6. CALCULATIONAL METHODS

6.1 Thermal and Fast Reactors

In the case of thermal and fast reactors, the presence of actinides does not change the calculational methods presently applied provided the nuclear data, in particular cross-sections are available in the required group structure. Self shielding effect and Doppler broadening are calculated in the usual manner.

Multigroup cross-section libraries are generated by retrieval and processing codes (such as NJOY) which depart directly from ENDFB/4, ENDFB/5, ENDFB/6, JEF or JEF2 and JENDL3. In the case of continuous cross-section libraries as used by some Monte Carlo codes, in particular MCNP, the ACER module of NJOY is applied.

Reactivity and flux calculations are carried out for thermal reactors by code systems like WIMS or APOLLO-KAFKA. Fast reactors are calculated by similar systems based on nodal methods or different SN codes. Burnup and fission product decay is determined by ORIGEN, ORIGINS, FISBIN or PEPIN.

6.2 Accelerator Driven Systems

In accelerator-driven systems, the neutron energy extends to several hundred MeV. In classical reactor codes the upper energy limit lies between 15 and 20 MeV. In accelerator driven systems, between 10% and 20% of the spallation neutrons are above this limit and therefore require to be considered in the calculations. Usually a classical Monte Carlo code like MCNP or MORSE is extended to higher energies by codes like HETEC (High Energy Transport Code,ORNL) or NMTC (Nucleon Meson Transport Code).

Several research institutes upgraded two of the above mentioned codes and tailored the combination to their own requirements. Brookhaven National Laboratory is for example using BNLF,a modified combination of NMTC and MORSE. A similar combination is used by JAERI and the KFA Julich. In the Rutherford Laboratory Atchison used experimentally adjusted parameters for the fission process and put this fission model into HETC. At LANL Prael developed a code system by combining an upgraded HETC with MCNP and called it LAHET. In LAHET the geometry transport capability is that of the Monte Carlo Neutron and Photon transport code MCNP. LAHET includes two models for fission induced by high energy interactions : the ORNL model and Rutherford Appleton Laboratory model. HETC treats all interactions by protons, pions and muons, but neutron interactions only above the cut-off energy of 20 MeV.

F. Atchison reviewed in detail "Data and Methods for the Design of Accelerator Based Transmutation Systems" [26].

6.3 Used Calculational Methods for Proposed Concepts

At the CEA, in the case of LWRS, nuclear data used is JEF. Neutronic calculation is made by two dimensional transport code APOLLO with 99 group cross-sections generated from JEF. The code is a modular one which solves the multigroup transport equation by the collision probability method,and a multicell approximation is available for 2D geometries. Burnup calculation is made by the three dimensional diffusion code CRONOS which allows pin by pin core calculations.

In the case of fast reactor, standard isotopes cross sections are provided from CARNAVAL. Minor actinides data are provided from JEF and added to the standard isotopes cross-sections. Neutronic calculations are made by two dimensional diffusion option of ERANOS (European Reactor ANalysis Optimised System) with 25 group cross sections. Burnup is calculated also by ERANOS.

In the case of accelerator-driven system, nuclear data source comes from JEF version 2. High and medium energy reaction calculations are made by HETC of ENEA version. Neutronic calculations are executed by two dimensional transport option of ERANOS code with 25 group cross-sections generated from JEF. Treatment of resonance self-shielding and condensation is performed by HETAIRE code.

AT the JAERI, nuclear data library JENDL-3 is commonly used for transmutation studies.

In the case of LWR, neutronic calculation is made by the two dimensional diffusion option of the modular code system SRAC with 107 group cross-sections generated from JENDL-3. However, resonance absorption are calculated accurately by the ultra-fine group method. Burnup calculation is carried out by zero dimensional burnup option of SRAC, where FP chain treats explicitly important 65 fission product nuclides.

In the case of fast reactors including burner reactors, neutronic calculations are carried out by the two dimensional diffusion option of the code system ABC-S or SRAC/COREBN, with 70 group cross-sections generated from JENDL-3. Burnup is calculated with burnup option of the above mentioned code systems.

In the case of accelerator-driven system,nuclear data source comes from JENDL-3 or ENDFB/5. High and medium energy reaction calculations are performed by NMTC/JAERI. Neutronic calculations are made by TWOTRAN-2 with 30 group cross-sections. Burnup is calculated by COMRAD of which flow chart is given in Fig.5.2.

The three Japanese organizations described below propose their LMFBR based transmutation systems.

At the PNC,neutronic and burnup calculations are carried out by the two dimensional diffusion code CITATION-FBR (a modified version of original CITATION) with 18 group cross sections generated from JENDL-2.

At the CRIEPI, standard isotopes cross-sections are provided from JFS 70 group cross-sections set and minor actinides cross sections are generated from JENDL-2 or ENDFB/5. Neutronic and burnup calculations are carried out by two dimensional diffusion code CITATION-TRU with 70 or 18 group cross-sections. The code is a modified version of CITATION which can easily calculate complex minor actinide nuclides burnup/decay chain.

At the Toshiba Corporation, JFS 70 group cross-sections set is used for standard isotopes and minor actinides cross-sections are generated from JENDL-3. Neutronics are calculated with 70 group two dimensional or 7 group three dimensional diffusion code. Burnup calculations are based on two dimensional code.

The research organizations described below propose their accelerator-driven transmutation systems.

At the BNL, Nuclear data source is ENDFB/4. High and medium energy reaction calculations are carried out by LAHET and NMTC/BNL. In the latter, a fission model based on the Fong's statistical model is adopted into the NMTC code. Neutronic calculations are performed by the continuous energy Monte Carlo code MCNP-4. Burnup calculations are based on the ORIGEN-2 code with associated cross-sections.

At the ENEA, nuclear data source is JEF or ENDFB/5. High and medium energy reaction is calculated by NMTC/JAERI and HETC/KFA2 codes. Neutronics are calculated with the Monte Carlo code MCNP-4 and burnup is calculated by the ORIGEN-1 and 2 codes.

At the Royal Institute of Technology, nuclear data source is ENDFB/5 or 6. High and medium energy reaction calculations are made by the LAHET code. Neutronic and burnup calculations are carried out by MCNP-4 and 0RIGEN–2, respectively.

At the ITEP, nuclear data is ENDFB/6. Neutronic and burnup calculations are performed by a two dimensional transport code with 26 group cross-sections and the three dimensional TRIFOB code, respectively.