, see Fig. 2b.

3. Results and discussion

An elementary goal of this work was to validate the ODM procedure on a mixed-mode configuration in order to obtain a reliable tool for further analysis of the stress field in quasi-brittle materials. Therefore, a plate with an angled edge-crack under uniaxial tension (AECT) has been investigated and higher-order terms coefficients estimated from the displacement field of the fifth ring nodes, see Fig. 2a. Data comparison can be found in Tab. 1; calculations were made under consideration of N = M = 14. Note that only first five terms are mostly available in literature. It can be seen in Tab. 1 that the coefficients calculated by means of the ODM correspond very well with the data published in the literature.

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	HCE	BCM	ODM			HCE	BCM	ODM
a ₁	1.3867	1.3918	1.3938		b ₁	-0.3762	-0.3777	-0.3784
a ₂	0.1463	0.1485	0.1493		b ₂			-1.6653
a ₃	-1.2416	-1.2681	-1.2724		b ₃	-0.2141	-0.2213	-0.2210
a_4	0.2400	0.2468	0.2472		b ₄	-0.1954	-0.1906	-0.1928
a ₅	-0.5226	-0.5422	-0.5433		b ₅	0.1888	0.1792	0.1807

Tab. 1: Higher-order terms coefficients determined by means of the ODM (3. column) in comparison to data published in literature obtained by means of: HCE (1. column), see (Xiao et al., 2004); and BCM (2. column), see (Xiao et al., 2004)

It has been shown that the higher-order terms up to fifth order fit to data published in literature and thus, more detailed analyses could be done. For the basic analysis the displacement field of 31 nodes of the fifth ring around the crack tip, see Fig. 2a, were used for investigation of higher-order terms convergence with increasing number of the Williams series expansion terms N and M. The dependences studied are introduced as 3D plots in Fig. 3 for the a_3 -term and b_2 -term.



Fig. 3: Higher-order terms a_3 and b_2 convergence in dependence on the number of Williams expansion coefficients N, M considered during calculations.

It can be seen in Fig. 3a that for mode I higher-order terms convergence is obviously more important the number of corresponding mode I terms N whereas the number of mode II terms M is rather irrelevant and vice versa for mode II higher-order terms b_n , see Fig. 3b. A detailed view on the dependences in Fig. 3 brings even harder conclusion, namely that there is no influence of the number

1304

of mode I terms N on the b_n -values and similarly M is not important for a_n -values, see Fig. 4a. Thus, it seems that as a consequence, only 2D plots can be considered for a_n and b_n convergence analysis. However, it has been found out that it is not so easy. This independence was observed only if the displacements data set was perfectly symmetrical. If only one node displacements were left out from the analysis, a non-constant dependence on the both values (N, M) developed, see Fig. 4b.



Fig. 4: Higher-order terms coefficients a_n dependence on the number of Williams expansion mode II coefficients considered during calculations; a) perfectly symmetrical set of the displacements field; b) non-symmetrical set of the displacements field (one node missing).

Fig. 4 shows that a non-symmetrical displacement field around the crack tip used for evaluation of higher-order terms causes a purposeless dependence that can be easily avoided. Therefore, it should be recommended to use a symmetrical mesh around the crack tip in order to eliminate this kind of dependence.

When the previous conclusion is known, the two-dimensional dependences of the higher-order terms $(a_n \text{ and } b_n)$ on the corresponding number of coefficients considered during calculations (*N* for a_n and *M* for b_n) can be studied instead of the more complicated 3D plots. For the sake of better comparison and data manipulation, a dependence of the normalized higher-order terms coefficients $(a_{n,norm} = a_n/a_{n,N=14} \text{ and } b_{n,norm} = b_n/b_{n,M=14})$ on the number of coefficients was investigated, see Fig. 5.



Fig. 5: Normalized higher-order terms coefficients convergence in dependence on the number of Williams expansion coefficients considered during calculations; a) mode I terms $a_{1,norm} - a_{5,norm}$; b) mode II terms $b_{6,norm}$, $b_{8,norm}$, $b_{12,norm}$, $b_{13,norm}$.

Fig. 5a shows that the coefficients a_n up to fifth order converge relatively fast; N = M = 11 seems to be enough (the same conclusion can be derived in the case of b_n coefficients). The dependences presented show that it holds, the higher *n*, the higher number of higher-order terms has to be considered in order to obtain reliable a_n and b_n values. It has been observed that it is possible to determine relatively accurately 12 higher-order terms coefficients under consideration of k = 31, see Fig. 5b. Then the uncertainty increases.

Further study was made on the same numerical model, the only difference was the number of nodes used for displacement field evaluation. The main effort was to find out if it is possible to calculate the Williams expansion term a_{14} and higher ones, which was not possible (with sufficient accuracy) with the data set of 31 nodes. Therefore, additional set of nodes was used with k = 62, see Fig. 2b. Several results are presented in Fig. 6.



Fig. 6: Higher-order terms coefficients convergence in dependence on the number of Williams expansion coefficients considered during calculations in the case of 62 nodes investigated around the crack tip; note that only the x-axis scale differs.

As it can be seen in Fig. 6a, the higher-order terms $a_{11} - a_{15}$ seem to converge with number of terms N = 22 (similar dependences exist for $b_{11} - b_{15}$ as well), but a more complex view on the whole curve in Fig. 6b provides an ambiguous dependence. The curve really looks like it converges between N = 20 and N = 30 but then it exhibits nearly random behaviour again. Thus, it is not sure if the a_n (and b_n) values are correct and more studies should be done in this direction.

4. Conclusion

A numerical study has been carried out in order to test and validate the so-called over-deterministic method suggested for determination of higher-order terms coefficients in Williams expansion describing the stress field near a crack tip. A very good agreement has been found between the mixed-mode coefficients calculated and data published in literature for a plate with an angled edge-crack under uniaxial tension. On the basis of a convergence study performed, a recommendation on a symmetrical mesh around the crack tip (and symmetrical displacements field, respectively) can be expressed in order to avoid the general 3-dimensional dependence of higher-order terms on the number of terms considered during calculations N, M. Further, it has been observed that only first several terms (let's say up to n = 12) converge clearly with the increasing number of terms considered during calculations; the higher ones are not sure and thus, additional studies should be done in this direction because these terms can be important for better understanding of fracture in quasi-brittle materials as well.

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Šestáková L.

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