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Adaptation of OCA-P, a Probabilistic Fracture-Mechanics Code, to a Personal Computer

D. G. Ball R. D. Cheverton

Prepared for the U.S. Nuclear Regulatory Commission
Office of Nuclear Regulatory Research
Under Interagency Agreements DOE 40-551-75 and 40-552-75

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FOR THE UNITED STATES
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ADAPTATION OF OCA-P, A PROBABILISTIC FRACTURE-MECHANICS CODE, TO A PERSONAL COMPUTER

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MARTIN MARIETTA ENERGY SYSTEMS, INC.
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CONTENTS

FOREWORD

The work reported here was performed at Oak Ridge National Laboratory (ORNL) under the Heavy-Section Steel Technology (HSST) Program, C. E. Pugh, Program Manager. The program is sponsored by the Office of Nuclear Regulatory Research of the U.S. Nuclear Regulatory Commission (NRC). The technical monitor for the NRC is Milton Vagins.

This report is designated HSST Report 84. Prior reports in this series are listed below:

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ADAPTATION OF OCA-P, A PROBABILISTIC FRACTURE-MECHANICS CODE, TO A PERSONAL COMPUTER

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ABSTRACT

The OCA-P probabilistic fracture-mechanics code can now be executed on a personal computer with 512 kilobytes of memory, a math coprocessor, and a hard disk. A user's guide for the particular adaptation has been prepared, and additional importance sampling techniques for OCA-P have been developed that allow the sampling of only the tails of selected distributions. Features have also been added to OCA-P that permit RTNDT to be used as an "independent" variable in the calculation of $P(F|E)$.

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1. INTRODUCTION

OCA-P, which is a probabilistic fracture-mechanics code, was developed for the Nuclear Regulatory Commission (NRC) to help in the evaluation of pressurized water reactor (PWR) pressure-vessel integrity during pressurized thermal-shock (PTS) transients. The code was originally written for a main-frame computer, but because of the popularity of personal computers (PC), OCA-P has now been adapted to a PC. The adaptation requires 512 kilobytes of memory, a math coprocessor, and a hard disk. These requirements were met with an IBM PC-XT and PC-AT, using the IBM Professional 1.0 compiler.[1]

This report provides the necessary user's guide information for running OCA-P on a PC. In addition, it describes improvements that have been made in the importance-sampling techniques that are used in OCA-P and discusses further the use of RTNDT as an independent variable in the probabilistic analysis. The original version of OCA-P is described in Ref. 2, and typical applications are found in Refs. 3 and 4.

2. USER'S GUIDE

OCA-P is composed of two parts: a one-dimensional heat transfer code (1-R) and a probabilistic fracture-mechanics code (PFM). A description of the input and output associated with OCA-P is given in Ref. 2. It should be noted that the plotting options are not yet available in the PC version.

The file names used by the PC version are given in Table 2.1. Although the digital output to each unit is routed to a specific file by the code, this may be overridden by using the DOS "SET" command. For example, during a run of the 1-R code, unit-1 output in a file named CASE1.BIN is obtained by issuing the commands:

```
SET ONER01.BIN=CASE1.BIN
ONER.
```

To obtain unit-6 output on the console during a run of the PFM code, issue the commands:

```
SET PFM.LPT=CON
PFM.
```

Due to its size, the load module for the PFM portion of the code must be stored on a 1.2 megabyte floppy disk for transmittal, or, the source or object modules may be included on a 360 kilobyte floppy.

Table 2.1. OCA-P file information

FORTRAN unit	File name	File type	Description
1-R Code:			
55	ONER.DAT	Formatted	Control input
6	ONER.LPT	Formatted	Digital output
1	ONER01.BIN	Binary	Data for input to PFM
PFM Code:			
55	PFM.DAT	Formatted	Control input
56	KICKIA.DAT	Formatted	Override toughness curves
1	ONER01.BIN	Binary	Output from 1-R code
2	LI860945.BIN	Binary	2-D axial influence coefficients
7	LI8603D.BIN	Binary	3-D axial influence coefficients
8	CI860945.BIN	Binary	2-D circ. influence coefficients
6	PFM.LPT	Formatted	Detailed digital output
17	CCD.LPT	Formatted	Deterministic summary
29	PFMSUM.LPT	Formatted	Probabilistic summary
19	Scratch	Formatted	

Using the PROFORT linker, the PFM load module may be constructed from the object modules by the command:

```
LINK PFM1+PFM2,PFM,CON;.
```

After the input files are set up, the codes are run by typing ONER for the I-R code and PFM for the PFM code. In addition, it is necessary to include the statement FILES=15 in the CONFIG.SYS file.

Input control data for a sample problem is contained in files ONER.DAT and PFM.DAT, which will be on the transmitted floppy disk. The problem is the same as that given in Appendix A of Ref. 2 with the exception that only one weld is analyzed in PFM using 10,000 trials. The execution times for the sample problem are given in Table 2.2 for different machines.

The PC version of OCA-P has a timing routine which writes the date and time of the run on unit 6. Also, the elapsed time of the run is calculated and included at the end of the unit-6 output.

Table 2.2. Timing information on sample problem

Code	Computer	Execution time (minutes)	(PC time)/(3033 time)
I-R	PC	62.37	83.7
	PC-XT (hard disk)	60.97	81.8
	PC-AT	52.32	70.2
	IBM 3033	0.745	
PFM	PC-XT (hard disk)	18.98	61.8
	PC-AT	16.98	[illegible].3
	IBM 3033	0.307	

3. IMPROVEMENTS TO OCA-P

Since the time that the OCA-P report was issued, several additions have been made to the code. This section discusses the additions and indicates the necessary corresponding changes in the user's manual. (These latter changes are included in detail in Appendix A.)

3.1 Inclusion of Improved Importance Sampling Capability

As discussed in Ref. 2, the OCA-P probabilistic model is based on Monte Carlo techniques; that is, a large number of vessels is generated, and each vessel is then subjected to a deterministic FM analysis to determine whether the vessel will fail. Each vessel is defined by randomly selected values of several parameters that are judged to have significant uncertainties associated with them. The calculated conditional probability of vessel failure [P(F|E)] is simply the number of vessels that fail divided by the total number of vessels generated. Thus,

$$P(F|E) = \sum_j \hat{P}_j \, V_j N_j \int_0^w f(a)B(a)da \ , \qquad (3.1)$$

where

$P_j = \frac{N'_{fj}}{N'_{vj}}$,

N'_{fj} = number of vessels with a flaw in the jth region that fail,

N'_{vj} = number of vessels simulated with a flaw in the jth region,

V_j = volume (or area) of jth region,

N_j = flaws of all depths per unit volume (or surface area) of the jth region,

a = flaw depth,

f(a) = flaw-depth density function,

B(a) = probability of nondetection,

w = wall thickness.

The parameters N and f(a) pertain to vessel conditions prior to preservice inspection and repair, and B(a) is derived on the basis of repairing or otherwise disposing of all detected flaws.

For very small values of P(F|E), the values of N'_{vj} required to achieve reasonable accuracy become quite large. Under some circumstances, the value of N'_{vj} can be reduced by using importance sampling techniques. This can be done in some cases by eliminating flaw depths that do not contribute significantly to initiation and by sampling only the tails of other distribution functions. The portion of the distribution function not sampled is accounted for by multiplying the number of simulated vessels, N'_{vj}, by a correction factor. Equation (3.1) then becomes

$$P(F|E) = \sum_j \frac{\hat{P}_j}{\Pi F_{kj}} N_j A_j \int_0^w f(a)B(a)da , \qquad (3.2)$$

where

F_{kj} = correction factor for kth simulated parameter.

Va ues of F_k are a function of the points on the distribution curve at which sampling is started and stopped (truncation point). When importance sampling is used for the flaw-depth density function given in Ref. 2, and only the first flaw-depth increment is omitted,

$$F_k \text{ (flaw depth density)} = \frac{1}{\int_{\Delta a_1}^{w} f(a)B(a)da} = 3.24$$

Table 3.1 includes values of F_k for several different starting points on a normal distribution curve that is truncated at 3σ. As indicated, if the distribution is sampled above 1σ, F = 6; if it is sampled above 2σ, F = 46. If just two normal distributions are sampled, if they are sampled above 1.25σ, and if the first crack-depth increment can be omitted, ΠF_{kj} = 300, which represents a significant savings in computer costs for the same accuracy in $P(F|E)$. Of course, this type of importance sampling can only be used when the first crack-depth increment does not contribute much to $P(F|E)$ and when $P(F|E)$ is small enough

Table 3.1. Values of F_k for a normal distribution

Identifying No. (NDLRS or NRTRS)	Start of sampling (number of standard deviations above mean)	Fraction of distribution not simulated[a]	F_2, F_3
1	1.0	0.8422	6
2	1.25	0.8954	10
3	1.50	0.9343	15
4	1.75	0.9611	26
5	2.00	0.9784	46
6	2.25	0.9891	92
7	2.50	0.9951	204
8	2.75	0.9983	588

[a]Assuming truncation at $\pm 3\sigma$.

that only the tails of the distribution functions contribute significantly to P(F|E). (At the time of this writing, importance sampling is applied to the crack-depth density function and to the normal distribution for RTNDT and ΔRTNDT.)

3.2 The Use of RTNDT as an Independent Variable

In some cases it is convenient to use $RTNDT_s$ as an independent variable in the probabilistic FM analysis, where $RTNDT_s$ is the nil ductility reference temperature at the inner surface. Values of RTNDT at any radial position in the wall can be estimated using Eq. (11) in Ref. 2 and the relation

$$RTNDT = RTNDT_o + \Delta RTNDT \ ,$$

where $RTNDT_o$ is the initial value of RTNDT, and ΔRTNDT is the increase in RTNDT due to radiation. However, since $\Delta RTNDT = f(F_o, Cu, Ni)$ [where F_o is the fast-neutron fluence at the inner surface, and Cu and Ni are the concentrations of copper and nickel in the vessel material (wt %)], RTNDT is not actually an independent variable; that is, the actual independent variables are $RTNDT_o$, F_o, Cu, and Ni. Thus, an error is introduced when RTNDT is used as the independent variable. This error is discussed below and in greater detail in Ref. 5.

A distribution function for $\Delta RTNDT_s$ can be obtained by performing a Monte Carlo analysis with

$$\Delta RTNDT\ (°C) = f(Cu, Ni, F) \ ,$$

in which case F, Cu and Ni are simulated. However, as discussed in Ref. 5, the distribution is somewhat sensitive to the mean values of F_o, Cu and Ni. Furthermore, for a given value of RTNDT, different combinations of $RTNDT_o$ and ΔRTNDT will result in somewhat different values of P(F|E). The size of the error depends on details of the transient and can be as large as an order of magnitude.[5]

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APPENDIX A. UPDATES TO ORIGINAL REPORT

Appendix A includes the revised probabilistic control input to the OCA-P code. The revised control input replaces pages 48-50 of Ref. 2. Also, a revised summary sheet for the probabilistic analysis (page 81 of Ref. 2) is included. There is a charge in the calculated probability of vessel failure that reflects the existence of an error in the code related to use of SI units in the Monte Carlo part of the analysis.

Card Type 6.0 - Probabilistic Control Parameters

S/R Name	Variable	Default	Description
RDPTSS	NSIM	0	Maximum number of trials to be generated for each weld if IACCEL > 0, ≠ 2; for each flaw depth if IACCEL < 0 or = 2. A positive value indicates use of fluence and copper on Card Type 6.2, whereas a negative value indicates the the use of $\Delta RTNDT_s$ on Card Type 6.3.
	IACCEL	0	Controls use of importance sampling on crack depth. = 0 no importance sampling = 1: first-increment flaw does not initiate but is counted in number of trials, thus accelerating convergence. = 2: uniform sampling of crack depths (NSIM trials used for each crack depth) = 3: first and second-increment flaws do not initiate but are counted in number of trials thus accelerating convergence. < 0: only one crack depth is sampled; for instance, for IACCEL =-2 the second depth would be the only depth sampled (see Table 4.2 in Ref. 2).
	VOLWLD	1	Volume of weld 1 on Card Type 6.2, or 6.3, m^3.
	WELDN	1	Number of flaws/m^3.
	CONVPC	10	Maximum percent error in P(F|E) for each weld at a 95% confidence level.
	FLWSTR	551.7	Flow stress for plastic instability determination, MPa.
	USKIA	220	$(K_{Ia})_{max}$, MPa·$\sqrt{m}$.
	NPCRK	9	Number of increments to be used for initial crack depth (maximum of 15).
	AWINT	4.3	Size of first crack-depth increment, mm.
	CDLIM	57.2	Extreme dimension of deepest crack-depth increment, mm. A geometric progression of NPCRK increments is generated between 0 and CDLIM to model initial crack depths. K_I values are sampled at midpoint of each increment.

Card Type 6.1 - Probabilistic Distribution Parameters

S/R Name	Variable	Default	Description
RDPTSS	SDFDRT	13	ΔRTNDT standard deviation, °C.
	SDFKIC	0.15	K_{Ic} standard deviation (fraction of mean). If positive, use ORNL mean curve, Eq. (3) (Ref. 2); if negative, use NRC mean curve, Eq. (5) (Ref. 2).
	SDFKIA	0.1	K_{Ia} standard deviation (fraction of mean). If positive, use ORNL mean curve, Eq. (4) (Ref. 2); if negative, use NRC mean curve, Eq. (6) (Ref. 2).
	SDLDRT	3.0	ΔRTNDT-standard truncation point (number of standard deviations).
	SDLKIC	3.0	K_{Ic}-distribution truncation point (number of standard deviations).
	SDLKIA	3.0	K_{Ia}-distribution truncation point (number of standard deviations).
	CONKIC	1.43	K_{Ic}-equation multiplier.
	CONKIA	1.25	K_{Ia}-equation multiplier.
	NDLRS	0	Controls use of importance sampling on $\overline{\Delta RTNDT_s}$: = 0: no importance sampling. > 0: sample only the tail of the distribution where NDLRS determines the starting point (see Table 3.1). Applies to all welds in Card Type 6.3.
	NRTRS	0	Controls use of importance sampling on RTNDT: = 0: no importance sampling. > 0: sample only the tail of the distribution where NRTRS determines the starting point (see Table 3.1). Applies to all welds in Card Type 6.3.

Card Type 6.2 - Weld Characteristics

Only required if NSIM > 0 (defined on Card Type 6.0).

S/R Name	Variable	Default	Description
RDPTSS	NWELDS	1	Number of welds to be simulated, NWELDS $\leq$ 6.
	PFO(I)	†	Mean inside-surface fluence, neutrons/cm^2.
	PCU(I)	†	Mean copper content, %.
	PNI(I)	†	Mean nickel content, %.
	PRTNO(I)	None	Mean initial reference temperature, °C.
	SIGFO(I)	0.3	Fluence standard deviation, fraction of mean.
	SIGCU(I)	0.025	Copper standard deviation, %.
	SIGNI(I)	0.0	Nickel standard deviation, %.
	SIGRTO(I)	9	Initial reference temperature standard deviation, °C.
	VOLFAC(I)	1.0	Fraction to adjust $P(F\|E)_i$ for weld I based on the volume of the weld relative to weld 1. VOLFAC(1) = 1.0.

The READ list is: NWELDS, [PFO(I), PCU(I), PNI(I), PRTNO(I), SIGFO(I), SIGCU(I), SIGNI(I), SIGRTO(I), VOLFAC(I), I = 1, NWELDS].

---

†If NWELDS = 1, these parameters are obtained from Card Type 4.0, if not provided here.

Card Type 6.3 - Weld Characteristics

Only required if NSIM < 0 (defined on Card Type 6.0).

S/R Name	Variable	Default	Description
RDPTSS	NWELDS	1	Number of welds to be simulated, NWELDS $\leq$ 6.
	PFO(I)	None	$\overline{\Delta RTNDT}_s$
	PRTNO(I)	None	Mean initial reference, temperature, °C.
	SIGFO(I)	0.14	$\overline{\Delta RTNDT}_s$ standard deviation, fraction of mean.
	SIGRTO(I)	9	Initial reference temperature standard deviation, °C.
	SIGNI(I)	None	Associated fluence (optional).
	VOLFAC(I)	1.0	Fraction to adjust $P(F\|E)_i$; for weld i based on the volume of the weld relative to weld 1. VOLFAC(1) = 1.0.

The READ list is: NWELDS, [PFO(I), PRTNO(I), SIGFO(I), SIGRTO(I), SIGNI(I), VOLFAC(I), I = 1, NWELDS].

TYPICAL POSTULATED TRANSIENT H=5678   1. FLAWS/M**3   FO = 1.500D+19

	UNADJUSTED					ADJUSTED			
WELD	P(F/E)	95%CI	%ERR	P(INITIA)	N*V	P(F/E)	%ERR	NFAIL	NTRIALS
1	1.60D-02	7.64D-04	4.79	1.60D-02	1.000	1.60D-02		1632	60000
2	6.25D-03	3.05D-04	4.88	6.27D-03	0.500	3.13D-03		1597	150000
					VESSEL	1.91D-02	4.08		

DEPTHS FOR INITIAL INITIATION (MM)

	2.16	6.68	11.62	17.03	22.95	29.42	36.51	44.25	52.72
NUMBER	37	2031	762	300	84	16	7	2	0
PERCENT	1.1	62.7	23.5	9.3	2.6	0.5	0.2	0.1	0.0

WEIGHTED TIMES OF FAILURE(MINUTES)

	0.0	10.0	20.0	30.0	40.0	50.0	60.0	70.0	80.0	90.0	100.0
PERCENT	0.0	0.0	0.0	5.7	37.3	45.5	11.5	0.0	0.0	0.0	

INITIATION T-RTNDT(DEG.C)

	-55.6	-41.7	-27.8	-13.9	0.0	13.9	27.8	41.7	55.6	69.4	83.3	97.2	111.1
NUMBER	0	14	239	1096	1432	442	18	0	0	0	0	0	
PERCENT	0.0	0.4	7.4	33.8	44.2	13.6	0.6	0.0	0.0	0.0	0.0	0.0	

ARREST T-RTNDT(DEG.C)

	-27.8	-13.9	0.0	13.9	27.8	41.7	55.6	69.4	83.3	97.2	111.1	125.0	138.9
NUMBER	0	0	2	6	3	0	0	1	0	0	0	0	
PERCENT	0.0	0.0	16.7	50.0	25.0	0.0	0.0	8.3	0.0	0.0	0.0	0.0	

KIC HISTOGRAM

	0.40	0.50	0.60	0.70	0.80	0.90	1.00	1.10	1.20	1.30	1.40	1.50	1.60
NUMBER	0	85	362	845	1011	662	241	32	3	0	0	0	
PERCENT	0.0	2.6	11.2	26.1	31.2	20.4	7.4	1.0	0.1	0.0	0.0	0.0	

ICRKTP = 1   IACCEL = 0   NDLRS = 0   NRTRS = 0   DATE: 10/03/85   TIME: 22.21.17

CPU TIME: 4 MIN 21 SEC

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The OCA-P probabilistic fracture-mechanics code can now be executed on a personal computer with 512 kilobytes of memory, a math coprocessor, and a hard disk. A user's guide for the particular adaptation has been prepared, and additional importance sampling techniques for OCA-P have been developed that allow the sampling of only the tails of selected distributions. Features have also been added to OCA-P that permit RTNDT to be used as an "independent" variable in the calculation of P(F|E).

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