



INTERNATIONAL ATOMIC ENERGY AGENCY  
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# INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

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## WORKING PARTY ON MODELLING THERMOMECHANICAL BEHAVIOUR OF MATERIALS (29 May - 16 June 1989)

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### BACKGROUND MATERIAL

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These are preliminary lecture notes, intended only for distribution to participants.

BACO is a code for the simulation of the thermo-mechanical and fission gas behaviour of a cylindrical fuel rod under operation.

Steady-state operation is simulated, as well as power/coolant transients lasting more than approximately 30 seconds. This means that transient due to on-power reshuffling in HWR and to load follow operation can be handled by the code. On the other side, severe accident transients (i.e. LOCA), are not in the scope of this code.

The code can be used for any type of fuel rod made with UO<sub>2</sub> pellets and Zircaloy cladding. However, its extension to FBR and MOX fuel is rather simple, due to the modular character of the code.

BACO simulates the fuel rod power history by time steps. The user only needs to define the power history; the code itself will automatically select the time step according to physical criteria. The Code calculates for each time step (that is, along the whole power history): the temperature distribution in the pellet and the cladding; the principal stresses at the pellet and the cladding; the principal stresses at the pellet and the cladding; the radial and axial crack pattern in the pellet, the principal strains and hot geometry of pellet and cladding; the changes in porosity, grain size and restructuring of the pellet; fission gas release to the free volumes in the rod, trapped gas distribution in the fuel and in the UO<sub>2</sub> grain boundaries, internal gas pressure and current composition of the internal gas. The distribution along the rod axis of this variables is given.

The modular character of BACO is based on having separate subroutines for each mechanism or phenomenon occurring at the fuel, at the cladding, and at the fuel rod. As an example, if the user wishes to simulate a MOX fuel, he will only have to add, at the corresponding subroutines, the physical properties of this fuel: creep, elasticity, fission gas release, etc., but the overall Code structure remains unchanged.

## 2-GENERAL DESCRIPTION OF THE FUEL ROD IN BACO.

### 2.1-REPRESENTATION OF THE FUEL ROD.

Symmetry of revolution around the fuel rod axis is assumed in the Code. This means that the angular coordinates does not exist in the modelling. However, angular-dependent phenomena - as radial cracking - are simulated via some angular averaging method.

With respect to the axial dependence of the fuel rod behaviour - arising usually from the axial dependence of power generation in the reactor - the fuel rod is divided in axial sections. This division is made by the user when preparing the data input, and will result of a compromise between having a detailed description at high computer cost (if many axial sections are considered), or a coarse description at a low computer cost (if the number of axial sections is small).

At each axial section, there is no axial dependence. This means that the equations solved in the Code only depend on the radial coordinate, and also that calculation is performed for the middle cross-section of each axial section. Axial section can have different lengths, thus enabling the user to model the effect of the maximum linear power along the fuel.

In the Code, the different axial sections are coupled by the fact that the internal gas pressure is the same in all of them. Moreover, gas pressure is assumed to be the same in all the free volumes of the rod: plenum, pellet-cladding gap, pellet cracks, pellet dishing and pellet central hole (as-fabricated or due to fuel restructuring).

# INPUT DESCRIPTION

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The input file for BACO must be prepared as follows :

LINE	VARIABLES and DESCRIPTION	FORMAT
1-8	Title to be printed at the beginning of the output.	Cols. 1-52
9	Blank line.	
10	KASE : -KASE=1 : standard models for fuel modelling. -KASE=2 : linear thermo-elastic problem.	10X, I2
11	Blank line.	
12	KFISI : -if KFISI=3 : no fission gas release in the fuel rod. -if KFISI # 3 : default model for fission gas release.	10X, I2
13	KREDI : -if KREDI=3 : Assmann and Stehle model for pellet densification. -if KREDI# 3 : default model for densification.	10X, I2
14	KCREEI : -if KCREEI=3 : Liu and Bement correlation for Zry steady state creep. -if KCREEI# 3 : default model for Zry creep.	10X, I2
15	KDISHI : -if KDISHI=3, pellet dishing will not affect stress/strain state. -if KDISHI# 3 : default model for pellet dishing.	10X, I2
16	KRELOI : -if KRELOI=3 : pellet relocation is not considered in gap conductance modelling. -if KRELOI# 3 : default model for gap conductance considering pellet fragments relocation.	10X, I2
17	Blank line.	
18	REXTO : pellet outer radius (cm).	10X, F10.0
19	HPEL : pellet height (cm).	10X, F10.0
20	HNDSH : number of dishing in the fuel rod. If pellets are single dished, enter number of pellets; if double dished, enter twice the number of pellets in the rod.	10X, F10.0

21	HDSHO : dishing depth, measured at the pellet centerline (cm).	10X, F10. 0
22	RDHO : radius of the dishing on the pellet flat end (cm) (Equal to: pellet radius minus pellet land width).	10X, F10. 0
23	DENS : pellet density as percent of Theoretical Density (%).	10X, F10. 0
24	PAB : pellet fractional open porosity (Fraction of pellet volume).	10X, F10. 0
25	GS : pellet grain size ( $\mu\text{m}$ ).	10X, F10. 0
26	SRF : pellet surface roughness (cm).	10X, F10. 0
27	Blank line.	
28	RGIO : cladding inner radius (cm).	10X, F10. 0
29	RGEO : cladding outer radius (cm).	10X, F10. 0
30	SRC : cladding surface roughness (cm).	10X, F10. 0
31	Blank line.	
32	PLENV : plenum volume ( $\text{cm}^3$ ).	10X, F10. 0
33	FUELC : pellet stack length (rod active length) (cm).	10X, F10. 0
34	CCO(1) : Helium molar fraction in rod filling gas.	10X, F10. 0
35	CCO(2) : Argon molar fraction in rod filling gas.	10X, F10. 0
36	CCO(3) : Krypton molar fraction in rod filling gas.	10X, F10. 0
37	CCO(4) : Xenon molar fraction in rod filling gas.	10X, F10. 0
38	CCO(5) : Nitrogen molar fraction in rod filling gas. (Note that $\text{CCO}(1)+\text{CCO}(2)+\text{CCO}(3)+\text{CCO}(4)+\text{CCO}(5)=1$ )	10X, F10. 0
39	RES : force constant of spring at top of stack ( $\text{MPa}\cdot\text{cm}=100 \text{ Newton/cm}$ ).	10X, F10. 0
40	GPRO : rod filling gas pressure at room temperature (MPa).	10X, F10. 0
41	Blank line.	
42	DLN : inverse diffusion length for neutrons in the pellets ( $1/\text{cm}$ ).	10X, F10. 0

43	FFIN : fractional porosity at the end of densification (default densification model).	10X, F10.0
44	BUS : burn-up at which densification ends (Mw*day/Ton(U)), (default densification model).	10X, F10.0
45	Blank line.	
46	SO2 : cladding stress for 0.2 % plastic strain (MPa).	10X, F10.0
47	B2R : stress exponent in cladding Norton law for plasticity ( $\epsilon_{eq}^{pl} = B1 * \sigma_{eq}^{B2R}$ )	10X, F10.0
48	AZ(1) : Hill anisotropy coefficient for the cladding. Convention :  $\sigma_{eq}^2 = AZ(1) * (\sigma_Y - \sigma_z)^2 + AZ(2) * (\sigma_r - \sigma_Y)^2 + AZ(3) * (\sigma_r - \sigma_z)^2$	10X, F10.0
49	AZ(2) : Hill anisotropy coefficient.	10X, F10.0
50	AZ(3) : Hill anisotropy coefficient.	10X, F10.0
51	Blank line.	
52	HFILM : coolant to cladding heat transfer coefficient (W/(cm2*sec)).	10X, F10.0
53	Blank line.	
54	RGHG : ratio between gamma heating of the cladding (W/cm3) and fuel linear power (W/cm). If cladding gamma heating neglectable, or if constant gamma heating GHG is to be used, enter any negative number.	10X, F10.0
55	GHG : gamma heating in the cladding (W/cm3), constant during the whole power history.	10X, F10.0
56	RFNR : ratio between fast neutron flux (E>1Mev) in the cladding (neutrons/(cm2*sec)) and fuel linear power (W/cm). When RFNR negative, a constant fast neutron flux of $10^{14}$ n/(cm2*sec) will be defined.	10X, F10.0
57	Blank line.	
58	Blank line.	

59	RPMF, FPMF : -RPMF is the radius (in $\mu\text{m}$ ) of the fine porosity in the pellet. -FPMF : volume fraction of fine porosity (defined as pores having diameter less than 0.1 $\mu\text{m}$ ). Used in the Assmann-Stehle densification model. If that model is not used (KREDI # 3), leave blanks in lines 59 to 72.	2F10.0
60	Blank line.	
61	NPOR : number of different pore sizes in the coarse porosity size histogram (NPOR: 10).	10X, 12
62	Blank line.	
63-72	RP(I), FP(I) : - RP(I) is the average radius ( $\mu\text{m}$ ) of coarse pores in size group I of the histogram. - FP(I) is the volume fraction of coarse porosity in size group I of the histogram. NOTE : I runs from 1 to NPOR. Nevertheless, even if NPOR<10, 10 lines must always be entered; leave the rest in blank.	2F10.0
73	Blank line.	
74	KREAD : -KREAD=1, power history is given as a function of time. -KREAD=2, power history is given as a function of burn-up.	10X, 12
75	KIMPRE : 1 condensed output 2 detailed output	10X, 12
76	KULON : 0 output every time step ≠0 condensed output (valid if KIMPRE=1) each KULON time steps.	10X, 12
77	Blank line.	
78	NZ : number of axial sections considered in the fuel rod (1: NZ : 7)	10X, 12
79	FUELCS(I), I=1,NZ : FUELCS(I) is the active length of axial section I (cm). Axial sections are numbered downstream, that is : axial section 1 at the coolant outlet, axial section NZ at the coolant inlet.	10X, 7F10.0
80	RINTO(I), I=1,NZ : Inner radius of the pellet at axial section I (cm). If pellet is solid at axial section I, enter 0.	10X, 7F10.0
81	KAGUJ(I), I=1,NZ : -KAGUJ(I)=0 if pellets at axial section I are solid. -KAGUJ(I)=1 if pellets at axial section I are hollow.	10X, 7I10

82 N(I), I=1,NZ : number of pellet mesh points at axial section I (for finite differences calculation)  
3: N(I) : 20. Value suggested: 18 10X,7I10

83 M(I), I=1,NZ : number of cladding mesh points at axial section I (for finite differences calculation)  
3: M(I) : 10. Value suggested: 6.  
If cladding is very thick, and/or if high pressure gradients are to be expected, use M(I)=8. 10X,7I10

84 Blank line.

NOTE :  
Now, the power history begins. The following blocks must be repeated as many times as necessary for describing all the power steps in power history.

LINE	VARIABLES and DESCRIPTION	FORMAT
85	NCICLO, KIMPRI : -NCICLO=1 if the step in power history to be read is a power or coolant ramp; -NCICLO=0 if the step is not a ramp. All power histories must begin with NCICLO=1 (the initial power up ramp at BOL). KIMPRI: value of KIMPRE for defining output of the present time step. If KIMPRI=0, the value of KIMPRE previously read from line 75 will be used.	7X,2I10

If NCICLO = 1, the ramp values must be entered as follows :

LINE	VARIABLES and DESCRIPTION	FORMAT
86	TREFE : inlet coolant temperature (deg K)	10X,F10.0
87	TREFS : outlet coolant temperature (deg K)	10X,F10.0
88	TREFO: average coolant temperature at reference average rod linear power CHM (deg K).	10X,F10.0
89	CHM :reference average rod lineal power for which the coolant temperature is TREFO (W/cm).	10X,F10.0
90	PREFR : coolant pressure (MPa).	10X,F10.0
91	TSUB : ramp length of time (day). That is, if the ramp starts at time To, it ends at time To+TSUB.	10X,F10.0
92	CHINOF(I), I=1,NZ : linear power at fuel rod axial section I at the end of the ramp (W/cm).	10X,7F10.0



If NCICLO = 0, the step in power input must be input as follow :

LINE	VARIABLES and DESCRIPTION	FORMAT
N	a) If KREAD=1 (line 74): TFIN, time at the end of the step in power history to be read (day), counted from BOL. b) If KREAD=2 (line 74): BFAV, fuel rod average burn-up at the end of the step in power history to be read (MW*day/Ton(U), counted from BOL.	10X,F10.0
N+1	CHINOF(I), I=1,NZ : linear power at fuel rod axial section I at the end of the step being read (W/cm). The code will, at each time step, interpolate the linear power at fuel rod section I between its value at the beginning of the present step in power history, and CHINOF(I).	10X,7F10.0

NOTE :

In the numeration previously followed, if the NCICLO=0, step immediately follows the initial power-up ramp read between lines 84 and 92, input would have been as follow :

LINE	VARIABLES and DESCRIPTION	FORMAT
93	Blank line	
94	NCICLO, KIMPRI (with NCICLO=0)	7X2I10
95	TFIN or BFAV, as defined by the value of KREAD	7X,F10.0
96	CHINOF(I), I=1,NZ	10X,7F10.0

At the beginning of the output, the general information, corresponding to the fuel rod being simulated is printed. If the user has changed some default model, models being used are indicated in the output.

Different outputs are possible:

a) *Overall rod information:*

- 1- Present time (days)
- 2- Gas composition (Molar fraction) in the rod free volume.
- 3- \* Internal gas pressure (MPa).
  - \* Volume of fission gases (cm<sup>3</sup> at STP) stored in the fuel rod since BOL (under title VG(TRAP)).
  - \* Volume of fission gases (cm<sup>3</sup> STP) stored in the grain boundaries since BOL (under title GAS(GB)). Note that GAS(GB) is part of VG(TRAP).
  - \* Total number of moles of gases filling the rod (under title GAS(MOL)), made up of initial filling gas and released fission gases.
- 4- \* Volume (cm<sup>3</sup> STP) of fission gases produced since BOL.
  - \* Volume (cm<sup>3</sup> STP) of fission gases released to the rod free volumes since BOL.
  - \* Fraction of the fission gases produced that has been released.
- 5- \* The plenum average temperature at present time (deg K, under title T(PLENUM)).
  - \* Hot plenum volume (cm<sup>3</sup>) at present time (under title V(PLENUM)).
  - \* Rod average burnup (MW\*day/Ton. (U)) at present time (under title B-UP(AV)).
- 6- \* Hot pellet stack length (cm) at present time (under title FUEL LENGTH).
  - \* Hot length of the part of the cladding that, in cold conditions, corresponded to the rod active length (under title CLAD LENGTH).
- 7- \* The pellet-cladding gap thermal conductance (W/cm<sup>2</sup> \* deg K) for each axial section.

b) *Detailed information for each axial section:*

Subroutine IMPRE prints, for each axial section:

- 1- \* Present time (day)

- \* Time step in this calculation (day).
- \* Step number.
- 2- \* Local generating power (W/cm and W/gr.).
- \* Local burnup (MW\*day/Tn (U)).
- \* Local fast neutron ( $E > 1$  MeV) flux in the cladding (neutrons/cm<sup>3</sup>\*sec)
- 3- \* Volume (cm<sup>3</sup> STP) of fission gases produced at the axial section since BOL.
- \* Volume (cm<sup>3</sup> STP) of fission gases released from the axial section since BOL.
- \* Fraction of fission gases released from the axial section since BOL.
- 4- \* Axial strain of the pellet stack at the axial section since BOL.
- \* Axial strain of the cladding at the axial section since BOL.
- 5- PELLET :
  - \* Radius (cm) of each mesh point.
  - \* Temperature (deg K) at each mesh point.
  - \* Von Mises equivalent stress (MPa) at each mesh point.
  - \* Radial, axial, and tangential stresses (MPa) at each mesh point.
  - \* Radial crack opening (cm) at each mesh point.
  - \* Axial crack opening per unit length at each mesh point.
  - \* Fractional porosity at each mesh point.
- 6- CLADDING :
  - \* Radius (cm) of each mesh point.
  - \* Temperature (deg K) at each mesh point.
  - \* Hill's equivalent stress (MPa) at each mesh point.
  - \* Radial, axial, and tangential stresses (MPa) at each mesh point.

c) *Reduced information for each axial section.*

Subroutine IMPRE1 prints for each axial section:

- \* Time.
- \* Pellet inner radius (cm).
- \* Pellet outer radius (cm).

- \* Cladding inner radius (cm).
- \* Cladding outer radius (cm).
- \* Local linear heat generating rate (W/cm).
- \* Local burnup (MW\*day / Tn(U))
- \* Von Mises equivalent stress (MPa) at the pellet center.
- \* Fractional porosity at the pellet outer radius.
- \* Fission gases stored at grain boundaries in the axial section since BOL (cm<sup>3</sup> STP).
- \* Pellet centerline temperature (deg K).
- \* Pellet surface temperature (deg K).
- \* Cladding inner surface temperature (deg K).
- \* Cladding outer surface temperature (deg K).
- \* Tangential (hoop) stress at the cladding inner surface (MPa).
- \* Pellet-cladding contact pressure (MPa).
- \* Fraction of fission gases released from the axial section since BOL.

d) *Pellet microstructural detailed information.*

- \* Volume fraction of fine porosity at each axial section.
- \* Average radius and volume fraction of each coarse porosity size group, at each pellet ring and at each axial section. (Only when KRED=3, that is, when Assmann & Stehle densification model is used)
- \* Radial distribution of pellet grain size (due to equiaxed grain growth) at each axial section.
- \* Radial distribution of the fraction of fission gases stored in the pellet since BOL, at each axial section.

Output Group a) will be printed whenever output groups b) or c) are printed.

Output Group b) will be printed:

- \* At the end of each time step if parameter KIMPRE or KIMPRI are set to 2 by the user. Beware that this will produce a large output.
- \* Always, at the end of a step in the power history.

Output Group c) will be printed:

- \* Each KULON time steps when parameters KIMPRE or KIMPRI are set to 1

by the user

Output Group d) will be printed:

\* Always at the end of a step in the power history.

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