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Calibration of Damage Parameters for Y5 and G91 Steels in Use of Genetic Algorithm

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1 ABSTRACT

Determination of fracture toughness is prerequisite to perform elastic-plastic fracture mechanics assessment, for instance, leak-before-break analyses of nuclear piping systems and integrity evaluation of low upper-shelf reactor vessels. However, sometimes, there are lacks of fracture toughness data especially for old vintage nuclear power plants and it is not easy to prepare standard specimens from archival materials or installed components. In these cases, damage mechanics is applicable as one of alternative approaches because several efficient models have been suggested to simulate ductile fracture behaviour during the last couple of decades. In the present paper, a multi-island genetic algorithm is adopted into well-known Rousselier model to resolve complexity of previous calibration methods since reliability of damage parameters is significantly dependent on the calibration method - trial and error method, neural network method and so on combined with notched bar tests or small punch (SP) tests - and analyzer's experiences. SP test data of typical nuclear materials such as a low alloy steel (Y5) and a high Cr steel (G91) are used to determine damage parameters and, then, resulting values are applied to predict fracture toughness of the material. Load-displacement curves and fracture resistance curves are compared with those obtained from experiments, which show effectiveness of the proposed method.

2 INTRODUCTION

The scatter of measured fracture toughness data and transferability of them have been dealt as one of crucial problems to investigate material's fracture behaviour relating to various flaw shapes and loading conditions. In this context, to predict failure of cracked structure, a local approach adopting micro-mechanical damage models are suggested and widely used. Advantages of the local approach are that material parameters are independent of loading mode as well as geometry and applicable to assess structures fabricated from the same material. The first step of the local approach starts from calibration of material specific parameters by comparing test data and finite element method (FEM) results. However, based on previous researches, the calibration methods such as trial and error method, neural network method and so forth require analyzer's proficient experience along with significant numerical efforts. In this paper, a genetic algorithm to optimally solve problems by imitating the evolutionary process based on Darwin's natural selection is introduced, which is able to reduce numerical burdens for determining the material specific parameters. To achieve this goal, damage parameters of Rousselier model are calibrated using multi-island genetic algorithm, in which load-displacement (*P*-) curves obtained from small punch (SP) tests are compared with those from the corresponding numerical simulation. Typical nuclear materials, namely, a low alloy steel denoted by Y5 and a high Cr steel denoted by G91 are used for case studies. Employing the calibrated parameters into the damage model, elastic-plastic fracture resistance (*J–R*) curves are predicted by detailed FE analyses, of which validity is demonstrated by comparing them with the experimental *J–R* curves obtained from the standard compact tension (CT) specimens.

3 DAMAGE MODEL AND GENETIC ALGORITHM

3.1 Brief review of Rousselier model

In order to describe ductile fracture behaviour based on the local approach, well-known Rousselier model was adopted. Rousselier model defines the yield surface as a function of hydrostatic stresses:

$$\Phi = \frac{\sigma_{eq}}{\rho} + D \cdot \sigma_1 \cdot f \cdot \exp\left(\frac{\sigma_m}{\rho\sigma_1}\right) - R(\varepsilon_{eq}^{p}) = 0 \tag{1}$$

where, $_1$ and D are fitting constants, $_{eq}$ is the equivalent von Mises stress, $_h$ is the hydrostatic stress, is the material density, f is the void volume fraction and R($^p{}_{eq}$) represents the work-hardening law. In the above equation, $_1$, D and f_f (void volume fraction at fracture) are selected as design variables for optimization of Rousselier model.

3.2 Multi-island genetic algorithm

Aforementioned multi-island genetic algorithm (MIGA) is adopted for the present work among diverse of genetic algorithms. The remarkable characteristic of MIGA is that the population in one generation is divided into several sub-populations called as islands. To avoid converging partial optimized result, each sub-population maintains independency during the iteration. Before a new iteration, the exchange of individual information, called migration, is performed between sub-populations. Fig. 1 shows schematic illustration of MIGA.

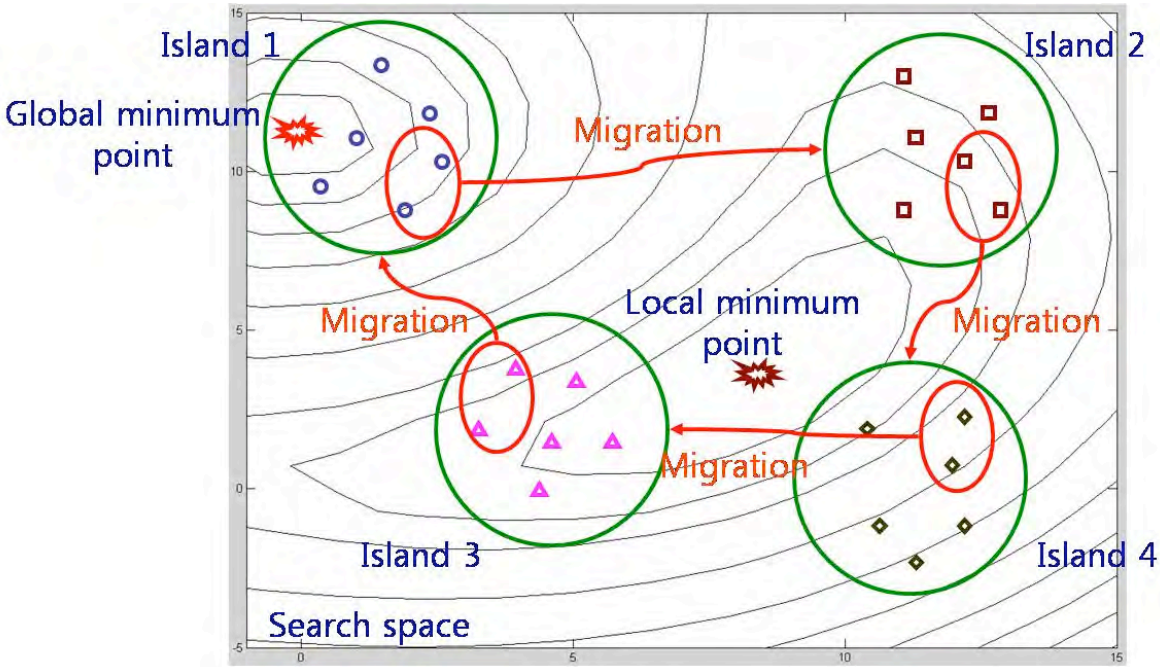


Figure 1. Schematic illustration of multi-island genetic algorithm

3.3 Optimized procedure for calibration of damage parameters

Fig. 2 illustrates the calibration procedure using MIGA, for which an objective function is set to minimize error sum between test and numerical data. The predescribed design variables ($_1$, D and f_f) of Rousselier model are extracted taking into account of upper and lower bounds based on the author's previous works. Table 1 represents optimization parameters such as number of island, number of generation, rate of migration, rate of cross over and etc. Also, Table 2 summarizes the objective function, design variables and their boundary conditions used in this work.

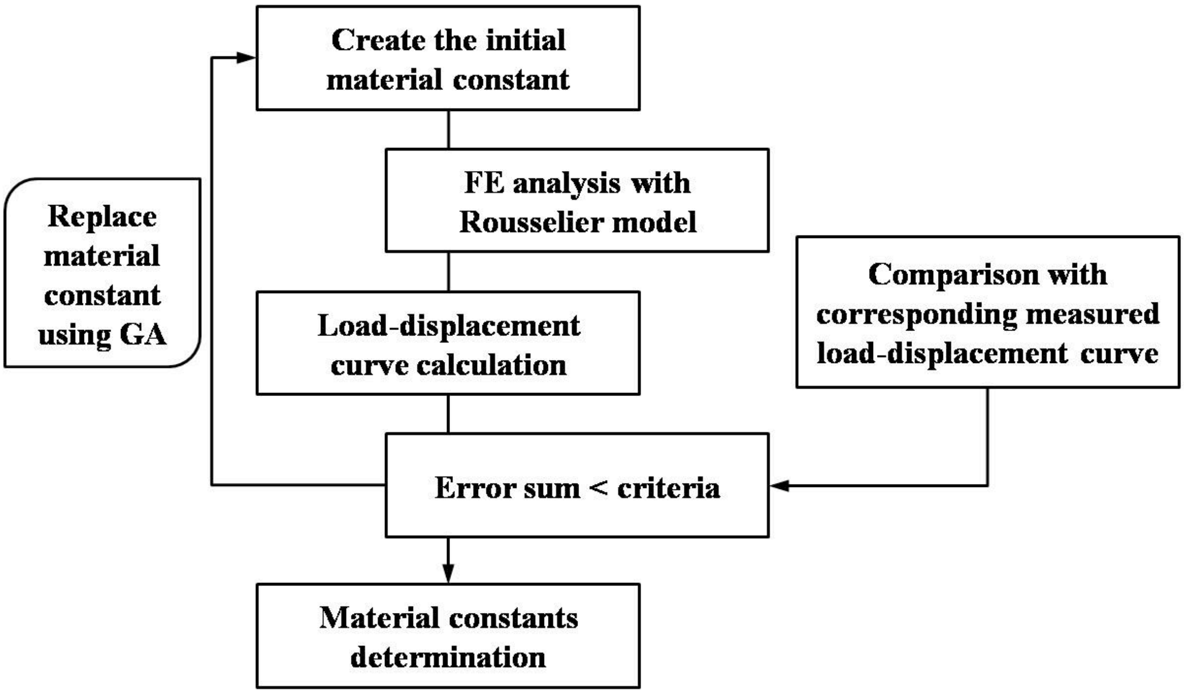


Figure 2. Calibration procedure using multi-island genetic algorithm

Table 1. Optimization parameters of multi-island genetic algorithm

Size of subpopulation	5	**Rate of Crossover**	1
No. of Island	5	**Rate of Mutation**	0.01
No. of Generations	10	**Rate of Migration**	0.5
Gene Size	32	**Interval Migration**	5

Table 2. Objective function and design variables

Objective Function	Minimize $\sum_{i=1}^{n}\left[f_i(f_f, f_0, D, \sigma_1) - y_i\right]^2$
Design Variables	f_f, f_0, D, $_1$
Boundary Condition	f_0=0.00007(Y5), 0.0003(G91) 0.01< f_f <0.5 1.0< D <5.0 400< $_1$ <1500

4 CALIBRATION OF DAMAGE PARAMETERS

4.1 Experimental raw data

In the author's previous works, small punch tests were performed to obtain load-displacement curves of the materials, Y5 and G91. Table 3 summarizes chemical compositions of Y5 and G91. Mechanical properties of the materials such as the values of yield strength ($_{YS}$) and ultimate tensile strength ($_{UTS}$) of Y5 are 400*MPa* and 596*MPa*, and the values of those of G91 are 480*MPa* and 687*MPa*, respectively. Fig. 3 depicts resulting experimental load-displacement curves. To calculate error sum between the SP test data and numerical data, polynomial equations of each material were developed as shown in Table 4.

Table 3. Chemical composition of Y5 and G91 (wt%)

Materials	C	Mn	P	S	Si	Ni	Cr	Mo	Cu	N	Al
Y5	0.210	1.360	0.007	0.002	0.240	0.920	0.210	0.490	0.030	-	0.005
G91	0.091	0.395	0.019	0.0003	0.314	0.093	8.916	0.915	0.093	0.035	0.026

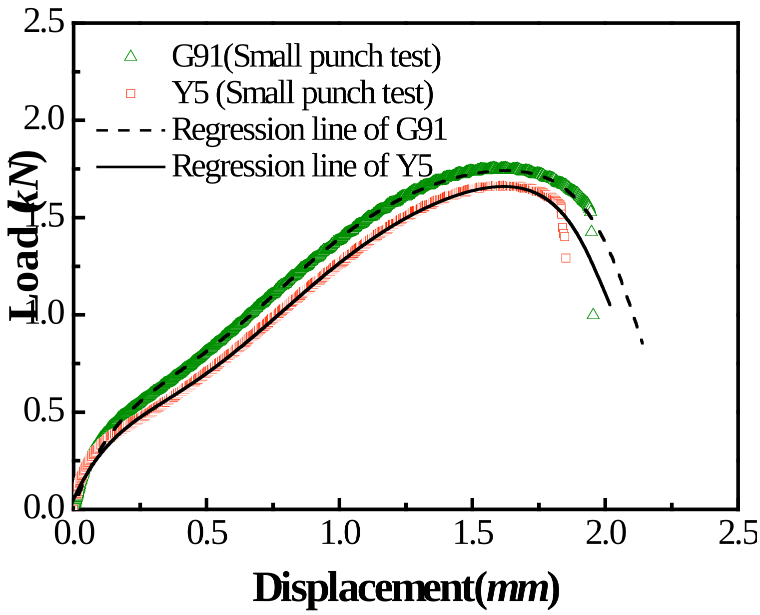


Figure 3. Experimental *P*- curves of SP specimens

Table 4. Polynomial equation of Y5 and G91 ($P=C_1\ ^6+C_2\ ^5+C_3\ ^4+C_4\ ^3+C_5\ ^2+C_6\ +C_7$)

Materials	C_1	C_2	C_3	C_4	C_5	C_6	C_7
Y5	-0.950	5.684	-13.327	14.927	-7. 954	2.801	0.088
G91	-0.914	5.778	-14.247	16.792	-9.653	3.587	0.057

4.2 FEA results based on SP simulation

FE analyses were implemented into ABAQUS/Standard combined with the user subroutine (UMAT) by using two-dimensional mesh of SP specimen generated from the author's previous work. Then, in order to determine damage parameters of Rousselier model, load-displacement curves obtained from the simulation were compared with those from the corresponding experiments.

4.3 Calibration results

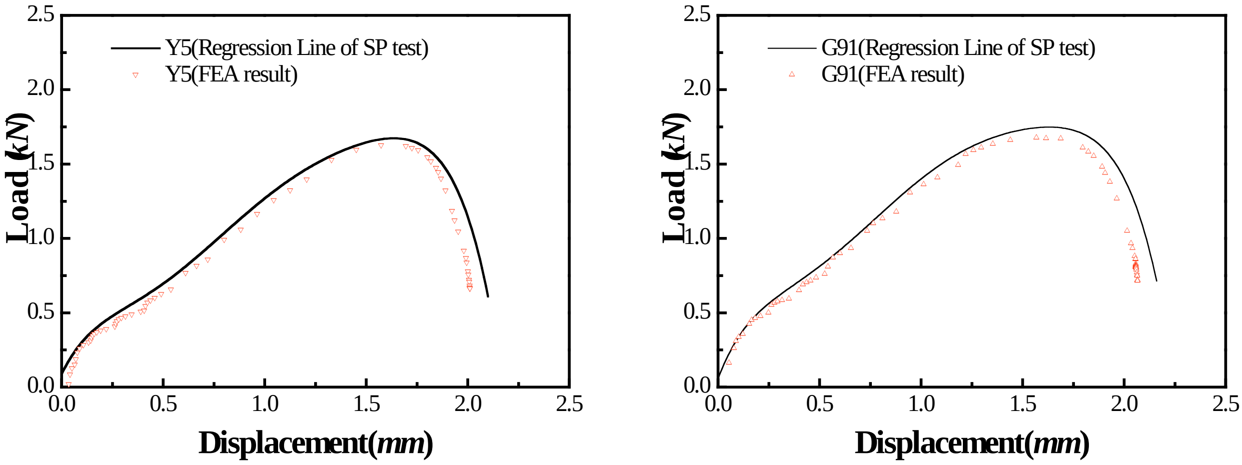
Franklin proposed a well-known formula to estimate the initial void volume fraction of particles (f_0) based on manganese and sulphur contents like the followed equation.

$$f_0 = f_v = 0.054\left(S\% - \frac{0.001}{Mn\%}. \right) \quad (2)$$

The f_0 value of Y5 was calculated as 0.00007 from Eq. (2) and used for prediction of *J-R* curve in the later section. On the other hand, the f_0 value of G91 calculated from the equation was too small. So, to simplify the complex calibration process, it was set to 0.0003 which was quoted from the author's previous research. Table 5 summarizes resulting values of the calibrated parameters and Fig. 4 depicts the estimated load-displacement curves of the SP specimens comparing with the corresponding experimental ones.

Table 5. Calibrated micro-mechanical parameters

Materials	$_1$	D	f_0	f_f
Y5	800	3.5	0.00007	0.45
G91	1220	3.0	0.00030	0.26



(a) Low alloy steel (Y5) (b) High Cr steel (G91)

Figure 4. Comparison of *P*- curves of SP specimens

5 VERIFICATION OF THE DAMAGE PARAMETERS

5.1 FE analyses of CT specimens

In order to verify the determined damage parameters, FE analyses employing two-dimensional model, were carried out to predict *J-R* curves of standard CT specimens for each material. Fig. 5 represents FE model of the specimen, which consists of 1,496 nodes and 1,378 elements (C3D8 in ABAQUS element library). With respect to the crack front mesh, as shown in the enlarged part of the figure, refined square elements just like those of the SP specimen were generated.

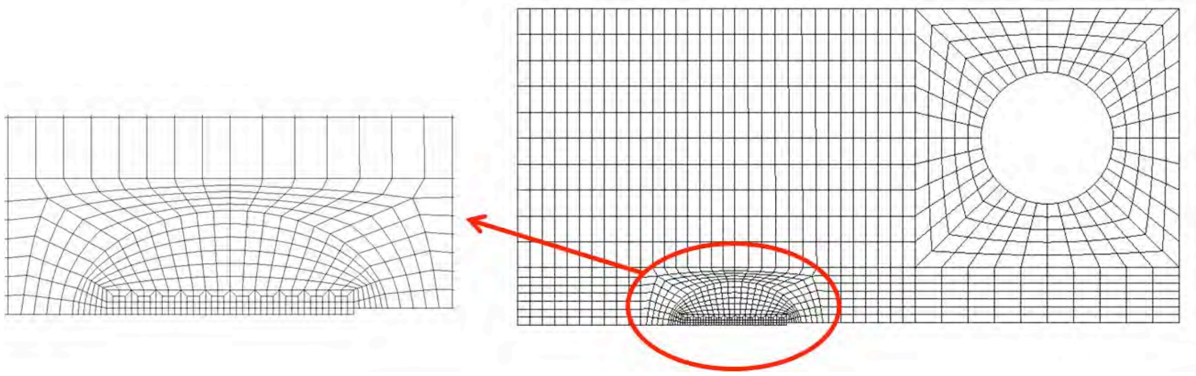
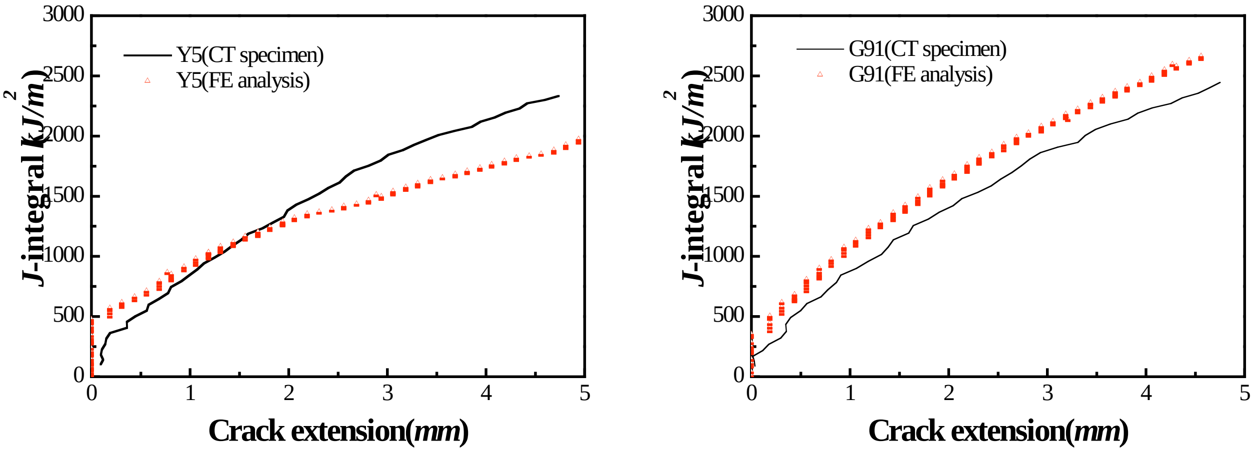


Figure 5. Two-dimensional FE model of CT specimen

5.2 FE analysis results

Fig. 6 shows *J-R* curves of CT specimens predicted by using Rousselier model compared with the corresponding experimental ones quoted from the author's previous paper. In case of Y5 material, maximal difference between estimated *J*-integral and corresponding experimental one was 25% and mean difference was 15%, approximately. In case of G91 material, maximal difference was 33% and mean difference was 21%, approximately. The discrepancy which may be caused by anisotropic feature of test data and so forth is somewhat larger than expected one. However, if taking into account different features between SP and CT tests, the estimated *J-R* curves seems reasonably good.



(a) Low alloy steel (Y5) (b) High Cr steel (G91)

Figure 6. Comparison of *J-R* curves of CT specimens

6 CONCLUSION

In the present paper, an optimized calibration procedure was introduced by employing multi-island genetic algorithm. The proposed method was applied to determine damage parameter of Rousselier model in use of small punch specimens for two types of typical nuclear materials – a low alloy steel and a high Cr steel. Then, FE analyses in conjunction with the damage model were carried out for standard CT specimens to demonstrate validity of the calibrated parameters and efficiency of the proposed method. Consequently, it was proven that the local approach by adopting the Rousselier model and MIGA algorithm is applicable to predict *J-R* curves when it is not easy to extract standard specimens from archival materials or installed components.

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