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V. S. O. P. (99) for WINDOWS and UNIX

Computer Code System for Reactor Physics and Fuel Cycle Simulation

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Computer Code System for Reactor Physics and Fuel Cycle Simulation

by

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Abstract

V.S.O.P. is a computer code system for the comprehensive numerical simulation of the physics of thermal reactors. It implies the setup of the reactor and of the fuel element, processing of cross sections, neutron spectrum evaluation, neutron diffusion calculation in two or three dimensions, fuel burnup, fuel shuffling, reactor control, thermal hydraulics and fuel cycle costs. The thermal hydraulics part (steady state and time-dependent) is restricted to HTRs and to two spatial dimensions. The code can simulate the reactor operation from the initial core towards the equilibrium core.

V.S.O.P.(99) represents the further development of V.S.O.P. (97). Compared to its precursor, the code system has been improved in many details. Major extensions have been included concerning the thermal hydraulic sections. Beyond that, the many modules of the code-system have been condensed to only 2 executables in the "99"-release of V.S.O.P., to be comfortably handled on a WINDOWS-PC or a UNIX-computer. The necessary data input as well as the handling and book-keeping of intermediate data sets has been condensed and simplified.

A 64 MB memory should be available for the execution of the code. The hard disk requirement for the executables and the basic libraries associated with the code amounts to about 7 MB.

Preface

The V.S.O.P.- system in its present form is the result of code development, which has continuously been performed since more than two decades. Multiple and continuous application for reactor development lead to various extensions of its capability. High temperature reactor programs for nuclear process heat production and for electricity generation gave important impulses for improvements of the code-system, specially in view of the research on inherent safety features, reactor operation and licensing requirements. The first two editions of the V.S.O.P.-code were published in 1980 and 1994, respectively /1,2/. During the current decade certain aspects of the fuel cycle of thermal reactors (waste assessment, proliferation resistance) gained in significance. Thus, in particular the demand for a more detailed treatment of the generation and depletion of the heavy metal isotopes including the minor actinides lead to a relevant further development of the code, which has been published as version V.S.O.P.(97) /3/.

Recent safety research for advanced Modular High Temperature Reactors required some major extension of the code concerning the thermal hydraulics as well as the modeling of neutronics for some special operating conditions. Furthermore, an increasing demand for a code version, which can be comfortably handled on current high-performance-PCs gave rise to basically restructure the code system in view of its optional use either on a "Windows"-PC or on a "Unix"-computer. These two aspects were the main incentives for further code development resulting in the version at issue, i.e.V.S.O.P. (99):

The authors express their thanks to the director of the "Institut für Sicherheitsforschung und Reaktortechnik", Professor K. Kugeler, who strongly promoted their development work by many suggestions and ideas. They also express their gratitude for many contributions resulting from the cooperation with many colleagues and guest scientists.

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1. Introduction

V.S.O.P. (Very Superior Programs) is a computer code system for the comprehensive numerical simulation of the physics of all types of thermal reactors. The code has widely been used for research in the course of the development of the High Temperature Reactor with spherical fuel elements. Thus, many tools have been included to cover very specific features of this reactor type. The application of the code implies processing of cross sections, the set-up of the reactor and of the fuel element, neutron spectrum evaluation, neutron diffusion calculation, fuel burnup, fuel shuffling, reactor control, and thermal hydraulics of steady states and transients (Fig. 2). The neutronic calculations can be performed in up to three dimensions. Thermal hydraulics is restricted to Pebble-bed HTRs in two spatial dimensions.

The V.S.O.P.-code enables the user to follow the reactor life from the initial core towards the equilibrium core. Repeated calculation of the different physics features ensures consistency in their feedback during the proceeding burnup, the simulation of the fuel shuffling, and variations of the core power rating. Accidental transients can be followed in a quasi-static nuclear approximation under repeated criticality evaluation. Characteristics of the life history of the fuel elements are used for the calculation of their individual decay power . Evaluation of fuel cycle costs over the reactor life time is made using the present worth method. Reprocessing and closure of the fuel cycle can be simulated under consistent control of the mass flow of the fuel, including the isotopic decay during periods of intermediate storage. Due to the basic revision and extension of the burnup section for the "97"-release of the code - replacing the hitherto applied heavy metal burnup chains by a more complete and more flexible structure (see /3/ for details)- the code since then also allows the assessment of the impact of the "minor actinides" on the physics of the reactors and on the characteristics of spent fuel.

Two aspects were the main incentives for further code development resulting in the version at issue, V.S.O.P. (99):

- Recent safety research on advanced Modular High Temperature Reactors required some major extension of the code concerning the thermal hydraulic treatment of specific fuel-moderator arrangements of the reactor core and a higher flexibility in the modeling of neutronics at incidents of water ingress into graphite-moderated reactor cores.
- Increasing demand for a code version, which can be comfortably handled on current high-performance-PCs gave rise to basically restructure the code system in the sense of a condensation of its numerous modules to only two executables. Thus, the necessary data input as well as the number of intermediate data sets to be identified and handled has been distinctly simplified and reduced, respectively. V.S.O.P.(99) can optionally be used either on a "Windows"-PC or on computers using the AIX 4.3 operating system.

Chapters 2 and 3 of this report give a survey of new features of the code, of its structure and organization. Chapters 4 and 5 are the manuals of the required data input for the code sections VSOP-MS and VSOP-ZUT, respectively. The APPENDIX contains more detailed information and comments on the code and, in essence, is an update of chapter "useful comments" of the VSOP(94)- and VSOP(97)-manuals /2, 3/.

2. New Features of the Code

2.1 Physics concerns

Using former versions of VSOP – including the "94" and the "97"- editions – two restrictions had to be observed, one concerning neutron physics and the other one concerning thermal hydraulics. These were the incentive for the following code improvements in the frame of setting up VSOP (99).

2.1.1 Neutron transfer cross sections

The code section GAM (see chapter 3) – after the evaluation of the fast and epithermal neutron spectrum – condenses the multi-group cross sections to few "broad" energy group values to be used at the evaluation of neutron diffusion. This procedure has to include the construction of transfer-cross sections, accounting for the down-scatter from a given broad energy group, g, to all groups of lower energy, g^*, i.e. $\sigma_S(g \rightarrow g^*)$. In the earlier VSOP-editions, the construction of this transfer matrix has been dropped from the GAM code section. Instead, the total amount of neutrons scattered out of energy group g was assumed to be the in-scatter source of the next lower, broad energy group, i.e. group $g^* = g + 1$, exclusively. This procedure produces correct results only as long as the maximum possible energy loss per scattering event is smaller than the energy width of group g^*. This again is true e.g. for a graphite-moderated system, calculated with typically 4 broad energy groups and energy boundaries at say ~2 eV, ~30 eV and ~100 keV. However, incorrect results would be produced regarding e.g. an ingress of water into this system, leading to neutron collisions with hydrogen. In other words, for the numerical research concerning HTRs at an incidental water ingress into the reactor core or concerning LWRs, the VSOP-diffusion calculation had to be restricted to 2 energy groups, the fast group covering the complete energy range above 2 eV.

In order to overcome this restriction for present and future research, a section constructing the neutron transfer cross section matrix has been added to the GAM-part of the code system according to the treatment at the original GAM-code /12/. Thus, a free choice of the number of fast and epithermal energy groups - independent of the given moderator material- is allowed in VSOP(99).

2.1.2 Thermal hydraulics

Another restriction of former VSOP-editions, which was to be eliminated with a view to research on current HTR-concepts, concerns the numerical simulation of pebble-beds, which are a mixture of fuel elements and so called 'dummy' elements. These are pure moderator (graphite) elements, containing no fuel and thus not producing any fission power. While the neutronics parts also of the precursors of VSOP(99) already could well handle the presence of such dummy elements with different fractions of them being at different local positions within the pebble-bed, a corresponding treatment in the calculation of the thermal hydraulic properties of the core was missing so far.

In VSOP(99) each mesh point of the grid used for the evaluation of the fuel and graphite temperature in the code section THERMIX (see following chapters) may have its specific mixture of fuel elements and dummy elements. The respective fractions are assigned according to those of the corresponding core region, which the regarded mesh point belongs to. The fraction of dummy elements is defined by data input for each pre-defined region. The temperature evaluation then is performed separately for the power producing fuel elements and for the dummy elements. The so derived local fuel temperature is fed back for the determination of the resonance cross sections. The graphite temperature, i.e. the average value of fuel elements and dummy elements, is used for the evaluation of the thermal neutron spectrum.

2.2 Using the code on PC or Workstation

The Fortran source of the code system is structured in two parts to be used for the construction of two executable codes by the compilation and linking procedure. The first executable is named VSOP-ZUT. This code section is used to set up a matrix of resonance cross sections to be used in following applications of the MAIN-section of the VSOP. The latter code section is available as the executable code VSOP-MS. The two executables should be positioned within the same directory of the permanent memory device. We name this directory the "Working Directory" (see Fig. 1). The working directory must have a subdirectory, which must be named "Libraries", containing the various library data files. Necessary read- and write- data transfer from and to these data sets – illustrated in Fig.1- is done automatically during the execution of the code via this path. The name (and possibly the path) of the card image input and of the printout data sets (this sequence) have to be given as arguments when starting the program. All other data sets –unless they are automatically scratched after the end of code execution- are written onto the working directory and they are available for further use (e.g. Restart-libraries, data to be graphically displayed etc.). A list of the data sets possibly produced or used is given in chapter 3.4.

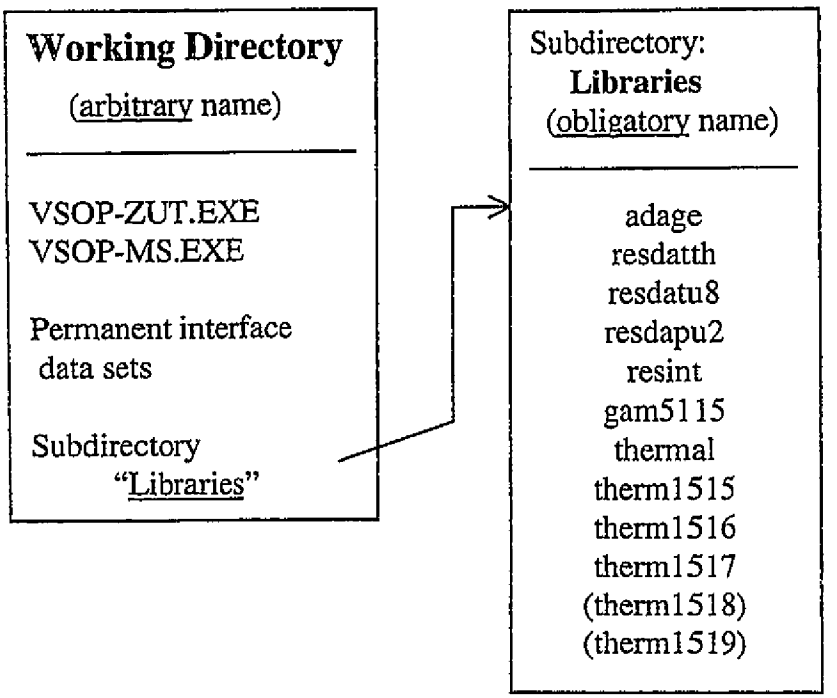

Fig. 1: Installation scheme of code executables and libraries

A 64 MB memory should be available for the execution of the code. The hard disk requirement for the executables and the basic libraries associated with the code amounts to about 7 MB. The source codes consist of about 65000 Fortran statements. They have been compiled and linked for use under the WINDOWS 95/98 and the AIX 4.3 operating systems.

3. Program Organization and Data Base

3.1 Structure of the code and program tasks

The structure of the V.S.O.P. - code system in terms of calculation tasks on the one hand and in terms of the programs and basic libraries on the other hand is illustrated in Fig. 2 and in Fig. 3, respectively.

Subroutines DATA-2 and ZDATA-2 use input data specifying the fuel element design to prepare detailed data to be used in different subroutines of V.S.O.P.

The BIRGIT code prepares the mesh pattern for a 2-d diffusion calculation and for the thermal hydraulics calculation. If experimental data for the flow of the fuel elements in a Pebble-bed reactor are available to the user, the code can generate a sophisticated flow pattern of finite batches of elements which move down to the discharge tubes in finite steps. It then provides the transformation between this pattern and the one used in the diffusion calculation for the macroscopic cross sections and for the neutron flux. Similar transformations may be performed for the thermal hydraulics calculations.

For a 3-d diffusion and burnup calculation the mesh pattern is prepared by use of subroutine TRIGIT in x-y-z -geometry.

The neutron spectrum is evaluated by means of GAM-I /12/ and THERMOS /13,14/ for a predefined, arbitrary number of spectrum zones, providing broad group cross sections for neutron absorption, neutron-induced fission and n,2n-reactions. The epithermal cross section library has a 68 group structure, corresponding to the GAM-I code. The thermal library fits in the 30 group structure of THERMOS. These libraries have been generated using ENDF/B-IV, -V and JEF-I data /6/. For some nuclides the cross sections within the resonance energy range are calculated prior to a VSOP-MS calculation by means of the VSOP-ZUT code section, which is based on the ZUT-DGL code /7,8/. This is done for ^{232}Th , ^{238}U and ^{242}Pu using resonance data also from ENDF/B-IV and -V. The resonance cross sections are stored on a permanent data set (see also chapter 3.4).

Two different sets of temperature dependent cross sections may be generated and used for each resonance absorber, both representing different absorber concentrations. Normally, these two concentrations should represent the highest and the lowest concentration, respectively, occurring in the fuel elements. The code then first constructs new resonance cross sections for these two states of burnup by interpolation between the values for different temperatures according to the calculated fuel temperature in each spectrum zone. It then gains the final cross sections by interpolation between these two sets for the highest concentration on the one

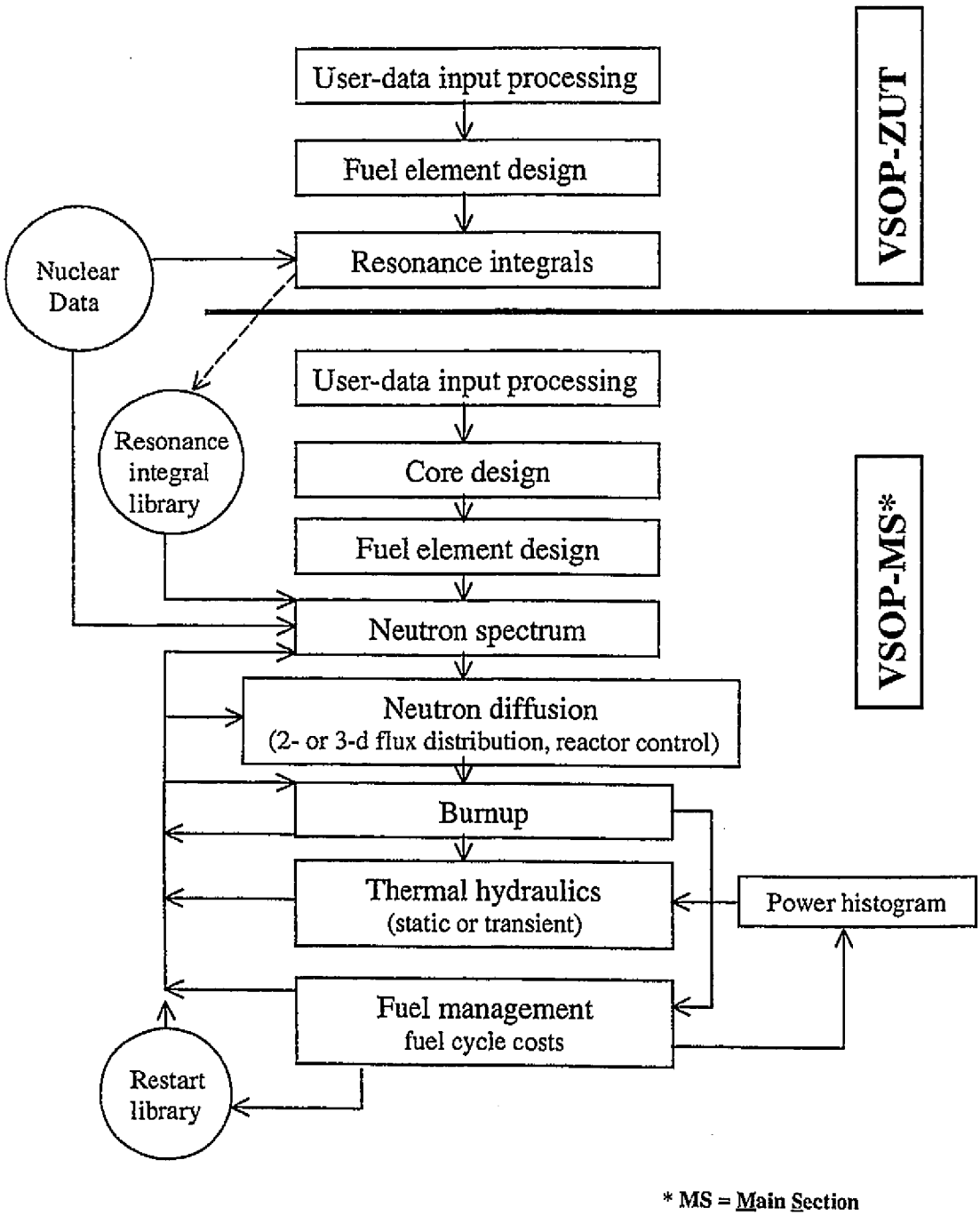

Fig. 2: Calculation tasks, V.S.O.P.-99

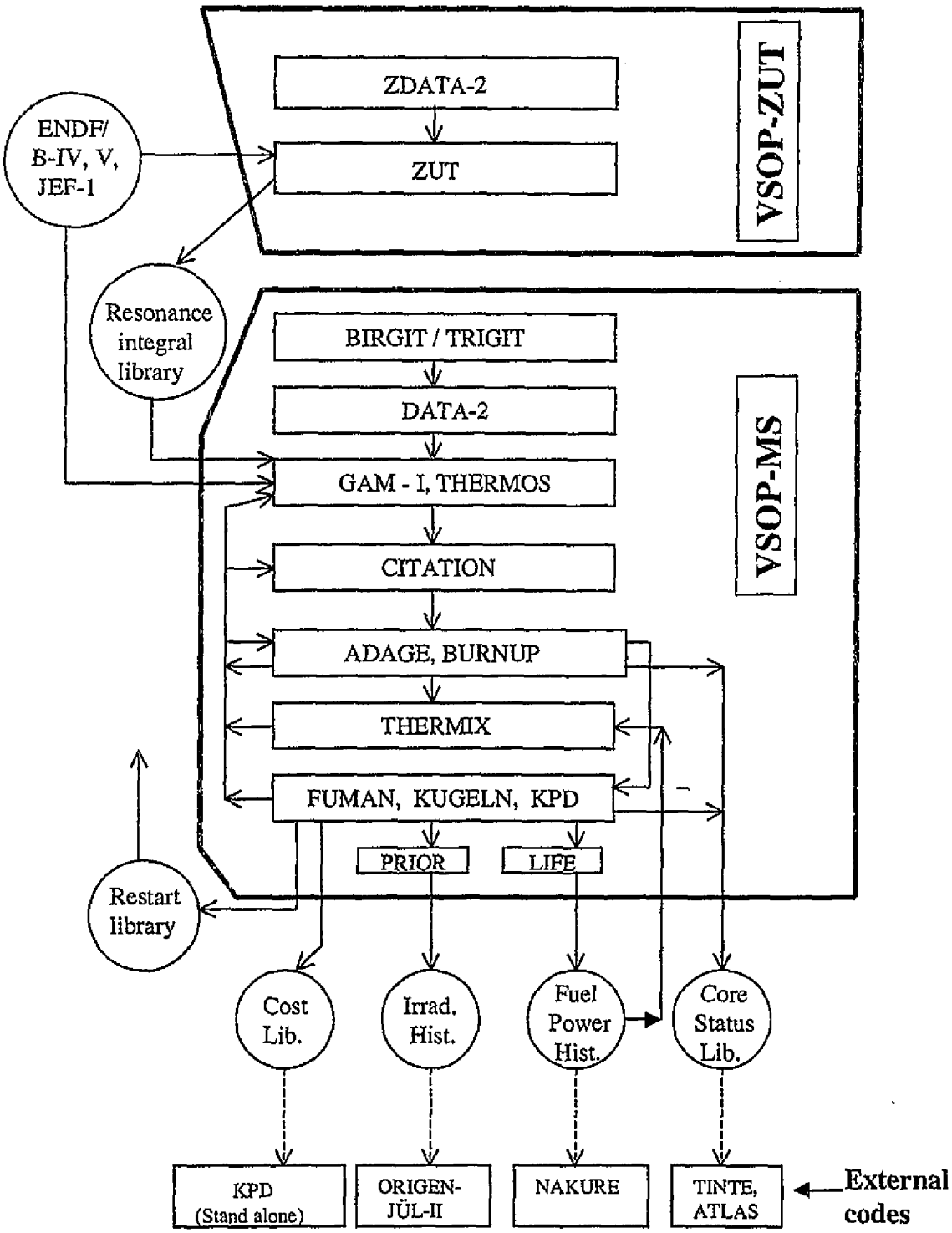

Fig. 3: The basic programs of the two code sections

hand and the lowest concentration on the other hand according to the true absorber concentration.

Graphite scattering matrices are based on the Young -Koppel spectrum in Graphite /9,10,11/.

Neutron diffusion is calculated by CITATION /15/ in its 2- or 3- dimensional version.

The burnup of -at present- 28 heavy metal isotopes in the numerous fuel batches (up to 9999) is evaluated by means of subroutine ADAGE. It includes the subroutines TERM, DECAY, EQUIL and parts of subroutines NUDATA and FLUXO, as they have been used in ORIGEN-JUEL-II /4/, which in its turn has been based on the ORIGEN code /5/. ADAGE uses the matrix exponential method in order to treat the decay and transition scheme. For this purpose it constructs a transition matrix for the group of heavy metals, whose size is determined by the number of isotopes defined in the ADAGE-library. This library contains an identification number for each nuclide to be treated. It also contains the decay constants and information about the possible nuclide transitions by α, β^-, β^+ - decay, by disintegration from an excited nuclear state to the ground state and by spontaneous fission. At present, the ADAGE-library defines the heavy metal chain from ^{232}Th through ^{244}Cm according to the cross section data available in the GAM-library (chapter 3.2). As burnup equations now are no longer fixed within the code, but the transition matrix is constructed according to the information contained in the ADAGE-library, the number of the considered materials in principle can easily be extended.

The burnup of the fission products and the simulation of the fuel shuffling are covered by subroutines BURNUP, FUMAN and KUGELN. These subroutines are a further development of the FEVER code /16/. A burnup chain for 44 fission products is included, which can optionally be supplemented. Collapsing the cross sections into broader energy groups can be made for 171 – at present- nuclides of the source libraries, as desired for a more detailed calculation of the isotopic composition of the fuel by means of the code ORIGEN-JUEL-II /4/.

The THERMIX code /17,21,22/ is included as program part for static and for time dependent thermal hydraulics. The resulting temperature values of the fuel and of the moderator regions may be fed back to the spectrum calculation in each spectrum zone for subsequent core neutronics calculations.

The economics code KPD /18/ performs the fuel cycle cost evaluation on the basis of the "present worth" method.

The status of the reactor at the end of each calculation can be preserved for a restart of the code. Further preservation of calculated reactor data may be provided for the purpose of joint evaluations beyond the capability of VSOP. The full irradiation history of the fuel batches is preserved for the calculation of the local and of the integral decay power of the fuel by means

of the NAKURE code /19/, which is included in VSOP as a subroutine and which is needed e.g. for the explicit following of reactor heat-up under loss-of-coolant conditions.

Internal restart facilities have been included for THERMOS and CITATION: After convergence of the first calculation the neutron flux fields are preserved as initial values for subsequent calculations, which results in a efficient reduction of the computing time.

The simulation of the fuel burnup is an alternation between the simulation of the fuel shuffling, the evaluation of the space and energy dependent neutron flux and the resulting local depletion and generation of the nuclides. In the nomenclature of the code the phase between two shuffling steps is named "Burnup Cycle". It is subdivided into "large burnup time steps". At its beginning the spectrum calculations and the diffusion calculation can be repeated. All flux values then are re-normalized to the demanded power level of the reactor. The large burnup time steps are subdivided again into "small burnup time steps". According to the proceeding burnup of the fuel, the height of the neutron flux is re-adjusted to the core power for each of these steps, whereas its spatial distribution remains unchanged till the start of the next large burnup time step.

For each small burnup time step, the subroutines ADAGE and BURNUP are called in order to solve the burnup equations for the fuel elements, using the re-normalized neutron flux at its local position.

3.2 Nuclear data

3.2.1 Libraries

Neutron spectrum calculations are performed using the GAM-I /12/ and the THERMOS /13,14/ code. The two respective libraries have been derived from the evaluated nuclear data files ENDF/B-V and JEF-1. The GAM-library data is given in an 68-energy group structure ranging from 10 MeV through 0.414 eV. It contains cross section data for 171 materials. In addition, there are 6 more heavy metal isotopes included (Id.-no. 185 through 190), which are part of the actinide build-up chain. These are short-lived isotopes, and only decay constants but no cross section data have been available to the authors for the time being. Their half-lives, however, are short enough (some minutes through 2 days) to dominate neutron capture rates by far. Thus, neutron capture may well be neglected. A list of the isotopes and of the origin of the nuclear data is given in Table II.

The THERMOS-library data are given in 30 energy groups ranging from 10^{-5} through 2.05 eV. The library (Tab. III) is subdivided into 2 parts: (1) The absorbers with identification numbers identical to those in the GAM-library. (2) The scatterers with identification numbers

made of 4 digits. For the scattering nuclides scattering kernels have formerly been constructed applying different scattering laws and different temperatures. Tab. III gives the respective information. The basic thermal library provides data in the form of the 96-energy group structure of the THERMALIZATION spectrum code. It has to be condensed to a THERMOS library using a neutron spectrum which is representative for the considered reactor. This may be done by use of the program part TTTT (see section 3.2.4). Modifications of the THERMALIZATION-library may easily be done using the auxiliary code MAKI /20/.

Some data concerning disintegration of the heavy metal isotopes by alpha emission, beta decay transitions, positron emission, spontaneous fission and isomeric transitions as well as their half-lives are provided by the ADAGE-library, which is used in the burnup section of the code.

3.2.2 Identification of the nuclides

The number of materials used in the VSOP-calculation is presently limited to 200. This is caused by the dimensioning of some data sets and may easily be extended, if required. The identification of each nuclide is defined by input on cards D2 (Section 4.3.1). Each nuclide of a VSOP-calculation is defined by the number IMAT(I), which is its Id.-no. in the GAM-library, as listed in Table II. A certain sequence must be observed for the designation of the nuclides, which is outlined in Table IV: The heavy metal isotopes (28 at present) are firmly assigned. They are followed by the fission products, with ^{135}Xe and the cumulative fission product in the positions 29 and 30, respectively. The order of the explicitly treated fission products must correspond with the chain definition (Fig. 4). Subsequently, control poisons represent absorbers of variable concentration. They are followed by absorbers of fixed concentrations. The scattering nuclides must be given at the end. Here, they are also identified by their GAM-Id.- numbers. Note that the code accepts several scattering matrices from the THERMOS-library for one and the same scattering nuclide, each for a different temperature of the scattering material. This information is given in the THERMOS data input.

3.2.3 Fission products

Yields are included in the code for 97 fission products (Tab. V). They have been taken partly from ENDF/B-IV, partly from ENDF/B-V. The built-in fission product chain and the sequence of the identification numbers are given in Fig. 4. The second number of this chain is a "non-saturating" fission product. It stands for the sum of many low absorbing fission products which are not included in the chain. The yields of the non saturating fission product were adjusted by comparison with results generated by the ORIGEN-JÜL-II code /4/ which comprises more than 800 fission products explicitly. In a typical HTR with a fuel burnup equal 80 MWd/kg $_{HM}$ the explicit fission products of the VSOP-chain were found to cover 98.02 % of the total neutron absorptions by fission products obtained by the ORIGEN-

calculation. The yields of the accumulative fission products have been adapted to cover the remaining 1.98 %.

It is possible to extend the fission product chain by defining new isotopes, new yields and new chain information on cards V4, V5. Similarly, the chain can be shortened, modified or even be fully replaced by the user of the code.

3.2.4 Preparing a THERMOS-library by means of TTTT

The basic thermal library of VSOP is given in 96 thermal energy groups ranging from 10^{-5} eV through 2.05 eV. It is made in the structure of the zero-dimensional thermal spectrum code THERMALIZATION. For normal use within VSOP this code has been replaced by the THERMOS code performing thermal cell calculations in one dimension and in 30 energy groups.

THERMOS requires a specific 30 group library. This can be generated by condensing the 96 groups THERMALIZATION-library with the neutron flux belonging to the considered problem. For this purpose the VSOP input must be prepared for the respective reactor design case with one representative spectrum zone. On input card T1 a blank space for variable CIDTHER tells the code to run THERMALIZATION instead of THERMOS, and the thermal neutron spectrum is preserved for the condensation of the cross sections (see input description of sections 4.4.5 and 4.4.11).

Table I: Available THERMOS libraries

Data set name	Neutron spectrum typical for:
therm1515	HTR
therm1516	LWR
therm1517	HWR
therm1518	*
therm1519	*

* reserved for additional libraries to be generated by the user, if desired

Table II: GAM-library

Id.-no.				Id.-no.				Id.-no.			
1	H-1	Mat 1301	ENDFB-V	64	Pd-105	Mat 4465	JEF-1	123	Gd-158	Mat 4648	JEF-1
2	H-2	Mat 4012	JEF-1	65	Pd-106	Mat 4466	JEF-1	124	Tb-159	Mat 4659	JEF-1
3	Be-9	Mat 1289	ENDFB-4	66	Pd-107	Mat 4467	JEF-1	125	Au-197	Mat 4797	JEF-1
4	B(nat)		JEF-1	67	Pd-108	Mat 9386	ENDFB-V	126	Pb	Mat 4820	JEF-1
5	C	Mat 1306	ENDFB-V	68	Pd-110	Mat 4460	JEF-1	127	Bi-209	Mat 4839	JEF-1
6	Th-232	Mat 4902	JEF-1	69	Ag-109	Mat 1373	ENDFB-V	128	Li-6	Mat 4036	JEF-1
7	Pa-233	Mat 1391	ENDFB-V	70	In-115	Mat 4495	JEF-1	129	Li-7	Mat 4037	JEF-1
8	U-233	Mat 4923	JEF-1	71	Cd	Mat 4480	JEF-1	130	B-10	Mat 4050	JEF-1
9	U-234	Mat 4924	JEF-1	72	Cd-110	Mat 4483	JEF-1	132	U-237	Mat 4927	JEF-1
10	U-235	Mat 4925	JEF-1	73	Cd-111	Mat 4484	JEF-1	133	Np-237	Mat 4937	JEF-1
11	U-236	Mat 4926	JEF-1	74	Cd-112	Mat 4485	JEF-1	134	V mit Cr-Streumatr.		GER
12	U-238	Mat 4928	JEF-1	75	Cd-113	Mat 4486	JEF-1	135	V	Mat 4230	JEF-1
13	Np-239	Mat 4939	JEF-1	76	Cd-114	Mat 4487	JEF-1	136	Nb mit Zr-Streumatr.		GER
14	Pu-239	Mat 1264	ENDFB-4	77	Te-126	Mat 4525	JEF-1	137	Ti	Mat 4220	JEF-1
15	Pu-240	Mat 4940	JEF-1	78	Te-128	Mat 4527	JEF-1	139	Ag-107	Mat 4477	JEF-1
16	Pu-241	Mat 4941	JEF-1	79	Te-130	Mat 4529	JEF-1	140	Nb-93	Mat 4413	JEF-1
17	Pu-242	Mat 1342	ENDFB-V	80	I-127	Mat 9606	ENDFB-V	141	W(nat)		JEF-1
22	N-14	Mat 4074	JEF-1	81	I-129	Mat 9608	ENDFB-V	142	Ru-105	Mat 4445	JEF-1
23	O-16	Mat 4086	JEF-1	82	Xe-128	Mat 4542	JEF-1	143	Rh-105	Mat 4455	JEF-1
24	Mg	Mat 4120	JEF-1	83	Xe-130	Mat 4544	JEF-1	144	Cs-134	Mat 4554	JEF-1
25	Al-27	Mat 4137	JEF-1	84	Xe-131	Mat 4545	JEF-1	145	Ce-144	Mat 4584	JEF-1
26	Si	Mat 4140	JEF-1	85	Xe-132	Mat 4546	JEF-1	146	Pr-142	Mat 4592	JEF-1
27	Cr	Mat 4240	JEF-1	86	Xe-134	Mat 4548	JEF-1	147	Pm-148	Mat 4612	JEF-1
28	Mn-55	Mat 4255	JEF-1	87	Xe-135	Mat 4549	JEF-1	148	Pm-148m	Mat 4613	JEF-1
29	Fe(nat)	Mat 4260	JEF-1	88	Xe-136	Mat 4551	JEF-1	149	Zr-95	Mat 4405	JEF-1
30	Co-59	Mat 4279	JEF-1	89	Cs-133	Mat 4553	JEF-1	151	Ru-103	Mat 4443	JEF-1
31	Ni	Mat 4280	JEF-1	90	Cs-135	Mat 4555	JEF-1	152	Xe-133	Mat 4547	JEF-1
32	Cu	Mat 4290	JEF-1	91	Cs-137	Mat 9669	ENDFB-V	153	Ce-141	Mat 9725	ENDFB-V
33	Se-82	Mat 4342	JEF-1	92	Ba-134	Mat 4564	JEF-1	154	Pr-143	Mat 4593	JEF-1
34	Br-81	Mat 4351	JEF-1	93	Ba-136	Mat 4566	JEF-1	155	Pm-149	Mat 4614	JEF-1
35	Kr-83	Mat 4363	JEF-1	94	Ba-137	Mat 4567	JEF-1	156	I-131	Mat 4536	JEF-1
36	Kr-84	Mat 4364	JEF-1	95	Ba-138	Mat 4568	JEF-1	160	Accum.fiss.prod.chain		44
37	Kr-85	Mat 4365	JEF-1	96	La-139	Mat 9707	ENDFB-V	164	B-11	Mat 4051	JEF-1
38	Kr-86	Mat 4366	JEF-1	97	Ce-140	Mat 4580	JEF-1	165	Hf-174	Mat 4724	JEF-1
39	Rb-85	Mat 4375	JEF-1	98	Ce-142	Mat 4582	JEF-1	166	Hf-176	Mat 4726	JEF-1
40	Rb-87	Mat 4377	JEF-1	99	Pr-141	Mat 9742	ENDFB-V	167	Hf-177	Mat 4727	JEF-1
41	Sr-88	Mat 4388	JEF-1	100	Nd-142	Mat 9763	ENDFB-V	168	Hf-178	Mat 4728	JEF-1
42	Sr-90	Mat 4380	JEF-1	101	Nd-143	Mat 4603	JEF-1	169	Hf-179	Mat 4729	JEF-1
43	Y-89	Mat 4399	JEF-1	102	Nd-144	Mat 4604	JEF-1	170	Hf-180	Mat 4720	JEF-1
44	Zr	Mat 4409	JEF-1	103	Nd-145	Mat 9766	ENDFB-V	171	W-182	Mat 4742	JEF-1
45	Zr-90	Mat 4400	JEF-1	104	Nd-146	Mat 4606	JEF-1	172	W-183	Mat 4743	JEF-1
46	Zr-91	Mat 4401	JEF-1	105	Nd-148	Mat 9769	ENDFB-V	173	W-184	Mat 4744	JEF-1
47	Zr-92	Mat 4402	JEF-1	106	Nd-150	Mat 4600	JEF-1	174	W-186	Mat 4746	JEF-1
48	Zr-93	Mat 4403	JEF-1	107	Pm-147	Mat 9783	ENDFB-V	175	Pm-151	Mat 4615	JEF-1
49	Zr-94	Mat 4404	JEF-1	108	Sm-147	Mat 9806	ENDFB-V	176	U-232	Mat 8232	ENDFB-V
50	Zr-96	Mat 4406	JEF-1	109	Sm-148	Mat 9807	ENDFB-V	177	Pu-238	Mat 1338	ENDFB-V
51	Mo	Mat 4420	JEF-1	110	Sm-149	Mat 1319	ENDFB-V	178	Am-241	Mat 1361	ENDFB-V
52	Mo-95	Mat 4425	JEF-1	111	Sm-150	Mat 9809	ENDFB-V	179	Am-242	Mat 8542	ENDFB-V
53	Mo-96	Mat 9283	ENDFB-V	112	Sm-151	Mat 4621	JEF-1	180	Am-242m	Mat 1369	ENDFB-V
54	Mo-97	Mat 4427	JEF-1	113	Sm-152	Mat 9811	ENDFB-V	181	Am-243	Mat 1363	ENDFB-V
55	Mo-98	Mat 9285	ENDFB-V	114	Sm-154	Mat 9813	ENDFB-V	182	Cm-242	Mat 8642	ENDFB-V
56	Mo-100	Mat 9287	ENDFB-V	115	Eu-151	Mat 4631	JEF-1	183	Cm-243	Mat 1343	ENDFB-V
57	Tc-99	Mat 1308	ENDFB-V	116	Eu-153	Mat 4633	JEF-1	184	Cm-244	Mat 1344	ENDFB-V
58	Ru-100	Mat 4440	JEF-1	117	Eu-154	Mat 4634	JEF-1	185	Th-233		0-SIGMA
59	Ru-101	Mat 4441	JEF-1	118	Eu-155	Mat 9832	ENDFB-V	186	U -239		0-SIGMA
60	Ru-102	Mat 4442	JEF-1	119	Gd-154	Mat 4644	JEF-1	187	Np-238		0-SIGMA
61	Ru-104	Mat 4444	JEF-1	120	Gd-155	Mat 4645	JEF-1	188	Np-240		0-SIGMA
62	Rh-103	Mat 1310	ENDFB-V	121	Gd-156	Mat 4646	JEF-1	189	Pu-243		0-SIGMA
63	Pd-104	Mat 4464	JEF-1	122	Gd-157	Mat 4647	JEF-1	190	Am-244		0-SIGMA

Table III: THERMOS-library

Id.-no.	Absorber
	H-1 ⎫
	H-2 ⎬ see Scatterer
	Be-9 ⎭
4	B(nat) JEF-1
	C see Scatterer
6 ⎫	
: ⎬	see GAM-Library
22 ⎭	
	O-16 see Scatterer
24 ⎫	
: ⎬	see GAM-library
190 ⎭	

Id.-no.	Scatterer
1001	Carbon 300°K P0 & P1 Summit to 1eV & Gas 739.32°K 1/V 3.88mb
1002	Carbon 600°K P0 & P1 Summit to 1eV & Gas 890.98°K 1/V 3.88mb
1003	Carbon 900°K P0 & P1 Summit to 1eV & Gas 1110.51°K 1/V 3.88mb
1004	Carbon 1200°K P0 & P1 Summit to 1eV & Gas 1363.14°K 1/V 3.88mb
1005	Carbon 1350°K P0 & P1 Gas kernel 1/V Absorption Sigma0=3.88mb
1006	Carbon 1500°K P0 & P1 Gas kernel 1/V Absorption Sigma0=3.88mb
1007	Hydrogen 300°K P0 & P1 Gas kernel 1/V Absorption Sigma0=.332b
1008	Hydrogen in H_2O 300°K P0 & P1 Gaker to 1eV & Gas 1153.26°K 1/V .332b
1009	Hydrogen 589°K P0 & P1 Gas kernel 600F 1/V .332b
1010	Hydrogen in H_2O 589°K 600F P0 & P1 Gaker to 1eV & Gas 1269.37°K 1/V .332b
1011	Hydrogen 1200°K P0 & P1 Gas kernel 1/V Sigma0=.332b
1012	Beryllium 980°K P0 & P1 Gas kernel 1/V Sigma0=10mb
1013	Beryllium 1366°K P0 & P1 Gas kernel 2000F 1/V Sigma0=10mb
1014	Beryllium 1422°K P0 & P1 Gas kernel 2100F 1/V Sigma0=10mb
1015	Oxygen 589°K P0 & P1 Gas kernel 600F
1016	Deuterium 293.4°K Gas-Kern Teuchert 18.5.1967
1017	Deuterium 493.4°K Gas-Kern Teuchert 18.5.1967
1018	Deuterium 593.4°K Gas-Kern Teuchert 18.5.1967
1019	Deuterium 693.4°K Gas-Kern Teuchert 18.5.1967
1020	Deuterium 593°K Gaker-Kira for Gr.1-55, 22-75 & Gas kernel Teu/Ha.67
1021	Oxygen 900°K Gas-Kern with BASK
1022	Beryllium in BeO 900°K Summit-BeO-Matr. minus O-Matr. Rest von 1012
1023	Berylliumoxyd 900°K Summit-BeO-Matr. XA=0.01/V XS=9.69 S=S(O) & S(Be)
1101	Hydrogen 293.6°K Nelkin-Kern (Gaker-Kira) IX.68 Darvas
1102	Hydrogen 323.6°K Nelkin-Kern (Gaker-Kira) IX.68 Darvas
1103	Hydrogen 373.6°K Nelkin-Kern (Gaker-Kira) IX.68 Darvas
1104	Hydrogen 473.6°K Nelkin-Kern (Gaker-Kira) IX.68 Darvas
1105	Hydrogen 573.6°K Nelkin-Kern (Gaker-Kira) IX.68 Darvas
1111	Deuterium 293.6°K Nelkin-Kern (Gaker-Kira) IX.68 Darvas
1112	Deuterium 323.6°K Nelkin-Kern (Gaker-Kira) IX.68 Darvas
1113	Deuterium 373.6°K Nelkin-Kern (Gaker-Kira) IX.68 Darvas
1114	Deuterium 473.6°K Nelkin-Kern (Gaker-Kira) IX.68 Darvas
1115	Deuterium 573.6°K Nelkin-Kern (Gaker-Kira) IX.68 Darvas
1121	Oxygen 293.6°K Brown-St-John-Freigas IX.68 Teuchert
1122	Oxygen 323.6°K Brown-St-John-Freigas IX.68 Teuchert
1123	Oxygen 373.6°K Brown-St-John-Freigas IX.68 Teuchert
1124	Oxygen 473.6°K Brown-St-John-Freigas IX.68 Teuchert
1125	Oxygen 573.6°K Brown-St-John-Freigas IX.68 Teuchert
1126	Oxygen 900°K Brown-St-John-Freigas XII.70 Teuchert
1127	Oxygen 1200°K Brown-St-John-Freigas XII.70 Teuchert
1128	Oxygen 1350°K Brown-St-John-Freigas XII.70 Teuchert
1500	Weißer Riese 1000°K Atomgewicht 1000000 22.XII.70
1600	Carbon 300°K Young Phon.-Spektr. Colli Punktwerte 2eV Schroeder 4.7.70
1601	Carbon 400°K Young Phon.-Spektr. Colli Punktwerte 2eV Schroeder 4.7.70
1602	Carbon 500°K Young Phon.-Spektr. Colli Punktwerte 2eV Schroeder 4.7.70
1603	Carbon 600°K Young Phon.-Spektr. Colli Punktwerte 2eV Schroeder 4.7.70
1604	Carbon 700°K Young Phon.-Spektr. Colli Punktwerte 2eV Schroeder 4.7.70
1605	Carbon 800°K Young Phon.-Spektr. Colli Punktwerte 2eV Schroeder 4.7.70
1606	Carbon 900°K Young Phon.-Spektr. Colli Punktwerte 2eV Schroeder 4.7.70
1607	Carbon 1000°K Young Phon.-Spektr. Colli Punktwerte 2eV Schroeder 4.7.70
1608	Carbon 1100°K Young Phon.-Spektr. Colli Punktwerte 2eV Schroeder 4.7.70
1609	Carbon 1200°K Young Phon.-Spektr. Colli Punktwerte 2eV Schroeder 4.7.70
1610	Carbon 1300°K Young Phon.-Spektr. Colli Punktwerte 2eV Schroeder 4.7.70
1611	Carbon 1350°K Young Phon.-Spektr. Colli Punktwerte 2eV Schroeder 4.7.70
1612	Carbon 1500°K Young Phon.-Spektr. Colli Punktwerte 2eV Schroeder 4.7.70

Table IV: Sequence of nuclides

	VSOP-Id.no.		GAM-Id.no.	
1.	Heavy metal isotopes are firmly assigned:			
	1	Th-232	6	
	2	Th-233	185	
	3	Pa-233	7	
	4	U -233	8	
	5	U -234	9	
	6	U -235	10	
	7	U -236	11	
	8	U -237	132	
	9	U -238	12	
	10	U -239	186	
	11	Np-237	133	
	12	Np-238	187	
	13	Np-239	13	
	14	Np-240	188	
	15	Pu-238	177	
	16	Pu-239	14	
	17	Pu-240	15	
	18	Pu-241	16	
	19	Pu-242	17	
	20	Pu-243	189	
	21	Am-241	178	
	22	Am-242m	180	
	23	Am-242	179	
	24	Am-243	181	
	25	Am-244	190	
	26	Cm-242	182	
	27	Cm-243	183	
	28	Cm-244	184	
2.	Fission products of chain definition:			
	29	Xe-135		
	30	Accumulative fission product		
	31 ...	Further isotopes of the chain		
		NO ≤ 49 fission products are allowed		
3.	Control poison:			
	subsequent	NC = 0-2 different nuclides are possible with concentrations adjustable to achieve given K_{eff}.		
4.	Non burning absorbers:			
	subsequent	Absorbers for which concentrations remain unchanged during burnup, e.g. structural materials		
5.	Scatterers:			
	subsequent	NKER = 1-5 scatterers must be given at the end.		

Table V: Fission product yields (values given in percentages)

Isotope	Type	U -233	U -235	Pu-239	Pu-241
Se- 82	t	0.56262	0.33405	0.21092	0.11602
Br- 81	t	0.31171	0.21005	0.1768	0.06469
Kr- 83	t	1.0178	0.53076	0.29608	0.20498
Kr- 84	t	1.7034	0.98786	0.48029	0.35393
Kr- 85	c	2.1946	1.314	0.56834	0.39618
Kr- 86	c	2.8581	1.9528	0.75863	0.61392
Rb- 85	i	6.5296-5	8.23-5	5.85-5	5.3024-7
Rb- 87	t	4.0088	2.551	0.94936	0.75709
Sr- 88	t	5.4953	3.6228	1.3703	0.97473
Sr- 90	c	6.7952	5.9137	2.1134	1.5363
Y - 89	t	6.2568	4.8469	1.7075	1.2146
Zr(nat)		6.4467	5.803	2.6405	2.645
Zr- 90	i	0.05	0.047	0.0164	0.0164
Zr- 91	t	6.5194	5.926	2.4941	1.8315
Zr- 92	t	6.5949	5.966	3.018	2.2781
Zr- 93	c	7.011	6.3703	3.9031	2.9643
Zr- 94	c	6.8076	6.4228	4.4431	3.4018
Zr- 95	c	6.2478	6.4678	4.9212	4.0456
Zr- 96	t	5.6694	6.2506	5.0958	4.4232
Mo- 95	c	9.5909-4	1.641-4	1.492-3	1.2927-5
Mo- 96	i	6.5-3	5.85-4	7.7-4	7.7-4
Mo- 97	t	5.4533	5.96	5.608	4.8208
Mo- 98	t	5.1587	5.7787	5.8542	5.2217
Mo-100	t	4.4094	6.3096	6.977	6.2311
Tc- 99	c	4.9573	6.1284	6.1405	6.2085
Ru-101	t	3.2258	5.0501	5.9135	6.0948
Ru-102	t	2.4492	4.2032	6.0201	6.4843
Ru-103	c	1.7066	3.1411	6.9845	6.2611
Ru-104	t	1.0276	1.8239	5.9539	6.9764
Ru-105		0.48	0.9	5.47	5.47
Rh-103	i	1.4219-9	1.858-9	1.358-7	5.6028-5
Rh-105	c	0.47126	1.0199	5.4261	6.2183
Pd-105	i	3.4998-11	9.83-11	2.03-8	1.6908-6
Pd-106		0.24063	0.37759	4.6234	4.6314
Pd-107	c	0.11417	0.16317	3.2361	5.3339
Pd-108	t	0.061481	0.071032	2.2319	4.0191
Pd-110	t	0.025376	0.022338	0.62204	1.2091
Ag-109	t	0.043363	0.029903	1.4115	2.2836
Cd-111	t	0.020268	0.019714	0.27428	0.57261
Cd-112	t	0.014602	0.012802	0.10707	0.23001
Cd-113	c	0.013152	0.012425	0.078216	0.15494
Cd-114	t	0.012268	0.011256	0.046789	0.075514
In-115		0.020052	9.9367-3	0.040467	0.040537
Te-126	t	0.24081	0.057818	0.19996	0.077127
Te-128	c	0.94592	0.35046	0.85079	0.35555
Te-130	c	2.3671	1.4466	2.4971	1.6617
I -127	t	0.67853	0.13037	0.49173	0.23046
I -129	c	1.616	0.65911	1.5039	0.77864
I -131	c	3.7089	2.8325	3.738	3.1411
I -135	c	4.8597	6.3482	6.3007	6.95
Xe-131	i	8.4795-5	1.54-6	1.652-5	1.3066-6
Xe-132	t	4.8038	4.2498	5.2688	4.6411
Xe-133	c	6.0307	6.7859	6.9758	6.741
Xe-134	c	5.7588	7.6825	7.389	8.1081
Xe-135	i	1.3374	0.2541	1.1517	0.22923
Xe-135	c	6.1971	6.6023	7.4524	7.1792
Xe-136	c	6.7934	6.2701	6.6153	7.2871
Cs-133	i	3.6998-5	5.08-5	1.61-5	4.302-7
Cs-134	i	1.1969-3	3.57-5	4.61-4	3.5416-5
Cs-135	c	6.1	6.45	7.22	7.8
Cs-137	c	6.7889	6.269	6.6834	6.698
Ba-138	t	5.8863	6.8272	5.7173	6.4446

continued.....

Continuation of Fission Product Yields

La-139	t	5.885	6.4933	5.6456	6.2283
Ce-140	t	6.4334	6.3229	5.5751	5.894
Ce-141		6.24	5.73	6.11	6.11
Ce-142	t	6.6304	5.9247	5.0173	4.815
Ce-144		4.5117	5.962	4.4514	4.8644
Pr-141	t	6.6224	5.8929	5.3634	4.8534
Pr-143	c	5.8513	5.971	4.5613	4.5017
Nd-142		0.	0.009	0.0009	0.0009
Nd-143	i	2.4799-8	9.5-11	4.9-10	1.2106-10
Nd-144	t	4.6495	5.4523	3.834	4.1564
Nd-145	t	3.4248	3.9339	3.0833	3.2046
Nd-146	t	2.5973	2.9912	2.5333	2.7401
Nd-148	t	1.2867	1.69	1.6982	1.9257
Nd-150	c	0.49846	0.64593	0.99451	1.196
Pm-147	c	1.7753	2.2701	2.0769	2.2601
Pm-148m	i	2.7899-5	7.49-7	2.09-6	5.4125-7
Pm-148g	i	9.4395-7	5.73-6	2.09-6	5.4125-7
Pm-149		0.76953	1.0888	1.2617	1.4635
Pm-151		0.32293	0.42044	0.7772	0.90238
Sm-147	i	2.0099-10	0.	2.43-12	0.
Sm-148	i	1.7999-8	6.95-11	2.8-10	4.272-11
Sm-149		0.	0.	0.	0.
Sm-150	c	2.5782-3	5.413-4	1.7009-3	3.9438-4
Sm-151		0.	0.	0.	0.
Sm-152	t	0.20784	0.27057	0.59618	0.71704
Sm-154	t	0.04558	0.074689	0.27682	0.37979
Eu-153	t	0.10686	0.16264	0.37224	0.52815
Eu-154	i	3.7198-5	1.63-6	3.54-5	5.5626-6
Eu-155	c	0.021252	0.033025	0.17082	0.23181
Gd-154		0.	0.	0.	0.
Gd-155	i	3.6198-7	4.41-9	2.83-7	1.9109-8
Gd-156	t	0.011737	0.013517	0.11989	0.16955
Gd-157	t	6.7747-3	6.4651-3	0.076297	0.13153
Gd-158	t	2.2298-3	3.2163-3	0.040955	0.086707
Tb-159	t	9.2311-4	1.0394-3	0.021205	0.046741

i = Independent fission yield
c = Cumulative fission yield
t = Total chain yield

Accumulative Fission Product:

U-233	U-235	Pu-239	Pu-241
112.3	94.76	115.6	110.4

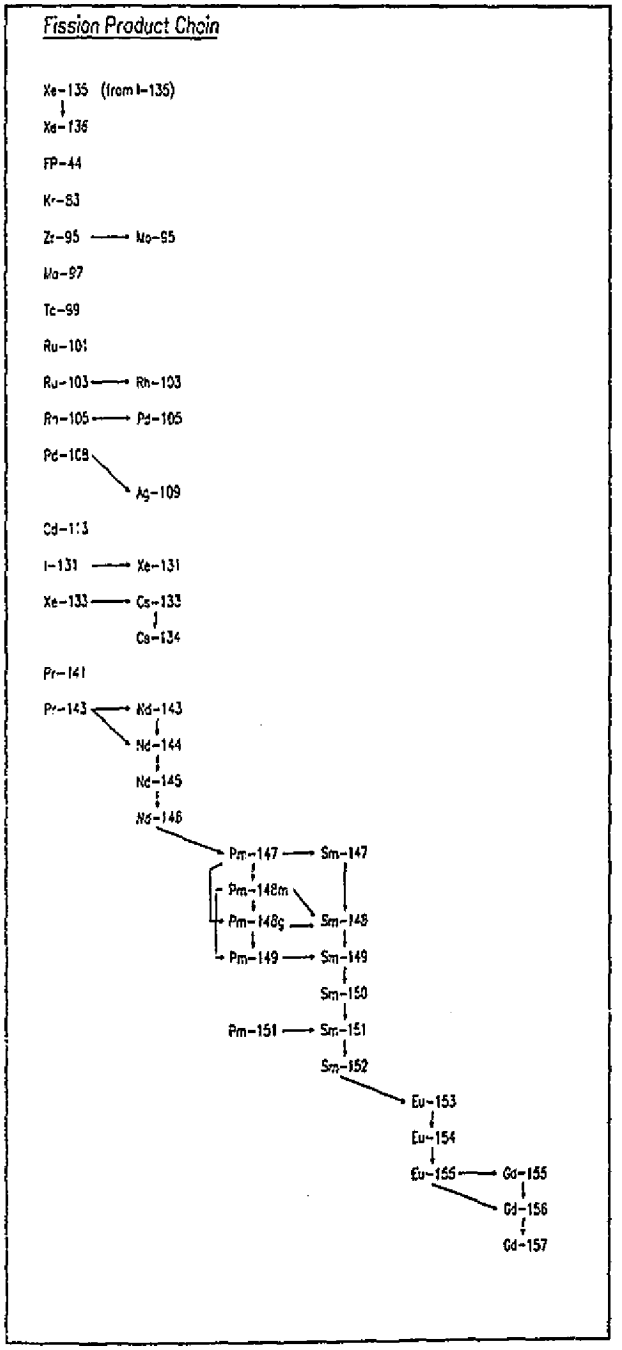

Fig.4: Built-in fission product chain

	VSOP-No	GAM-No
^{135}Xe	29	87
FP-44	30	160
^{136}Xe	31	88
^{83}Kr	32	35
^{95}Zr	33	149
^{95}Mo	34	52
^{97}Mo	35	54
^{99}Tc	36	57
^{101}Ru	37	59
^{103}Ru	38	151
^{103}Rh	39	62
^{105}Rh	40	143
^{105}Pd	41	64
^{108}Pd	42	67
^{109}Ag	43	69
^{113}Cd	44	75
^{131}I	45	156
^{131}Xe	46	84
^{133}Xe	47	152
^{133}Cs	48	89
^{134}Cs	49	144
^{141}Pr	50	99
^{143}Pr	51	154
^{143}Nd	52	101
^{144}Nd	53	102
^{145}Nd	54	103
^{146}Nd	55	104
^{147}Pm	56	107
^{148}Pm-m	57	148
^{148}Pm-g	58	147
^{147}Sm	59	108
^{148}Sm	60	109
^{149}Pm	61	155
^{149}Sm	62	110
^{150}Sm	63	111
^{151}Pm	64	175
^{151}Sm	65	112
^{152}Sm	66	113
^{153}Eu	67	116
^{154}Eu	68	117
^{155}Eu	69	118
^{155}Gd	70	120
^{156}Gd	71	121
^{157}Gd	72	122

3.3 Properties of reactor materials (particularly Graphite) and of the Pebble Bed

The thermal conductivity λ of graphite is a function of four parameters:

1. The type of graphite material due to its fabrication techniques
2. Its temperature *T*
3. The exposure to fast neutrons *D*
4. The temperature at which this exposure occurred

Broad experimental research on this matter has been performed by L. Binkele /23/.

As an example Fig. 5 (left part) gives λ(T,D) for the NUKEM/A3-3 graphite having been exposed to fast neutrons at the temperature 950 °C. Measurements were made at ten different temperature values (100.....1000 °C) and for 5 different status of fast neutron exposure (0.....$6.09*10^{21}$ cm^{-2}, E>0.1 MeV). For T>1000 °C experimental values have been missing. Therefore, these data have been constructed by extrapolation. The function λ (T,D) is included in the code as default, but it can be replaced by any other function to be defined as data input.

For many other materials the functions λ (T) are also included in the code. A survey of these functions is given in Tab. VII. For more detailed information we refer to subroutine XLAMT. Similarly, the included functions of the heat capacity (Tab. VI) are given in the subroutine WKPT.

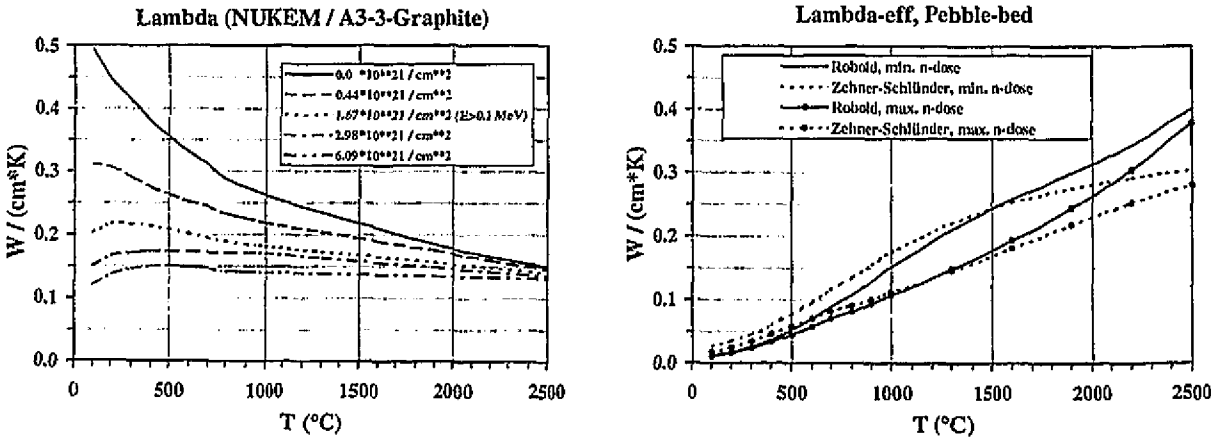

Fig. 5: Thermal conductivity

The heat transport through the bed of pebbles takes place partly by thermal conduction through the pebbles and partly by thermal radiation from one pebble to the other. Theoretical

models have been developed for the description of the mechanism of heat transport. At the end an effective thermal conductivity λ_{eff} (T,D) is defined which can be applied in the normal equation (4) (chapter A.6.1) of thermal conduction.

The model of Zehner-Schlünder accounts for the heat transport from one pebble to the next one. His finding is represented in the Heat Atlas /24/. It has been verified in experiments, and it is recommended for the pebble-bed at low and medium temperature levels.

The model of Robold /26/ takes special care of the heat transport through the openings between the pebbles of the bed by radiation. Again it derives an λ_{eff} (T,D) which is preferred at higher temperatures, i.e. for T > 1400 °C.

The effective thermal conductivity of the pebble-bed for both the models is illustrated in Fig. 5 (right part). It is drawn for the highest and for the lowest neutron dose corresponding to the function λ (T,D) of the graphite. In current calculations the code evaluates both models of Zehner-Schlünder and of Robold, respectively, and it applies the respective maximum of the two models.

Tab. VI: Available formulae of heat capacity

Id.no.	*Material function of temperature dependent heat capacity*	
6	Steatite	
7	Reactor graphite	density 1.75 gr. / cm^3
8	Carbon bricks (like Reakt. graph.)	density 1.55 gr. / cm^3
11	V2A - Steel (Hoesch)	DIN 4541
12	Thermal shield	
13	Reactor graphite (HRB)	density 1.70 gr. / cm^3
14	Reactor graphite (HRB)	density 1.60 gr. / cm^3
15	Reactor graphite (HRB)	density 1.80 gr. / cm^3
16	Al_2O_3	not a function of temperature

Tab. VII: Available formulae of thermal conductivity

Id.no.		*Material function*
1	Sodium (liquid)	
2	Graphite (Matrix)	T = irradiation temperature
3	Graphite (Reflector)	Interpolation from tables (see Subroutine GFIT)
4	EPS > 0.: Helium EPS = 0.: Static Helium	LAM0 = pressure (bar) 1 bar
5	Pebble bed	Extrapolation from experiments (Barthels)
6	Zehner- Schlünder for Steatite	Experiment (K. Verfondern)
7	Reactor graphite	LAMDA(0) = LAM (Comp.)
8	Carbon bricks	"Lukascewicz"
9	Static air	1 bar
10	Thermal shield (HRB)	
11	V2A - Steel (Thyssen	DIN 4541
12	Pebble bed	Breitbach/Barthels
13	Steatite	for heterogeneous calculation
14	Graphite balls	Experiment (Robolt)
15	Armed concrete	
16	Prismatic core	axial
17	Carbon-felt	in vacuum
18	Carbon-felt	in Ar- or N_2 atmosphere
19	Anti-friction bearing steel	100CR6
20	Static Nitrogen	
21	Kaowool-mat	in air (Jül 992RB)
22	H A W-glass	
23	Pebble bed	Schürenkrämer (II.84)
24	Ball graphite, Binkele/A3 graphite	Function of temperature and neutron dose (explicit)
25	LAMDA-eff., pebble bed	Function of temperature and neutron dose (Robolt)
26	Lambda eff., pebble bed	Function of temperature and dose (Zehner- Schlünder)
27	Lambda eff., pebble bed	Function of temp. and dose (Robolt+Zehner-Schlünder)
28	Al_2O_3	linear (Salmang/Scholz "Keramik")
29	Gilsonit coke (AGL-IE 1-24)	Irradiated at 760 °C (Binkele)

3.4 List of data sets

In the following all those units for intermediate or long-term storage of data are listed, which are not automatically scrapped at the end of a VSOP calculation:

a) VSOP-MS

Log. Unit No.	Data set name	Description
5	not fixed	Card image data input. DS-name to be defined by the user at the start of program execution.
6	not fixed	Print output. DS-name to be defined by the user at the start of program execution.
14	'rstold'	Read restart data (status of reactor operation, i.e. broad group cross sections, atom densities of the batches, shuffling scheme etc.), which were produced by a previous VSOP-calculation as data set 'rstnew' (see unit 15).
15	'rstnew'	Restart data written at the end of the last calculated burnup cycle, to be read from unit 14 as data set 'rstold' in a following restart.
16	'gam5115'	GAM-library data.
17	'thermal'	THERMALIZATION-library data.
18	'thermxxxx'	with 'xxxx' according to table I: THERMOS-library data.
19	'thermix'	Results of THERMIX are stored onto this data set in a steady-state calculation. They are retrieved from this data set in a subsequent time-dependent calculation.
20	'rstslib'	Restart data: Basic information on the spectrum calculation, i.e. libraries, group structure, cell structure etc. The data are written after the first fuel shuffling operation of the first VSOP calculation of a series. They are read in all subsequent restarts.
28	'nucdens'	Optional storage of atom densities of each batch.
30	'resint'	Effective resonance integrals (GAM-group structure) produced and stored in case of a VSOP-ZUT-calculation. To be read and used in a VSOP-MS-calculation.
33	'costdata'	Cost data library.
35	'rstflux'	Restart data (neutron flux map etc.).
37	'geomcit'	Restart data (geometry data for diffusion section).
42	'macsig'	Macroscopic cross sections are stored on this DS.
43	'geomther'	Restart data (geometry data for thermal hydraulics section)
44	'atlas'	Data set for external use in code 'ATLAS'.
53	'phiunfor'	Printout of point-flux values by group is copied to this data set (optionally). Unformatted data.

54	'powunfor'	Like unit 53, but for point power density
58	'therlist'	and →
59	'temunfor'	Some results of the transient THERMIX calculation are stored on data sets 58 and 59 for further use e.g. in external plot routines. (Unformatted data, see FORTRAN code for details, if required).
61	'nakure'	Power histogram of the fuel batches for use in subroutine NACHW (decay power evaluation).
63	'adage'	Contains the ADAGE-library.
64	'tinte'	Preserves data for external use (TINTE code).
66	'inpcit'	CITATION input data. Written at the start to be read in all subsequent restarts.
67	'origen'	Preserves data for external use (ORIGEN-JUEL-II – code).
68	'phiform'	Like unit 53, but formatted data.
69	'origmod'	ORIGEN-JÜL-II library (MEDUL-reactors).
70	'thxnew'	THERMIX-restart data to be written.
71	'thxold'	THERMIX-restart data to be read.
75	'birgplot'	Plot data (core geometry), 2-d, unformatted.
76	'birgexcl'	Plot data (core geometry), 2-d, formatted.
77	'trigplot'	Plot data (core geometry), 3-d,unformatted.
80	'powform'	Like unit 54, but formatted data.
98	'tempform'	Like unit 59, but formatted data.

b) VSOP-ZUT

25	'resdapu2'	Resonance parameters of ^{242}Pu
26	'resdatu5	Resonance parameters of ^{235}U
27	'resdatth'	Resonance parameters of ^{232}Th
28	'resdatu8'	Resonance parameters of ^{238}U

5, 6, 30: see a) VSOP-MS

4. Input Manual V.S.O.P.-MS

4.1 Steering the execution mode. S1 – S3

Card S1		Format (A4,2I4)
1	MODE	= vsop: Complete V.S.O.P.-calculation. Data input may consist of the following parts: card types S, BI or TR (see variable I3D), D, V, G, T, C, K, R, LF, P, TTTT, TX and KX. = geom: Provide geometric reactor design only. Data input consists of cards S, BI (2-d -) or TR (3-d - calculation), exclusively. = fuel: Provide fuel elements design only. Data input consists of cards S and D, exclusively.
2	I3D	= 0: 2-dimensional diffusion calculation in r-z - geometry (cards BI required). = 1: 3-dimensional diffusion calculation in x-y-z - geometry (cards TR required).
3	ITTT	= 0: No effect. > 0: Calculate TTTT (section 4.4.11) in order to prepare a new 30 groups THERMOS-library out of the 96 groups THERMALIZATION-library.

Card S2		Format (A72)
		Literal description of case.

Card S3 only if MODE = 'vsop' on card S1.

Card S3		Format (3I4)
1	JTPE7	= 0: Normal start. > 0: Restart. JTPE7 is the identification number of restart data to be retrieved from data sets 'rstold' and 'rstslib'. Data input continues with cards R6 (optionally, see IRR9 below) or R7.
2	JTPE9	= 0: No effect. > 0: Prepare restart data with id. no. JTPE9 from this calculation, write them onto data sets 'rstnew' and 'rstslib' to be used for a following restart.
3	IRR9	= 0: No effect. > 0: For restart only: Card R6 will be given to re-define the options for the first cycle of the restart.

4.2 Geometric reactor design
(only if MODE = 'vsop' or 'geom')

4.2.1 2-dimensional (r-z – geometry). BI1 - BI11

Cards BI only if I3D = 0 on card S1.

Card BI1		Format (4I6)
1	NCASE	= 0: Parallel flow of spherical fuel elements in vertical flow channels, or no movement of the fuel during reactor operation. Read cards BI1 - BI5. = 1: Flow of fuel pebbles with different speed in various radial channels and/or along non-vertical trajectories. Read cards BI1 - BI9. = 2: Like = 1; prepare geometric data for THERMIX, in addition. Read cards BI1 - BI11. (In case of vertical, parallel fuel element flow, no data for THERMIX needs to be prepared).
2	IPUT	= 0: Normal output. = 1: Test output in addition.
3	IPLOT	= 0: No effect. > 0: Store data for plots on unformatted data set 'birgplot'. < 0: Store same data, but formatted on data set 'birgexcl'.
4	KANAL	Pebble bed: Number of flow channels inside the core. (≤ 15) (see NCASE) Non-moving fuel: Number of radial coarse meshes (equal IMAX resulting from card BI3).

For each of the KANAL channels one card BI2.

Card BI2		Format (3I6)
1	KANTYP	= 1: For the outermost core channel. = 0: For all other core channels.
2	KAN	> 0: Number of axial regions in this channel (≤ 100). For each region a set of macroscopic cross sections will be generated. For use in the diffusion calculation, these data are transferred to the grid which is defined on cards BI4. The total number of regions (core + reflector area) is restricted to 1500. = 0: One region only.
3	IBATCH	> 0: Number of batches per region. = 0: One batch only.

Coarse meshes define the CITATION-material compositions (= regions), the fine meshes define the grid for the neutron flux calculation.

One card BI3 for each radial coarse mesh I.

Card BI3		Format (I6,E12.5,I6)
1	IOP(I)	= 0: Coarse mesh is situated within the core area. = 1: Coarse mesh is situated outside the core. = -1: End of input for radial coarse meshes.
2	DR(I)	Thickness of the I-th radial coarse mesh (cm). Within the core the width of the respective channel is a good choice in most cases.
3	MR(I)	Number of fine radial meshes in this coarse mesh.
	I=1, ...	The number of given radial coarse meshes defines IMAX (see card BI5).

One card BI4 for each axial coarse mesh N.

Card BI4		Format (I6,E12.5,I6)
1	NOP(N)	= 0: Coarse mesh is situated within the core area. = 1: Coarse mesh is situated outside the core. = -1: End of input for axial coarse meshes.
2	DZ(N)	Thickness of the N-th axial coarse mesh for the diffusion calculation. (cm)
3	MZ(N)	> 0: Number of fine axial meshes in this coarse mesh. < 0: This coarse mesh represents the void above a pebble-bed core. |MZ| is the number of fine meshes.
	N=1, ...	The number of given axial coarse meshes defines NMAX (see card BI5).

Each of the NMAX axial coarse meshes N requires one card BI5.

Card BI5		Format (18I4)
1 . IMAX	LAYVC (I,N), I=1,IMAX	> 0: Id.no. of CITATION composition (region), which coarse mesh I is to be assigned to, starting with no. "1" for the first composition outside the core. (The numbers are preliminary and will be renumbered successively after the id. numbers of the core area have been internally defined). = 0: Core area, id. numbers are defined by the code for the fine grid.

Cards BI6 - BI9 only if NCASE > 0 on card BI1.

Card BI6		Format (3I6,3E12.5)
1	KONUS	= 0: No effect. = 1: An outer cone at the bottom of the core structural material is present. = 2: A central reflector column with another cone towards the core bottom is present.
2	IZFEIN	Number of axial meshes of a superposed fine grid for cross section and flux transfer matrix (see also section A.2.1).
3	JRFEIN	Number of radial meshes of the superposed fine grid.
4	EPSY	Convergence criterion for the iteration on the radial position of the mesh points defining the flow channel curves (about 1.E-5).
		Only if KONUS > 0:
5	RKONUS	Radial thickness of the cone. (cm)
6	ZKONUS	Height of the cone. (cm)

For each of the KANAL channels one set of cards BI7 - BI9.

Card BI7		Format (I12,E12.5)
1	IJR	> 0: Number of axial mesh points for the definition of the outer limiting curve of this channel. Only for the inner core channels (KANTYP = 0). IJR = 1 defines a straight vertical line. = -1: The value of IJR is taken from the preceding channel. Drop card BI8. = 0: Last core channel. Drop cards BI8, BI9. Limiting curve is internally defined by the information of card BI3.
2	VEKA	> 0.: Only when KANTYP = 0. Ratio of the volume of this channel per volume of the core. Radial mesh points of the limiting curve will be adapted to meet this volume of the channel. = 0.: No adaptation of the limiting curve.

Card BI8 only if IJR > 0 on card BI7.

Card BI8		Format (6E12.5)
1 . IJR	XWE(J), J=1,IJR	Axial position of the coarse mesh points for the outer limiting curve of this channel (cm), starting from the top of the core (XWE = 0.) down to the bottom (positive values).

Card BI9 only if IJR ≠ 0 on card BI7.

Card BI9		Format (6E12.5)
1 . IJR	YWE(J), J=1,IJR	Radial position of the coarse mesh points for the outer limiting curve of this channel (cm). In case of an annular core, YWE(J) must be given as the distance from the inner limiting curve of the first core channel.

Cards BI10 - BI11 only if NCASE = 2 on card BI1.

For the THERMIX calculation, the fine mesh grid only of the core has to be defined. It must be identical to that of the THERMIX input on cards TX8, TX9.

Card BI10		Format (I3 / (4(E12.5,I6)))
1	IMAXT	Number of radial coarse meshes I within the core.
2	DR(I)	Thickness of the I-th radial coarse mesh. (cm)
3	MR(I)	Number of fine radial meshes within this coarse mesh.
	I=1,IMAXT	

Card BI11		Format (I3 / (4(E12.5,I6)))
1	NMAXT	Number of axial coarse meshes N within the core.
2	DZ(N)	Thickness of the N-th axial coarse mesh. (cm)
3	MZ(N)	Number of fine axial meshes within this coarse mesh.
	N=1,NMAXT	

4.2.2 3-dimensional (x-y-z - geometry). TR1 - TR5

This part of code defines the 3-dim. pattern of compositions in the reactor. VSOP-regions and CITATION-compositions must be identical. They are assigned with the same id. numbers. (See also chapter A.2.1).

Cards TR only if I3D = 1 on card S1.

Card TR1		Format (3I5)
1	MYX	= 0: 1 batch per region. > 0: Number of batches per region. Note: The total number of regions as well as of batches is limited to 9999 !!
2	IPL	= 0: No effect. > 0: Plot data for plane no. IPL is written onto data set 'trigplot'. (For special purposes only).
3	ICORE	= 0: Normal. > 0: Just for plot data: = 2: Data of ½ core-plane are transmuted to 1/1 core-plane. = 4: Data of ¼ core-plane are transmuted to 1/1 core-plane.

Meshes in X-direction.

Card TR2		Format (6(I3,F9.3))
1	MX(I)	Number of fine meshes in the I-th coarse mesh in X-direction.
2	DX(I)	> 0.: Thickness of the I-th coarse X-mesh. (cm) = 0.: End of the input of coarse X-meshes.
	I=1, ...	The number of given coarse X-meshes defines IMX.

Meshes in Y-direction.

Card TR3		Format (6(I3,F9.3))
1	MY(J)	Number of fine meshes in the J-th coarse mesh in Y-direction.
2	DY(J)	> 0.: Thickness of the J-th coarse Y-mesh. (cm) = 0.: End of the input of coarse Y-meshes.
	J=1, ...	The number of given coarse Y-meshes defines JMY.

Meshes in Z-direction.

Card TR4		Format (6(I3,F9.3))
1	MZ(K)	Number of fine meshes in the K-th coarse mesh in Z-direction.
2	DZ(K)	≠ 0.: |DZ(K)| gives the thickness of the K-th coarse Z-mesh. (cm) < 0.: Core regions. > 0.: Non-core regions (e.g. reflectors). = 0.: End of the input of coarse Z-meshes.
	K=1, ...	The number of given coarse K-meshes defines KMZ.

Definition of the pattern of compositions:

For each of the planes (Z) K = 1,KMZ one set of cards TR5.
For each of the rows (Y) J = 1,JMY one card TR5.

Card TR5		Format (15I5)
1 . IMX	LAY3(I,J,K) I=1,IMX	Only for the core: > 0: Composition id. number of the I-th mesh (X) in this row and plane. In the upper plane the code evaluates the maximum number NPL of core compositions. = 0: Id. no. of this composition is internally defined by adding NPL to the LAY3(I,J,K-1) of the foregoing plane.

.....

Continuation of card TR5		
		Only for the non-core-compositions (reflectors etc.): < 0: Id. no. of this composition is internally defined by adding the maximum number of core compositions to the absolute of |LAY3(I,J,K)|. Reflector id. numbers must be given in an unbroken sequence starting with "-1".

4.3 Fuel Element Design. D1 – D17
(only if MODE = 'vsop' or 'fuel')

4.3.1 Specifications. D1 – D4

Card D1		Format (4I4)
1	KMAT	Sum of nuclides - except the heavy metal isotopes (see Table IV) to be included in the VSOP calculation (i.e. fission products, control poisons, non burning absorbers, scatterers). (≤ 172)
2	NHOM	= 0: Normal. = 1: Drop heterogeneous evaluation of fuel elements. Read homogenized atom densities on cards D17. The input sequence is : Cards D1, D2, D5, D6, D17, D5.
3	KOSTDA	Only when NHOM = 0: > 0: Input data for fuel element fabrication and reprocessing will be specified on cards D3, D4. ≤ 0: Drop cards D3, D4.
4	NDANC	Only when NHOM = 0: = 0: No effect. > 0: Definition of lattice type according to card Z11 (variable K) of VSOP-ZUT- input (section 5.3.3). Some values are calculated and printed, which should be used as input data for the Dancoff factor calculation in VSOP-ZUT.

Card D2		Format (18I4)
1 . KMAT	IMAT(I), I=1,KMAT	GAM-library identification numbers for the KMAT (card D1) nuclides in the sequence of Table IV, starting with the fission products (drop the heavy metal isotopes!). Note: Nuclide id. numbers beyond the library can be used (i.e. IMAT(I) > 190). These nuclides must be identified on the cards V3.

Cards D3, D4 only if KOSTDA > 0 on card D1.

Card D3		Format (A4,2I4,10F6.0)
1	CURCY	Literal abbreviation for the monetary unit MU.
2	NC	Number of different coated particle fabrication cost data. (≤ 6)
3	NF	Number of different fuel element fabrication cost data. (≤ 3)
4 . 9	FC(I), I=1,6	Fabrication costs of the I-th coated particle variant. (MU/ fuel element)
10 . 12	FF(I), I=1,3	Fabrication costs of the I-th fuel element variant. (MU/ fuel element)
13	DK	Fabrication costs of dummy elements. (MU/ element)

Card D4		Format (3E12.5)
1	HK	Costs of head end and transportation. (MU/kg_C)
2	AK	Costs of reprocessing. (MU/kg_{HM})
3	EK	Costs of waste treatment and disposal per 10% Fima. (MU/kg_{HM})

4.3.2 Design of fuel element-types and -variants. D5 - D17

One set for each variant of each desired fuel type (limited to 27 different sets).
Calculation is terminated by one last card D5.

Card D5		Format (18A4)
1 . 18	TITLE(I), I=1,18	Literal description of fuel element-types and –variants. TITLE(1) = 'stop': This terminates the sequence of cards D5 – D17.

Card D6		Format (5I4,E12.5)
1	NTYP	= 0: Spherical fuel elements. = 1: Prismatic block fuel element.
2	NFUTP	Identification of the fuel elements in 4 digits IJKL: IJ : Type (characterizes design and cost data), increasing numbers. ($\leq$ 10) KL: Variant (e.g. for different enrichments), increasing numbers, starting from 01 for each type IJ.
3	NFCP	Input option for the coated particle: = 2: Read cards D7 - D11. = 1: Read card D7 only. = 0: Data from preceding design, or when NHOM = 1 (card D1).
4	NFBZ	Input option for the fuel element: = 1: Read cards D12 - D13 or D14 - D16, respectively. = 0: Data from preceding design, or when NHOM = 1 .
5	NZUS	= 0: No effect. > 0: Number of nuclides for which atom densities will be specified on cards D17. ($\leq$ 30) Previously calculated values are replaced.
6	FF3	Variable is used for spherical fuel elements only (NTYP=0). > 0: Volumetric filling fraction of spherical fuel elements in the core. = 0: Default value (0.61) is used.

4.3.2.1 Coated particles. D7 - D11

Card D7 only if NFCP > 0 on card D6.

Card D7		Format (6E12.5)
1	ANR	Fissile enrichment of the fuel (fissile/heavy metal). > 0.: Atom fraction. < 0.: Weight fraction = |ANR|. = 0.: If INDBS (card D8) = 7 .
2	U53	= 0.: Fissile uranium is ^{235}U. = 1.: Fissile uranium is ^{233}U.

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Continuation of card D7		
3	FIMA	Envisaged heavy metal burnup for reprocessing cost calculation. (FIMA)
4 .	FRC(I), I=1,NC	> 0.: Fraction of coated particle variant I in this fuel element. = 0.: Coated particle variant I (card D3) is not present.

Cards D8 - D11 only if NFCP = 2 on card D6.

Card D8		Format (4I4)
1	INDBS	Fuel identification: = 1: UO_2 = 2: UC = 3: UC_2 = 4: UO_2 - ThO_2 = 5: UC - ThC = 6: UC_2 - ThC_2 = 7: PuO_2 = 8: PuO_2 - ThO_2 = 9: PuO_2 - UO_2
2	NCT	Total number of coating layers (≤ 5), to be numbered with increasing radius.
3	NSIC1	Number of the 1. SiC coating layer, if present.
4	NSIC2	Number of the 2. SiC coating layer, if present.

Card D9		Format (4E12.5)
1	RK	Radius of the coated particle kernels. (cm)
2	ROBR1	Density of the kernels. (g/cm^3)
3	ROBR2	Density of 2. type of kernels, if present. (g/cm^3) Only if INDBS = 4, 5, 6, 8, 9 on card D8.
4	BETA	Enrichment of the uranium N_{U5} / N_U if INDBS = 4, 5, 6, 9 on card D8. For U53 = 1. (card D7) program uses ^{233}U instead of ^{235}U.

Card D10 only if INDBS = 7, 8 or 9 on card D8.

Card D10		Format (4E12.5)
1 . 4	PU(I), I=1,4	Atom fractions of the isotopic composition in plutonium: ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu. If required, an additional ^{238}Pu concentration may be defined on card D17.

Card D11		Format (6E12.5)
1,3,5	DCT(I),	Thickness of the I-th coating layer. (cm)
2,4,6	ROCT(I), I=1,NCT	Density of the I-th coating layer. (g/cm3) (Numbered with increasing radius, NCT on card D8).

4.3.2.2 Spherical fuel elements. D12, D13

Cards D12 - D13 only if NTYP = 0 and NFBZ = 1 on card D6.
Only a selected set of the following parameters of the cards D12 and D13 is required. Possible combinations are given in Table VIII.

Card D12		Format (6E12.5)
1	R1	Outer radius of fuel zone. (cm) (Fuel zone consists of coated particles and graphite matrix).
2	R2	Outer radius of the sphere. (cm)
3	FF1	Volume fraction: coat.part. / (coat.part. + matrix).
4	VMOD	Moderation ratio N_C / N_{HM}.
5	INDBK	= 0: No dummy elements. = 1: Dummy elements existing.
6	BK	Volume fraction: dummy elements / (fuel + dummy) elements.

Table VIII: Alternative specifications of spherical fuel elements

No.	1	2	3	4	5	6	7	8	9	10	11
INDBK	0	0	0	0	0	0	0	1	1	1	1
R1	x	x	x	x	x			x	x	x	x
R2	x	x	x			x	x	x	x	x	x
FF1		x			x		x		x		x
VMOD			x	x	x	x	x	x	x		
ROSM	x			x		x		x		x	
BK										x	x

Card D13		Format (4E12.5,4E6.1)
1	ROSM	Density of heavy metal, homogenized in the fuel zone. (g/cm^3)
2	ROMTX	Density of graphite in the matrix. (g/cm^3)
3	ROSCH	Density of graphite in the outer shell. (g/cm^3)
4	ROBK	Only relevant for INDBK = 1: > 0.: Density of graphite in the dummy elements. (g/cm^3) = 0.: Density of graphite in the dummy elements equals ROSCH.
5	SR0	Inner radius of the matrix. (cm) (normally = 0.) > 0 for "shell ball" design.
6 .	FRF(I), I=1,NF	= 0.: Fabrication costs of the I-th fuel element variant (card D3) are dropped. > 0.: Fabrication costs of the I-th fuel element variant are used and multiplied by FRF(I). (Usually = 1.)

4.3.2.3 Prismatic fuel elements. D14 – D16

Cards D14 - D16 only if NTYP = 1 and NFBZ = 1 on card D6.

Card D14		Format (6E12.5)
1	R(1)	Radius of central graphite zone. (cm)
2	R(2)	Outer radius of inner cooling channel. (cm)
3	R(3)	Outer radius of inner graphite tube. (cm)
4	R(4)	Outer radius of the fuel zone. (cm)
5	R(5)	Outer radius of the outer graphite tube. (cm)
6	R(6)	Outer radius of the outer cooling channel. (cm) If FFUEL > 0. (card D15) insert "thickness" instead of "radius".

Only a selected set of the following parameters of the cards D15 and D16 is required. Possible combinations are given in Table IX.

Card D15		Format (6E12.5)
1	FF1	Volume fraction: coat.part. / (coat.part. + matrix).
2	VMOD	Moderation ratio N_C / N_{HM}.
3	BETA	Volume fraction of gaps (other than cooling channels) in the core relative to the bulk graphite volume.
4	GKAN	Number of fuel elements per square meter. ($1/m^2$)
5	FFUEL	= 0.: No effect. > 0.: Cross section of the fuel zone (cm^2). Use R(4) = 0. on card D14 and insert "thickness" instead of "radius".
6	ACTIV	Active length of the fuel rods in the core. (cm)

Card D16		Format (4E12.5)
1	ROSM	Density of heavy metal, homogenized in fuel zone. (g/cm^3)
2	ROMTX	Density of graphite in the matrix. (g/cm^3)
3	ROSTR	Density of graphite in the cooling channel. (g/cm^3)
4	ROHR	Density of graphite in the tubes. (g/cm^3)

Table IX: Alternative specifications of fuel rods

No.	1	2	3	4	5
FF1	x	x			negative guess
VMOD	x		x		x
GKAN		x		x	x
ROSM			x	x	

4.3.2.4 Additional nuclides. D17

Card(s) D17 only if NZUS > 0 on card D6.

Card D17		Format (I4,4X,E12.5)
1	NRGAM	GAM-lib. identification no. of nuclide with additionally given atom density.
2	DENG	Atom density (atoms / (barn cm), homogenized). Note: Use 1 card for each of the NZUS (≤ 30) additional nuclides.

4.4 Reactor and fuel cycle. V1 - KX5
(only if MODE = 'vsop')

4.4.1 Set up dimensions. V1

Card V1		Format (16I4)
1	NXS	Number of different spectrum zones, comprising a combination of one or more batches.
2	N26	Number of energy groups in the diffusion calculation.
3	MMAF	Maximum number of burnup cycles.
4	MBATCH	Maximum number of batches to be filled into storage boxes. * (See card R21).
5	MSTOB	Maximum number of storage boxes to be filled. * (See card R21).
6	JTYP	Number of different fuel element types in the system. (≤ 10) (See card R3).
7	MREP	Number of reprocessing mixtures, if present. (≤ 10) * (See card R3).
8	JABOX	Total number of aging boxes and jumble boxes as explicitly specified on card R5 (only if MREP > 0). *
		* See also chapter A.2.2 .
		Dimensions for thermal hydraulics (see cards TX and KX):
9	KMAZ	> 0: Maximum number of THERMIX-compositions. = 0: Default value = 35 .
10	IMAZ	> 0: Maximum <u>total</u> number of radial meshes (rows) for THERMIX. = 0: Default value = 50 .
11	NMAZ	> 0: Maximum <u>total</u> number of axial meshes (columns) for THERMIX. = 0: Default value = 80 .
12	ICO	> 0: Maximum number of radial meshes <u>inside the core area</u> for THERMIX. = 0: Default value = 30 .
		.....

Continuation of card V1		
13	NCO	> 0: Maximum number of axial meshes inside the core area for THERMIX. = 0: Default value = 30 .
14	KOMAX	> 0: Maximum number of KONVEK-compositions. = 0: Default value = 20 .
15	KONI	> 0: Maximum number of radial meshes for KONVEK. = 0: Default value = 30 .
16	KONN	> 0: Maximum number of axial meshes for KONVEK. = 0: Default value = 50 .

4.4.2 Definition of materials. V2 – V5

Card V2		Format (4I4)
1	NO	Number of fission products (≤ 49): = 0: Default value = 44, code uses the built-in fission product chain (see Fig. 4). 0<NO<44: The code drops the last surplus ones of the built-in chain. > 44: See KETT and card V4. (See also cards D1 (KMAT) and D2).
2	KETT	= 0: No effect. > 0: Chain information of the last KETT fission products will be defined on cards V4. This option can be used to extend the chain structure or to define a new one.
3	NLT	= 0: No effect. > 0: Number of fission products, for which new yields and decay constants will be defined on card V5.
4	NC	Number of control poison nuclides. (≤ 2)

Card(s) V3 only if some nuclides of the library shall be duplicated and used with new id. numbers IMAT(I) > 190 for special purposes. One card V3 for every new id. number.

Card V3		Format (2I4)
1	JNEU	GAM-Id. number to be assigned to the new nuclide.
2	LMAT	GAM-Id. number of the original library nuclide of which the cross sections are to be duplicated.

Card(s) V4 only if KETT > 0 on card V2.
A total of KETT cards required, starting with the card for the fission product nuclide
N = NO - KETT + 1.

Card V4		Format (4E12.5)
1	DIRAC(N,1)	Fractional production of nuclide N from N-1. > 0.: By capture. < 0.: By decay.
2	DIRAC(N,2)	Fractional production of nuclide N from N-2.
3	DIRAC(N,3)	Fractional production of nuclide N from N-3.
4	DIRAC(N,4)	Fractional production of nuclide N from N-4.

Card(s) V5 only if NLT > 0 on card V2.
A total of NLT cards is required, one for each fission product for which the yields are defined or altered.

Card V5		Format (I6,6X,5E12.5)
1	N	VSOP identification no. of a selected fission product nuclide.
2	YIELD1(N)	^{233}U fission yield of nuclide N.
3	YIELD2(N)	^{235}U fission yield of nuclide N.
4	YIELD3(N)	^{239}Pu fission yield of nuclide N.
5	YIELD4(N)	^{241}Pu fission yield of nuclide N.
6	XLAM(N)	Decay constant of nuclide N. (1/sec)

4.4.3 Design and operations. V6 – V17

4.4.3.1 Case identification. V6

Card V6		Format (8I4,2E12.5)
1	JSER	= 0: Diffusion calculation, control poison adjustment, burnup. = 1: Diffusion calculation, burnup. = 2: Diffusion calculation. = 3: Same as 0, but control poison adjustment also in the reflector. = 4: Cell burnup calculation (no diffusion calculation, K_{inf} and group fluxes by means of subroutine KINF). = 5: Same as 4, with control poison adjustment.
2	NRSTRT	= 0: No effect. = 1: Fuel shuffling. = 2: Fuel shuffling and iteration of the enrichment. * = 3: Fuel shuffling and reprocessing. = 4: Fuel shuffling, reprocessing and iteration. * * (Cards R28 - R31).
3	NKOST	= 0: No effect. > 0: Fuel cycle cost calculations (cards K1 - K12).
4	IBUCK	= 0: No feedback of leakage from diffusion to spectrum calculation. = 1: Feedback of broad group bucklings to GAM, and thermal leakage to THERMOS. = 2: Feedback of an average epithermal buckling to GAM, and thermal leakage to THERMOS.
5	MUHU(3)	= 0: Drop streaming correction in pebble bed. = 2: Streaming correction LIEBEROTH /27/ in power generating batches (only for pebble bed).
6	LOBNEW	= 0: Normal. = 2: Life history is preserved for ORIGEN-JÜL-II (all NON-MEDUL-reactors, see /4/), starting from the first burnup cycle (data set 'origen').
7	IBASCH	= 0: No effect. > 0: For x-y-z - geometry: Number of batches in the upper plane of the core. Will be used only in connection with variable MULT on card V7.
8	IPRIN2	≥ 0: Print layout of batches at startup. = -1: No output.
9	SERCON	Convergence criterion for K_{eff} when adjusting control poison or other atom concentrations. (≅ 0.0001)

.....

Continuation of card V6		
10	ERR	> 0.: Truncation error limit to be used for the burnup calculation. = 0.: Default value = 1.E-25 .

4.4.3.2 Definition of reactor batches. V7 – V9

Each batch (see output of "Geometric reactor design" - section) requires one set of cards V7-V9.
The sequence has to be as follows:
1) In-core batches, numbered from 1 through ....
2) Cone regions (= batches), numbered from (in-core batches + 1) through ....
3) Other non-power generating regions, numbered from 1 through ....
(The number of in-core + cone batches is automatically added up).

Card V7		Format (5I6,E12.5,18X,2I6)
1	NREAD	≤ 100: Number of atom densities to be specified on subsequent cards V8. > 100: Atom densities of fuel type IJ, variant KL are used. (*NFUTP* on card *D6*).
2	NCH1	NCH1 = 0, if NREAD ≠ 0 . NCH1 ≠ 0, if NREAD = 0: > 0: Number of a previously specified batch with the same atom densities. < 0: Read new atom densities from data set 'nucdens', which have been stored in an earlier VSOP calculation (comp. variable LIB < 0 on card R7).
3	NCH5	> 0: Number of a previously specified batch with the same control poison data. = 0: Use data of batch no. 1. < 0: Read card V9.
4	NHOT	> 0: Number of the spectrum zone this batch belongs to. = 0: Use *NHOT of the preceding batch.*
5	NFTST	Only if NREAD ≤ 100: Definition of fuel type id. no. of this batch. Only if fuel is defined by cards V8, otherwise the id. no. is taken from batch no. NCH1. In reflector regions the id. no. is 0 .
6	WPART	Fraction of *the volume of this batch per region:* = 0.: In the batches of the first region the code makes WPART = 1. / (number of batches per region). In the other batches of the .....

Continuation of card V7

		core the code copies WPART of the corresponding batch of the preceding region. In the regions of the reflectors the code makes WPART = 1. > 0.: Redefinition of the volume fraction of this batch. If redefinition is specified, it must be given for all batches of this region, and it holds for all subsequent ones until redefined.
7	MULT	= 0: No effect. > 0: The id. no. of this batch is defined by KD18 = KD18 + MULT * IBASCH (Card V6). (Useful in x-y-z geometry for the batches in the lower planes).
8	KD18	> 0: Id. no. of the batch for which the information of this card is to be applied. It will also be applied for all subsequent batches until redefined. Note: The sequence of the reflector batches (= regions) must correspond to the numbering defined on input cards BI5. < 0: Last card V7, holding for the batch |KD18|.

Atom densities: Card V8 only if 0 < NREAD ≤ 100. A total of NREAD cards is required.

Card V8 Format (I4,4X,E12.5)

1	L	VSOP-identification number of the nuclide with atom density > 0.
2	DEN	Atom density (atoms per barn cm). All densities must be given homogenized.

Control poison: Card V9 only if NC > 0 on card V2, and if NCH5 < 0 on card V7. One card V9 for each control poison nuclide.

Card V9 Format (2E12.5)

		The control poison nuclide(s) in all batches of one region have the same limitations.
1	POISM	Minimum atom density of control poison in this region. (e.g. = 0.)
2	POISL	Maximum atom density of control poison in this region.

4.4.3.3 Data for the burnup calculation. V10, V11

Cards V10-V11 only if JSER ≠ 2 on card V6.

Card V10		Format (4E12.5)
1	DELDAY	Length of large burnup time steps (time between possible diffusion calculations). (days)
2	POWER	Thermal core power. (watts)
3	FIWATT	Initial value of Fissions/Ws: = 0.: Starting value = 3.087E+10 (^{235}U) > 0.: Optional starting value. Note: In the course of the proceeding burnup, an actual value of FIWATT is calculated by the code according to DIN 25485 /25/. This value then depends on the fraction of the fission rates of the different fissile isotopes.
4	ZKFIND	Minimum allowed value of K_{eff}. The present burnup cycle is terminated, when K_{eff} equals ZKFIND. Fuel shuffling is then performed, if specified. In case of control poison adjustment, ZKFIND is the target K_{eff}.

Card V11		Format (2I4)
1	JNSTOP	Last large burnup time step in one burnup cycle. (≤ 95)
2	JNUM	Number of small time steps in one large step. Renormalization of the neutron flux to the specified reactor power is done for each small time step.

4.4.3.4 Control poison search. V12 - V14

Cards V12-V14 only if JSER = 0, 3, 5 on card V6.

Card V12		Format (18I4)
1	JSMAX	Maximum number of control poison iterations for any region at one time step. All batches of the region are treated simultaneously. (≅50)
2	JSSMAX	Maximum number of control poison iterations for the total core at one time step. (≅ 200)
3	LSIM	Number of regions, for which the control poison is adjusted simultaneously. LSIM regions form a poison area for simultaneous poison adjustment.
4	KSS	Length of the list of regions for control poison adjustments. The ratio KSS / LSIM gives the number of poison adjustment areas.
5 .	NPOIS(I), I=1,KSS	This list gives the sequence of regions in which the adjustments are performed.

Card V13		Format (6E12.5)
1 . KSS	PINMIN(I), I=1,KSS	Minimum fraction of control poison insertion in the I-th region to be adjusted. (e.g. = 0.)

Card V14		Format (6E12.5)
1 . KSS	PINMAX(I), I=1,KSS	Maximum fraction of control poison insertion in the I-th region to be adjusted. (e.g. = 1.)

4.4.3.5 Print-out options and steering. V15

Card V15		Format (5I4)
1	IPRIN(1)	Spectrum calculation: = 0: Thermal selfshielding factors, only. = 1: Same as 0, plus averaged thermal cross sections. = 2: Same as 1, plus fine group neutron fluxes. = 3: Same as 2, plus broad groups averaged cross sections for materials with concentration > 0. = 4: Same as 3, for all materials.
2	IPRIN(2)	= 0: No output. = 1: Print layout of batches before shuffling. = 2: Same as 1, plus atom densities (only in combination with IPRIN(3) ≥ 0).
3	IPRIN(3)	Burnup calculation: = -1: Global neutron balance. = 0: Detailed neutron balance. = 1: Same as 0, plus characteristic data for all fuel batches.
4	IPRIN(4)	= 0: Skip spectrum calculation if a set of cross sections is available. Instructions on card V16 are neglected. = 1: Repeat spectrum calculation as defined on card V16. = 3: Same as 1, but not for zones without heavy metal (reflectors).
5	IPRINO	Burnup calculation (ADAGE): = 0: No output. = 1: Short output (cross sections + total flux). = 2: Detailed output.

4.4.3.6 Steering the performance for spectrum and diffusion calculation. V16, V17

Card V16		Format (18I4)
1	ISPEKT(1)	≥ 0: No. of the first large burnup time step in which the spectrum calculation is to be repeated prior to the diffusion calculation.

Continuation of card V16		
2 . 18	ISPEKT(I), I=2,18	> 0: No. of further time steps for spectrum calculation. = 0: If all ISPEKT = 0, spectrum calculation is performed in every time step.

Card V17 only if JSER < 4 on card V6.

Card V17		Format (18I4)
1 . 18	IDIFF(I), I=1,18	If all IDIFF(I) = 0: Diffusion calculation is performed at every time step. If at least one IDIFF(I) ≠ 0: The IDIFF(I) give the time steps at which diffusion calculation is to be performed.

4.4.4 Fast and epithermal neutron spectrum. G1 - G12

Card G1		Format (A7,5X,7I6)
1	CIDGAM	Data set name of GAM-library. Only present choice: = gam5115
2	IDZUT	Id. no. of the resonance integral library. (180)
3	IDESIN	Number of different fuel element designs (≤ 10). Only for different resonance integral data on cards G3-G5. The differentiation of fuel element designs for the resonance calculation is normally the same as for the thermal cell calculation, i.e. IDESIN = NBER on card T6.
4	JJGM	= 0: Cylindrical fuel element. = 1: Spherical fuel element.

.....

Continuation of card G1		
5	MSTU	Fission source spectrum: = 3: ^{233}U. = 5: ^{235}U. = 11: ^{239}Pu. = 13: ^{241}Pu. = 0: Unit fission source.
6	MGHUS	Only if MSTU = 0: GAM group no. in which the unit fission source is located.
7	NSSS	= 0: No selfshielding factors applied. > 0: Number of sets of selfshielding factors (cards G7-G12). = -1: One single set of selfshielding factors to be applied in all spectrum zones (cards G8-G12).
8	IPRSEL	Output option of the selfshielding factors: = 0: Broad energy group definition. = 1: Selfshielding factors for the different nuclides.

Card G2		Format (6E12.5)
1 . NXS	TEMZUT(I), I=1,NXS	Temperature of the resonance absorbers in the NXS different spectrum calculations. (°C) (NXS on card V1) (= 0., if no fuel in the regarded spectrum zone).

Card(s) G3 only if IDESIN > 1 on card G1.

Card G3		Format (12I6)
1 . NXS	NDES(I), I=1,NXS	Cell design number in the spectrum calculation I.

For each design (IDESIN on card G1) 3 sets of cards G4-G5, the first set for ^{232}Th, the second set for ^{238}U, the third set for ^{242}Pu.

Card G4		Format (2E12.5,I6)
		Two values of homogenized atom densities of the resonance absorber nuclide, for which sets of resonance integrals are available on data set 'resint'. These values should represent the highest and the lowest densities, occurring within the reactor, respectively.
1	SM1	≥ 0.: Highest density of the absorber nuclide. [barn^{-1} cm^{-1}] = -1.: Density is taken from data set 'resint'.
2	SM2	≥ 0.: Lowest density of the absorber nuclide. [barn^{-1} cm^{-1}] = -1.: Density is taken from data set 'resint'.
3	NZ	Number of sets of resonance integrals for each SM1 and SM2 densities. These sets represent different temperatures of this absorber nuclide.

2 cards G5, the first one for SM1, the second one for SM2.

Card G5		Format (12I6)
1 . NZ	IZUT(K), K=1,NZ	Id. numbers of the resonance integral sets to be read from data set 'resint'.

Definition of broad energy groups.

Card G6		Format (6E12.5)
1 .	CEG(I), I=1,N26-1	Desired lower energy limit of the fast energy group(s). (eV)

Individual epithermal selfshielding factors. G7 - G12

Card G7 only if NSSS > 0 on card G1 (see also section A.1.3).

Card G7		Format (12I6)
1 . NXS	NSET(I), I=1,NXS	Id. no. of the set of selfshielding factors to be applied in the spectrum zone I.

Cards G8 - G12 only when NSSS ≠ 0 on card G1:
For each of the |NSSS| sets of selfshielding factors one set of cards G8-G12.

Card G8		Format (3I6)
1	MOBG	> 0: Number of broad epithermal energy groups for input of self-shielding factors (card G9). (Up to 67 groups can be defined). = 0: Broad energy groups same as defined on card G6 (the code sets MOBG = N26 - 1). < 0: Same broad energy groups as defined before.
2	LSUB	> 0: Number of subsets of cross section-selfshielding factors SC (cards G10). (≤ 9) = 0: No input of SC.
3	NK	> 0: Number of cell zones for neutron flux-selfshielding factors SF (cards G11). (≤ 6) = 0: No input of SF.

Card(s) G9 only if MOBG > 0 and MOBG ≤ 67.

Card G9		Format (12I6)
1 . MOBG	MGBN(J), J=1,MOBG	Id. number of the GAM group with the highest energy in the broader energy group J.

Card(s) G10 only if LSUB > 0 on card G8.
A set of (J=1,MOBG) cards G10 must be given for the MOBG broad energy groups.

Card G10 Format (6E12.5)

1 . LSUB	SC(L,J), L=1,LSUB	Broad energy group J: Cross section-selfshielding factor of subset L.

Card(s) G11 only if NK > 0 on card G8.
A set of (J=1,MOBG) cards G11 must be given for the MOBG broad energy groups.

Card G11 Format (6E12.5)

1 . NK	SF(K,J), K=1,NK	Broad energy group J: Neutron flux-selfshielding factor of cell zone K.

A card G12 is required for each nuclide (simplification of input can be defined on the cards).

Card G12 Format (I6,2I2,6E10.4)

1	IDG	> 0: Id. no. of nuclide in the GAM library in rising sequence. Nuclides standing before the first given id. no. are assigned with selfshielding factors equal 1.0 . < 0: This is the last card G12.
2	JT	= 0: Information of this card applies also for all following nuclides, unless revised. = 1: Information of this card applies only for this nuclide.
3	LSC	= 0: No cross section-selfshielding factors applied. > 0: Id. no. of cross section-selfshielding factors (SC(LSC,J), J = 1, MOBG) to be applied for this nuclide.
4 .	ANT(K), K=1,NK	Fraction of the homogenized atom density to be assigned to the cell zone no. K (only when NK > 0).

4.4.5 Thermal cell spectrum - T1 - T13

Card T1		Format (A9,3X,6I6)
1	CIDTHER	Data set name of THERMOS-library to be used (one of the existing according to chapter 3.2, Table I, or a new one, which must have been generated before by means of TTTT). Blank value: Calculate TTTT with THERMALIZATION (ITTT > 0 on card S1). It shall be made only for one spectrum zone. The following variables must have a zero value, if no data set name is assigned to variable CIDTHER.
2	NKER	Number of scattering nuclides (≤ 5). (See also Tables III and IV)
3	NKERAB	Number of absorber materials for which a scattering matrix is calculated internally (Brown St. Johnes). (≤ 10)
4	NUTTE	= 1: THERMOS calculation, no subsequent calculation of self-shielding factors. = 2: Calculation and print-out of selfshielding factors.
5	NUCT	Maximum number of scattering matrices - according to different temperatures - per one scattering nuclide to be used for interpolation (cards T3). (≤ 11)
6	ITY	Identification of fuel element type (see FUTYP on card T7) of which the geometry data are used for streaming correction. = 0: Use the first fuel element type (for which the first set of cards T7-T12 is given). > 0: Use the ITY-th fuel element type. = -1: Define the geometry data to be used for the streaming correction on card T13. This is necessary if THERMOS cell definition is different from fuel element size, which may have been defined by input cards D.
7	MUP	= 0: Normal. > 0: Number of broader thermal groups (to be read on card(s) T2) for given individual selfshielding. (≤ 30)

Card(s) T2 only if MUP > 0 on card T1.

Card T2		Format (6E12.5)
1 . MUP	EMU(I), I=1,MUP	Upper limit (eV) of the I-th thermal broader group for the given individual selfshielding, starting with the lowest thermal group.

For each of the NKER scattering nuclides one set of cards T3-T4, in sequence of VSOP nuclides on card D2.

Card T3		Format (1 1I6)
1 . NUCT	IKER(J), J=1,NUCT	Id. no. of the J-th scattering matrix to be used for interpolation according to the actual temperature of this scattering nuclide.
Card T4		Format (6E12.5)
1 . NXS	TCELS(J), J=1,NXS	Temperature of this scattering nuclide for spectrum calculation J. (°C)

Card T5 only if NKERAB > 0 on card T1.

Card T5		Format (E12.5,10I6)
1	TKG	Relative temperature in the calculation of scattering matrices for absorber nuclides. (°K/293.6)
2 .	IDTA(I), I=1,NKERAB	GAM-identification no. of nuclide I for which a scattering matrix is calculated internally.

Card T6		Format (12I6)
1	NGEOM	= 0: Cylindrical fuel element. = 1: Spherical fuel element.
2	NBER	Number of different cell definitions for the thermal spectrum calculation. Normally same as IDESIN on card G1.
3 .	NTYSP(I), I=1,NXS	Identification no. of the cell definition used for spectrum calculation I.

For each of the NBER cell definitions one set of cards T7 - T12 required.

Card T7		Format (6E12.5)
1	TKG	Temperature for the initial guess of Maxwell neutron spectrum, relative to T0. (See STRT0 on this card). ≅ 1.5
2	FUELL	Ratio: Volume of the cell / homogenized volume. (E.g. volumetric filling fraction of fuel balls in the core).
3	FUTYP	> 0.: Fuel element type identification IJ as specified by NFUTP on card D6. = 0.: All design specifications must be given on cards T8-T9.
4	STRT0	> 0.: Identification of the most important scattering nuclide. Its temperature will be used as base temperature T0, as required for TKG. STRT0 = 1., 2. .... identifies the first, second .... scatterer in sequence of VSOP nuclide list (cards D2, T3). = 0.: T0 = 293.6 °K.
5	PNORM	= 0.: Average cross sections are based on the average cell flux. > 0.: Average cross sections are based on the flux at the mesh point PNORM. < 0.: Average cross sections are based on the flux at the outer edge of the cell.
6	TLEAK	= -1.: Isotropic boundary condition. Read card T12. = 1.: White boundary condition.

Card T8		Format (20I1,2I2,4E12.5)
1 . 20	MTBL(J), J=1,20	Cell zone no. in which mesh point J is located. E.g. 11122223330000000000. The highest digit defines the number of cell zones NCZ (≤ 9). Each cell zone must contain a scattering nuclide.
21	IBRENN	Skip if FUTYP > 0. Cell zone no. in which the fuel is located.
22	ICOAT	Skip if FUTYP > 0. > 0: Cell zone no. in which the coated particles are located. = 0: No calculation of coated particles heterogeneity.
23	COA(1)	Skip if FUTYP > 0. or ICOAT = 0 . Radius of the coated particle kernel. (cm)
24	COA(2)	Skip if FUTYP > 0. or ICOAT = 0 . Outer radius of the coating. (cm)
25	COA(3)	Skip if FUTYP > 0. or ICOAT = 0 . Volume fraction: coat. part. / (coat. part. + matrix).
26	COA(4)	Skip if FUTYP > 0. or ICOAT = 0 . Ratio: Density of matrix / density of coating.

Card T9 only if FUTYP = 0. on card T7.

Card T9		Format (6E12.5)
1 .	RED(I+1), I=1,NCZ	Outer radius of cell zone no. I. (cm) Inner radius of cell zone no. 1 is set to 0. (See variable MTBL on card T8 for NCZ).

A card T10 is required for each nuclide. For simplified input see below.

Card T10		Format (I5,I4,I1,10F6.3)
1	IDISO	> 0: Id. no. of nuclide in the THERMOS-library, starting with absorber nuclides in sequence of increasing THERMOS-library numbers. Followed by the scatterers with modified numbers 1000+J. Here, J = 1, 2 .... identifies the first, second .... scatterer in sequence of VSOP nuclide list, see cards D2 ,T3. < 0: -IDISO terminates the input of cards T10.

.....

Continuation of card T10		
2	MUPN	= 0: Normal. > 0: Individual thermal selfshieldings of this isotope are given on cards T11.
3	JT	= 0: The fractional densities VB specified on this card are also valid for all subsequent nuclides, unless revised. This holds also for the selfshielding SFMU (card T11), if defined. = 1: The VB are valid only for this nuclide.
4	VB(1)	≥ 0.: Fraction of the homogenized atom density to be assigned to the 1. cell zone. < 0.: Fractions are derived from data input of cards D (only if NHOM = 0 on card D1). = -1.: Nuclide distributed like fuel. = -2.: Nuclide distributed like moderator.
5 .	VB(L), L=2,NCZ	Only if VB(1) ≥ 0.: Fraction of the homogenized atom density to be assigned to the L-th cell zone. L = 2 ... NCZ.
	VB(NCZ+1)	The fraction of the nuclide assigned to the coated particle fuel zone ICOAT on card T8 must be further subdivided between kernel, coating and matrix. VB(NCZ+1) gives the fraction in the kernels.

Card(s) T11 only if MUPN > 0 on card T10.

Card T11 Format (6E12.5)

1 . MUP	SFMU(K), K=1,MUP	Individual selfshielding of this isotope in the MUP broader thermal energy groups as defined on card(s) T2.

Card(s) T12 only if TLEAK = -1. on card T7.

Card T12 Format (6E12.5)

1	ALBEDO(1)	Albedo at the outer edge of the cell for the lowest energy group no. 1. .....

Continuation of card T12		
2	ALBEDO(2)	Albedo for the group no. 2 . = 0.: Use ALBEDO(1) for all energy groups. ≠ 0.: Read Albedos for all groups.
3 . 30	ALBEDO(J), J=3,30	Skipped if ALBEDO(2) = 0. Otherwise the group dependent Albedos must be given.

Card T13 only if ITY = -1 on card T1.

Card T13		Format (5E12.5)
1	FF(1)	Volumetric filling fraction of fuel elements in the core.
2	FF(2)	Inner radius of the fuel zone of the elements. (cm) (normal = 0.)
3	FF(3)	Outer radius of the fuel zone. (cm)
4	FF(4)	Outer radius of the element. (cm)
5	FF(5)	Fraction of pure graphite balls (only spherical elements).

4.4.6 Diffusion calculation. C1 - C21

4.4.6.1 Title card

Card C1		Format (18A4)
1 . 18	B(I), I=1,18	Literal description of case.

4.4.6.2 General control. C2 – C6

Card C2		Format (I3)
1	IOPT	001

Control options.

Card C3		Format (3I3)
1	NGC10	Type of eigenvalue problem. = 0: Effective multiplication factor calculation. = -5: Fixed source (read cards C18 – C21).
2	NGC15	Termination option (applied only to the flux iteration calculation). = 0: Terminate calculation and proceed as if converged if machine time or iteration count is exceeded (see also card C5). = 1: If limits are exceeded, terminate calculation and proceed as if converged only if the iterative process is converging. = 2: If limits are exceeded, terminate calculations.
3	NGC24	= 0: No effect. = -1: Define - possibly unisotropic - diffusion constants on cards C11 – C17.

Edit options.

Card C4		Format (8I3)
1	IEDG3	= 0: No effect. > 0: Print macroscopic group-to-group transfer cross sections.
2	IEDG4	= 0: No effect. > 0: Print macroscopic reaction rate cross sections.
3	IEDG5	= 0: No effect. > 0: Print gross neutron balance over system by group.
4	IEDG6	= 0: No effect. > 0: Print gross neutron balance by zone by group.
5	IEDG9	= 0: No effect. > 0: Print zone average flux values by group (IEDG6 = 0).
6	IEDG10	= 0: No effect. = 1: Print point flux values by group, write them onto unformatted data set 'phiunfor'. = 2: Like = 1, but formatted data set 'phiform'.
7	IEDG12	= 0: No effect. > 0: Print zone average power densities.
8	IEDG14	= 0: No effect. = 1: Print point power densities, write them onto unformatted data set 'powunfor'. = 2: Like = 1, but formatted data set 'powform'.

General iteration count and machine time limit.
Problems are terminated when the iteration count reaches the limit and the calculation proceeds as per NGC15 (see card C3).

Card C5		Format (3I3)
1	ITMX1	> 0: Maximum number of initial eigenvalue problem iterations. (≤ 999) = 0: Default value = 200 The following items are machine time limits (min). Generally, calculations continue if time is exceeded as if convergence criteria had been satisfied. .....

Continuation of card C5		
2	ITMX19	> 0: Limit for the initial eigenvalue problem. = 0: Default value = 60
3	ITMX20	> 0: Limit for all other eigenvalue problems. = 0: Default value = 30

General restraints.

Card C6		Format (2E12.5)
		Any calculation will be terminated if the following restraints are not met.
1	GLIM1	> 0.: Maximum multiplication factor. = 0.: Default value = 1.5
2	GLIM2	> 0.: Minimum multiplication factor. = 0.: Default value = 0.5

4.4.6.3 Description of neutron flux problem. C7 – C10

Card C7		Format (I3)
1	IOPT	003

General description.

Card C8		Format (12I6)
1	NUAC5	Geometry option. = 7: Two-dimensional cylinder. (r,z) = 11: Three-dimensional slab. (x,y,z) .....

Continuation of card C8

		Note: 2-dim.: r = left → right z = top → bottom 3-dim.: x-y-z x = left → right y = top → bottom z = front → back
2	NUAC11	Left boundary condition (required for 2-d, 3-d). = -1: Periodic. = 0: Extrapolated (vacuum). = 1: Reflected.
3	NUAC12	Top boundary condition (required for 2-d, 3-d). = 0: Extrapolated. = 1: Reflected.
4	NUAC13	Right boundary condition (required for 2-d, 3-d). Set to -1 if NUAC11 = -1 = 0: Extrapolated. = 1: Reflected.
5	NUAC14	Bottom boundary condition (required for 2-d, 3-d). = 0: Extrapolated. = 1: Reflected.
6	NUAC15	Front boundary condition (required for 3-d). = 0: Extrapolated. = 1: Reflected.
7	NUAC16	Back boundary condition (required for 3-d). = 0: Extrapolated. = 1: Reflected.
8	NUAC17	Number of zone to be an internal black absorber and to have the non-return boundary condition applied at its edges (see XMIS2 on card C10; this zone will be black to all groups unless additional data are supplied).
9	NUAC18	= 0: Only positive neutron flux allowed. > 0: Option to allow negative neutron flux.
10	NUAC19	= 0: No effect. > 0: Override use of Chebychev polynomials in adjusting the acceleration parameters.

.....

Continuation of card C8		
11	NUAC20	= -1: Force alternating direction line relaxation on rows and columns, and also fore and after for 3-d. = -2: Use only on rows and columns. > 0: Line relaxation only on rows. = 0: The code selects line relaxation on rows only with one inner iteration for all problems involving upscattering, otherwise three inner iterations for 3-d problems without I/O and five with data I/O during iteration, and alternating direction line relaxation for all 2-d problems.
12	NUAC23	Number of inner iterations. Normally not specified (see NUAC20 above).

Iteration convergence criteria

Card C9		Format (2E12.5)
1	EPI1	> 0.: Maximum relative flux change for the last iteration of each initialization eigenvalue problem. = 0.: Default value = 0.0001
2	EPI2	> 0.: Maximum relative change in the eigenvalue for the last iteration of eigenvalue problems. This applies to the multiplication factor calculation. = 0.: Default value = 0.00001

Miscellaneous data

Card C10		Format (3E12.5)
1	XMIS1	External extrapolated boundary constant. = 0.: The code will use the built-in value for all extrapolated boundaries. (0.4692) > 0.: Specifies the constant for all extrapolated boundaries for all groups (see NUAC11 - 16 on card C8).

Continuation of card C10		
2	XMIS2	Internal black absorber boundary constant for the zone NUAC17. * = 0.: In connection with NUAC17 > 0 on card C8 the code will use the built-in value for all groups and the absorber will be black over all energy. (0.4692) > 0.: The constant for all groups applying to zone NUAC17.
3	XMIS6	Initial overrelaxation factor. Normally calculated by the code and not specified here.

* $= -\frac{D}{\Phi} \cdot \frac{\partial \Phi}{\partial x}$

4.4.6.4 Simulation of control devices and void areas. C11 – C17

Cards C11 – C17 only if NGC24 = -1 on card C3

Card C11		Format (2I6)
1	JH	Number of regarded areas (card(s) C12). (≤ 200)
2	KH	Number of different cross section sets to be applied (cards C13 - C15). (≤ 5)

Card C12		Format (18I4)
1	IZONE(J),	Id. no. of cross section set to be applied to the J. area.
2	M1(J,1),	First CITATION zone located in the J. area.
3	M1(J,2), J=1,JH	Last CITATION zone located in the J. area.

One set of cards C13 – C17 for each of the K = 1,KH cross section sets.

Card C13		Format (6E12.5)
1 . N26	RDK(K,I), I=1,N26	Diffusion constants of the energy groups I.
Card C14		Format (6E12.5)
1 . N26	SGA(K,I), I=1,N26	Macroscopic absorption cross sections of the energy groups I.
Card(s) C15 for each energy group I = 1,N26. Card C15		Format (6E12.5)
1 . N26	SGTR(K,I,J), J=1,N26	Macroscopic transfer cross sections from energy group I to energy groups J.
Card C16		Format (2E12.5,I3)
1	V2(K,1)	Factor to be multiplied to the diffusion constants in radial dimension.
2	V2(K,2)	Factor to be multiplied to the diffusion constants in axial dimension.
3	IKEN	= 0: No effect. > 0: Group dependent factors will be defined on card C17.
Car C17 only if IKEN > 0 on card C16. Card C17		Format (6E12.5)
1 . N26	FKEN(K,I), I=1,N26	Energy group dependent factors to be multiplied to the V2 of card C16.

4.4.6.5 Fixed source, specified by zones. C18 – C21

Cards C18 – C21 only if NGC10 = -5 on card C3

Card C18		Format (I3)
1	IOPT	026

Card C19		Format (I3)
1	NFX2	= 0: Short output. > 0: Source (n/sec) will be edited by mesh points.

Card C20		Format (6E12.5)
1 . N26	V1F(I), I=1,N26	Fractions of the fixed neutron source distributed into each group starting with the highest energy group. These should sum to unity but are normalized to unity by the code.

One card C21 for each zone having a fixed neutron source. Fixed source input is terminated by a 'blank' card C21.

Card C21		Format (6(I3,E9.3))
1	N2F(I),	> 0: Zone number. = 0: End of the 'fixed source' input
2 .	V2F(I), I=1, ...	Fixed source. (n/sec-cm^3)

4.4.7 Fuel cycle costs calculation. K1 - K12

Cards K1-K12 only if NKOST > 0 on card V6.

Card K1		Format (9I4,A4,I4,A4)
1	IDCOST	Identification number for the cost library to be prepared. It will contain the reactor burnup history for KPD-cost calculations.
2	NCD	= 0: No cost library will be prepared. > 0: Prepare cost library on data set 'costdata'.
3	NMAF	Number of burnup cycles for which burnup data are supplied. The length of approach to equilibrium phase is assumed to be equal to NMAF burnup cycles. NMAF may be overridden by information contained within burnup data. (See also variable NPUFD and card(s) K11!).
4	MXTYP	Number of different fuel types in the system (≤ 10). For each type a set of cards K7-K10 is required.
5	ND2O	= 0: Normal. > 0: Heavy water moderated reactor. D_2O expenditures included in cost calculation. Card K12 required. (This option may be used to simulate capital costs of power plant).
6	NPUFD	= 0: Normal. > 0: Pu feed cycle, for each period a Pu equivalence value is calculated according to specified FCC for uranium feed cycle on card K11.
7	IPRINT	= 0: Print-out without materials balance for each batch. = 1: Print-out includes materials balance.
8	IQ	= 0: Normal. > 0: Calculate average equilibrium FCC over the last IQ periods (Ref. /18/, Section A.5). Recommended when the accounting period is shorter than the irradiation time of the fuel to obtain representative FCC for the equilibrium cycle.
9	NEWCO	= 0: Neglect financing cost of fresh out-of-pile batches. (Normal when appropriate lead-times are used). = 1: Calculate financing cost of fresh out-of-pile batches for the time TOUT on card K4. This option only for cases with out-of-pile batches, i.e. KUGL > 0 on card R2.
10	$	Monetary unit in which input is supplied. The user specifies the 4 character alphanumeric designation to be used in print-out, e.g. DM or US$.

Continuation of card K1		
11	X	The energy cost is calculated in units of $$ (see below) and X is the conversion from $ to $$. E.g. 100 means $ = 100 $$.
12	$$	Monetary unit in which energy costs are calculated and printed in output, e.g. DPf or Mill.

Card K2		Format (4E12.5)
1	F	Annual load factor. Same as AAAA on card R2.
2	ETA	Net efficiency of power plant.
3	GLD	> 0.: Total lifetime of the power plant (a). Average FCC are calculated for GLD years assuming an approach to equilibrium phase of NMAF periods. For the rest of the lifetime the last (or the IQ last) calculated periods are defined to be the equilibrium period and repeated till the end of plant operation. For D_2O cost calculation GLD is taken as amortization time for heavy water investments. < 0.: Drop average FCC calculation.
4	GMZ	Number of installments of electricity revenues within a period. Normally = 1., but for longer operation periods monthly or quarterly intervals of payment should be assumed.

Card K3		Format (6E12.5)
1	Z1	Pre-irradiation interest rate (1/a) on fuel expenditures.
2	Z2	Pre-irradiation interest rate (1/a) on fuel fabrication and D_2O replacement costs.
3	Z4	Interest rate (1/a) on all capital, incl. electricity revenues during irradiation.
		.....

Continuation of card K3		
4	Z3	Post-irradiation interest rate (1/a) on capital to finance fuel credit (in effect discount rate).
5	Z5	Post-irradiation interest rate (1/a) on reprocessing and shipping costs.
6	ZL	Discount rate (1/a) for present worth leveling of all expenditures and revenues over reactor lifetime. In most cases all interest rates will be chosen the same with the possible exception of the present worth discount rate. The code offers the flexibility to model most of the economic situations arising for those special cases where this might be needed.

Card K4		Format (5E12.5)
1	SS	Tax rate (1/a) on fissile investments.
2	RES	Reserve factor (RES = 1. + reserve) to account for additional fabrication costs for reserve elements in the initial core. In later cycles program sets RES = 1. The capital charges arising from a reserve store are contained in the appropriate defined lead-times TIN and TFAB on card K9. Blank = 1.0 .
3	VERL	Recovery factor for reprocessing. (0.97 - 0.99)
4	YPA	Fraction of discharged ^{233}Pa decaying into ^{233}U during out-of-pile storage (normally = 1.0). If storage and reprocessing time are defined on card R2, the amount of ^{233}U reaching the reprocessing plant has already been explicitly accounted for, then YPA = 0. (^{239}Np is assumed to decay completely into ^{239}Pu).
5	TOUT	Storage time (days) before reuse of out-of-pile batches. Financing cost with interest rate Z4 is calculated during time TOUT. Also for fresh fuel if not NEWCO on card K1 is specified = 0. TOUT = -1. will cause the code to specify TOUT = cycle length for each cycle.

Card K5 is always required. The data for uranium ore and enrichment will be used to calculate the price of ^{235}U for different fuel types and the changing value during depletion. If this option is to be by-passed, CU8(K) for all fuel types > 0. and CU5(K) specified accordingly, see cards K7.

Card K5		Format (6E12.5)
1	CU3O8	Cost of uranium ore as U_3O_8 ($/lb U_3O_8). The price is given as per lb corresponding to common use in literature.
2	CO8F6	Cost of conversion of U_3O_8 to UF_6 ($/kg U). The enriched end product is in the form UF_6, the costs of converting the hexafluoride into UO_2 or any other compound, are included in the fabrication costs.
3	CTRENN	Separation cost. ($/SWU)
4	TAIL	Tail enrichment, i.e., ^{235}U content in discarded uranium from enrichment plant.
5	XLOSS1	Fraction of losses in conversion of U_3O_8 to UF_6 (typically 0.005 - 0.01).
6	XLOSS2	Fraction of losses in conversion of enriched UF_6 to UO_2 or UC and in fabrication (typically 0.005 - 0.01).

Card K6 is always required. The costs of fresh ^{232}Th, ^{233}U and fissile plutonium are assumed to be the same for all types of fuel. The discharge value may, however, vary according to composition and subsequent utilization and for each fuel type depreciation factors are specified on cards K8.

Card K6		Format (3E12.5)
1	CTH232	Cost of ^{232}Th. ($/kg)
2	CU233	≥ 0.: Cost of fissile ^{233}U. ($/kg) < 0.: Cost of ^{233}U is calculated relative to cost of 93% enriched ^{235}U with |CU233| as parity value. Cost(^{233}U) = |CU233| * Cost(93% ^{235}U).
3	CPUFIS	≥ 0.: Cost of fissile ^{239}Pu and ^{241}Pu. ($/kg) < 0.: Cost of Pu_{fiss} relative to cost of 93% ^{235}U with parity value |CPUFIS|.

One set of cards K7 - K10 for each fuel type.

Card K7		Format (5E12.5)
1	ANSM	Type of heavy metal: 1.: Th(met.), 2.: ThO_2, 3.: ThC, 4.: ThC_2 5.: U(met.), 6.: UO_2, 7.: UC, 8.: UC_2
2	CU5	If CU8 (next variable) ≤ 0.: Initial reference enrichment of ^{235}U in uranium. All cost calculations are performed with the actual enrichment of a batch regardless of the reference enrichment for the type. Cost data on card K5 are used. If CU8 > 0.: Cost of ^{235}U ($/kg). Price kept constant during calculation.
3	CU8	≤ 0.: Cost of ^{238}U = 0., and cost of ^{235}U calculated from batch enrichment and card K5. > 0.: Cost of ^{238}U ($/kg). Supply ^{235}U cost as specified above. This option operates only if CU8 > 0. for <u>all</u> types!
4	CFAB	≥ 0.: Fuel fabrication cost ($/kg HM) excluding cost of heavy metal. Monetary unit is variable $ as specified on card K1 and given per kg initial HM in fuel element. < 0.: Data for this fuel element type is calculated by the code itself using basic cost data as specified on card D3.
5	CAUF	≥ 0.: Total costs of reprocessing, shipping and storage ($/kg HM) payable at time TAUF (card K9) after discharge. Cost per kg discharged HM. < 0.: Data for this fuel element type is calculated by the code itself using basic cost data as specified on card D4. Interests on HM during fabrication and reprocessing are calculated separately by the program for lead and lag times TIN and TEX on card K9.

Card K8		Format (4E12.5)
1	CHITH	= 0.: Irradiated and discharged fertile material (Th, U) has no value. > 0.: Cost of discharged fertile material depreciated by the factor CHITH.
2	CHIU3	= 0.: Discharged ^{233}U has no value. > 0.: Discharged ^{233}U cost depreciated by the factor CHIU3.

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Continuation of card K8		
3	CHIU	= 0.: Discharged ^{235}U has no value. > 0.: Discharged ^{235}U cost - for actual enrichment in depleted fuel - depreciated by the factor CHIU.
4	CHIPU	= 0.: Discharged fissile ^{239}Pu and ^{241}Pu has no value. > 0.: Discharged Pu_{fiss} cost depreciated by the factor CHIPU.
Card K9		Format (5E12.5)
1	TORE	Lead-time (d) for payment of uranium ore for replacement fuel. Lead-time is counted prior to the time of loading the fuel into the reactor and start of irradiation.
2	TIN	Lead-time (d) for payment of enrichment service and conversion costs for fuel replacement relative to fuel loading. Also lead-time for purchase of ^{233}U and fissile plutonium.
3	TFAB	Lead-time (d) for payment of fabrication costs for replacement fuel relative to fuel loading. The lead-time for D_2O replacement is taken the same as TFAB for fuel type 1.
4	TEX	Lag time (d) for credit for discharged fuel relative to time of discharge at end of irradiation. No difference between lag times for replacement and initial fuel.
5	TAUF	Lag time (d) for payment of reprocessing and shipping costs for discharged fuel relative to end of irradiation. Same for replacement and initial fuel.
Card K10		Format (3E12.5)
1	TORE	Lead-time (d) for payment of uranium ore for initial core.
2	TIN	Lead-time (d) for payment of enrichment service and conversion costs for initial core.
3	TFAB	Lead-time (d) for payment of fabrication costs for initial core. In general the lead-times for purchase of initial core will be longer than for replacement fuel as the amount of ore and the number of elements to be manufactured are larger.

Card K11 only if NPUFD > 0 on card K1.

Card K11		Format (6E12.5)
1 . NMAF	UUKOST(1) . . UUKOST (NMAF)	Fuel cycle cost ($\$/kW_h$) for the first period for the corresponding uranium feed cycle. A Pu price is evaluated for this period to yield FCC equal to UUKOST(1). The FCC for the U-cycle must be specified for all periods NMAF. This calculation allows for NMAF < 30 only.

Card K12 only if ND2O > 0 on card K1.

Card K12		Format (6E12.5)
1	DOUTIN	Weight (kg) of total D_2O in-pile and out-of-pile inventory. (D_2O cost calculations may be used to simulate amortization of capital investment for the plant. The capital is then paid in installments at the beginning of each cycle or accounting period, in such a way that the installments leveled over the lifetime GLD give the total present worth value at the time of start-up. In this case DOUTIN could be interpreted as kW_e of the power plant.)
2	CDNEU	Cost ($/kg) of new D_2O. (Capital cost including interest during construction at time of start-up in $/$kW_e$.)
3	CDALT	Cost ($/kg) of old D_2O (0., i.e. no value of station end-of-life).
4	ZD	Interest rate (1/a) on D_2O investments (or capital costs).
5	SD	Tax rate (1/a) on D_2O investments (or capital costs).
6	VD	D_2O losses per year (normally 0.01). It is assumed that the D_2O replacement expenditures have the same lead-time and interest rate as fabrication costs. (0.0 in case of plant cost).

4.4.8 Fuel management. R1 - R34

Cards R1 - R34 only if NRSTRT > 0 on card V6.

4.4.8.1 General definitions. R1 - R2

Card R1 only if NRSTRT = 3 or 4 on card V6, i.e. for fuel management with reprocessing.

Card R1		Format (6E12.5)
1 . KTOT	XREPRO(I), I=1,KTOT	Reprocessing factor for material no. I. The reprocessing plant is simulated by reprocessing factors multiplied to the different nuclide quantities. The decay of the heavy metal isotopes is calculated for period TREPRO (card R2). The reprocessing factors are defined as: 1.00 = No losses. 0.00 = Complete removal. 0.95 = 5% loss during reprocessing, etc. Data must be specified for all nuclides [KTOT = 28 (i.e. no. of heavy metal isotopes) + KMAT (card D1) non-heavy metal nuclides]. The same reprocessing factors are applied to all batches.

Card R2		Format (7E10.3)
1	KUGL	= 0.: Reactor without out-of-pile cycle. = 1.: Pebble bed reactor with out-of-pile fuel management: Fresh fuel stores for each type, reusable discharged fuel batches, and handling of discarded scrap fuel. = 2.: Reactor with out-of-pile cycle: As above, fuel may be replaced in any core position.
2	TDOWN	Length of downtime during reload (days). The isotopic decay of the heavy metals is calculated for all in-core batches.
3	TSTORE	Length of out-of-pile storage time (days) before reuse of the fuel. Decay is calculated for all out-of-pile batches, except for the fresh and for the scrap fuel. Financing costs are paid during time TSTORE.

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Continuation of card R2		
4	TREPRO	Length of cooling, shipping and reprocessing time (days) of discharged fuel. Decay is calculated during this period for scrap fuel batches and reprocessed fuel batches.
5	AAAA	Load factor of power plant. When fuel cycle costs are evaluated, same as F on card K2 in cost input.
6	BRUCH	Failure rate of discharged fuel (pebble bed reactor only). In each discharged batch a fraction BRUCH is assumed non-reusable and is added to the scrap batches.
7	AGEBOX	= 0.: No effect. = 1.: Aging boxes for reprocessing mixtures will be specified. Card R5 is required.

4.4.8.2 Data for individual fuel types. R3 - R4

Cards R3-R4 only if KUGL > 0. on card R2. The cards are supplied as a set for each fuel type, i.e. JTYP (card V1) sets.

Definition of fresh fuel store.

Card R3		Format (2(I6,E12.5))
1	NTP1	Id. no. of the fuel type.
2	PARVL1	Volume (cm^3) of fuel store. The choice of fuel volume is arbitrary as long as no financing costs of fresh fuel store are calculated. In many cases it is advantageous to define the volume equal to the volume of one fuel element and when reloading specify the fraction of the store as no. of elements in the batch. If more fuel from the store than actually present is required, the store is regarded as unlimited. Fuel removed from the store does not change the remaining volume, neither does the isotopic composition change during the reactor life.
3	NISO	> 0: Number of isotopes on the following card(s) R4. The composition of fresh fuel is specified by the number NISO and by the card(s) R4. The rest of the isotope concentrations equals zero. .....

Continuation of card R3

4	XMARX	= 0: Card(s) R4 are skipped for this fuel type, and PARVL1 = 0. < -100: Isotope composition of the fresh fuel store has been defined by variable NFUTP on card D6. INISOI = NFUTP. No. of the reprocessing mixture to which the scrapped fuel of this type is transmitted. Each mixture may consist of one or more fuel types. After each reload the discharged fuel is volume averaged to form a mixture, which at the next reload may be reprocessed and be used for refueling. XMARX ≤ 10. If AGEBOX > 0. (card R2) this reprocessing mixture is transferred to its corresponding aging box(es). If for all types XMARX = 0., no reprocessing mixtures are prepared.

Card(s) R4 only if NISO > 0 on card R3.

Card R4 Format (4(I6,E12.5))

1	L	Id. no. according to VSOP list of first nuclide with atom density ≠ 0.
2	DAV(L)	Atom density of nuclide L in fresh fuel store for type NTP1.
3	L	Id. no. of second nuclide.
4	DAV(L)	Atom density of second nuclide.
.		
.		Data for all NISO isotopes in fresh fuel store.

4.4.8.3 Aging boxes for discharged fuel. R5

Card R5 only if AGEBOX > 0. on card R2.

Card R5		Format (10I4)
1 . MREP	NAJB(J), J=1,MREP	Number of aging boxes including one jumble box to be defined for the J-th reprocessing mixture. MREP is the total number of reprocessing mixtures defined by the XMARX sequence on card R3. NAJB ≤ 10. Note: 1. Scrap fuel discarded from the reactor is loaded into the reprocessing mixture box J. 2. It is transferred to the corresponding first aging box. 3. Aging boxes are stepwise transferred to the next higher ones. 4. Those with an age ≥ TREPRO (card R2) are transferred to the corresponding jumble box J. 5. If NAJB(J) = 1, the reprocessing mixture box J is immediately given to the jumble box. 6. A fraction FOJB(J) (card R11) of the jumble box is loaded into the reprocessing mixture box J. It is ready for use after that reload, which will be performed after the following burnup cycle. 7. That fraction which is not used, is returned to the jumble box J.

4.4.8.4 Instructions for the burnup cycles. R6 - R27

These cards will be read at the end of each burnup cycle. They define the fuel management prior to the subsequent cycle and give some new options for the next cycle.

Card R6 only if IRR9 > 0 on card S3, and only at the beginning of a restart. The preceding run ended after a fuel management performance. The restart starts at the beginning of the new burnup cycle. This card allows to change some options for this first cycle, which were given at the last card R7 of the preceding run.

Card R6		Format (12I3,3E12.5)
1	IPRIN(1)	Same as on card R7.
2	IPRIN(2)	Same as on card R7. .....

Continuation of card R6		
3	IPRIN(3)	Same as on card R7. (-2: Doesn't work).
4	IPRIN(4)	Same as on card R7.
5	NNSTOP	= 0: No effect. > 0: Number of large time steps per burnup cycle, i.e. redefinition of JNSTOP (cards V11 and R10).
6	NNUM	= 0: No effect. > 0: Number of small time steps per large time step, i.e. redefinition of JNUM (cards V11 and R10).
7	NIAVC	= 0: No change of the option of average fuel cycle cost calculation. = 1: Drop average FCC calculation. = -1: Calculate average FCC.
8	IBUC	= 0: Leakage feed back option unchanged. = 1: Feedback of broad group bucklings to GAM and thermal leakage to THERMOS. = 2: Feedback of average epithermal buckling to GAM and thermal leakage to THERMOS. = 3: No feed back at all.
9	MUHU3	= 0: Streaming correction option unchanged. = 2: Streaming correction LIEBEROTH /27/ in power generating batches (only for pebble bed). = 3: No streaming correction at all.
10	NOCPA	= 0: Option of control poison adjustment unchanged. < 0: If in the preceding run control poison adjustment was calculated, it can be stopped here.
11	IVSP11	= 0: No change of diffusion calculation option. < 0: Drop diffusion calculation. > 0: Repeat diffusion calculation as defined by the IDIFF on cards V17 / R13.
12	INGC24	= 0: No effect. > 0: Value of option NGC24 (if previously defined equal -1 on card C3) is reset to zero value, starting with the next diffusion calculation.
13	XDAY	Same as DELDAY on cards V10 and R10.
14	XPOW	Same as POWER on cards V10 and R10.
15	XKAY	Same as ZKFIND on cards V10 and R10.

Card R7		Format (10I3,15I2,I12)
1	IVSP(1)	≤ 1: The information of this card holds only for this shuffling and for the following burnup cycle. > 1: The information of this card holds for IVSP(1) shufflings and burnup cycles. The items 2 ... 10 are kept, the others are set to 0. Output options:
2	IPRIN(1)	Spectrum calculation (same as on card V15): = 0: Thermal selfshielding factors, only. = 1: Same as 0, plus averaged thermal cross sections. = 2: Same as 1, plus fine group neutron fluxes. = 3: Same as 2, plus broad groups averaged cross sections for materials with concentration > 0. = 4: Same as 3, for all materials.
3	IPRIN(2)	= 0: No output. = 1: Printout of the irradiation time of the batches. = 2: Same as 1, plus atom densities (only in combination with IPRIN(3) ≥ 0).
4	IPRIN(3)	Burnup calculation (same as on card V15): = -2: All output dropped except K_{eff}. = -1: Global neutron balance. = 0: Detailed neutron balance. = 1: Same as 0, plus characteristics of all batches.
5	NPRINT	Fuel management operations at this reload: = -1: No fuel management output. = 0: Short summary. = 1: List of all operations. = 2: Detailed printout including atom densities in all batches before and after reload (very much!).
6	IPRINT	Fuel cycle costs calculation (same as on card K1): = 0: Printout without materials balance for each batch. = 1: Printout includes materials balance.
7	JTIK	VSOP - THERMIX: = 0: Minimum output. = 1: List of properties of the VSOP regions.
8	IN2	= 0: No effect. > 0: No. of the burnup time step for which a list of performance data will be printed. < 0: Print neutron balance averaged over the cycle.

Continuation of card R7		
		Steering the calculation performance:
9	IPRIN(4)	= 0: Skip spectrum calculation if a set of cross sections is available. Instructions on cards V16 / R12 are neglected. = 1: Repeat spectrum calculation as defined on cards V16 / R12. = 3: Same as 1, but not for zones without heavy metal (reflectors).
10	IVSP(11)	= 0: Drop diffusion calculation. > 0: Repeat diffusion calculation as defined by the IDIFF on cards V17 / R13. = 2: Read card R32 for this fuel shuffling in order to redefine the CITATION edit options. (Does not work for the first diffusion calculation of a restart).
11	NCYC	= 0: No effect. = 1: After this fuel management some fuel of the jumble boxes can be loaded into reprocessing mixtures. Here it is available for the fuel management after the next burnup cycle. Read card R11.
12	NKEEP	= 0: Use the previously defined fuel management scheme. = 1: Read a new fuel management scheme on the cards R21. = 2: Generate a new fuel management scheme with all batches staying in their position (no cards R21 are required). = 3: Generate a new fuel management scheme. Batches with individual fuel management instructions will be identified on cards R21. Non identified power generating batches will be shuffled to the next region. Non-power generating batches (e.g. reflectors) stay in their position. = 4: Same as 3. Also the power generating batches stay in their position. = 5: Generate a new fuel management scheme. For power generating batches: Fuel management instructions given for a batch on card R21 are also valid for all subsequent batches until redefined by a new card R21. Non-power generating batches (e.g. reflectors) stay in their position. = 6: Same as 3, but shuffling of each non identified power generating batch to the following batch within the same region.
13	IK	= 0: Normal. = 1: Fuel management is preserved for ORIGEN after large time step 1 (equilibrium cycle treatment for MEDUL-reactors - see input description of ORIGEN-JUEL-II /4/) on data set 'origmod'. = 2: Power histogram is preserved for decay heat calculation in thermal hydraulics part (THERMIX) or NAKURE-code /19/ starting from next cycle (data set 'nakure').
		.....

Continuation of card R7		
		= 3: Stop the preservation of the data for decay heat calculation. Last preserved data are from preceding cycle. Read cards LF after the very last card R (last burnup cycle, IVSP(24) > 0 on this card R7).
14	LK	= 0: Normal. = 2: Life history is preserved for ORIGEN-JUEL-II (all NON-MEDUL-reactors, see /4/), starting from next cycle (data set 'origen'). = 3: Stop the preservation of the data for ORIGEN-JUEL-II. Last preserved data are from preceding cycle. Read card P after the very last card R (last burnup cycle, IVSP(24) > 0 on this card R7) and cards LF, if present.
15	NTIK	= 0: No effect. > 0: Perform temperature calculation: = 1: Read new time steps ITEMP on card R14, and read new input for THERMIX on cards TX and KX. = 2: Read new ITEMP on card R14, use previous THERMIX input. = 3: Use previous ITEMP, and give new THERMIX input. = 4: Use previous ITEMP, previous THERMIX input.
16	NJ	Only if NTIK > 0: = 1: One single THERMIX calculation at each time step given by the ITEMP (steady state). > 1: Time dependent THERMIX parallel to the VSOP (cards TX and KX, see also Fig. 10): = 2: Power for THERMIX is only the decay heat. = 3: Power for THERMIX is the decay heat plus the fission power of the individual time step.
17	NI	= 0: No effect. Use the information of the given THERMIX-KONVEK input. = 1: Submit new KONVEK input.
		Redefinitions:
18	IVOID	= 0: No effect. = 1: Redefinition of void areas for CITATION on card R8.
19	IREDEF	= 0: No effect. = 1: Redefinition of time steps, power, criticality constraints etc. on card R10.
		.....

Continuation of card R7		
20	IVSP(16)	= 0: No effect. = 1: Redefinition of time steps for spectrum calculation. Give ISPEKT on card R12 (same as card V16).
21	IVSP(17)	= 0: No effect. = 1: Redefinition of time steps for diffusion calculation. Give IDIFF on card R13 (same as card V17).
22	IRETEM	= 0: No effect. = 1: Redefinition of temperatures of the spectrum zones. Read cards R15-R16 (same as card G2 and cards T4). = 2: Read new resonance integral definition on cards R17-R18 (same as cards G4-G5). = 3: Includes both options 1 and 2.
23	LIB	= 0: No effect. > 0: Write data set 'tinte' ("status of core") for TINTE /28/ at time step LIB prior to the spectrum and diffusion calculation. Read card R34. < 0: For each batch write atom densities on data set 'nucdens'.
24	MUHU(1)	= 0: No effect. > 0: Extracted number of nuclides (≤ 20) for the output of atom densities at the end of the burnup cycle. Read id. numbers NUPRI(I) on card(s) R33. Transfer to data set 'atlas' according to MUHU(8) (only for 3-dim. cases).
25	MUHU(8)	= 0: No effect (2-dim. cases). > 0: No. of burnup time step. Batch data of 3-dim. cases are written onto data set 'atlas' which can be evaluated in the display code ATLAS. Power, burnup, and thermal flux are written for the given burnup time step, atom densities (see MUHU(1)) and weight of materials for the end of the burnup cycle.
26	IVSP(24)	= 0: No effect. > 0: Terminate the run after this fuel shuffling. The following burnup cycle will be the first cycle in a restart case.

Card R8 only if IVOID = 1 on card R7 (only for the CITATION diffusion calculation).

Card R8		Format (18I4)
1	JH	Number of void areas. For each void area the following set of items:
2	IZONE(I),	Id. no. of a void cross section set to be inserted in the I-th void area (the cross section sets are defined on the cards C13 – C17 of CITATION. - see section 4.4.6.4).
.	M1(I,1),	First CITATION region located in the I-th void area.
.	M1(I,2), I=1,JH	Last CITATION region located in the I-th void area.

Card R9 only if NJ > 1 on card R7 and only at the beginning of time dependent THERMIX.

Card R9		Format (2I6,2E12.5)
1	JRESTW	= 0: No effect. > 0: THERMIX restart data will be written onto data set 'thxnew'.
2	JRESTR	= 0: No effect. > 0: THERMIX restart data will be read from data set 'thxold'.
3	PSPALT	= 0.: No effect. > 0.: Redefinition of the pressure in the gap compositions of THERMIX.
4	URZ	= 0.: No effect. < 0.: Minimum THERMIX output.

Card R10 only if IREDEF = 1 on card R7.

Card R10		Format (3I4,3E12.5,4E6.0)
1	JNSTOP	= 0: No effect. > 0: Redefinition of the number of large burnup time steps per burnup cycle (see card V11).

.....

Continuation of card R10		
2	JNUM	= 0: No effect. > 0: Redefinition of small burnup time steps in one large step (see card V11).
3	IVSP(27)	= 0: Streaming correction as defined before. = 2: Streaming correction by LIEBEROTH /27/.
4	DELDAY	= 0.: No effect. > 0.: Redefinition of the length of one large time step (days) (card V10).
5	POWER	= 0.: No effect. > 0.: Redefinition of thermal core power, Watts (card V10).
6	ZKFIND	= 0.: No effect. > 0.: Redefinition of end of cycle - K_{eff} (card V10).
7	HNUC	= 0.: No effect. > 0.: Number of new atom densities to be read on card R19. ($\leq$ 12)
8	HPOS	Only if HNUC > 0.: > 0.: Number of batches to be loaded with the new atom densities (read card R20). = 0.: Load additional materials into all power generating batches.
9	XTDOWN	= 0.: No effect. > 0.: Redefinition of length of down time during reload (TDOWN on card R2). < 0.: Set TDOWN = 0.
10	CONPOI	= 0.: No effect. > 0.: Read control poison adjustment data on cards R24 - R27. CONPOI gives the number of regions with control poison data. < 0.: Stop the control poison adjustments.

Card R11 only if NCYC = 1 on card R7.

Card R11		Format (6E12.5)
1 . MREP	FOJB(I), I=1,MREP	> 0.: Volumetric fraction of the I-th jumble box which shall be loaded into the reprocessing mixture I for the use at the reload after the following burnup cycle. < 0.: Volumetric fraction is calculated by the code. |FOJB(I)| gives the ratio: Volume to be loaded into the reprocessing mixture I / volume of the scrap fuel, which is discharged to the first aging box.

Card R12 only if IVSP(16) = 1 on card R7.

Card R12		Format (18I4)
1	ISPEKT(1)	≥ 0: No. of the first large burnup time step in which the spectrum calculation is to be repeated prior to the diffusion calculation.
2 . 18	ISPEKT(I), I=2,18	> 0: No. of further time steps for spectrum calculation. = 0: If all ISPEKT = 0, spectrum calculation is performed in every time step.

Card R13 only if IVSP(17) = 1 on card R7.

Card R13		Format (18I4)
1 . 18	IDIFF(I), I=1,18	If all IDIFF(I) = 0: Diffusion calculation is performed at every time step. If at least one IDIFF(I) ≠ 0: The IDIFF(I) give the time steps at which diffusion calculation is to be performed.

Card R14 only if NTIK = 1 or 2 on card R7.

Card R14		Format (18I4)
1 . 18	ITEMP(I), I=1,18	If all ITEMP(I) = 0: THERMIX temperature calculation at every time step. If at least one ITEMP(I) ≠ 0: The ITEMP(I) give the time steps at which temperature calculation is to be performed.

A set of cards R15 - R16 only if IRETEM = 1 or 3 on card R7.

Card R15		Format (6E12.5)
1 . NXS	SEMZUT(I), I=1,NXS	> 0.: Temperature of the resonance absorbers in the NXS different spectrum calculations. (°C) (See NXS on card V1). = 0.: Temperature of the I. spectrum calculation stays unchanged.
For each of the NKER scattering nuclides one set of cards R16. Card R16		Format (6E12.5)
1 . NXS	SCELS(I), I=1,NXS	> 0.: Temperature of this scattering nuclide for spectrum calculation I. (°C) (See NKER on card T1). = 0.: Temperature of the I-th one stays unchanged.

Cards R17 - R18 only if IRETEM = 2 or 3 on card R7.
For each design (IDESIN on card G1) 3 sets of cards R17-R18, the first set for ^{232}Th, the second set for ^{238}U, the third set for ^{242}Pu.

Card R17		Format (2E12.5,I6)
		Two values of homogenized atom densities of the resonance absorber nuclide, for which sets of resonance integrals are available on data set 'resint'. These values should represent the highest and the lowest densities, occurring within the reactor, respectively.
1	SM1	≥ 0.: Highest density of the absorber nuclide. [barn^{-1} cm^{-1}] = -1.: Density is taken from data set 'resint'.
2	SM2	≥ 0.: Lowest density of the absorber nuclide. [barn^{-1} cm^{-1}] = -1.: Density is taken from data set 'resint'.
3	NZ	Number of sets of resonance integrals for each SM1 and SM2 densities. These sets represent different temperatures of this absorber nuclide.

2 cards R18, the first one corresponds to SM1, the second one to SM2.

Card R18		Format (12I6)
1 . NZ	IZUT(K), K=1,NZ	Id. numbers of the resonance integral sets to be read from data set 'resint'.

Card R19 only if HNUC > 0. on card R10.

Card R19		Format (4(I6,E12.5))
1	INEW(I),	VSOP id. no. for the I-th new material.
2 .	DNEW(I), I=1,HNUC	Atom density for the I-th new material.

Card R20 only if HPOS > 0. on card R10.

Card R20		Format (12I6)
1 . HPOS	IBAE(I), I=1,HPOS	New materials only in the individual batches IBAE(I). (≤ 999)

When NKEEP = 1 on card R7 one full set of cards R21 - R23 for each of the different reload batches is required. This defines the FM-scheme. When NKEEP = 3, 4, 5 or 6, these cards are only required for batches with important instructions. Batches which are only shuffled to the next region (NKEEP = 3) or to the next batch within the same region (NKEEP = 6) or stay in their position (NKEEP = 2 or 4) do not need the card R21.

FM means "Fuel Management".
TBP means "This Batch Position".
OPB means "Out of Pile Box".
RPM means "Reprocessing Mixture".

Card R21		Format (2I5,I2,6I4,3E12.5)
1	IX1	= 0: Normal. > 0: When NKEEP = 3, 4, 5 or 6: No. of batch position to which this card R21 (and R22, R23) refers. < 0: Last card R21 holding for the batch |IX1|.
2	NRX	= 0: Refueling of this batch position TBP with fresh fuel specified by I7. > 0: Id. no. of a batch which is shuffled into TBP. > 10000: Load storage box no. (NRX - 10000) into TBP. (This storage box must have been filled up at a previous reload!). < 0: New atom densities are loaded into TBP. A set of |NRX| densities are defined on cards R22. The fuel type identification is unchanged (not a recommended option).
3	NSB	= 0: Normal. > 0: No. of storage box into which this batch is to be filled. Data can be retrieved in the following reload. (See chapter A.2.2)
4	NREP	= 0: No reprocessing. = 1: Reprocessing before loading into TBP. This option only when NRSTRT = 3 or 4 on card V6 and after having supplied cards R1.

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Continuation of card R21		
5	NSPALT	Number of materials for enrichment or reenrichment. A card R23 must follow.
6	MAKEUP	If NREP > 0 and/or NSPALT > 0: VSOP id. no. of the isotope used as make up material in reprocessed and/or reenriched fuel. The heavy metal density of the new batch is adjusted to the initial value of the loaded fuel type. If MAKEUP = 0: No material is added. Thus a new heavy metal loading is defined.
7	MANAGE	= 0: Load fuel without any change into TBP. = 1: Treated is the content of a reprocessing mixture which is the considered OPB. It can optionally be loaded from a jumble box (comp. card R5 and NCYC on card R7). The content has been formed from the disloaded fuel of one or more fuel types (XMARX on card R3) and has been summed up over previous cycles.
The following part of card R21 is dependent on the option MANAGE.		
MANAGE = 0:		
8	I7	= 0: Fuel type no. same as batch NRX. > 0: Fuel type to be loaded into TBP (only with out of pile FM, KUGL > 0 on card R2).
9	I8	Dummy.
10	R1	= 0.: Fissile enrichment stays unchanged. > 0.: R1 defines a new enrichment for the loaded fuel. Only relevant if fresh fuel is used.
11	R2	When NRX > 0 and use of in-core batches: = 0.: New volume of TBP is defined by the batch NRX, which is loaded. > 0.: R2 is the fraction of the in-core batch to be loaded into TBP. When NRX > 0 and use of storage boxes: = 0.: The total storage box volume is used for loading into TBP. By this way a new volume is assigned to TBP. A maximum is given .....

Continuation of card R21		
		by filling up of the region's volume. > 0.: R2 is the fraction of the storage box to be loaded into TBP. When NRX = 0: > 0.: Fraction of the total volume of the out of pile fuel of type I7 to be loaded into TBP. If KUGL = 1 (on card R2) the volume of all batch positions in the upper region is automatically limited to the region's volume. The fresh fuel store is unlimited.
12	R3	= 0.: Normal. > 0.: TBP will be integrated within a different spectrum zone, numbered R3. (≤ NXS on card V1).
MANAGE = 1:		
8	I7	New fuel elements are formed in the following way: The identification number and the total heavy metal content are taken from the fresh fuel type numbered by I7. The isotopic composition of the new fuel elements is taken over from the reprocessing mixture numbered by I8.
9	I8	Id. no. of the used reprocessing mixture.
10	R1	Enrichment N_{fiss}/N_{HM} for the new formed elements.
11	R2	> 0.: Fraction of the total reprocessing mixture (RPM) volume to be treated and loaded into the volume of TBP. < 0.: The RPM volume fraction |R2| is related to that part of the total volume, which has been left over from preceding loading procedures during the present fuel management step. If depletion would be necessary, the program reduces the RPM volume fraction R2 instead.
12	R3	= 0.: New volume of TBP is that one which has been made available from the RPM. > 0.: New volume of TBP is R3 * volume of the upper region which the presently considered batch belongs to. = 1.: The upper region is filled up. The new definition of the TBP volume immediately causes a corresponding change in the used RPM volume fraction R2. < 0.: The specified fraction of the RPM volume is reprocessed. No

.....

Continuation of card R21		
		fissile material is added or removed. Only make up material is added or removed in order to achieve the required enrichment R1 for the defined fuel type I7. The presently considered TBP volume is modified. For the presently considered TBP a volume WERA = |R3| * volume of the upper region is made available. If the prepared new volume of fuel elements is larger than WERA, the fraction R2 will be reduced. If it is smaller, the WERA will be reduced correspondingly.
Card(s) R22 only if NRX < 0 on card R21.		
Card R22		Format (4(I6,E12.5))
1,3,5 . 2,4,6 .	NPX(J), CPX(J), J=1,|NRX|	VSOP id. no. of the J-th nuclide with the atom density ≠ 0. Atom density of the J-th nuclide. If = 0., the nuclide needs not to be specified.
Card(s) R23 only if NSPALT > 0 on card R21.		
Card R23		Format (4(I6,E12.5))
1,3,5 . 2,4,6 .	IDFISS(J), FICOMP(J), J=1,NSPALT	VSOP id. no. of the J-th nuclide used for reenrichment. Relative fraction of the J-th nuclide in the enrichment composition. The sum of all FICOMP in the composition must be equal 1. Only the fissile isotopes in FICOMP are used to calculate enrichments, so the composition may also contain fertile materials, for instance 0.93 ^{235}U and 0.07 ^{238}U. The original fissile / HM ratio in the batch before re-enriching be YSPALT, the code distinguishes two different cases: Case 1: R1 > YSPALT, new material with the relative composition specified in FICOMP is added to make up the difference (R1 - YSPALT). .....

Continuation of card R23		
		Case 2: R1 < YSPALT, the original HM composition in the batch is unchanged, but the densities of all HM are reduced to obtain the fissile/HM ratio R1. The out of pile volume fraction R2 (card R21) is reduced correspondingly. To maintain the correct HM density the designated make up material (normally a fertile isotope) is added. Here, the FICOMP data are obsolete.
.	IXTYPE	= 0: Normal. > 0: The fuel in this batch position is given a new fuel type no. after reprocessing and/or reenrichment. Redefinition of types may be necessary in order to use pertinent cost data for recycled fuel.
.	HMETAV	= 0.: Normal. > 0.: New heavy metal density for use in this batch position, only of significance in connection with the MAKEUP option (on card R21). For some types of reactors the heavy metal loading in a particular batch position may have to be varied during the lifetime of the reactor, for instance during the running-in phase.

Cards R24 - R27 only if CONPOI > 0. on card R10.
One card R24 for each of the CONPOI regions with control poison data.

Card R24		Format (I12,2E12.5)
1	KR	Id. number of the considered region.
2	POISL(1)	Maximum atom density of the first control poison nuclide.
3	POISL(2)	Maximum atom density of the second control poison nuclide (if defined).

Cards R25 - R27 like cards V12 - V14 !!!

4.4.8.5 Criticality search for the reloads. R28 - R31

Cards R28 - R31 only if NRSTRT = 2 or 4 on card V6.

Card R28		Format (18I4)
1	JARIT	= 0: No iteration for this reload, skip cards R29 - R31. > 0: Total number of batches to be iterated, length of following list of batch id. no's. The atom densities of the materials specified on card R30 are iterated to give reactivity K-search.
2 .	NCOL(I), I=1,JARIT	Id. no. of the I. batch.
.	ITVAR	= 0: No effect. > 0: Use different sets of materials to increase resp. decrease enrichment to obtain correct K_{eff}. Two sets of cards R29 - R30: First set in case K-search > K_{eff} core, second set in case K-search < K_{eff} core. Code reads both sets of cards and selects the required one in each case.
.	IR16	= 0: Normal. > 0: Read card R31 with new heavy metal densities for iteration batches. IR16 is the number of batches in which the HM density is redefined and used to determine the amount of make up material to be added. The option may be necessary for reactors where the moderation ratio and HM loading in the fuel types vary during reactor life, for instance during the running-in phase.

If JARIT > 0 on card R28: At least one set of cards R29 - R30.
If ITVAR > 0 on card R28: Two sets of cards R29 - R30.

Card R29		Format (2(I6,E12.5))
1	ITMAT	Total number of materials iterated, i.e. length of materials list on card R30. (≤ 28)
2	XKEFF	> 0.: k(o), reactivity specification for iteration search in cycle i. = 0.: Use same k(o) as beginning of last cycle, $k^i(o) = k^{i-1}(o)$. < 0.: Determine a k(o) value for beginning of next cycle so that the end of cycle reactivity k(min) is reached after the specified number of time steps JNSTOP. The extrapolation is made from .....

Continuation of card R29		
		$k^i(o) = (k^{i-1}(o) - k^{i-1}(JNSTOP)) + k(min) * \|XKEFF\|$ and k(min) = ZKFIND (card V10). The value of XKEFF may be used to adjust for uncertainties in k(min). This is black magic.
3	MAKEUP	VSOP id. no. of nuclide to adjust heavy metal density in batches to either initial value in batch or as specified on card R31.
4	XTYPE	= 0.: Fuel type no. of batches is not altered. > 0.: New fuel type no. for batches. Same no. is given to all batches for which iteration is performed.

Card R30		Format (4(I6,E12.5))
1	IDIT(1)	VSOP id. no. of first nuclide used in iteration.
2	COMPIT(1)	Relative fraction of first nuclide.
3	IDIT(2)	VSOP id. no. of second nuclide.
4	COMPIT(2)	Relative fraction of second nuclide.
.		
.		The relative fractions of all ITMAT (card R29) nuclides must be equal 1. If all COMPIT = 0., the existing relative fractions in the batches remain unaltered during iteration.

Card R31 only if IR16 > 0 on card R28.

Card R31		Format (I6,E12.5)
1	IR	Batch no. for which the following HM density is specified. The specification on this card only for those batches for which the HM density differs from the initial one.
2	HMETAV (IR)	New heavy metal density in batch no. IR, to be used when adjusting the make up material. One card for each specified batch: I=1,IR16.

4.4.8.6 Re-definition of CITATION edit options. R32

Card R32 only if IVSP(11) = 2 on card R7.

Card R32		Format (8I3)
		Redefinition of edit options. Same as card C4 (see input section 4.4.6.2).

4.4.8.7 Extracted nuclides for printout and/or transfer to data set 'atlas' (for 3-dim. display code ATLAS). R33

Card R33 only if MUHU(1) > 0 on card R7.

Card R33		Format (12I6)
1 .	NUPRI(I), I=1, MUHU(1)	VSOP id. no. of nuclide for which printout and/or transfer to data set 'atlas' is desired. Up to 20 nuclides can be specified.

4.4.8.8 "Status of core"- data set for TINTE. R34

Card R34 only if LIB > 0 on card R7.

Card R34		Format (18A4)
1 . 18	TITEL(I), I=1,18	Literal description of the case to be transferred to the TINTE code /28/ via data set 'tinte'.

4.4.9 Fuel power histogram for decay power evaluation. - LF1 - LF3

Only if IK = 3 on any card R7

Card LF1 sets up the dimensions.

Card LF1		Format (3I6)
1	KMAX	Number of VSOP burnup cycles required for the set-up of the full irradiation history of the individual batches (compare KT5 > 0 on card LF2).
2	LMAX	Number of all VSOP time steps of the KMAX burnup cycles.
3	MTMAX	Number of graded time steps to be generated (≤ 49).

Card LF2		Format (5I6)
1	IOUT	Output option: = 0: Short output. = 1: Recommendable. = 2: Additional test output.
2	ICOMPA	= 0: The generated library of all batches in the graded time steps is printed out from batch no. 1. > 0: Print out starts from batch no. ICOMPA.
3	ICOMPE	= 0: Print out ends at the last batch. > 0: Print out ends at batch no. ICOMPE.
4	LT0	= 0:Default. Evaluation starts from the last time step of the given cycle. > 0: Time step of the given cycle, from which the precursory history evaluation begins.
5	KT5	= 0: No effect. = 1: Preserve only the last VSOP cycle and prepare KMAX identical cycles out of it. > 1: Preserve only VSOP cycle with id. no. KT5 and prepare KMAX identical cycles out of it.

Card LF3		Format (4E12.5)
1	TN	Time span (days) to be covered by the coarse new intervals (≥ maximum fuel element residence time + out of pile times).
2	DT	First coarse time interval (days). Normally the same as the last VSOP time step.
3	TOOP	MEDUL-fueling only: Time span (days) between fuel discharge from the core and its reload onto the core. Zero power is assumed during this shuffling procedure.
4	TEPS	> 0.: Convergence limit for iterative calculation of the incremental parameter of the coarse time steps. = 0.: Default value = 0.1 .

4.4.10 Fuel irradiation histogram for entire isotope generation. - P

Only if LK = 3 on any card R7

Card P		Format (3I6)
1	LXS	Number of time steps with spectrum calculation (for dimensioning only).
2	LT0	= 0: Normal. Evaluation starts from the last time step of the given cycle. > 0: Time step of the given cycle, from which the precursory history evaluation begins.
3	IOUT	Output option: = 0: Recommendable. = 1: Additional test output.

4.4.11 Preparing THERMOS-library. TTTT1 - TTTT5

Only if ITTT > 0 on card S1

Sequence of input cards:

S1 - G6: VSOP input of case identification.

TTTT1, TTTT2: THERMALIZATION input without selfshielding factors.

T1: Blank card.

TTTT3 - TTTT5: Preparing (condensing) new THERMOS library.

Card TTTT1		Format (12I6)
1	JNTAPE	Id.no. of the thermal 96 groups THERMALIZATION-library on data set 'thermal'. Only choice at present: JNTAPE = 115 .
2	NKER	Number of different scattering nuclides for the present spectrum run.
3	IDKER(1,I)	VSOP-id.no. of the first scatterer.
4	IDKER(2,I)	Thermal library-id.no. of scattering matrix to be applied.
.		
.	I=1,NKER	NKER different pairs of id. numbers and scattering matrices.

Card TTTT2		Format (3E12.5)
1	TOM	Temperature in calculation of Maxwellian neutron energy distribution for starting iterations of thermal spectrum. (°K)
2	EPSI	Criterion of convergence of flux iteration. (≅ 0.0001)
3	WAT	Acceleration of convergence: 0. = no, 1. = yes.

Card TTTT3		Format (A9,I3,4I6,E12.5)
1	DSIDTP	Data set name of the THERMOS library to be replaced or to be generated in addition to existing libraries. For possible choices see Table I.
2	ITTTT	> 0: Reduced output.
3	IEBE	Nuclide no. with full output.
4	ITUTEU	> 0: Print out of scattering matrices.
5	KERNE	Number of scattering matrices to be condensed for the THERMOS library. = 1000: Condensing of all scattering matrices.
6	ITOT	> 0: All absorbers.
7	T	Temperature (°K) for Maxwellian flux for eventually condensing absorbers.

Card TTTT4 only if KERNE ≠ 1000 on card TTTT3.

Card TTTT4		Format (12I6)
1	IDKER(1,J)	GAM-id.no. of the J-th scattering matrix.
2	IDKER(2,J)	VSOP-id.no. of the J-th scattering matrix.
.	J=1,KERNE	

Card TTTT5		Format (10I5)
1 . 30	NG(I), I=1,30	Number of the lowest THERMALIZATION group within the I-th THERMOS group to be formed.

4.4.12 2d-Thermal hydraulics. TX1 - KX5

Only if NTIK = 1 or 3 on card R7.

Card TX1		Format (18A4)
1 . 18	TITLE(I), I=1,18	Literal description.

Card TX2		Format (13I4,6I3)
		Steering the calculation:
1	IFKON	= 0: THERMIX calculation only, no KONVEK. Note: The input of KONVEK is needed anyway. ≠ 0: THERMIX-KONVEK coupling: = -1: Coupling between the temperatures of gas and solid material by heat transfer coefficient α. Recommended for steady state calculations, not valid in transient runs. = 1: Coupling via the source/sink distribution.
2	IHMAX	Used only for transient calculation: = 0: Temperature calculation in fuel elements by matrix elimination (Gauss). > 0: Approach by iteration (Gauss-Seidel). Not to be applied, if dummy elements (pure graphite spheres) are present!
3	IPRINT	= -2: Minimum output. = 1: Recommendable output. = 2: Maximum output.
4	IPUN	= 0: No effect. Steady state calculation only: = 3: Preserve temperature fields on data set 'thermix' as start-up values for a transient calculation.
5	IFRSTA	= 0: No effect. = 3: Read temperature fields from data set 'thermix' as start-up values for a transient calculation.

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Continuation of card TX2		
6	INTVAL	= 0: Steady state run. = 1: Transient calculation: The time steps are given by the burnup scheme (JNSTOP, DELDAY on card R10).
7	IFRED	= 0: For steady state calculation. > 0: Calculation of the decay power according to DIN 25485, using the fuel life history (see cards LF). Iterations:
8	MITMAX	> 0: Maximum number of iterations of temperature calculation. = 0: Default value = 2000
9	IKORM	> 0: Maximum number of changes of the relaxation factor. = 0: Default value = 100
10	IFREL	= 0: Inner iteration in radial direction (I). = 1: Inner iteration in axial direction (N).
11	ITLAM	> 0: Repeat calculation of temperature dependent material data for every ITLAM-th time step (only for steady state THERMIX-KONVEK iteration). = 0: Default value = 10
12	NLOOP	> 0: Maximum number of THERMIX-KONVEK ("Loop") iterations (steady state). = 0: Default value = 100
13	IEXPR	= 0: No effect. = 1: Write temperature fields (e.g. for 2d-plots) onto unformatted data set 'temunfor'. = 2: Write them onto formatted data set 'tempform'. Read card TX3.
14 . 18	ICODEF(I), I=1,5	= 0: Must be = 0 in steady state calculations. > 0: Id. numbers of one or more (≤ 5) THERMIX-compositions, whose properties shall be redefined for the transient calculation. Read a new card TX11 for each of these compositions, following card TX5.
19	IDE	= 0: No dummy (pure graphite) elements in the core. = 1: Fraction of dummy elements, identic in all core regions. Read card TX15 for the steady state calculation. = 2: Individual fraction of dummy elements in each core region (as defined on card BI2). Read card TX16 for the steady state calculation. For a transient calculation, cards TX15 or TX16, respectively, have to be dropped. Data then is automatically assigned.

Card TX3 only if IEXPR = 2 on card TX2.

Card TX3		Format (2E12.5)
1	PHIA	Start of temperature table at axial position PHIA (lower value according to THERMIX mesh point positions). (cm)
2	PHIE	End of temperature table at axial position PHIE. (cm)

Card TX4		Format (10F6.1)
1	QNORM	> 0.: Total power (MW). Input power field is normalized to QNORM. In a transient run the QNORM must be the reactor power, for which the life histogram was calculated. = 0.: Drop normalization.
2	ETHA	> 0.: Convergence criterion for local THERMIX temperature field. (°C) = 0.: Default value = 0.01
3	OVMAX	> 0.: Maximum relaxation factor. = 0.: Default value = 1.7
4	OVMIN	> 0.: Minimum relaxation factor. = 0.: Default value = 0.6
5	TDIFF	> 0.: Relative convergence criterion of the time independent THERMIX-KONVEK iteration. = 0.: Default value = 0.0005
6	EFAK	> 0.: Multiplication factor for maximum allowable error level, which stops the run. = 0.: Default value = 1.
7	DTVOR	> 0.: Maximum allowed relative temperature change $\Delta T / T$ in a time interval Δt of a transient run. The time intervals Δt are correspondingly adapted. = 0.: Default value = 0.05
8	ZEITMI	Minimum length of the time intervals Δt in a transient run. (sec)
9	EPSST	= 0.: Emission coefficient of graphite spheres from internal function GREPS(T). > 0.: New emission coefficient (e.g. for coated spheres).
10	ZEITNW	= 0.: (Special option).

Card TX5 only if INTVAL = 1 (transient calculation) on card TX2.

Card TX5		Format (F6.1,2I2,E10.3,F6.1)
1	DZEIT1	Length of the first small time interval. (sec)
2	NPRIN1	> 0: Print the fields of temperature and streaming for all NPRIN1 small time steps. = 0: Default value = 50 .
3	NKONV1	> 0: Run the KONVEK calculation every NKONV1 small time steps (only if IFKON ≠ 0 on card TX2). = 0: Default value = 1
4	ZEI1	End of the first large time interval. (hours) The following large time intervals are defined by variable DELDAY (card R10). The small intervals are defined by DZEIT.
5	DZEIT	= 0.: Free choice of the small intervals. < 0.: Also free choice, but maximum = |DZEIT|. (sec)

Cards TX6 – TX19 only if INTVAL = 0 (steady state calculation) on card TX2.

Card TX6		Format (E12.5,4I4)
1	PHI0	Height of the sum of all compositions above the core. (cm) Note: The upper edge of the core is located at the position 0. The axial core dimension is counted from top to bottom.
2	IFRFI	= 0: Default. = 1: Adiabatic boundary condition in the first radial mesh.
3	IFRFA	= 0: Default. = 1: Adiabatic boundary condition in the last radial mesh.
4	IFRFL	= 0: Default. = 1: Adiabatic boundary condition in the first axial mesh.
5	IFRFR	= 0: Default. = 1: Adiabatic boundary condition in the last axial mesh.

Card TX7		Format (2I4)
1	NTHX	= 0: Default (NCASE ≠ 2 on card BI1). > 0: Read data set 'geomther'. (Necessary if NCASE = 2 on card BI1).
2	IFTEST	= 0: Default = 1: Test option. For checking the input, the code runs without iterations.

Cards TX8 – TX10 define the coarse mesh grid and its subdivision into a fine grid, and the positions of KONVEK- and THERMIX-compositions in the coarse grid.

Card TX8		Format (6(I3,F9.0))
1	IC(1)	Number of fine mesh intervals in the 1. coarse radial interval.
2	C(1)	Width of the 1. coarse radial interval. (cm)
.	.	
.	.	
	IC(I)	> 0: Number of fine mesh intervals in the I-th coarse radial interval. = 0: End of radial mesh definition.
	C(I)	Width of the I-th coarse radial interval. (cm)

Card TX9		Format (6(I3,F9.0))
1	NC(1)	Number of fine mesh intervals in the 1. coarse axial interval.
2	C(1)	Width of the 1. coarse axial interval. (cm)
.	.	
.	.	
	NC(I)	> 0: Number of fine mesh intervals in the I-th coarse axial interval. = 0: End of axial mesh definition.
	C(I)	Width of the I-th coarse axial interval. (cm)

Two sets of cards TX10:
First set defines the KONVEK compositions to be described on cards KX3. One card TX10 is required for each axial coarse mesh "N" (even when no KONVEK composition is present in this mesh).
Second set defines the THERMIX compositions to be described on cards TX11 - TX14.

Card TX10		Format (24I3)
1	KOC(1,N)	> 0: Id. no. of composition in the 1. radial coarse mesh. = 0: No composition is present.
.	.	
.	.	
	KOC(I,N)	> 0: Id. no. of composition in the I-th radial coarse mesh. = 0: No composition is present.

One card TX11 (optionally followed by TX12 - TX14) for each THERMIX composition numbered continuously increasing.

Card TX11		Format (A3,6I3,9E5.0,E6.0)
1	BEM	Literal description of this composition,.3 digits. Free choice, except for: = HET: Temperatures are calculated in the inner of the fuel elements. Analysis of temperature/volume. = DBH: In a transient calculation the average and the maximum temperature of this composition is displayed as a function of time. = END: Termination of cards TX11, drop all other items of this card. Code sets variable KMAX = number of THERMIX compositions equal to highest value, which was assigned to variable I1.
2	I1	Id. no. of this composition.
3	IFTV	= -1: "Solid material zone". Temperature calculation comprises the heat exchange with the coolant of KONVEK by source/sink heat transfer within the meshes of this zone. = 0: "Solid material zone". No heat exchange with the coolant is involved. = 1: "Fluid zone". No temperature calculation is performed for this zone. Coupled with the neighbors by the heat transfer coefficient ALP on this card. Note: For instance these zones are used as a heat sink at the outer boundary of the system. At the top and right of the reactor one mesh is sufficient for this zone. At the bottom two meshes are required.

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Continuation of card TX11

4	IFWKT	= 0: Heat capacity given by C on this card. > 0: Identification no. of the material function for temperature dependent heat capacity (see Tab. VI).
5	IFLT	= 0: Thermal conductivity λ given by LAM on this card. > 0: Identification no. of the material function for temperature and dose dependent λ (see Tab. VII). = 7: The temperature dependent function of id. no. = 7 uses LAM0 of this card as λ(T = 0°C). = 4: In case of EPS1 and EPS2 > 0. (see below) the function uses LAM0 of this card as pressure (bar) of the gas in the gap. In case of EPS1 and EPS2 = 0. the function uses helium at the pressure 1 bar. No heat radiation.
6	IDIR	Only if EPS > 0.: = 0: Radiation in radial direction. = 10: Exclusively in radial direction. = 1: Radiation in axial direction. = 11: Exclusively in axial direction.
7	NTVAR	= 0: No effect. > 0: In case of fluid zone (IFTV = 1) provide time dependent temperatures on card TX14.
8	RHO	Volumetric fraction of solid material in this composition. RHO is used for calculation of the heat capacity.
9	C	= 0.: When IFWKT > 0. > 0.: Heat capacity of the solid material. (J/cm^3/°K)
10	LAM	= 0.: When IFLT > 0. > 0.: Thermal conductivity in solid material zones (only if IFTV = 0 or -1). (W/cm/°K)
11	LAM0	= 0.: Default. > 0.: When IFLT = 7, LAM0 is λ(T = 0°C). When IFLT = 4 and EPS1 > 0. and EPS2 > 0., LAM0 is the pressure of the gas in this composition.
12	EPS1	= 0.: No heat radiation. > 0.: Coefficient of emission for heat radiation; inner wall of the gap. (Maximum number of compositions with heat radiation = 19).
13	EPS2	Like EPS1, for outer wall.
14	R1R2	Horizontal gap: = 0. Radial gap: Ratio: inner radius / outer radius.

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Continuation of card TX11

15	TVOR	= 0.: Start-up temperature field results from the input temperature field of the cards TX17 - TX19. > 0.: Start-up temperature of this composition (°C) superior to the start-up temperatures of the cards TX17 - TX19.
16	WPRR	= -1.: Field of power density results from VSOP. It will be normalized to QNORM (card TX4). ≥ 0.: Power density of this composition. (W/cm^3)
17	ALP	= 0.: No effect. > 0.: Heat transfer coefficient in fluid zones (only if IFTV = 1). ($W/cm^2/°K$) Note: ALP ≅ 0.5: Temperature at the boundary close to that of this fluid zone. ALP ≅ 0.01: Temperature at the boundary close to that of the adjacent zone.

Cards TX12, TX13 only if BEM = "HET" on card TX11.

Card TX12 Format (2E10.3,I5)

1	HEPS	> 0.: Void fraction in the pebble bed. = 0.: Default value = 1. - RHO (on card TX11).
2	HKUG	Diameter of the spherical fuel element. (cm)
3	NHZON	Number of radial mesh intervals in the sphere. (≤ 5)

I = 1,NHZON cards TX13.

Card TX13 Format (E10.3,2I5,E10.3)

1	DI(I)	Inner diameter of the I-th radial mesh interval. (cm) Caution: I = 1 ... counts from the outer shell towards the inner.
2	NH1(I)	Id. no. of temperature dependent thermal conductivity (see IFLT on card TX11).
		.....

Continuation of card TX13		
3	NH2(I)	Id. no. of temperature dependent heat capacity (see IFWKT on card TX11).
4	XFW(I)	Shielding factor of the power density in the I-th shell (normally = 1. in the fuel shells, = 0. in the outer graphite zone).

Card TX14 only if NTVAR > 0 on card TX11.

Card TX14		Format (14F5.2)
1	TKV(I),	Temperature. (°C)
2 .	ZEIV(I), I=1,NTVAR	Time. (h)

Card TX15 only if IDE = 1 on card TX2.

Card TX15		Format (E12.5)
1	DEC	Fraction of dummy elements to be assigned to <u>all</u> core regions.

Card TX16 only if IDE = 2 on card TX2.

Card TX16		Format (6E12.5)
1 . .	BLIND(I), I=1,LAYER	Fraction of dummy elements in the I-th core <u>region</u> (definition of core regions according to the definition on card BI2) continuously numbered beginning with region 1 of channel 1 through the last region of the last channel. Thus, LAYER is the total number of regions in the core.

Card TX17		Format (2I5,6E10.3 / 7E10.3)
1	IPOLI	= 0: Linear interpolation of temperature input of cards TX19. = 1: Logarithmic interpolation (radial).
2	IE	= 0: Drop cards TX18, TX19. > 0: Number of radial mesh points for start-up temperature input.
3 .	RE(I), I=1,IE	Radial mesh points for start-up temperature input on cards TX19. Continuation cards according to given FORMAT.

Cards TX18 - TX19 only if IE > 0 on card TX17.

Card TX18		Format (2I5,6E10.3 / 7E10.3)
1	IPOLN	= 0: Linear interpolation of temperature input of cards TX19. = 1: Logarithmic interpolation (axial).
2	NE	Number of axial mesh points for start-up temperature input.
3 .	PHE(I), I=1,NE	Axial mesh points for start-up temperature input on cards TX19. Continuation cards according to given FORMAT.

One card TX19 for each of the N = 1,NE axial mesh points.

Card TX19		Format (7E10.3)
1 . IE	T(I,N), I=1,IE	Start-up temperature at mesh point I, N.

Card TX20		Format (2I6,5E12.5)
1	MZNORM	= 0: No effect. > 0: Start the time counting from the present THERMIX-restart (see card R9).
2	MC2	= 0: No effect. > 0: Read card TX21 with definition of THERMIX compositions for time dependent output of the "heat storage". (Also stored on data set 'therlist'). The following items only in transient calculations with evaluation of the decay power:
3	SIG	= 0.: Default value = 1. > 0.: Factor to be multiplied with the explicitly evaluated decay power function.
4	RL	Avg. power density. (MW/m^3)
5	SM	Avg. heavy metal content per fuel element (incl. pure graphite spheres). (g/sphere)
6	BURN	Avg. burnup of spent fuel. (MWd/kg_{HM})
7	A0	Initial fissile enrichment of the fuel. (w%)

Card TX21 only if MC2 > 0 on card TX20.

Card TX21		Format (70I1)
1 . KMAX	IKO(I), I=1,KMAX	"Heat storage" fraction id. no. to which the heat of THERMIX composition I shall be added up. Possible "heat storage" fraction numbers: 1 - 5 (core data is always stored). IKO(I) = 0 means no storage.

Card TX22		Format (5E12.5)
1	DELTAT	Desired temperature interval (ΔT) for the numerical integration inside the fuel elements (°K). Up to 200 intervals are possible between TU and TO.
2	TU	Lowest surface temperature of fuel elements.
3	TO	Highest temperature at center of the fuel elements.
4	WRIT	= 0.: Program uses standard data of the thermal conductivity as a function of fast neutron dose and temperature. > 0.: Like = 0, but various test output of temperature integration inside the fuel elements in addition. < 0.: Thermal conductivity as a function of fast neutron dose and temperature will be given on the cards TX23 - TX26.
5	R0	= 0.: No effect. > 0.: Inner radius of the fuel matrix (if shell ball is considered).

Cards TX23 - TX26 only if WRIT < 0. on card TX22.

Card TX23		Format (5I6)
1	NSCH	Number of different functions of the thermal conductivity. (≤ 2)
2	KTEM(N), N=1,NSCH	Number of temperature mesh points for which the thermal conductivity will be given. (≤ 10)
.	LFAD(N), N=1,NSCH	Number of fast neutron dose mesh points for which the thermal conductivity will be given. (≤ 10)

For each of the NSCH thermal conductivity functions one set of cards TX24 - TX26.

Card TX24		Format (6E12.5)
1 . KTEM	TSTUE(K), K=1,KTEM	Temperature mesh points.

Card TX25		Format (6E12.5)
1 . LFAD	DSTUE(L), L=1,LFAD	Mesh points of fast neutron dose.

For each of the LFAD mesh points of the fast neutron dose one card TX26.

Card TX26		Format (6E12.5)
1 . KTEM	WLSTUE(K) K=1,KTEM	Thermal conductivity at the temperature mesh points. (W/cm/°C)

Card KX1		Format (5E10.3,3I5)
1	EPSI1	> 0.: Relative criterion of convergence for gas temperature. = 0.: Default value = 1.E-5
2	EPSI2	> 0.: Criterion of convergence for mass flow. = 0.: Default value = 0.01
3	OVM1	> 0.: Extrapolation factor for iterations on mass flow (every 10 iterations an extrapolation is provided with 1 + OVM1). = 0.: Default value = 0.5
4	OVM2	> 0.: Relaxation factor for iterations on mass flow. = 0.: Default value = 1.0
5	EPSI4	> 0.: Relative criterion of convergence of the avg. gas temperature in the outer iterations between gas temperature and mass flow. = 0.: Default value = 0.02
6	ITM1	> 0: Maximum number of iterations for gas temperature. = 0: Default value = 100
7	ITM2	> 0: Maximum number of iterations for mass flow. = 0: Default value = 500
8	ITM3	> 0: Maximum number of outer iterations between gas temperature and mass flow. = 0: Default value = 5

Card KX2		Format (5E10.3,I5)
1	DKUG	> 0.: Diameter of the spheres. (cm) = 0.: Default value = 6.0
2	EPSI	> 0.: Void fraction in the core. = 0.: Default value = 0.39
3	CP	> 0.: Specific heat capacity of the gas. (J/kg/°K) = 0.: Default value = 5195.
4	PRAN	> 0.: Prandtl-constant of the gas. = 0.: Default value = 0.66
5	DRUCK	Pressure of the gas. (bar)
6	IFZDR	= 0: Pressure of the system is constant. = 2: Pressure changes according to temperature. Gas inventory is constant.

One card KX3 for each of the KONVEK compositions as defined on the first set of cards TX10.

Card KX3		Format (5I6,7E6.0)
1	KR	Id.no. of this composition.
2	IFBQ	= 0: When IFTV = -1 on card TX11. Convective heat source is computed in the meshes of this composition. = -1: No convective heat source evaluation (e.g. in voids).
3	IFBR	Type of composition: = 0: No gas streaming. = 1: Pebble bed. = 2: Vertical pipes. (Total number of such compositions ≤ 8) = 5: Horizontal void (no more than one mesh over its thickness).
4	IFZST	= 0: No time dependent mass flow. = 1: Given by input on cards KX4, KX5. = 2: Mass flow according to conservation law (heat sink).
5	IFZTF	= 0: No time dependent gas inlet temperature. = 1: Given by input on cards KX4, KX5.

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Continuation of card KX3		
6	PVOR	> 0.: Pressure at beginning of iterations. (bar) = -1.: Pressure = pressure of the gas (see DRUCK on card KX2).
7	XKON	Additional pressure drop relative to computed pressure drop over the length of the channel (only if IFBR = 2). (1/cm)
8	ALPHA	= 0.: Internal calculation of the coefficient of heat transition. In voids (IFBR = 5) use ALPHA = 0. > 0., ≠ 1: No internal calculation of ALPHA. Use the given value. ($W/cm^2 K$) = 1.: For the pebble bed.
9	EPSIL	Volumetric fraction of void in this composition.
10	DHYD	Hydraulic diameter (cm). Only if IFBR ≥ 2.
11	STZUK	Source of mass flow. (kg/s)
12	TFLVOR	Temperature of inlet gas. (°C)

Cards KX4, KX5 only if at least one of the IFZST and/or IFZTF = 1 on cards KX3. Up to 100 time steps can be defined by cards KX5. Linear interpolation is provided between the time steps.

Card KX4		Format (4I10)
1	IZK1	Number of compositions with time dependent input of mass flow and/ or gas inlet temperature. (≤ 3)
2 .	IZKOM(I), I=1,IZK1	Id. no. of the I-th composition.
Card KX5		**Format (8F9.3)**
1	ZVOR	> 0.: Time. (min) = 0.: End of the input of cards KX5.
2	ZDR	Pressure. (bar) .....

Continuation of card KX5		
3	ZST(I)	Source of mass flow of the composition no. IZKOM(I). (kg/s) (Only if IFZST(I) = 1).
4 .	ZTF(I), I=1,IZK1	Temperature of inlet gas of the composition no. IZKOM(I). (°C) (Only if IFZTF(I) = 1).

5. Input Manual V.S.O.P.-ZUT

5.1 Steering the execution mode. ZS

Card ZS		Format (A8)
1	MODE	= data2zut: For spherical fuel elements only (coated particle fuel). Read cards DZ and Z. = zutalone: All other fuel element geometries. Read cards Z only.

5.2 Fuel element design. DZ1 – DZ9
(only if MODE = 'data2zut')

One set for each variant of each desired fuel type (limited to 27 different sets).
Calculation is terminated by one last card DZ1.

Card DZ1		Format (18A4)
1 . 18	TITLE(I), I=1,18	Literal description of fuel element-types and –variants. TITLE(1) = 'stop': This terminates the sequence of cards DZ1–DZ9.

Card DZ2		Format (3I4,E12.5)
1	NFUTP	Identification of the fuel elements in 4 digits IJKL: IJ : Type (characterizes design), increasing numbers. (≤ 10) KL: Variant (e.g. for different enrichments), increasing numbers, starting from 01 for each type IJ.
2	NFCP	Input option for the coated particle: = 2: Read cards DZ3 - DZ7. = 1: Read card DZ3 only. = 0: Data from preceding design.
3	NFBZ	Input option for the fuel element: = 1: Read cards DZ8 - DZ9. = 0: Data from preceding design.
4	FF3	> 0.: Volumetric filling fraction of spherical fuel elements in the core. = 0.: Default value = 0.61

Card DZ3 only if NFCP > 0 on card DZ2.

Card DZ3		Format (E12.5)
1	ANR	Fissile enrichment of the fuel (fissile/heavy metal), atom fraction. = 0.: If INDBS (card DZ4) = 7 .

Cards DZ4 - DZ7 only if NFCP = 2 on card DZ2.

Card DZ4		Format (5I4)
1	INDBS	Fuel identification: = 1: UO_2 = 2: UC = 3: UC_2 = 4: UO_2 - ThO_2 = 5: UC - ThC = 6: UC_2 - ThC_2 = 7: PuO_2 = 8: PuO_2 - ThO_2 = 9: PuO_2 - UO_2
2	NCT	Total number of coating layers (≤ 5), to be numbered with increasing radius.
3	NSIC1	Number of the 1. SiC coating layer, if present.
4	NSIC2	Number of the 2. SiC coating layer, if present.
5	IU8TH	Preparation of ZUT-data for: = 1: ^{232}Th = 2: ^{238}U = 3: ^{242}Pu = 4: ^{235}U

Card DZ5		Format (4E12.5)
1	RK	Radius of the coated particle kernels. (cm)
2	ROBR1	Density of the kernels. (g/cm^3)
3	ROBR2	Density of 2. type of kernels, if present. (g/cm^3) Only if INDBS = 4, 5, 6, 8, 9 on card DZ4.
4	BETA	Enrichment of the uranium N_{U5} / N_U if INDBS = 4, 5, 6, 9 on card DZ4.

Card DZ6 only if INDBS = 7, 8 or 9 on card DZ4.

Card DZ6		Format (4E12.5)
1 . 4	PU(I), I=1,4	Atom fractions of the isotopic composition in plutonium: ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu.

Card DZ7		Format (6E12.5)
1,3,5	DCT(I),	Thickness of the I-th coating layer. (cm)
2,4,6	ROCT(I), I=1,NCT	Density of the I-th coating layer. (g/cm3) (Numbered with increasing radius, NCT on card DZ4).

Cards DZ8 – DZ9 only if NFBZ = 1 on card DZ2.
Only a selected set of the following parameters of the cards DZ8 and DZ9 is required. Possible combinations are given in Table VIII.

Card DZ8		Format (6E12.5)
1	R1	Outer radius of fuel zone. (cm) (Fuel zone consists of coated particles and graphite matrix).
2	R2	Outer radius of the sphere. (cm)
3	FF1	Volume fraction: coat.part. / (coat.part. + matrix).
4	VMOD	Moderation ratio N_C / N_{HM}.
5	INDBK	= 0: No dummy elements. = 1: Dummy elements existing.
6	BK	Volume fraction: dummy elements / (fuel + dummy) elements.

Table VIII: Alternative specifications of spherical fuel elements

No.	1	2	3	4	5	6	7	8	9	10	11
INDBK	0	0	0	0	0	0	0	1	1	1	1
R1	x	x	x	x	x			x	x	x	x
R2	x	x	x			x	x	x	x	x	x
FF1		x			x		x		x		x
VMOD			x	x	x	x	x	x	x		
ROSM	x			x		x		x		x	
BK										x	x

Card DZ9		Format (5E12.5)
1	ROSM	Density of heavy metal, homogenized in the fuel zone. (g/cm^3)
2	ROMTX	Density of graphite in the matrix. (g/cm^3)
3	ROSCH	Density of graphite in the outer shell. (g/cm^3)
4	ROBK	Only relevant for INDBK = 1: > 0.: Density of graphite in the dummy elements. (g/cm^3) = 0.: Density of graphite in the dummy elements equals ROSCH.
5	SR0	Inner radius of the matrix. (cm) (normally = 0.) > 0. for "shell ball" design.

5.3 Resonance integral calculation. Z1 - Z20

Note:
If MODE = 'data2zut' on card ZS and resonance parameters provided from a library, the input is reduced to the cards Z1 - Z6.

In order to open a new direct access data set 'resint' for storage of the resonance integral values read cards Z18 - Z20, Z6.

5.3.1 Short input. Z1 - Z6

Cards Z1 - Z5 can be repeated for N different cases. The input stream is terminated by the card Z6.

Card Z1		Format (I1,I5,I1,E9.4)
1	IEND	9
2	JI	00000
3	KI	1 (Number of items on this card).
4	RNRESO	1.) Perform ZUT calculation: = 1.: Read resonance parameters for ^{235}U from data set 'resdatu5'. = 2.: Read resonance parameters for ^{232}Th from data set 'resdatth'. = 3.: Read resonance parameters for ^{238}U from data set 'resdatu8'. = 4.: Read resonance parameters for ^{242}Pu from data set 'resdapu2'. = 5.: Read resonance parameters from input cards Z7 - Z10. 2.) Prepare resonance parameter (r.p.) data set: = 6.: Read r.p. from input cards Z7-Z10 for ^{235}U, write onto data set 'resdatu5'. = 7.: Read r.p. from input cards Z7-Z10 for ^{232}Th, write onto data set 'resdatth'. = 8.: Read r.p. from input cards Z7-Z10 for ^{238}U, write onto data set 'resdatu8'. = 9.: Read r.p. from input cards Z7-Z10 for ^{242}Pu, write onto data set 'resdapu2'. From the value of RNRESO result different sequences of the following input cards: For RNRESO = 1. - 4. the sequence is: a) MODE = 'data2zut': Z1 - Z6 b) MODE = 'zutalone': Z1, Z2, Z4, Z5, Z11 - Z17 .....

Continuation of card Z1		
		For RNRESO = 5. the sequence is: Z1, Z2, Z4, Z7-Z9, Z5, Z10-Z17 MODE must have the value 'zutalone'. For RNRESO = 6. – 9. the sequence is: Z1, Z7 - Z10

Card Z2		Format (7E10.4)
1	ETEMP	Temperature of the resonance absorber. (°K)
2	ENERGU	Lower energy boundary for the set of resonance data to be respected. (eV)
3	ENERGO	Upper energy boundary for the set of resonance data to be respected. (eV)
4	ESOLVE	Five digits IJKLM.0 as specification of the calculation method: I : Specifies the geometry of the absorber regions: = 0: Infinite size or numerical computation of the geometric escape probability P(E). (Coated particle grain structure, see section A.1.2) = 1: Cylindrical geometry = 2: Slab. = 3: Spherical, analytic formula of P(E). J : Specifies the method for scattering by the absorber: = 1: Down scattering based on the computed neutron flux. = 2: NR-approximation. = 3: IM-approximation. K : In case of "double heterogeneous calculation" plus calculation of unresolved resonances (IEND=6 on card Z8), the coating material of the particles must be specified as moderator 1. = 0: Moderator no. 1 is not present. = 1: Down scattering in moderator no. 1 uses the computed neutron flux. = 2: Down scattering assumes 1/E flux. .....

Continuation of card Z2		
		L = 0: Moderator no. 2 is not present (cp. item K). = 1: Down scattering in moderator no. 2 uses the computed neutron flux. = 2: Down scattering assumes 1/E flux. M = 0: Normal output option. > 0: More output.
5	TESTA	These three digits IJK.0 for output options. (Use 001.0) I ≥ 1: Control data of the energy fine structure for each resonance. J ≥ 1: Partial probabilities at the mesh points of the P(E) – calculation. K ≥ 1: Mesh points of P(E), Dancoff factors and data of homogenization of the matrix zone.
6	EW(13)	Number of mesh points for P(E)-calculation. (≅ 20)
7	VAZVG	Volume of absorber / total cell volume.

Card Z3 only if MODE = 'data2zut' on card ZS.

Card Z3		Format (6E12.5)
1	FUTYP	Fuel type and -variant specification to be applied. See variable NFUTP on card DZ2).
2	EAMOD1	Atomic weight of moderator material 1, which is admixed with the absorber. (e.g. Carbon) (only if K > 0 in ESOLVE on card Z2).
3	ESIGM1	σ_s of the moderator 1 (only if K > 0 in ESOLVE).
4	EAMOD2	Atomic weight of moderator material 2, which is admixed with the absorber (e.g. Oxygen) (only if L > 0 in ESOLVE).
5	ESIGM2	σ_s of the moderator 2 (only if L > 0 in ESOLVE).
6	ECDANC	Dancoff factor. = 0.: For infinite absorber size or numerical computation of P(E) for the spherical fuel elements. > 0.: Dancoff-Ginsburg factor. Required for the cylindrical fuel element. This ECDANC has higher priority than the internally calculated one, which can optionally be ordered by the card Z11.

Card Z4		Format (11I6)
1	IDSATZ	Identification number of this set of resonance integrals to be stored on data set 'resint' for further use in GAM-calculations (VSOP-MS).
2	IDNUCL	GAM-library identification no. of the absorber nuclide.
3 . 11	LOESCH(J), J=1,9	Id.-numbers of existing resonance integrals on data set 'resint' to be deleted prior to creating the new set.

Card Z5		Format (4A3,24X,12A3)
1 . 4	HEAD(J), J=1,4	Literal heading, e.g. date.
5 . 16	HEAD(J), J=5,16	Literal heading, e.g. case identification.

Termination of the input sequence by card Z6.

Card Z6		Format (I1,I71)
1	IEND	9
2		Blank: Terminates the sequence of resonance integral calculations.

5.3.2 Resonance parameters. Z7 - Z10

Cards Z7 - Z10 only if RNRESO = 5., 6., 7., 8. or 9. on card Z1.

Note:
The input of resonance parameters on cards Z7 - Z9 must be terminated by a blank-card.

One card Z7 for each resolved resonance. In rising sequence of the energy EZERO.

Card Z7		Format (I1,I5,I1,5E9.4)
1	IEND	2
2	JI	00005
3	KI	5
4	EZERO	Energy at the center of the resonance. (eV)
5	GAMN	Γ_n (eV)
6	GAGM	Γ_γ (eV)
7	R	= 0.: Mesh spacing under the resonance decided by the code. > 0.: Mesh spacing under the resonance.
8	S	Ratio: Range of integration / effective width. Give S = 5.

Cards Z8, Z9 for the unresolved resonances.

Card Z8		Format (I1,I5,I1,6E9.4)
1	IEND	6
2	JI	00000
3	KI	6
4	EC	Lower energy of the range of unresolved resonance evaluation. (eV)
5	GAMNO	Avg. [Γ_n°] (eV)
		.....

Continuation of card Z8		
6	GMGM	Avg. [Γ_γ] (eV)
7	G	Statistical weight.
8	D	Avg. spacing between the resonances. (eV)
9	EO	Upper energy of the range of unresolved resonance evaluation. (eV)

Card Z9 only if one of the input figures for the unresolved resonances differs from the corresponding value, which has been defined for the resolved resonances.

Card Z9		Format (I1,I5,I1,4E9.4)
1	IEND	6
2	JI	00000
3	KI	4
4	SIGPZ	σ_s . Potential scattering cross section of the absorber.
5	SIGM1	σ_s of moderator 1.
6	SIGM2	σ_s of moderator 2.
7	C	Dancoff factor. = 0.: For infinite absorber size or numerical computation of P(E) for the spherical fuel elements. > 0.: Dancoff-Ginsburg factor. Required for the cylindrical fuel elements. This C has higher priority than the internally calculated one, which can optionally be ordered by the card Z11.

Card Z10		Format (I1,I5,I1,4E9.4)
1	IEND	1
2	JI	00001
3	KI	4
4	AZERO	Atomic weight of the absorber.
5	G	Statistical weight factor. (= 1. for ^{232}Th, ^{238}U and ^{242}Pu)
6	SIGPZ	σ_s . Potential scattering cross section of the absorber.
7	TEMP	Temperature. (°K)

5.3.3 Explicit fuel element design. Z11 - Z17

Cards Z11 - Z17 only if MODE = 'zutalone' on card ZS.

Card Z11 only if Dancoff factor calculation by subroutine DANC3.

Card Z11		Format (I1,I5,I1,7E9.4)
i	IEND	7
2	K	Type of lattice: 00010: Square lattice up to the 4. neighbor. 00014: 4 x 4 bundle. } 00015: 5 x 5 bundle. } Finite lattice 00016: 6 x 6 bundle. } 00020: Triangular lattice up to the 4. neighbor. 00022: 2 - rods bundle. 00023: 3 - rods bundle. 00027: 7 - rods bundle. 00029: 19 - rods bundle.
3	KI	7
4	A	Radius of the rod. (cm)
		.....

Continuation of card Z11		
5	B	Pitch. (Distance between the center lines of the rods). (cm)
6	DHUE	Cladding thickness. (cm)
7	DSP	Thickness of the gaps between the bundles (for K = 14, 15, 16) (cm)
8	SMOD	Σ_{tot} of the moderator. (cm^{-1})
9	SHUE	Σ_{tot} of the cladding. (cm^{-1})
10	SSP	Σ_{tot} in the gaps. (cm^{-1})

Card Z12		Format (I1,I5,I1,3E9.4)
1	IEND	1
2	JI	00010
3	KI	3
4	SOLVE	Same value as ESOLVE on card Z2 must be given here.
5	ABAR	Radius (cm), for cylindrical or spherical fuel. Half thickness (cm), for slab. = 0.: Infinite absorber size, or explicit calculation of $P(\sigma_a)$.
6	C	Dancoff factor. = 0.: For infinite absorber size or numerical computation of P(E) for the spherical fuel elements. > 0.: Dancoff-Ginsburg factor. Required for the cylindrical fuel elements. This C has higher priority than the internally calculated one, which can optionally be ordered by the card Z11.

Card Z13		Format (I1,I5,I1,7E9.4)
1	IEND	1
2	JI	00013
3	KI	7
4	EDZERO	N_{abs} atom density of absorber (atoms / (barn*cm)).
5	EAMOD1	Atomic weight of moderator no. 1.
6	ESIGM1	σ_s of moderator 1. (barn)
7	EDIQU1	$N_{mod\,1}$ / N_{abs} ratio.
8	EAMOD2	Atomic weight of moderator no. 2.
9	ESIGM2	σ_s of moderator 2. (barn)
10	EDIQU2	$N_{mod\,2}$ / N_{abs} ratio.

Cards Z14, Z15 only if numerical evaluation of P(E) is required (I = 0 in ESOLVE on card Z2).

Card Z14		Format (I1,I5,I1,6E9.4)
1	IEND	5
2	JI	00018
3	KI	6
4	R1	Radius of the kernel of a coated particle. (cm)
5	R2	> 0.: Outer radius of a coated particle. (cm) = 0.: Coated particles and matrix are treated homogenized.
6	R4	Outer radius of the matrix. (cm)
7	R5	> 0.: Outer radius of a spherical fuel element. (cm) = 0.: Cylindrical fuel element.
8	F	Volumetric filling fraction coat.part. / (coat.part. + matrix); (matrix including possible inner coolant / graphite zones)
9	H	= 0.: Default > 0.: Fraction of dummy graphite spheres in the pebble bed.

Card Z15		Format (I1,I5,I1,4E9.4)
1	IEND	5
2	JI	00025
3	KI	4
4	SI2	Avg. Σ_{tot} of the coatings. (cm^{-1})
5	SI4	Σ_{tot} in outer shell of a spherical element. (cm^{-1})
6	SI5	Σ_{tot} in dummy graphite spheres. (cm^{-1})
7	ALPH	Ratio of: (Σ_{tot} of the matrix / average Σ_{tot} of the coatings).

Card Z16		Format (I1)
1	IEND	8: Termination of input of this resonance integral calculation.

Card Z17		Format (A3)
1	HEAD(1)	REP: Another input case will follow (possible only for the same resonance absorber). END: Termination of the calculation.

5.3.4 Opening of a new resonance integral data set ('resint'). Z18 - Z20

Card Z18		Format (1X,I5)
1	JI	= - 30: Opening of direct access data set 'resint' for the resonance integrals in GAM-group-structure.

Card Z19		Format (2I6)
1	IDENTI	= -180 .
2	IZAHL	Number of sets to be reserved for the resonance integral sets. (Use 170)

Card Z20		Format (3I2)
1 . 3	K(I), I=1,3	= -1-1-1: Special key word.

A. Appendix (Comments)

A.1 Neutron spectrum calculation

Spectrum calculations are made by means of the codes GAM-I /12/ and THERMOS/13,14/. They are allowed for an unlimited number of spectrum zones.

GAM-I performs neutron spectrum evaluation in 68 energy groups ranging from 10 MeV to 0.414 eV. It uses the materials homogeneously distributed and it applies the P1-approximation. Heterogeneity effects can be included by defining selfshielding factors. Resonance cross sections can be generated for ^{232}Th, ^{238}U and ^{242}Pu by means of the ZUT-DGL code/7,8/, which is part of the V.S.O.P-section VSOP-ZUT. Leakage of neutrons from/to the adjacent spectrum zones is included by buckling terms which are generated from the diffusion calculation over the whole reactor.

The THERMOS code performs a 1-dimensional cell calculation in 30 energy groups ranging from 10^{-5} eV to 2.05 eV. Again input of selfshielding factors allows to account for additional heterogeneity. The effect of coated particle grain structure can be included by evaluation of the collision probability for a neutron which travels through a coated particle. Neutron coupling to other spectrum zones is accounted for by calculating albedos by use of the leakage terms.

The resulting neutron fluxes are applied to form broad group cross sections for the subsequent diffusion calculation. In the thermal energy range only one broad group is allowed.

A.1.1 Resonance integrals

For the isotopes ^{232}Th, ^{238}U and ^{242}Pu resonance integrals are evaluated by the VSOP-ZUT-section. The corresponding cross sections can be transferred to the GAM code. They are added to the background absorption cross sections of the GAM-library. This background is independent of lumping effects and temperature. (The GAM-I cross sections in the region of the unresolved resonances are treated as infinitely diluted and are included in the background data. They have to be corrected by means of selfshielding factors in case of high lumping of the resonance absorber).

Prior to do a VSOP-MS task, the resonance absorption cross sections must be prepared for the considered fuel assemblies for different absorber concentrations at different temperatures. They are stored on the permanent data set 'resint'. VSOP-MS applies these sets for the different spectrum calculations during the following of the reactor operation. The dependence of the cross sections on the temperature and on the fuel burnup is achieved by linear interpolation between the respective cross section sets.

A.1.2 Coated particle grain structure

At energy ranges with λ_a (E) smaller than the mean cord length **l** of a coated particle, the grain structure is of importance in spectrum calculations. This is true in the resonances and at the lower end of the thermal spectrum. Therefore, the capability of grain structure effect has been included in the ZUT and THERMOS codes.

The resonance integral calculation of the standard ZUT code is made for a homogeneous distribution of the resonance absorber in the finite volume of a lump. The transport equation is solved in very fine groups over the energy range of each resonance. The calculation also includes the neutrons which are born in the lump, leave it, and are absorbed or scattered down in any other lump of the same configuration. Excluded are those neutrons which leave the lump and undergo scattering reactions outside. Nordheim excludes these neutrons by the geometric escape probability

$$P(E)=\frac{P_0(E)\cdot(1-C)}{1-(1-l\cdot\Sigma_a(E)\cdot P_0(E))\cdot C}$$

in which C is the Dancoff factor and P_o (E) is the probability for a neutron to escape from the lump of its birth. This method has proven to be a good approximation for lumps of all degrees of grayness.

In case of coated particles inside a fuel element the absorber lump is the inner kernel of a representative coated particle. Because of the smallness of a particle, the escape probability P_0(E) is close to 1, even for neutrons with energy close to the peak of strong resonances. The neutron can travel through many coated particles without any collision, whether through the coatings or stripping through the kernels. It can meet the boundary of the fuel matrix, pass through the outer shell of the fuel element, enter another matrix, and undergo collision in any of its coated particles or somewhere between them. Fig. 6 gives the different possibilities to escape from a coated particle.

For such a "double heterogeneous" composition of the absorber lumps a Dancoff factor is hard to define. Therefore in ZUT-DGL /8/ the escape probability P(E) is directly evaluated by a numerical method.

The possible path of a neutron is subdivided into parts for which the probability of traversing can rigorously be evaluated by a numerical treatment. This requires the evaluation of 8 different probabilities W_1 - W_8 as indicated in Fig. 6. For instance, W_1 is the probability for a neutron to undergo a collision in the coating of the coated particle in which it was borne. Finally, the geometric escape probability is

$$P(E) = W_1 + W_2(W_3 + W_4) + W_2 W_5 \frac{W_6 + W_7}{1 - W_8}$$

This formula can replace the P(E) of Nordheim in the version ZUT-DGL. It has been derived for spherical and for cylindrical elements. The outline of the numerical treatment is given in Ref. /8/.

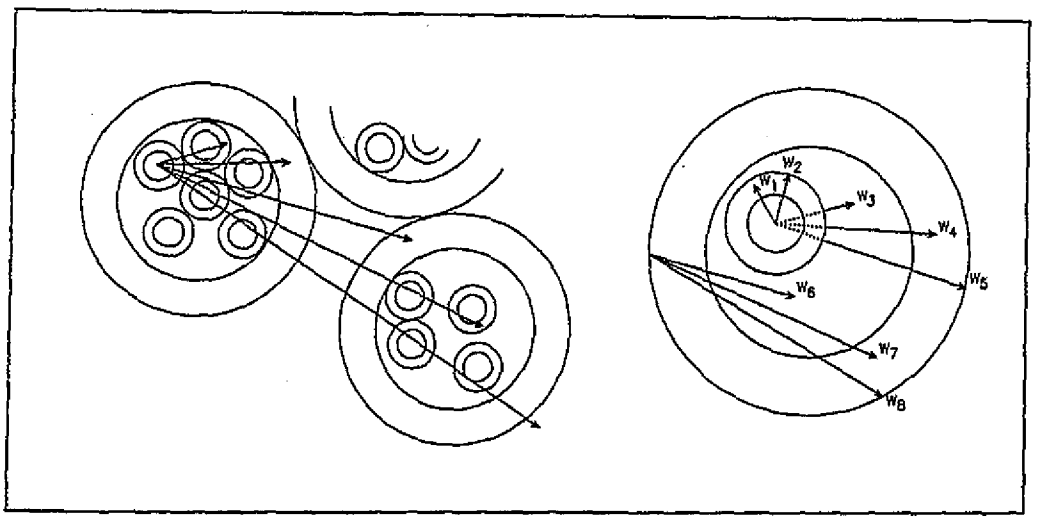

Fig. 6: Break down of the neutron escape probability.

In the thermal energy range - i.e. in the THERMOS code- the grain structure is treated analogously: in the fuel matrix the mean path of a neutron from one coated particle to the next one be *L*. Its magnitude results from the diameter and from the volumetric filling of the particles in the matrix. For a neutron at the energy *E* the probability *W(E)* of traversing one coated particle and the corresponding amount of matrix material is calculated by a direct numerical integration as outlined in Ref. /14/. Thereupon, *W(E)* is used to define an effective macroscopic total cross section $\Sigma_e(E)$ by the equation

$$W(E) = e^{-\Sigma e(E) \cdot L}$$

$\Sigma_e(E)$ is used to replace the homogenized $\Sigma(E)$ of the mixture of matrix and coated particles in the THERMOS calculation. The individual reaction rates of the different materials are defined correspondingly.

A.1.3 Selfshielding factors in the epithermal energy range

The GAM code performs epithermal spectrum calculations for the nuclide composition resulting from a homogenization of the respective spectrum zones. Selfshielding factors can be applied for the many nuclides. They can be given in coarse energy groups or in the 68 group structure of the GAM library. Two types of selfshielding factors can be submitted:

SC: Cross section selfshielding factors allow modification of the microscopic cross sections of the library. This might be desired to account for resonance shielding effects, for changes of the neutron energy spectrum within a fine group g, or for improved measurements of cross sections, respectively. The code allows input of LSUB different subsets of cross section-selfshielding factors SC_g. They can be applied for any nuclide in any spectrum zone. The SC_g are multiplied to the respective cross sections σ_g of the energy group g.

SF: Neutron flux-selfshielding factors allow to bring the cell structure local neutron flux in relation to the average cell flux.

Assuming a space and energy dependent cell calculation, the reaction rate per volume V_0 of the cell is given by

$$R = \sum_{g=1}^{NG} \sigma_g \cdot SC_g \cdot \sum_{k=1}^{NK} N_k \cdot V_k \cdot \Phi_{kg}$$

being:

g, NG	energy groups of the GAM library
k, NK	cell zones
σ_g, SC_g	cross section and corresponding selfshielding factor
V_k	volume of cell zone k
ϕ_{kg}	neutron flux

(Note: R represents the reaction rate of any nuclide in any spectrum zone. Respective subscripts have been dropped.)

In view of the homogeneous treatment of the cell in the GAM code, the neutron reaction rate per cell volume can be formed in terms of the average cell flux ϕ_{0g}:

$$R = \sum_{g=1}^{NG} \sigma_g \cdot SC_g \cdot N_0 \cdot V_0 \cdot \phi_{0g} \cdot \sum_{k=1}^{NK} \frac{N_k \cdot V_k \cdot \phi_{kg}}{N_0 \cdot V_0 \cdot \phi_{0g}} \cdot$$

with the following cell zone averaging applied

$$V_0 = \sum_{k=1}^{NK} V_k \qquad N_0 = \sum_{k=1}^{NK} N_k \cdot \frac{V_k}{V_0} \qquad \phi_{0g} = \sum_{k=1}^{NK} \phi_{kg} \cdot \frac{V_k}{V_0}$$

With the definition of the neutron selfshielding factors of the different cell zones

$$SF_{kg} = \frac{\phi_{kg}}{\phi_{0g}}$$

the reaction rate can be written in the form

$$R = \sum_{g=1}^{NG} \sigma_g^* \cdot N_0 \cdot V_0 \cdot \phi_{0g}$$

where the cross section is modified by the selfshielding factors SC and SF

$$\sigma_g^* = \sigma_g \cdot SC_g \cdot \sum_{k=1}^{NK} \frac{N_k \cdot V_k}{N_0 \cdot V_0} \cdot SF_{kg}$$

These modified cross sections σ^*_g are applied in the GAM spectrum calculation. They are further applied to form the broad group cross sections which are turned to the diffusion and burnup calculations.

The selfshielding factors SC_g and SF_{kg} are defined by the data input according to cards G10 - G12. They may be given in few broad energy groups *J*. The code books them into the respective fine groups *g*.

A.1.4 Leakage feedback

The 2 / 3-dimensional diffusion calculation by the CITATION module provides leakage terms L_{SI} for the different spectrum zones *S* and coarse energy groups *I* (option IBUCK >0 on card V6). They are available for the subsequent spectrum calculation. For the first one at the beginning of the reactor operation all leakage terms have a zero value. Startup leakage terms can be generated by running a dummy initial cycle of a very short time interval with practically zero-burnup.

For the epithermal coarse groups the leakage terms are transformed into bucklings

$$B_{SI}^2 = \frac{L_{SI}}{D_{SI} \cdot \phi_{SI} \cdot V_S}$$

which are needed by the P1 approximation of the GAM code. In case of option IBUCK=1 the bucklings are directly booked into the corresponding fine groups. If IBUCK = 2, the code prepares one average epithermal buckling to be booked into all fine groups of the GAM. In some cases the use of multiple coarse group bucklings led to unreliable results strongly depending on the coarse energy group structure. Stable results, however, have always been obtained by the application of one single averaged buckling.

For the thermal cell code THERMOS the thermal leakage is transferred into the albedo at the surface of the cell:

$$a = \frac{j_-}{j_+}$$

This is the ratio of the current density j_- of neutrons entering the cell divided by j_+ leaving the cell. The partial currents are given by

$$j_- = \frac{\phi_0}{4} - \frac{j_0}{2} \qquad\qquad j_+ = \frac{\phi_0}{4} + \frac{j_0}{2},$$

$j_0 = j_+ - j_-$ being the net current leaving the cell per cm^2. The net current of the cell is equal to the ratio of the leakage L_c of the cell per surface S_c:

$$j_0 = \frac{L_c}{S_c}$$

On the average, the leakage of one cell is equal to the leakage of the whole spectrum zone divided by the number of cells (n_c) in the spectrum zone:

$$L_c = \frac{L_s}{n_c} \qquad \text{and} \qquad n_c = \frac{V_s}{V_c} \cdot (1-e)$$

being
- L_c: Leakage of the cell
- L_s: Leakage of the spectrum zone
- V_c: Volume of the cell
- V_s: Volume of the spectrum zone
- e: Void fraction between the cells, if present

Approximating the neutron flux at the surface of each cell by the average neutron flux Φ_s of the spectrum zone then leads to the albedo

$$a = \frac{1 - \frac{2}{\phi_s} \cdot \frac{L_s}{V_s(1-e)} \cdot \frac{V_c}{S_c}}{1 + \frac{2}{\phi_s} \cdot \frac{L_s}{V_s \cdot (1-e)} \cdot \frac{V_c}{S_c}}$$

A.2 Design specifications

A.2.1 Reactor layout (input cards BI and TR)

The geometric design of the reactor is provided in the subroutines BIRGIT (2-d) or TRIGIT (3-d). In VSOP the basic unit of reactor material compositions is named a "batch". For the first core loading the reactor design must be subdivided into batches. They all must be loaded with fuel material or - outside the active core- with the materials of the reflectors etc. The calculation is performed individually for each batch: For the in-core batches it is the follow of the burnup, of the fuel shuffling, cost evaluation, and of the decay power production in transient temperature calculations.

In many cases different types of fuel elements, or elements of a different irradiation age form a nearly homogeneous mixture within the reactor core. They are exposed to the same local neutron flux. For this purpose a mix of the respective batches can be put together forming a "region". These regions represent volume parts *V(I)* of the reactor, which provide the distribution of materials (and of their cross sections) for the calculation of the spatial neutron flux distribution. Further, some larger number of batches are grouped together forming "spectrum zones". Spectrum calculations are based on the averaged atom densities of these zones. They provide the broad group cross sections for the respective batches.

In the pebble bed reactor the fuel elements move downward from the top towards the bottom of the core. Here, the shape of the regions and their shuffling must fit into the flow pattern. On the other hand the calculation of the neutron flux is performed by means of the code member CITATION /15/, and this is confined to a pattern of "CITATION-compositions" *W(J)* with perpendicular boundaries in r-z coordinates. Similarly the thermal hydraulics code member THERMIX /17/ is subject to a mesh lattice of perpendicular r-z coordinates. Transfer of the relevant data of the "regions" to CITATION compositions and back is provided by a volume matrix which is generated in subroutine BIRGIT.

The subroutine generates both reactor "regions" *V(I)* and CITATION compositions *W(J)*. It then synthesizes a matrix of volumes *VW(I,J)*, which is the overlapping set of the *V(I)* and *W(I)* as shown in Fig. 7.

The transfer of the nuclear data proceeds as follows:

- Macroscopic cross sections Σ are made for the "batches" and thereafter for the "regions": $\Sigma(I)$.
- The $\Sigma(I)$ are converted into macroscopic cross sections $\Sigma(J)$ of the CITATION compositions by

$$\Sigma(J) = \frac{\sum_I \Sigma(I) \cdot VW(I,J)}{W(J)}$$

- Code section CITATION provides the criticality and neutron flux calculation.
- Neutron fluxes Φ(J) of the CITATION compositions are transformed to fluxes Φ(I) of the "regions" by

$$\Phi(I) = \frac{\sum_J \Phi(J) \cdot VW(I,J)}{V(I)}$$

and this is applied for the further burnup calculations of the "batches".

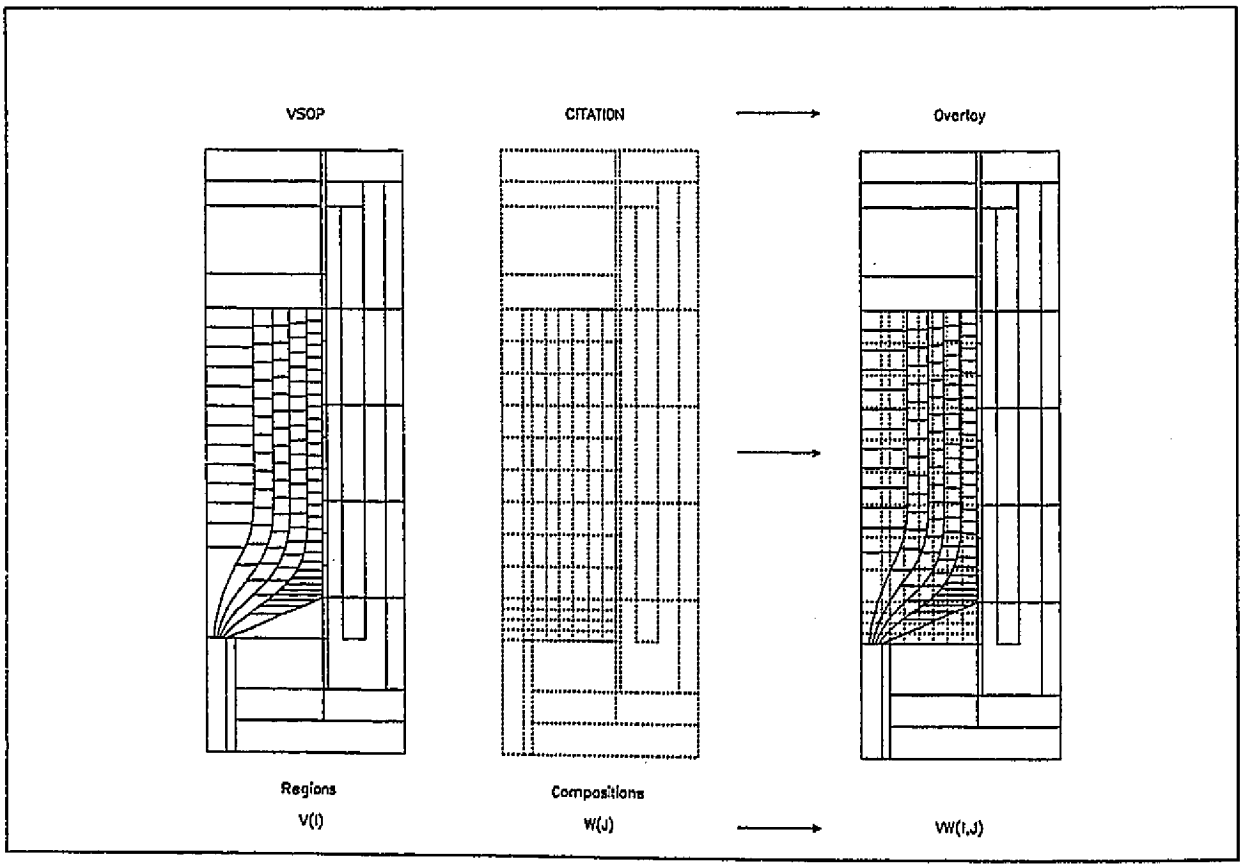

Fig. 7: Overlay of reactor-regions and CITATION-compositions

Analogously, a transfermatrix *VW(I,K)* between the "regions" *V(I)* and the fine mesh volumes *W(K)* of the code member THERMIX can be provided. Here, the power distribution, the fast neutron dose, the local decay power, and spectrum zones identification numbers are transferred to the THERMIX. The temperatures of the fuel and of the moderator of the different spectrum zones are turned back.

As seen from Fig. 7, the two different mesh grids overlap in the area of the core. But they are congruent in the reflectors.

In case that parallel movement of the fuel elements from the top to the bottom of the core may be assumed as a sufficient approximation the data input is restricted to cards BI-1 through BI-5, and thus is rather short and simple. A more sophisticated simulation of the movement of the fuel elements can be defined by input according to cards BI-6 through BI-9 in addition. Here, a more complex geometry of the core bottom of a pebble-bed core and very special flow patterns of the fuel - resulting from experimental data or from theoretical research - can be considered. The limiting curves of "flow channels" are defined by few coarse points, and the curves are gained by interpolation. The radial position of the coarse points can internally be modified in order to adjust the channel volume to a predefined value. Each channel is subdivided into regions *V(I)*, which are numbered by the code from top to bottom starting with the first inner channel. Subsequent upon the highest region number within the core, the reflector regions are numbered in the order as given on the input card BI-5.

The matrix of volumes *VW(I,J)* is derived in the following way: A very fine mesh grid of an elementary volume of few cm^3 is superposed over the given grids. For every small mesh the code identifies the respective *V(I)* and *W(J)* in which it is located. It adds the elementary volume to the corresponding element of the *VW(I,J)* volume matrix.

In case of a non-parallel movement of the fuel elements an overlay also for THERMIX is to be defined in the same way for the THERMIX-meshes, but only for the core area. The return of the temperatures to the reflector spectrum zones is made by the code independently of the transformation of the subroutine BIRGIT.

Similarly, subroutine TRIGIT prepares the geometric design in 3 dimensions (x-y-z). Here, "regions" and CITATION compositions must be identical.

A.2.2 Out-of-pile fuel positions

During the burnup cycle the data for the many batches of the reactor (core, reflectors etc.) are stored in an array in the common. The atom densities within the core area are subject to burnup.

Beyond the batches of the reactor itself, there are numerous further positions reserved, which represent out-of-pile fuel positions. They serve as storage for fresh fuel, and for the disloaded fuel which can be reloaded to the reactor, or stored, or reprocessed, or removed and sold, respectively. Four different types of out-of-pile positions can be defined:

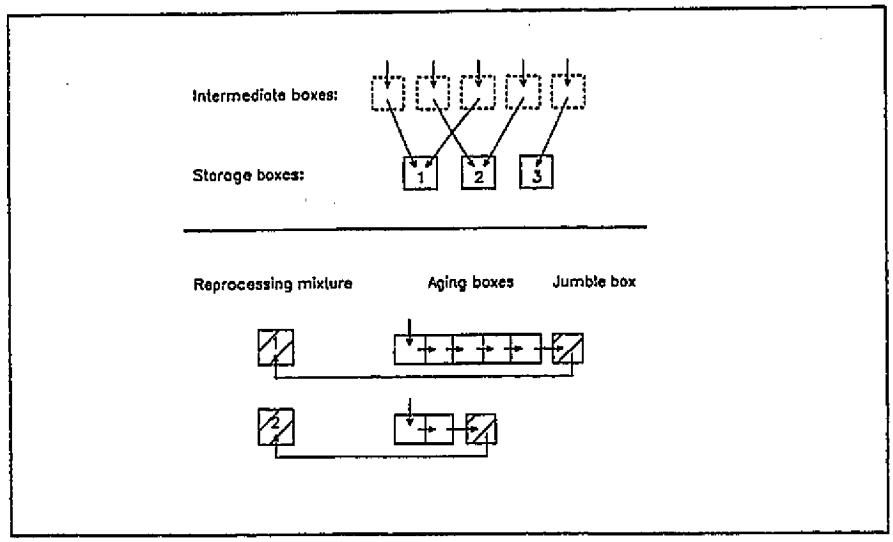

Fig. 8: Out-of-pile fuel positions

1. Fuel types. In the course of the shuffling the reactor batches can be loaded with fuel from these fuel positions. 1 through 10 different fuel types can be defined.

   When the shuffling of the batches of the reactor is complete, all the fuel is considered which has not been used in the shuffling specifications. It is available for use in the next shuffling step.

2. "Storage boxes". Shuffling specifications from cards R21 can also direct fuel into storage boxes. Temporarily it is stored in intermediate boxes, because the content of the storage boxes stems from the preceding shuffling and is available for reload at the present shuffling procedure.

   After the shuffling has been finished the remaining fuel of the storage boxes is turned to the scrap fuel of the respective fuel types. Thereupon, the content of the intermediate boxes is directed into the storage boxes, then being ready for use at the subsequent shuffling.

3. "Reprocessing mixtures". The scrap fuel of one or more fuel types can be directed into reprocessing mixtures. Here, the amount of fuel adds up from cycle to cycle, and parts of it can be used for recycling. Re-use of the fuel can be defined with reprocessing and with re-fabrication of new fuel elements.

4. "Aging boxes". This is an extension of the reprocessing mixture option, which simulates an intermediate storage for isotopic decay. This option allows real bookkeeping of the out-of-pile inventories with given decay periods prior to reprocessing. It has been developed for the simulation of closed fuel cycles.

The scrap fuel is first turned to a sequence of "aging boxes" in which the decay proceeds over a given time period. During this period the fuel is bound to the out of pile storage and is not available for re-use. The last box (named jumble box) is reserved for accumulation of the fuel which has gone through the aging period. At every shuffling step its content is turned to the respective mixture for the purpose of re-use. After the end of the shuffling procedure the amount of unused fuel is turned back to the jumble box.

A.3 Simulation of reactor operation

As seen from the input manual, the design of reactor life time follow requires information about many different physical events which are mutually coupled with each other. The user should be familiar with the respective physical laws and with their representation by the calculation model. Beyond the input description the following comments might give a further help in setting up a reactor simulation.

For the repeated calculation of the thermal neutron spectrum an efficient acceleration is included in the code: It preserves the field of the neutron flux and provides it as initial guess for the subsequent calculation. The same is done for repeated diffusion calculation. If during the burnup periods in between the isotopic concentrations change only slightly, the number of iterations is reduced this way by about 90% or more.

A.4 Restart

When the option to prepare restart data is defined, the code prepares several data sets to be used at the restart of the calculation (see chapter 3.4 for details). Using the restart option, parametric research can easily be made at different time steps during the simulation of reactor operation, i.e. at selected time steps of the running-in period or at different time steps of an annual fueling cycle, e.g. for power transients, shut-down procedures, ingress of water / air or loss of coolant etc.

A.5 Fuel cycle costs

Evaluation of the fuel cycle costs is based on the present worth method. It is performed by means of the module KPD /18/. Before and after each step of fuel shuffling, the code accepts the inventory of the heavy metal isotopes of all in-core batches and of the out-of-pile fuel. All fuel which enters the system is regarded as bought, and the fuel leaving the system is regarded as sold. Basing on this knowledge the code evaluates expenditures and revenues individually for each of the examined cycles. From this result the fuel cycle costs of each cycle dated to the start of the cycle.

Life time fuel cycle costs are derived from the individual cycle costs, which are re-dated to the start up of the reactor operation. For this evaluation the last calculated cycle is considered as an equilibrium cycle. It is considered to be identically be repeated until the end of reactor operation.

An important role is played by the delay times of payments and revenues, especially for the costs of fabrication and of spent fuel, respectively. The many choices of lead and lag times are illustrated in Fig. 9 (left hand side). They are grouped together as shown on the right hand side of the figure.

Break down of the fuel cycle costs is evaluated in four different terms:

1. Fuel costs include the expenditures for the fuel and working capital costs.

2. Revenue for the spent fuel assumes reprocessing. In case of final storage it can be nullified by depreciation factors (input card K8).

3. Fabrication costs, which also include the re-fabrication in closed cycles

4. Reprocessing costs, which more accurately should be named "spent fuel handling costs", because they could also be the costs of final disposal if an adequate value is given for the input variable CAUF on card K7.

The whole history of the reactor life time can be written onto a data set "costdata" (See Fig. 3 and chapter 3.4).

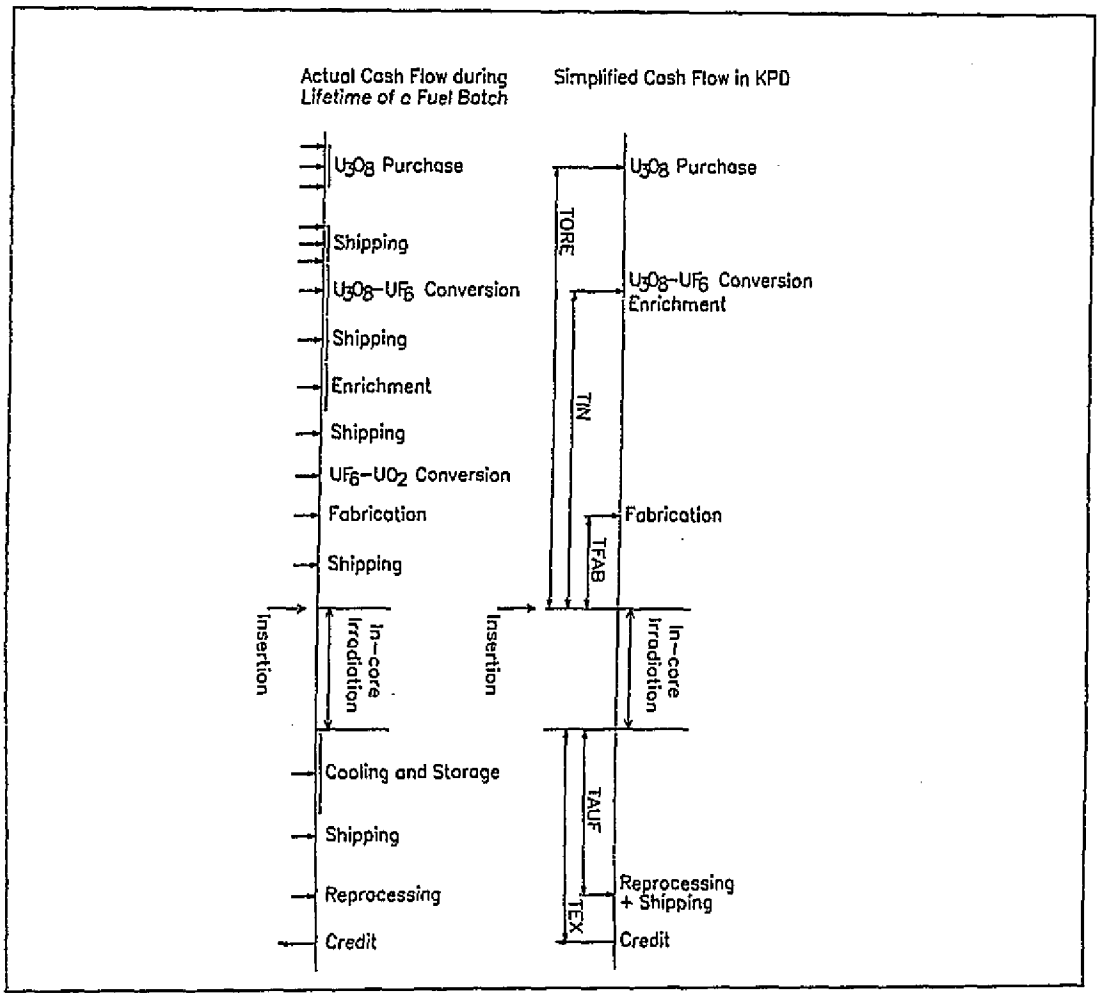

Fig. 9: Lead and lag times of payments

A.6 Thermal hydraulics (THERMIX code)

The THERMIX-KONVEK code has been developed for the thermal hydraulics evaluation of the pebble-bed HTR in two dimensions (r-z geometry) /17,21,22/. The code may simulate steady state and transient conditions. It is linked into VSOP (see Fig.2 and Fig. 3). It receives the power distribution of the reactor core from the nuclear code modules at given points in time. It then returns the corresponding temperatures of the fuel and of the moderator averaged over the volumes of the reactor spectrum zones to be used for further neutronics evaluation (Fig. 10).

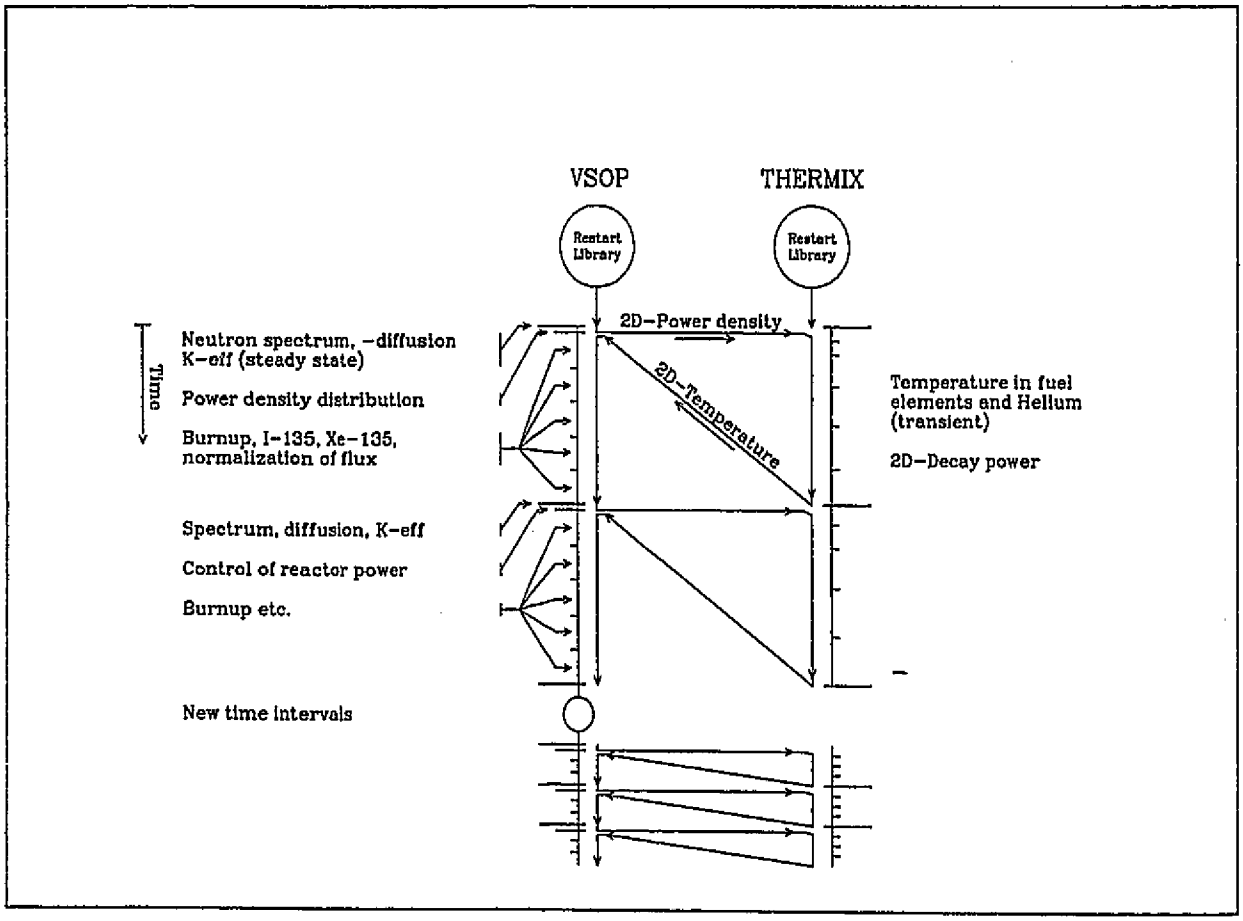

Fig. 10: Coupling between neutronics and thermal hydraulics

A.6.1 Basic equations

The calculation of the overall heat transmission is synthesized of the coupling of different equations which represent conservation laws. These equations are solved individually and the synthesis is made by a superposed iteration. (Fig. 11).

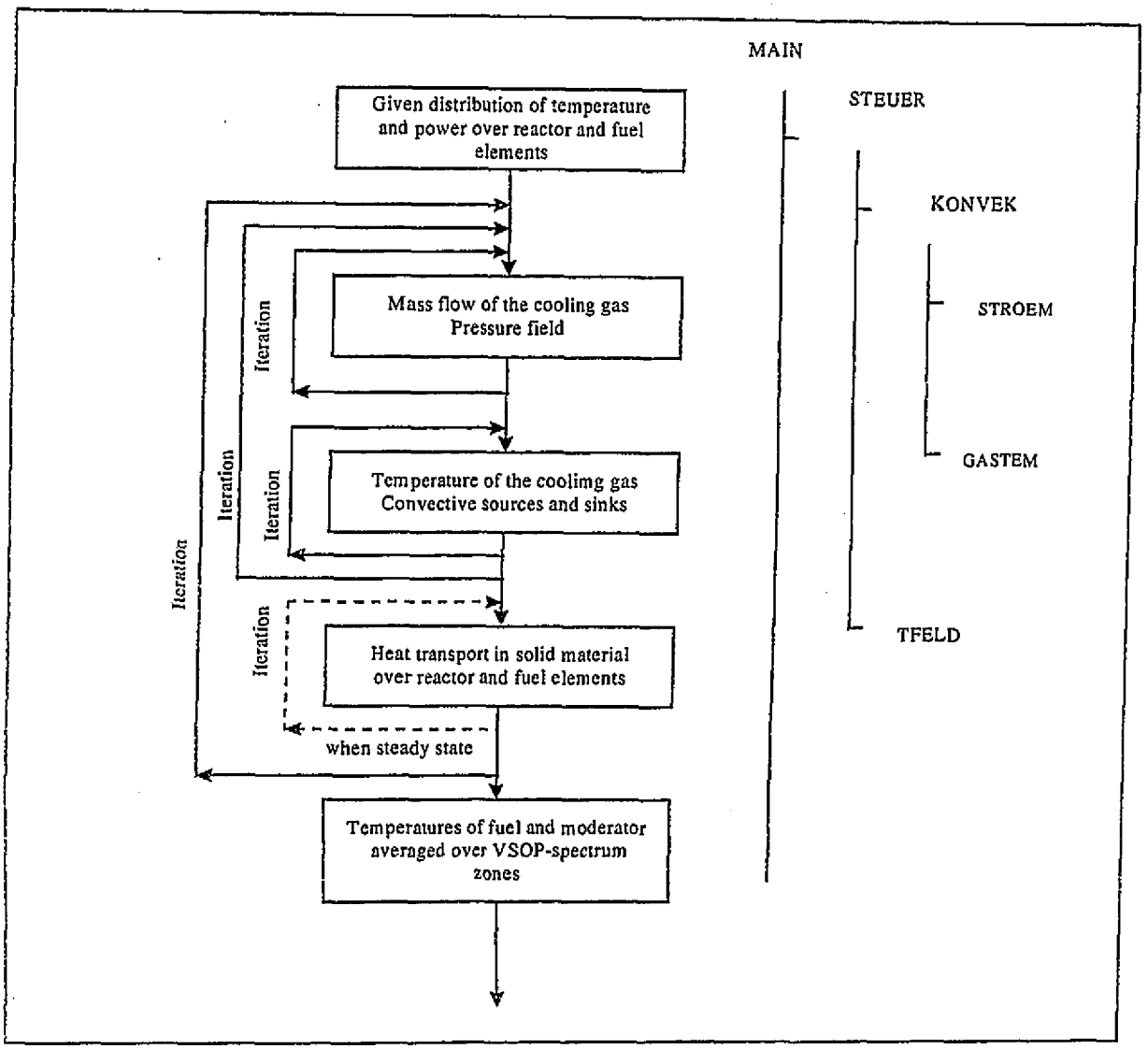

Fig. 11: Flow scheme of the THERMIX

The conservation of mass of the cooling gas in quasi-static representation yields the mass flow vector $G = \rho_G \cdot \mathbf{v}$ over the circuit. It is given by

$$\nabla \rho_G \cdot \mathbf{v} = q \qquad (1)$$

where

ρ_G = density of the cooling gas [kg/m^3]

v = velocity [m/s]

q = mass source rate density [kg/s/m^3]

The conservation of momentum quasi-static representation yields the pressure field p over the circuit. It is given by

$$\nabla p - \rho_G \cdot \mathbf{g} + \mathbf{R} = 0 \qquad (2)$$

where

ρ = static pressure
$\mathbf{g}$ = gravity
$\mathbf{R}$ = frictional force

Eq. (2) gives the balance of the gradient of the pressure, the hydrostatic force of the gravity, and the frictional force per unit volume. The spatial acceleration and inertia are neglected. According to Ref. /29/ the frictional force is given by

$$\mathbf{R} = \frac{\psi}{d} \cdot \frac{1-\varepsilon}{\varepsilon^3} \cdot \frac{|G|}{2\rho_G} \mathbf{G}$$

where

ψ = pressure loss coefficient for flow through pebble bed
(given in Ref. /29/ as a function of the Reynolds number
d = pebble diameter

Evaluation of the equations (1) and (2) is done in the subroutine STROEM.

The conservation law of the energy in quasi-static representation yields the gas temperature field T_G :

$$\nabla \lambda_G \nabla T_G - \nabla(\rho_G \cdot \mathbf{v} \cdot c_p \cdot T_G) + \alpha \cdot \frac{F}{V} \cdot (T - T_G) = 0 \qquad (3)$$

where

c_p = gas specific heat capacity
λ_G = effective thermal conductivity of the gas due to dispersion
T = temperature of the solid, e.g. at the surface of the fuel elements
$\alpha \frac{F}{V}$ = coefficient of heat transition between the solid and the gas

In eq.(3) the first term gives the heat transport in the gas by thermal conduction. The second term is the heat transport according to the mass flow of the gas. The third term is the heat source or sink due to heat transition between the gas and the fuel elements. The compressive

work term and the time dependent energy storage are neglected. Eq.(3) is evaluated in the subroutine GASTEM.

For given temperature field T of the solid material, the quasi static status of the gas is derived by the code member KONVEK. It contains an iterative procedure between the subroutines STROEM and GASTEM.

The conservation law of energy in the solid material is evaluated in the dynamic representation. It yields the temperature field T:

$$\rho \cdot c \cdot \frac{\partial T}{\partial t} = \nabla \lambda_{eff} \nabla T + \alpha (T_G - T) + Q \qquad (4)$$

where

T = $T(\mathbf{r},t)$ temperature of the solid, i.e. at the surface of the fuel elements, in reflectors, etc.
ρ = density of the solid
c = heat capacity
λ_{eff} = effective thermal conductivity, which includes thermal conduction and radiation
α = coefficient of heat transition between gas and solid
Q = $Q(\mathbf{r},t)$ nuclear heat source

In eq. (4) the time dependent change of the energy per volume results from the balance of the heat transport by thermal conduction (first term), from the heat sink due to the heat transition to the gas (second term), and from the heat source due to the nuclear power production and decay power (third term). In the inner of the fuel elements the temperature distribution T_F is also given by the conservation law of energy in time dependent representation:

$$\rho \cdot c \cdot \frac{\partial T_F}{\partial t} = \nabla \lambda \cdot \nabla T_F + Q \qquad (5)$$

where c and λ are dependent on the local temperature T_F. At the surface of the fuel element the temperature T_F is equal to T of eq.(4) at the respective position in the reactor.

Both eq.(4) and (5) are solved in the subroutine TFELD. Under steady state condition an iterative procedure is between the TFELD and KONVEK routines, which yields a consistent solution for the temperatures of the solid and the gas. Under dynamic condition the time dependent changes of T and T_F are explicitly followed. Here, the time dependent change of the heat source Q is also included which is due to given changes of the power of the isotopic decay power. At any time step the status of the gas is solved in the static representation.

A.6.2 Coupling with nuclear routines

In VSOP the included THERMIX is operated by its own input section. In principle, the input is that of the stand-alone version. Major changes have been made for the geometric design and for the data to be transmitted between the code members. The transfer is made via a matrix of partial volumes VW(I,K) internally or by BIRGIT, as explained in section A.2.1.

The transmission from VSOP to THERMIX is done for the following data fields:

- The power density of the VSOP-regions is converted into a power density of the THERMIX grid, applying the matrix VW(I,K). Here it is normalized to the given integral power, or, by option, to any other integral value.

- The fast neutron dose is transformed analogously. It is applied for the calculation of the thermal conductivity of the fuel elements, which can be given as a function of the temperature and of the dose of fast neutrons.

- The decay power can be individually evaluated for every VSOP-batch during a thermal transient. The transformation is made analogously to the power density.

- Assignment of spectrum zones of the VSOP-batches is also transmitted in this way.

Out of the local heterogeneous temperature calculation the THERMIX prepares the temperatures of the fuel and of the moderator for each mesh. Average values are prepared for the areas of the spectrum zone assignments. They are returned to VSOP for subsequent neutron spectrum calculations.

A.7 Decay power for transient THERMIX calculations

In case of a shut down of the reactor under normal conditions or by a loss of cooling event the power of the core is reduced to the decay power of the unstable isotopes. As the decay power of each unit of fuel depends on its power histogram, it is not only a function of the decay time but also of space and should be evaluated individually for each fuel batch within the reactor core. For this purpose the code NAKURE /19/ has been included as subroutine NACHW into the THERMIX code.

A.7.1 Power histogram of the fuel batches

The core is subdivided into regions, which again are composed out of a mixture of one or more batches (Section A.2.1). These batches go through burnup and fuel shuffling. For the

analysis of e.g. a loss-of-coolant incident the knowledge about the decay power of every batch is required as a function of its preceding irradiation history.

In a VSOP calculation subroutine LIFE prepares a power histogram of the fuel batches, which is the basis for the evaluation of the local decay power by means of the NAKURE code and by subroutine NACHW of THERMIX, respectively. This histogram contains the relevant data of the prehistory of every batch in coarser time intervals, i.e. the power, the burnup, the fractions of fissions of ^{233}U, ^{235}U, ^{239}Pu, ^{241}Pu, and the rate of neutron capture by ^{232}Th and ^{238}U.

Most complex is the compiling of the irradiation history for the multiple passes of the elements through the reactor. It is made by analogy to the fuel shuffling. In the calculations the length of a shuffling cycle can vary, shutdown periods may be included, and the residence time in the out-of-pile boxes normally is variable, too. In order to form averages of different histories a standardized set of time intervals must be defined. The code transforms the history data from the given pattern of time steps into the standardized intervals. This transformation is made for the irradiation history of every batch.

The present version of the code allows to subdivide the whole burnup period into 49 intervals of graded length. The first interval DT should be selected as short as the last cycle was prior to reactor shut down at time t_0. The time steps are made from a geometrical progression for the intervals I:

$$TG(I)=TG(I-1)+DT*(1+E1)^{I-1}$$

E1 is an incremental parameter derived iteratively by the condition

$$\frac{TG(MTMAX)-TN}{DT}<TEPS$$

being

MTMAX: Given number of graded time steps (≤ 49)

TN: Space of time to be covered by the graded time steps (≥ maximum fuel residence time)

TEPS: Criterion of convergence (e.g. = 0.1)

By this way intervals of high importance for the evaluated decay power are small and those of minor importance become longer.

The code prepares the histogram according to any fuel management scheme applied in VSOP. It can evaluate the running-in period of a reactor and any load follow prior to the shut-down time t_0.

By option it is also possible to evaluate an equilibrium cycle. In this case it prepares an equilibrium operation by copying one designated cycle many times. Then it proceeds as described above.

On the basis of this power histogram the values of the decay heat production of the fuel for use in THERMIX are then calculated by means of the subroutine NACHW. It employs the methods of the German Standard DIN 25485 /25/, which has been established for the evaluation of the decay heat production of High-Temperature-Reactor fuel.

A.7.2 Decay power of the fission products

The contribution P_s of the fission products to the decay power - calculated as the sum of the separate contributions of the considered fissile isotopes i - is given as:

$$P_s(t,T)=\sum_i P_{si}(t,T)$$

T being a time period of reactor operation and t being the cooling down time.

In /25/ the decay power P_{si} of the fission products resulting from fissions of each fissile isotope i is approximated by the sum of 24 exponential functions. The energy release rating f_i (τ) of the fission products of one single fission of isotope i is calculated as:

$$f_i(\tau)=\sum_{j=1}^{24}\alpha_{ij}\cdot e^{-\lambda_{ij}\cdot\tau} \qquad (1)$$

where τ is the time elapsed since the fission occurred. The coefficients α_{ij} and λ_{ij} for fissions of ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu are listed in /25/. In case of fuel containing thorium, the coefficients of the ^{235}U are also applied for the bred ^{233}U in subroutine NACHW.

Subdividing the power histogram of the fuel into a series of small time periods K with the length T_k , the decay heat rating of the fission products related to one fission per second is calculated as:

$$F_i(t_k,T_k)=\int_0^{T_k} f_i(T_k-T'+t_k)dT' \qquad (2)$$

with t_k being the cooling down time, i.e. the elapsed time since the end of the time interval T_k. Integrating equation (2) using equation (1) for f_i results in

$$F_i(t_k,T_k)=\sum_{j=1}^{24}\frac{\alpha_{ij}}{\lambda_{ij}}(1-e^{-\lambda_{ij}\cdot T_k})\cdot e^{-\lambda_{ij}\cdot t_k}$$

and the contribution of the fission products to the decay power at time t after reactor shut down amounts to

$$P_s(t,T)=\sum_i\sum_k\frac{P_{ik}}{Q_i}\cdot F_i(t_k,T_k)$$

with

P_{ik} Thermal power of the fissile isotope i during the time interval T_k
Q_i Total thermal energy release of one fission of isotope i
T Total time of fuel operation in the reactor from the initial loading until the last considered shut down.

A.7.3 Decay power of ^{233}Th, ^{233}Pa, ^{239}U and ^{239}Np

The decay power P_b of these isotopes as precursors of the bred fissile materials ^{233}U and ^{239}Pu, respectively, is shown to be /25/:

$$P_b(t,T)=\sum_k\left[\frac{P_k}{Q}\sum_I F_I(t_k,T_k\right]$$

being

$$\frac{P_k}{Q}=\sum_i\frac{P_{ik}}{Q_i}$$

and I = ^{233}Th, ^{233}Pa, ^{239}U and ^{239}Np, respectively.

The values of F_I are to be calculated as follows:

$$F_U(t_k,T_k)=E_U\cdot R_{Uk}\cdot(1-e^{-\lambda_U\cdot T_k})\cdot e^{-\lambda_U\cdot t_k}$$

$$F_{Np}(t_k,T_k)=E_{Np}\cdot R_{Uk}\cdot\left[\frac{\lambda_U}{\lambda_U-\lambda_{Np}}\cdot(1-e^{-\lambda_{Np}\cdot T_k})\cdot e^{-\lambda_{Np}\cdot t_k}-\frac{\lambda_{Np}}{\lambda_U-\lambda_{Np}}\cdot(1-e^{-\lambda_U\cdot T_k})\cdot e^{-\lambda_U\cdot t_k}\right]$$

The same equations hold for the decay power of Th and of Pa when using the indices *Th* and *Pa* instead of *U* and *Np*.

The meanings of the variables are:

E_U	mean decay energy of ^{239}U	(0.474 MeV)
E_{Np}	mean decay energy of ^{239}Np	(0.419 MeV)
E_{Th}	mean decay energy of ^{233}Th	(0.442 MeV)
E_{Pa}	mean decay energy of ^{233}Pa	(0.408 MeV)
λ_U	decay constant of ^{239}U	$(4.91*10^{-4}/s)$
λ_{Np}	decay constant of ^{239}Np	$(3.41*10^{-6}/s)$
λ_{Th}	decay constant of ^{233}Th	$(5.18*10^{-4}/s)$
λ_{Pa}	decay constant of ^{233}Pa	$(2.97*10^{-7}/s)$

$R_{U,k}$ and $R_{Th,k}$ are the neutron capture rates of ^{238}U and ^{232}Th, respectively, divided by the total fission rate during the time interval *K*.

A.7.4 Contribution of neutron capture in fission products and in actinides

An example for neutron capture in the fission products and in the actinides is given in Fig. 12.

Note, that the P_b actinides are treated according to section A.7.3.

The contribution of the decay power due to neutron capture in fission products (P_e) is calculated as a function of the decay time:

$$P_e(t,T) = P_S(t,T) * H(t)$$

using table 4 of /25/ for $H(t)$.

Not included in P_e is the contribution of the long-lived fission product ^{134}Cs. This is calculated separately as P_{Cs} according to equations 32 - 38 of Ref. /25/.

The contribution to the decay power by neutron capture in the heavy metal nuclides, P_a , is evaluated using equation 19 and table 3 of /25/:

$$P_a(t,T) = P_S(t,T) * f(\text{heavy metal density, heavy metal burnup, power density, } t)$$

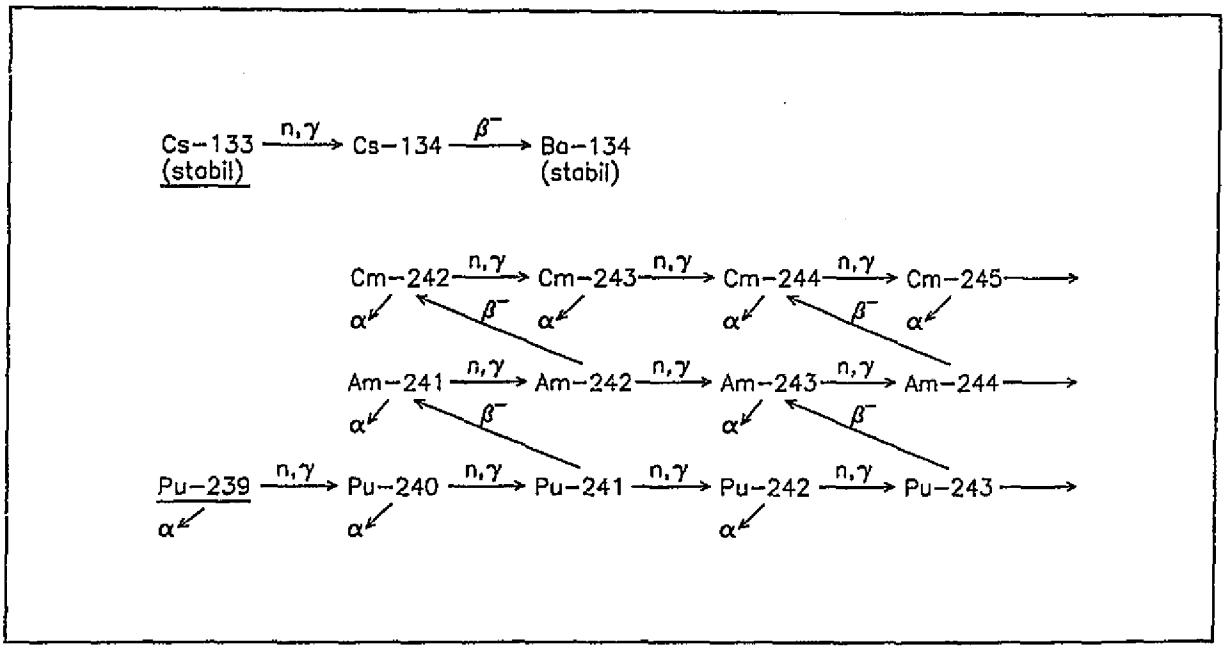

Fig. 12: Neutron capture in fission products and in actinides

The total decay power is finally summed up:

$$P_n = P_S + P_b + P_e + P_{Cs} + P_a$$

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