VERY FAST ISOTOPIC AND MASS BALANCE CALCULATIONS USED FOR STRATEGIC PLANNING OF THE NUCLEAR FUEL CYCLE

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ABSTRACT

Owing to the prevalence in France of nuclear generated electricity, the French utility, EDF focusses much research on fuel cycle strategy. In this context, analysis of scenarios combining problems related to planning and economics, but also reactor physics, necessitate a relatively thorough understanding of fuel response to irradiation. The main purpose of the fuel strategy program codes is to predict mass balance modifications with time for the main actinides involved in the cycle, including the minor actinides associated with the current back end fuel cycle key issues.

Considering the large number of calculations performed by a strategy code in an iterative process covering a range of about a hundred years, it was important to develop basic computation modules for both the "reactor" and "fabrication" items. These had to be high speed routines, but on an accuracy level compatible with the strategy code efficiency.

At the end of 1992, the EDF Research and Development Division (EDF/DER) developed a very simple, extremely fast method of calculating transuranian isotope masses. This approach, which resulted in the STRAPONTIN software, considerably increased the scope of the EDF/DER fuel strategy code TIRELIRE (1) without undue impairment of machine time requirements for a scenario.

1 BACKGROUND ON FUEL STRATEGY REACTOR PHYSICS MODELLING AT EDF

The elaboration of a nuclear fuel utilization scenario raises two basic questions (Fig. 1):

- how will irradiation in the reactor affect the isotopic composition of the main actinides ?
  what proportion of fissile isotopes would be required in the core load to sustain an energy production duty cycle of specified length ?

With a view to finding answers to these two questions, EDF/DER developed towards the end of the eighties a methodology based on a statistical approach involving :

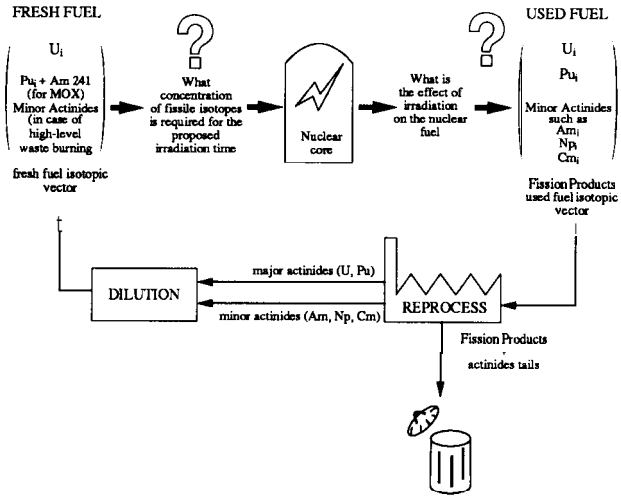

Figure 1 - Mimic diagram of fuel cycle strategy problems

calculating once and for all a transfer matrix giving the unloading mass/loading mass ratio for isotopes U235, U236, U238, Pu238, Pu239, Pu240, Pu241, Pu242 and Am241:

$$\begin{pmatrix} U_i \\ Pu_i \\ Am\ 241 \end{pmatrix}_{\substack{\text{discharged} \\ \text{fuel}}} = (\alpha_{ij}) \begin{pmatrix} U_j \\ Pu_j \\ Am\ 241 \end{pmatrix}_{\substack{\text{fresh} \\ \text{fuel}}}$$

determining an "equivalence" formula giving the total plutonium content versus the isotopic composition of available plutonium in the case of uranium-plutonium mixed oxide fuels (MOX) and the intended duty cycle length. This will solve the "fabrication" aspects of the problem.

However, matrix methods imply a certain number of major drawbacks :

they do not indicate the masses of the minor actinides particularly highlighted in current investigations on back end fuel cycle issues and incineration

their accuracy does not exceed 2% for uranium, 5% for plutonium and uncertainty can even be as high as 10% for americium 241

their scope of application is more or less limited to the reference plutonium presently obtained after reprocessing a uranium oxide having a 3.25910 U235 content, with a burnup of 33 GWd/t, cooled for 3 years and stored for 2 years after reprocessing(a).

fresh fuel, by definition, cannot contain other isotopes than those listed , thereby eliminating minor actinide incineration

finally, no fuel management modifications can be integrated without changing the matrix, which is an extremely penalizing factor in view of the ever-increasing number of fuel management possibilities in a nuclear power plant population.

2 THE "STRAPONTIN" METHOD FOR ACCURATE HIGH SPEED ISOTOPIC CALCULATIONS ON SPENT FUEL

In order to solve these different problems, EDF/DER developed at the end of 1992 an original isotopic calculation method based on :

a semi-empirical formulation of absorber and fission self-shielded microscopic cross sections, condensed to a single energy group. This formulation is obtained by statistical analysis of these cross sections as calculated by the French cell code APOLLO 1 (2) used as a reference in the EDF official reload calculation scheme

optimized numerical resolution of the Bateman differential equation governing the isotopic evolution of heavy nuclei :

$$\sim = A.N(t)$$

This approach culminated in the writing of the STRAPONTIN(b) software (STRategy with APO11O for Neutronics and for the Treatment of Installed Nuclear plants).

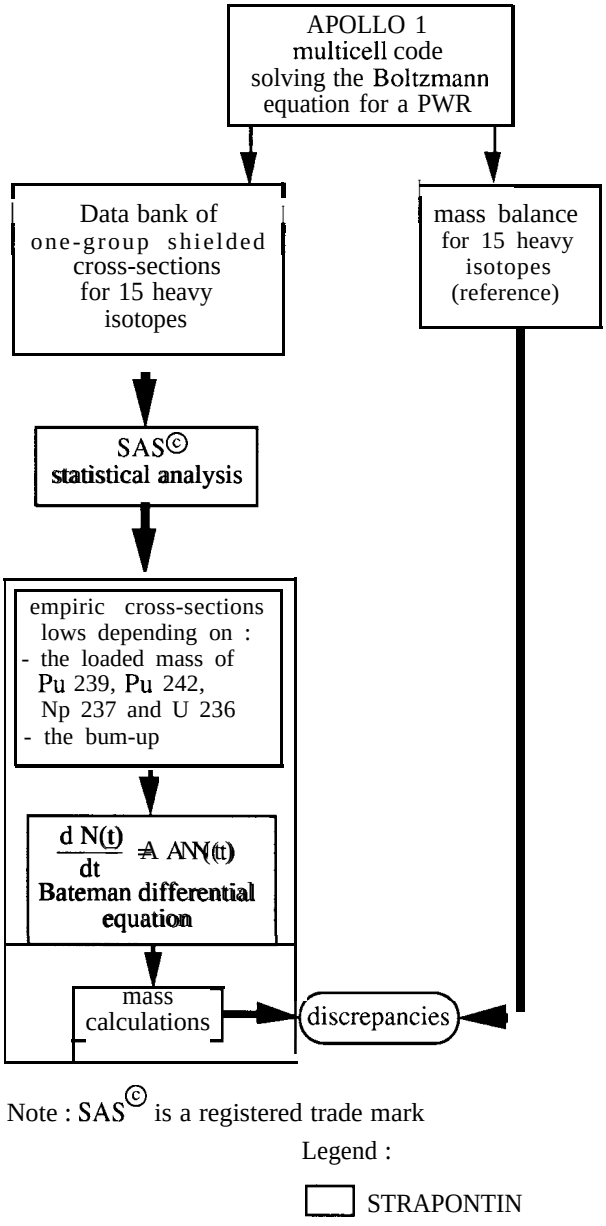

Figure 2- THE STRAPONTIN METHOD

A. Calculating the cross sections

The equations of state for one-group cross sections are calculated in two stages :

- first of all, a cross section database is constructed, using an APOLLO 1 calculation package, covering a wide range of fuels :
  - * enriched uranium oxides (UOX)
  - * mixed oxides (MOX) on a depleted, natural or even enriched uranium support
  - * oxides containing reprocessed uranium (URT)
  - * oxides initially comprising minor actinides (especially Np 237 which raises serious radiotoxicity problems)

(a) i.e. an isotopic vector corresponding to : Pu 238: 1.83% Pu 239: 57.93% Pu 240: 22.50% pu 241: 11.06% Pu 242: 5.60% Am 241: 1.08%

(b) A STRAPONTIN in French is a flap-scat : quick and easy to use

secondly, the empirical laws interpolating the database are determined. These laws give the actinide cross section variations versus the significant parameters for the problem considered :

* bum up
* total plutonium content
* uranium enrichment of the support
* isotopic composition of the plutonium and minor actinides loaded.

The accuracy with which these laws are determined is in the region of 5% for all situations encountered (tables la and lb).

Uox	Absorption cross-section in barns	Disc. in %	Fission cross-section in barns	Disc. in %
U234	18	± 0,3	-	-
U235	40 < σ <80	± 1	35 < σ < 65	± 1
U236	9	± 0,5	0.3	± 1
U238		± 0,4	0.1	± 0,2
Np237	30<rs <40	± 0,8	-	-
Pu238	25 < σ < 50	± 1,5	-	-
Pu239	140< σ <250	± 2	90 < σ < 160	± 1,5
Pu240	100<0<250	± 2	0.5	± 0,5
Pu241	88<0 <160	± 1,2	88 <0σ < 160	± 1,1
Pu242	25	± 2	0.5	± 0,4
Am241	105< σ <160	± 1,5	1.4	± 0,8
Am242	600<0<1200	± 1,5	500 < σ < 1000	± 1,5
Am243	38 < σ < 45	± 0,6	0.4	± 0,4
Cm242	8.5	± 0,015	-	-
Cm244	17	± 0,8	1.6	± 1,1

MOX	Absorption cross-section in barns	Disc. in %	Fission cross-section in barns	Disc. in %
U234			-	-
U235	14 < 0 < 30	± 3	12 < σ < 24	± 3
U236	9	± 1.7	0.3	± 0,6
U238	0.9	± 0,6	0.1	± 1
Np237	17 < σ < 27	+2, -12	–	
Pu238	8 < σ < 19	± 3.5	–	
Pu239	26 < σ < 76	± 7	16 < σ <50	± 7
Pu240	22 < σ < 64	+9, -1	0.6	± 0,8
Pu241	30 < σ < 76	+6, -5	24 < σ < 56	+6, -5
Pu242	15 < σ < 25	+9, -3	0.5	± 1.1
Am241	36 < σ < 72	+6, -3	1	+2, -1
Am242	I1O<O<38O	± 5	100 < σ < 310	± 5
Am243	24 < σ <38	+5, -2	0.4	+2, -1.6
Cm242	8.4	± 0.15	-	-
Cm244	14 < σ < 18	+2, -3	1.7	± 1

Tables 1 and 1 b - Accuracy of th empirical laws

B . Solving the isotope evolution equations

STRAPONTIN comprises two numerical models:

the conventional matrix exponential method:

$$N(t) = e^{At} N(0)$$

where N(t) is the actinide isotopic vector

the Runge-Kutta method (4.4) with automated time step calculation according to maximum authorized error.

It is the latter method, which is both extremely fast and endowed with exceptional computing efficiency, which is used when STRAPONTIN is coupled with the TIRELIRE prediction code.

3 ST RAPONTIN SCOPE AND PERFORMANCES

The scope of the code depends on the range of fuels included in the cross section database.

A. ST RAPONTIN COMPATIBILITY CRITERIA

STRAPONTIN is so designed as to cover present fuel requirements :

the burnup range covered is O -64 GWd/t
- for UOX or URT fuel, U235 enrichment must be below 6% and U 236 enrichment below 3.2%
- for MOX fuel, the total plutonium content must be comprised between 2% and 11% and U235 enrichment of the support must be below 4% of the total uranium content
- finally, the initially present Np237 concentration must be below 2% of the total mass of the assembly considered.

It is important to note that a wide range of fuels, even some of the more unusual varieties which can be encountered in certain scenarios, can be dealt with by STRAPONTIN.

B . ACCURACY ON THE ACTINIDE MASSES

Table 2 shows a comparison between four typical fuels with a 35 GWd/t burnup :

a 3.25% U 235 UOX fuel (standard fuel for a 3-batch uranium core)
a 5.30% Pu MOX fuel on a depleted uranium support. The Pu comes from the preceding UOX, cooled for 3 years, reprocessed and stored for 2 years
a URT fuel, comprising 3.55% U 235 and 1.15% U 236, with an equivalent core cycle length to that of the reference UOX (3.25%)
a MOX fuel containing 8.7% degraded Pu (from a 3rd multirecycling period)(c) on a depleted uranium support.

(c) Pu 238: 3.o9% Pu 239: 42.06% Pu 240 : 28.39% Pu 241: 14.52% Pu 142: 10.47% Am 241 : 1.47%

	UOX 3,25'%			URT 3,55%			MOX 5,30%			MOX Bad Plutonium 8,70%		
ISOTOPES	Mass STRAPONTIN in KG	Mass APOLLO in KG	Disc. in %	Mass STRAPONTIN in KG	Mass APOLLO in KG	Disc. in %	Mass STRAPONTIN in KG	Mass APOLLO in KG	Disc. in %	Mass STRAPONTIN in KG	Mass APOLLO in KG	Disc, in %
U_{234}	0,086	0,086	0,47	0,272	0,274	-0,96						
U_{235}	3,825	3,822	0,08	4,679	4,702	-0,49	0,495	0,496	-0,14	0,570	0,568	0,42
U_{236}	1,833	1,840	-0,38	6,681	6,704	-0,34	0,102	0,101	1,32	0,087	0,087	0,12
U_{238}	433,870	433,864	0,0	427,477	427,333	0,03	424,515	424,519	0,0	409,799	409,647	0,04
Np_{237}	0,278	0,278	-0,14	0,647	0,660	-1,89	0,099	0,098	0,41	0,095	0,096	-0,55
Pu_{238}	0,094	0,095	-0,80	0,244	0,250	-2,40	0,329	0,329	0,06	0,949	0,948	0,05
Pu_{239}	2,658	2,673	-0,56	2,710	2,790	-2,89	7,658	7,649	0,12	11,788	11,468	2,79
Pu_{240}	1,078	1,064	1,30	1,044	1,033	1,11	5,136	5,131	0,10	9,150	9,238	-0,95
Pu_{241}	0,679	0,675	0,53	0,666	0,672	-0,99	3,359	3,360	-0,03	5,656	5,881	-3,83
Pu_{242}	0,287	0,283	1,34	0,257	0,253	1,51	1,892	1,904	-0,63	4,208	4,287	-1,85
Am_{241}	0,017	0,017	0,54	0,017	0,017	-1,26	0,236	0,236	0,05	0,568	0,575	-1,26
Am_{242}	0,000	0,000	NS	0,000	0,000	NS	0,007	0,005	NS	0,021	0,014	NS
Am_{243}	0,051	0,050	1,23	0,044	0,043	0,88	0,622	0,623	-0,22	1,206	1,238	-2,56
Cm_{242}	0,007	0,007	NS	0,006	0,006	NS	0,077	0,077	-0,13	0,129	0,135	-4,31
Cm_{244}	0,013	0,012	5,32	0,011	0,010	5,43	0,256	0,245	4,40	0,404	0,410	-1,59
Pu_{238B} *	0,006	0,006	NS	0,005	0,005	NS	0,181	0,181	0,01	0,326	0,338	-3,56
Pu_{240B} *	0,000	0,000	NS	0,000	0,000	NS	0,009	0,006	NS	0,014	0,012	NS

N.S.: No significant discrepancy

* Note : APOLLO makes a difference between the initial Pu_{238} and Pu_{240} in the fresh fuel and the ones created by a decay of the Cm 242 and Cm 244. We did the same with STRAPONTIN for comparison.

Table 2- Discrepancies (in %) on mass (in kg) between STRAPONTIN and the APOLLO reference code

A. EXTENDED NUCLEAR PHYSICS CAPACITY

Provision has already been made for a certain number of developments in the code's nuclear physics capacity:

- first of all, recalculation of the cross section equations of state, based on the more recent multigroup cross sections, using to begin with the "CEA 86-1" cross section library[3] and subsequently the just out french "CEA 93" based on the JEF 2 basic nuclear data library

  then, inclusion of the moderator-to-fuel ratio in the cross section equation of state data. This would extend the scope to advanced over- or under-moderated LWR's.

B . FUTURE USE OF STRAPONTIN

as an all-purpose prospection tool for back-end fuel cycle and incineration investigations

as a "reactor" calculation module in the other EDF fuel management and strategy codes.

It should be borne in mind that discrepancies of a few % are perfectly compatible with the accuracy requirements of these strategy scenarios devised to predict fuel stock evolution trends and estimate the relevant isotopic data.

C . MACHINE TIME EFFICIENCY

STRAPONTIN's main targets are speed and accuracy. These are achieved, since a standard 35 GWd/t burnup is performed in 0.225 s on a SUN SPARC station IPC, which means that for a scenario covering about a hundred years of plutonium multirecycling comprising 108 STRAPONTIN calls, the extra computation time required will be 24.36 s, i.e. 30% of the total scenario time (the mass balance calculation time by the matrix method being practically negligible, amounting to 0.1 s for the 108 calculations). This additional machine time is a reasonable price to pay, considering the improved scope and accuracy of the STRAPONTIN spent fuel calculations as compared with those of the former, less flexible, mass balance matrix method.

4 PROSPECTS

On the basis of the high quality results obtained, a number of improvements are envisaged for STRAPONTIN together with its future use.

5 CONCLUSION

The STRAPONTIN software is an industrial tool for high speed accurate calculation of the mass balances of the main PWR spent fuel actinides.

The originality of the model stems from the well targetted cross section equations of state and the optimized numerical resolution. STRAPONTIN is designed to deal with fuels as varied as:

enriched natural uranium
enriched reprocessed uranium
mixed oxide (U02-PU02) fuels, of highly vaned isotopic compositions, on slightly or highly enriched uranium supports
identical fuels incinerating minor actinides.

With these characteristics, it will constitute a powerful basic module for the processing of the "reactor" aspects in nuclear fuel management strategy codes.

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