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C^{4}P-TRAIN NEUTRONICS TOOL FOR SUPPORTING SAFETY STUDIES OF INNOVATIVE FAST REACTORS

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ABSTRACT

For studies of innovative nuclear reactors, an advanced safety code, SIMMER, is used at KIT and other institutions. SIMMER generates macroscopic cross-sections for coupled neutronics and thermal-hydraulics transient simulations from a multigroup cross-section library with f-factors. For fuel behavior models coupled to SIMMER, also inventories of He and gaseous fission products are needed. C^{4}P-TRAIN is a neutronics tool for generation of SIMMER cross-section libraries and their benchmarking, for computation of isotopic inventories and decay heat. C^{4}P-TRAIN consists of C^{4}P and TRAIN. C^{4}P includes general-purpose fine-group cross-section libraries in the CCCC format and tools for generation of coarse-group libraries for SIMMER from fine-group ones. C^{4}P also includes a capability for producing multigroup cross-sections with f-factors for isotope mixtures from data for the isotopes. TRAIN can employ C^{4}P data for generation of macroscopic cross-sections; then these cross-sections can be used by an "external" neutron transport code for computing cell/reactor neutron fluxes, which can be used then by TRAIN for fuel burn-up simulations. Recently TRAIN was extended and used for burn-up simulations in a molten salt fast reactor as described in the paper. The computed decay heat values agree well with those obtained in the past with Monte-Carlo codes.

Key Words: Multigroup cross-sections, reactor safety, fuel burn-up simulation, molten salt reactor, decay heat

1. INTRODUCTION

For studies of innovative nuclear systems, an advanced safety code, SIMMER [1], is developed and applied by JAEA, CEA, KIT and their partners. SIMMER was initially used for simulation of accidents in sodium fast reactors. More recently it was extended and applied to safety analyses of other reactors types, including molten salt reactors. SIMMER employs multigroup cross-section libraries with f-factors in the CCCC format [2] for generation of self-shielded cross-sections used in transient neutron transport calculations. The cross-sections are usually computed in SIMMER by using smear nuclear densities and temperatures of isotopes in reactor sub-regions; techniques for taking into account heterogeneous effects were established in the past and will be further developed in the future.

Earlier an 11-group XS library [3] for SIMMER was developed at Karlsruhe. This library is employed at KIT for studies of fast reactors with solid fuel cooled by liquid metal or gas, but not used for other systems. To reduce uncertainties in SIMMER results related to the limited number of groups in the mentioned library and to extend the SIMMER application area, a new code and data system, C^4P, was developed [4]. It includes fine-group cross-section data in the extended - for including thermal scattering data - CCCC format, according to which cross-sections and f-factors are stored in two files: ISOTXS and BRKOXS. C^4P also includes tools for production of coarse-group libraries for SIMMER from fine-group ones.

C^4P libraries can be also used by another code, TRAIN, which was developed for burn-up simulations [5] and later extended by including a module for generation of macroscopic and microscopic self-shielded cross-sections from CCCC libraries. TRAIN is usually used in combination with an "external" neutron transport code, such as DANTSYS [6]. For reactor physics calculations performed at KIT/IKET in support of safety studies, the ERANOS code [7] is mainly used; but for some tasks, such as decay heat calculations, the use of C^4P-TRAIN in combination with a neutron transport code is preferable and also contributes to the benchmarking of C^4P libraries.

Additional information on C^4P and TRAIN is provided in Sections 2 and 3. Initially burn-up simulations with TRAIN were not possible for systems with online fuel reprocessing, but recently the code was extended for this purpose. This extension and results of decay heat calculations for a Molten Salt Fast Reactor (MSFR) model are described in Sections 4 and 5. These results agree with those obtained in the past [8] with Monte-Carlo-based tools.

2. C^4P code and data system

A two-step approach is used for generation of SIMMER libraries. First, fine-group libraries are generated from evaluated nuclear data files with codes like NJOY [9] and GRUCON [10]; in the latter a model for resonance Doppler scattering effect was recently included. We have chosen a 560-group structure for the fine-group libraries, which is an intermediate structure between the 172-group and 1968-group structures used in ERANOS.

For establishing the 560-group structure, we considered several possible fine-group options and a number of simplified homogeneous models representing systems with different coolants, including molten salt fast reactors with thermal and fast spectrum. For each model and its modifications (higher temperature, removal of moderator/coolant) we computed k-inf values with C^4P-TRAIN and compared these values to those obtained with a continuous-energy Monte-Carlo code. The 560-group structure has been chosen, because it provides sufficiently accurate results: the deviations between the 560-group and continuous-energy k-inf values - obtained with the same evaluated nuclear data - do not exceed a value about 200 pcm, while the Monte-Carlo statistical uncertainties are below 50 pcm [4]. Using of finer group structures, such as the 1968-group one, does not reduce the deviations for the considered homogeneous models appreciably. Using of a coarser group structure, such as the 172-group one, may lead to much larger uncertainties in the results. The 3 mentioned group structures, with 172, 560, 1968 groups, are not currently used at KIT with SIMMER, which employs coarse-group libraries with 72 or

less groups: to reduce the computation time. But establishing a reference fine-group structure is important, because the possibility of using fine-group data with TRAIN and transport codes may facilitate analyses of possible deviations between criticality and reactivity effects computed with SIMMER and reference neutronics tools, such as Monte-Carlo codes and ERANOS. These analyses may help to produce a better coarse-group library for SIMMER. In Figure 1, one may see group widths in lethargy units for the three mentioned fine-group structures.

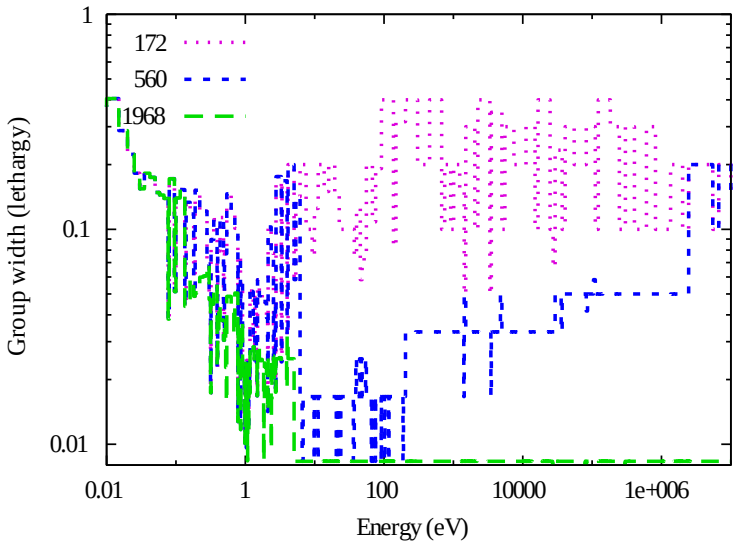

Figure 1. Group widths for 172-group, 560-group and 1968-group structures.

In addition to homogeneous models, we also investigated the performance of the 560-group structure for cells with heterogeneous arrangements of fuel and non-fuel isotopes. With TRAIN one can employ a simple method based on the rational approximation for computing background cross-sections for fuel isotopes in heterogeneous cells. According to this method, the cross-sections of the non-fuel region for a particular group are divided by the value equal to 1+EMCL*XSM when their contribution to the total background cross-sections for a fuel isotope is computed, XSM being the total macroscopic cross-section for this group in the non-fuel region, EMCL being the Effective Mean Chord Length computed in advance.

As an example, we describe here the computation of EMCL for a PWR cell performed in the past. This was done by employing the following procedure. A 400-group library, with coarser groups in the resonance region between 5 eV and 4 keV, was produced from the 560-group library by merging pairs of adjacent fine groups into coarser ones. Then the 400-group and 560-group libraries were used for computation of k-inf values. The differences between the "heterogeneous" EMCL-dependent k-inf values and k-inf values for the homogenized cell can be considered as k-inf heterogeneity corrections. These corrections are near-linear functions of EMCL, depending on ECML stronger when the number of groups is smaller. For a certain EMCL value, these corrections are the same. We employed this EMCL value for computing the results shown in Table I.

It shows relative deviations, %, between k-inf values computed for a PWR cell with two deterministic options, denoted as “560 group” and “ECCO” and with a continuous-energy Monte-Carlo code. We considered the following fuel compositions: UOX fuel at the Beginning Of Life (BOL), UOX fuel at the End Of Life (EOL), MOX fuel at BOL. EOL corresponds to the burn-up of 60 GWd/t.

We also computed relative deviations, %, between the average cross-sections computed with the deterministic options and with the Monte-Carlo one. These average cross-sections are: U235 fission and capture, U238 fission and capture, Pu239 fission and capture, Pu240 fission and capture, the deviations for these cross-sections being given in Table I as f35, c35, f38, …, c40, respectively. The first deterministic option is denoted as “560 group”. The results are obtained with a C^4P 560-group library, TRAIN and DANTSYS, while employing the EMCL values given in Table I in cm; in particular, EMCL is 4.1 cm for UOX at BOL. DANTSYS was used for cell flux calculations in 1D geometry with the S16 flux discretization in angle. The second deterministic option is denoted as “ECCO”, because ECCO is a cell module of ERANOS. For this option, results obtained with the ECCO module and the 1968-group library, based on the same evaluated data as the 560-group one and the files used for Monte-Carlo simulations, are given. One may conclude that both deterministic options provide quite accurate results assuming that the Monte-Carlo results can be considered as reference. The deviations from the reference values are similar for both options, but the maximum one is higher for the 560-group case.

Table I. Relative deviations, %, from continuous energy results for 560-group-based values obtained with TRAIN/DANTSYS and for 1968 –group-based values obtained with ECCO

	UOX, BOL		UOX, EOL		MOX, BOL	
	560 group EMCL=4.1	ECCO	560 group EMCL= 4.1/3.7	ECCO	560 group EMCL=4.1/4.3	ECCO
k_{inf}	-0.1	-0.5	-0.6/-0.6	-0.6	-1.0/-0.9	-0.6
f35	-0.7	0.8	-3.4/-3.5	-1.6		
c35	0.0	1.0	-1.9/-2.0	-1.1		
f38	-1.7	-0.8	-0.8/-0.8	2.8	-1.2/-1.2	2.7
c38	0.2	2.7	-0.7/-0.4	1.9	0.4/0.2	2.2
f39	0.6	2.3	-2.1/-2.1	0.3	-1.9/-1.8	-0.5
c39	0.9	2.8	-1.4/-1.4	1.0	-1.4/-1.4	-0.3
f40	-1.0	-0.1	-0.4/-0.4	1.2	-0.8/-0.8	1.3
c40	0.0	-0.1	2.0/1.9	2.3	1.9/1.9	1.8

The EMCL value for UOX EOL - evaluated with the described above procedure - is 3.7 cm. This value differs from the value of 4.1 cm for UOX at BOL. On the other hand, one may see in Table I that the results are not very sensitive to variations of EMCL. Therefore for burn-up simulations we employ burn-up-independent EMCL values, obtained at BOL. This approach was used at KIT while performing burn-up calculations with TRAIN/DANTSYS for a PWR-cell benchmark proposed in the past by CEA for an OECD-NEA project on fuel cycle. The calculated at KIT

isotopic inventories at EOL for UOX and MOX cases are close to those provided by CEA and by other codes employed at KIT. Using of a 612-group library instead of the 560-group one, with more groups, mainly below 5 eV, does not reduce the deviations appreciably.

More results of benchmarking of 560-group libraries for criticality and reactivity effects are provided in [4], where agreement with results obtained with continuous energy data is demonstrated for different reactor models, including a MSR with fast spectrum.

C4P includes a capability for computing multigroup cross-sections, including f-factors, for isotope mixtures from multigroup data for particular isotopes, e.g., cross-sections with f-factors for iron from data for iron isotopes, such as Fe54, Fe56, etc., that helps to reduce the time for cross-section generation during SIMMER transient simulations. The capability is based on application of the extended probability table (PT) method [11]. Unlike conventional PT (or subgroup) method, several total cross-section values are considered for a probability bin, one value per each partial cross-section, such as the elastic or capture one. This approach facilitates production of PT parameters used for computing of f-factors for mixtures of isotopes, but cannot be applied without a modification to neutron transport calculations. The use of produced with the extended PT method data for isotope mixtures, may give more accurate results compared to the use of data for isotopes if the conventional procedure for background cross-section iteration is applied in self-shielding calculations, because this procedure is often less accurate than the extended PT method [4].

3. TRAIN code

The TRAIN code consists of modules, including two major ones: (1) for self-shielded cross-section generation, ZMIX, and (2) for burn-up simulations, TRAM. It also includes smaller ones, such as a module for reading nuclear densities. Data are exchanged between the modules via files. The code input includes names of the modules, followed by module-dependent input values, such as nuclear densities and a file number for storing these data. This number is then referred in the input for ZMIX and TRAM. The file numbers are linked to files by commands of TRAIN or by default. The TRAIN input may also include Linux commands, that are used, e.g., for execution of codes, such as DANTSYS. It may also include “DOn” and “ENDDO” commands for repeating the input part between these commands n times.

ZMIX employs isotope-wise ISOTXS and BRKOXS text files, while SIMMER employs binary files containing data for all isotopes; C4P is used for data transfer between different formats. If ZMIX is used for computing cross-sections for cell components, the neutron transport calculations are performed for the cell; then ZMIX is called again and employed for cross-section homogenization and condensation. For burn-up simulations, self-shielded cross-sections are usually prepared for about 100 most important isotopes, including 60 fission products (FPs), the contribution of which to the total FP capture cross-section usually exceeds 90%.

A special module of TRAIN, DATR, is used for preparation of a larger set of infinitely-diluted multigroup data from a continuous energy activation cross-section file, a decay data file and a FP yield data file. These files can be downloaded from the Internet. A capability to process by DATR and employ by TRAM spontaneous fission data was also developed, but is not used for

reactor studies. DATR averages continuous energy data for a multigroup structure, which is the same or coarser than that for the neutron flux.

DATR prepares data for isotopes from the list given by the user. This list can be automatically extended by DATR for including FPs of the considered actinides, if their yields exceed a certain input value, e.g. 1.e-6. In this way, a file with data for about 1000 nuclides is usually created by DATR. In burn-up simulations all these 1000 isotopes are considered, but the cross-sections for about 100 important isotopes are replaced or renormalized by those produced by ZMIX. Taking into account of more isotopes is possible in ZMIX and in DATR, but we usually see no appreciable variation of the results when we use more isotopes.

For a particular isotope, the file with infinitely-diluted cross-sections may contain data for a larger number of reactions than the file with self-shielded cross-sections. Then the self-shielded cross-sections are used for renormalization of several infinitely-diluted ones together. For example, a file with infinitely diluted multigroup cross-sections usually contains data for production of Am242 and Am242m from Am241 by neutron capture, but the file with self-shielded cross-sections would contain those for production of Am242 and Am242m together. The Am241 infinitely-diluted cross-sections are used in TRAM for computing energy-dependent branching ratios for Am241 neutron capture applied to the self-shielded cross-sections.

The numerical scheme considered for one burn-up step in time is based on automatic generation of chains with lengths determined by input parameters, for all possible transitions due to nuclear reactions, data for which are available in the DATR file. For each chain an analytical formula is employed. A matrix - that contains transition probabilities from each isotope to other ones after application of all chains mentioned above for a time interval - can be generated first for a small time interval and then used many times for the same time intervals; this technique makes the computations more efficient. The FP yields are normalized by 2 without taking into account light FPs, such as He. The information on normalization is printed and the user may see that the FP yields employed in calculations are practically the same as in the initial data file. Due to this approach, the total amount of heavy atoms is kept with a very high accuracy: if a pair of non-light FPs is considered as a heavy atom. This accuracy is checked by the code.

The data on nuclear inventories of about 1000 isotopes are saved in a special file after first TRAM step and then TRAM reads these data at the next step, after optional recalculations of self-shielded cross-sections and fluxes. The nuclear densities for about 100 important nuclides are saved in the file used by ZMIX. These nuclear densities can be partly adjusted: the ones for FPs can be multiplied by a factor that is usually between 1 and 1.1. This factor is computed as the ratio of the total capture cross-section of all FPs considered in TRAM to the total capture cross-section of 60 FPs considered in ZMIX.

We have tested the TRAIN burn-up capability for a number of benchmarks. In Figure 2 one may see a comparison of results obtained for the benchmark on decay heat. This benchmark was organized for a European project [12] and contributed by 6 institutions: CEA, CIEMAT, ENEA, FZK (now KIT), PSI, and SCK-CEN. TRAIN results are denoted as FZK-TRA. Figure 2 shows the ratios of the results of participants to the average values of all participants for the decay heat

in MOX fuel in a fast reactor. The computed average value at zero cooling time is 5.535% of the total power.

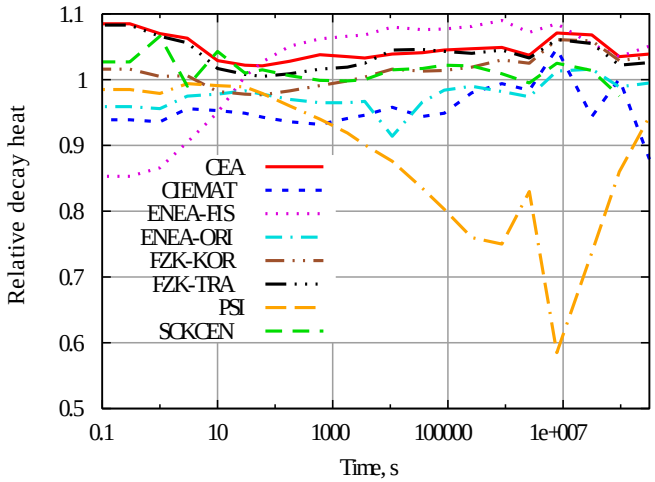

Figure 2. Ratios to average values of participants for decay heat in MOX vs. cooling time

One may observe that the results, except for a few ones at particular cooling times, are in general agreement.

4. TRAIN extension for MSFR burn-up simulations

For simulating reactor operation with bubbling and online fuel reprocessing in a batch manner, two modules were added to TRAIN. One module modifies the file produced by DATR by adding pseudo-decays with the specified half-lives for gaseous and noble FPs to pseudo-isotopes: in order to simulate the bubbling and its influence on the nuclide inventory in the reactor. These pseudo-isotopes are excluded from consideration till the time when the next batch step is simulated.

Another module simulates fuel transfer between the reactor and batch, fuel, waste storages. First, fuel from the batch storage is distributed, if it is present in this storage, to waste and fuel storages, depending on reprocessing losses for particular actinides, while all fission products go to waste. Then the fuel is transferred from reactor sub-regions, e.g. first from the core and then from the blanket, to the batch storage, this transfer is considered independently for each reactor sub-region. Optionally, different bins for different fuel batches can be used in the batch, fuel, and waste storages. When a batch from a sub-region arrives to the batch storage, a batch with the same amount heavy atoms is transferred from the fuel storage to the sub-region. For calculation of the amount of heavy atoms, a pair of FPs is considered as a heavy atom; light FPs, such as He, being not considered. The user provides maximum possible values of enrichment in the batch transferred to the sub-region for all considered actinides and identifies the “fertile” isotope that is added to keep the balance. This isotope and some amount of fissile ones should be available in the storage when the storage model is initialized, otherwise the simulation may stop due to lack

of material in the fuel storage. This restriction helps to control that the total number of heavy atoms, with the mentioned weights for FPs, is kept the same in the reactor and storage together. Decay in the storage can be simulated with TRAIN in parallel or independently of burn-up simulations in the reactor.

5. Decay heat computation for MSFR

Earlier, a MSFR benchmark was proposed and the results were reported in several publications, including [8]; it is shortly described in the following in an approximate manner, i.e. omitting or simplifying some details. A cylindrical reactor model is considered. The core and blanket volumes are 18000 liters and 7700 liters, respectively. The reactor power is 3 GWth, a He-bubbling device permanently removes gases and noble metals, so that their half-lives in the reactor due to bubbling are equal to 30 seconds. The salt initially contains the following heavy nuclides: U233 and Th232 (fertile). The online reprocessing facility removes 40 liters of salt per day from the core and the same volume of salt per day from the blanket. Then actinides are extracted from the removed salt and fully or partly (uranium) introduced into the core, the heavy atom inventory in the core and blanket being maintained by adding a fertile material, Th232. After extraction of minor actinides, the salt with FPs goes to reprocessing, that is done either completely for the salt from the core, or partly, only 1%, for the salt from the blanket, meaning that 99% of FPs extracted from the blanket return back.

A C^4P library for a 50-group structure, which is an intermediate structure between the 560-group one and the 40-group one described in Ref. [4], was established by C^4P from the 560-group JEFF 3.1.1 library with data for all important isotopes. The 50-group library is used as an intermediate one in generation of 40-group data, because it includes fine groups for first resonances of U238 and Th232, for which averaging to coarse 40 groups is done using neutron collision density spectra for a LWR model, while for other energy intervals, standard spectra, such as thermal, Fermi, or fission one, are used. A file with about 1000 isotopes was produced by DATR for the same 50-group structure.

Then the DATR file was modified by including pseudo-isotopes and pseudo-decays related to bubbling; about 300 pseudo-isotopes were added. The storage file was initialized with a larger amount of Th232 in view of the long period of simulations, about 100 years. From the published results [8], one may see that at this time, close to equilibrium nuclide inventories of most important isotopes are established in MSFR.

In the simulations we considered a batch reloading scheme, which is done every 45 days, so that 1800 liters of salt or 10% of core heavy atoms is replaced by one batch The current version of TRAIN does not allow the return of FPs to the reactor. This restriction prevents us from simulating the blanket reloading scheme exactly. Therefore we considered two options for the blanket fuel reprocessing: (1) 40 liters per day, which is correct for actinides and (2) 4 liters per day, which is closer, but not completely correct for FPs. The calculation of self-shielded cross-sections and 2D transport calculations with DANTSYS were done every 45 days.

The obtained results on inventories of most important nuclides are similar to those published in Ref [8], but not the same, in particular in view of the modified treatment of the blanket. The

uranium inventory of Ref [8] after 100 years is between the values obtained with the two mentioned options, the relative difference between the latter values being less than 8%. For the first blanket reloading option, 40 l/day, the system produces ca. 440 g/day of U within first 50 years, ca. 360 g/day within first 100 years. For the second option, 4 l/day, the production is ca. 10 g/day less.

The decay heat values are almost for the same for both options, they are given in Table II, which also includes the values after 45 days of operation, with and without bubbling.

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Table II. Decay heat values in MSFR, % of the total power

Cooling time	After ca. 100 years, 40 l/day	After ca. 100 years, 4 l/day	After 45 days	After 45 days, no bubbling
0	4.313	4.313	4.177	5.460
1s	3.993	3.993	3.870	5.153
1 min	2.270	2.271	2.200	3.373
1 hour	0.936	0.937	0.841	1.355
1 day	0.441	0.442	0.345	0.493
1 month	0.173	0.174	0.120	0.135
1year	0.010	0.010	0.002	0.002

The difference between the latter two values shows the reduction in the decay heat due to bubbling. At zero cooling time this reduction is about 1.3% of the total power. The obtained results agree with those published earlier. The decay heat value at zero cooling time for the case without bubbling is 5.460 %, close to the mentioned one for the MOX decay heat.

6. Conclusions

C4P-TRAIN is a system for supporting reactor safety studies, in particular with the SIMMER code. The system includes modern cross-section libraries and tools for their processing. It can be used together with neutron transport codes for cell and reactor calculations, including burn-up simulations. The computed isotopic inventories and decay heat values are employed in safety studies. These computations support benchmarking of libraries used with SIMMER. A new option was introduced for simulation of burn-up in molten salt reactors. The decay heat values obtained for a molten salt fast reactor model agree with earlier published results.

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