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ACCELERATOR-DRIVEN TRANSMUTATION REACTOR ANALYSIS CODE SYSTEM — ATRAS —

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Accelerator-driven Transmutation Reactor Analysis Code System -ATRAS -

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JAERI is proceeding a design study of the hybrid type minor actinide transmutation system which mainly consist of an intense proton accelerator and a fast subcritical core. Neutronics and burnup characteristics of the accelerator-driven system is important from a view point of the maintenance of subcriticality and energy balance during the system operation. To determine those characteristics accurately, it is necessary to involve reactions at high-energy region, which are not treated on ordinary reactor analysis codes. The authors developed a code system named ATRAS to analyze the neutronics and burnup characteristics of accelerator-driven subcritical reactor systems. ATRAS has a function of burnup analysis taking account of the effect of spallation neutron source. ATRAS consists of a spallation analysis code, a neutron transport codes and a burnup analysis code. Utility programs for fuel exchange, pre-processing and post-processing are also incorporated.

Keywords: Accelerator-driven System, Transmutation, Spallation, Neutron Transport, Burnup

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加速器駆動消滅処理炉心解析コードシステム
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日本原子力研究所東海研究所中性子科学研究センター
佐々　敏信・辻本　和文・滝塚　貴和・高野　秀機

（1999年２月１日受理）

日本原子力研究所では、大強度陽子加速器と未臨界炉心から構成されるハイブリッド消滅処理システムの設計研究を進めている．加速器駆動システムの核特性及び燃焼特性の解析は、炉心の未臨界度及びエネルギーバランスの維持という点から、重要である。これらの特性を正確に解析するには、従来の原子炉解析コードでは解析できない高エネルギー領域の反応を考慮する必要がある。著者らは、加速器駆動未臨界炉システムの核特性及び燃焼特性を解析するＡＴＲＡＳコードシステムを開発した。ＡＴＲＡＳは核破砕中性子源を考慮した燃焼特性解析の機能を持つ。ＡＴＲＡＳは核破砕解析コード、中性子輸送コード、燃焼解析コードから構成される。また、燃料交換、前／後処理等のユーティリティコードも組み込んだ。

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Contents

目　　次

1. Introduction

The Japan Atomic Energy Research Institute (JAERI) has carried out the conceptual design study of the hybrid type minor actinide (MA) transmutation system which combines a high intensity proton linear accelerator and a fast subcritical core under the national OMEGA program[1,2]. A design study of the experimental facilities for accelerator-driven system development is also underway in the framework of the Neutron Science Project proposed by JAERI[3]. In addition, there are several other projects of hybrid systems proposed by several foreign research institutes[4].

Those hybrid systems are driven by a high energy proton accelerator. High-energy protons from the accelerator are injected into the spallation target that usually consists of heavy metal such as tungsten, lead, lead-bismuth alloy, uranium and mercury. About twenty to thirty neutrons are generated by spallation reaction, evaporation and high-energy fission and are used to drive the subcrtitical core.

Those proposed accelerator-driven systems were designed to keep their core in subcritical condition under the system operation condition. The depth of subcriticality, that depends on the safety and economy of the system, must be carefully determined from the detail neutronics and burnup analyses. To perform the analysis with a high accuracy, energy and angular distribution of the spallation neutron source must be treat adequately.

The authers developed a code system named "ATRAS" (Accelerator-driven Transmutation Reactor Analysis Code System) to perform the neutronics and burnup analysis of the accelerator-driven systems. ATRAS mainly consists of a spallation analysis code, a fixed neutron source calculation code, a neutron transport code and a burnup analysis code. Utility codes for the pre-processing, post-processing and fuel exchange are also developed and incorporated in the code system. In this report, the outline, structure and input instructions of ATRAS are described.

2. The ATRAS code system

2.1 Structure and function of ATRAS

ATRAS is an integrated code system which consists of following analysis codes and programs:

- NMTC/JAERI[5,6] Spallation analysis above 20 MeV,
- FSOURCE Creation of fixed spallation neutron source,
- SCALE-4[7] Generation of effective cross section below 20 MeV,
- TWODANT[8] Neutron transport analysis below 20 MeV,
- BURNER[9] Burnup analysis below 20 MeV,
- ATRAS Driver Production of input data files and control a calculation,
- ATRAS Utility Post-processor of the analysis results, and
- CHFUEL Simulation of the fuel exchange at the end of each burnup step.

Figure 2.1 shows the structure of ATRAS. By using ATRAS, following neutronics and burnup characteristics can be analyzed:

- Spallation neutron yield from the spallation target,
- Spatial and energy distribution of the spallation neutrons,
- Heat deposition distribution in the spallation target,
- Time evolution of the subcriticality and isotope composition of the fuel,
- Reaction rate of the target, fuel and structural materials,
- One group cross section of the target, fuel and structural materials,
- Transmutation rate of MA,
- Particle flux and power density distribution in the subcritical core,
- Energy spectrum of the particles in the target and the fuel,
- Decay heat of the spallation target and fuel,
- Radiotoxicity of the spallation target and fuel,

- Required accelerator beam current for rated thermal power,
- Coolant void reactivity, and
- Doppler coefficient.

2.2 Spallation analysis code -NMTC/JAERI-

NMTC/JAERI calculates the spallation reaction of the high energy particle and nuclides in the energy range above 20 MeV. The code includes the calculation models of the intranuclear cascade reaction (BERTINI model and ISOBAR model), evaporation reaction, high-energy fission reaction and preequilibrium process. Latest data of the nucleon-nucleon reaction cross section and level density parameters are also adopted. NMTC/JAERI simulates spallation process by using the Monte Carlo method in the energy range from 20 MeV to 3.5 GeV. Proton, neutron, π^+, π^- and π^0 are transported. The neutron production yield of a proton, which is important to determine the proton beam power, can be also obtained.

In the energy range below 20 MeV, there are many nuclear data libraries which are well verified and revised. These nuclear data libraries can also be used in existing deterministic analysis codes which solve neutronics characteristics faster than the Monte Carlo codes. In ATRAS, when the neutrons transported by NMTC/JAERI have slowed down below a cut-off energy, which is arbitrary defined by user, neutrons are transfered to the transport calculation by the deterministic analysis code. Position, angle, energy and weight of the cut-off neutrons are scored into the intermediate data file.

2.3 Fixed neutron source calculation code -FSOURCE-

The FSOURCE code was provided to create a fixed neutron source data for deterministic neutron transport analysis from the intermediate data file that created by NMTC/JAERI. A fixed neutron source data generated by the FSOURCE contains the spatial, energy and angular distributions of the low energy neutrons. Angular distribution of the low energy neutrons is expressed in the form of the Legendre polynomial. The order of the Legendre polynomial can be selected from zero to three. By a default, the number of neutron group is set to 73 which is

the same as the ATRAS original cross section set. When the another cross section set are used, energy structure of the fixed neutron source file can be changed. Two types of normalization factor are prepared: one is normalized by a source particle of spallation analysis and the other is incident proton current in unit of mA. When the fixed neutron source is normalized by 1-mA current, the required beam current for a rated thermal power at each burnup step is determined automatically by the ATRAS Utility. FSOURCE can handle the intermediate file from the NMTC/JAERI, the NMTC/JAERI97 and the LAHET code system[10].

2.4 Low energy neutron transport code -TWODANT-

For the neutron transport analysis below 20 MeV, the two-dimensional discrete ordinate analysis code TWODANT is included in ATRAS.

In the accelerator-driven system, accelerated protons are injected into the spallation target through the beam duct. Inside the beam duct is always kept in a vacuum or near vacuum during the system operation. In case of liquid target, beam duct is inserted near the center of the subcritical core. In such case, leakage of neutron through the beam duct must be considered to obtain the neutron flux distribution in whole subcritical core. Therefore, for the analysis of the accelerator-driven systems, it is desirable to handle the large void region in the calculation model of the transport calculation. We selected TWODANT for the low energy neutron transport below 20 MeV which can accurately treat both large void regions like proton beam duct and volumewise unisotropic neutron source.

2.5 Burnup analysis code -BURNER-

One unique function of ATRAS is a capability of burnup analysis for the accelerator-driven subcritical systems. It is important to determine the burnup characteristics of the accelerator-driven subcritical system accurately, because it should be ensured that the subcriticality of the core must not exceed the critical. Moreover, the core subcriticality is directly influence the energy balance of the system. If the core has a deep subcriticality, although it must be safe from the viewpoint of neutronics, it requires a very high power beam

and is difficult to supply the electricity to generate such a very high power beam. A BURNER code, the burnup calculation code in the VENTURE code system[11], is included into ATRAS. When user uses BURNER together with TWODANT, it is possible to obtain the burnup characteristics by using the energy spectrum and flux distribution taking account of the spallation neutron source. In the BURNER code, user can modify the data for burnup and decay chains of the nuclides. Default burnup chain which is stored in master chain data file is illustrated in Fig. 2.3.

2.6 Fuel exchange simulation code -CHFUEL-

At the analysis of the core burnup characteristics, it is necessary to obtain a long-term burnup characteristic based on the fuel cycle strategy. Then, a code is required for simulating a fuel exchange. The program CHFUEL was developed to simulate the fuel exchange at the end of each burnup cycle. After the burnup calculation by BURNER, CHFUEL reads an atomic number density file (ZNATDN file) at the end of cycle. Then, the atomic number densities of spent fuel are changed to those of fresh fuel. The latest CHFUEL is based on the JAERI proposed transmutation system:

1) Nuclides specified in the input data of CHFUEL are extracted from the spent fuel

2) CHFUEL determines the total mass of the extracted nuclides

3) Nuclides specified in the input are added as a same amount of the extracted nuclides.

Ratio of the added nuclides and the decontamination factor of the extracted nuclides can be also specified in the input data of CHFUEL.

2.7 Effective cross section formation -SCALE-4-

The effective cross sections for deterministic neutron transport and burnup calculation in the energy range below 20 MeV are prepared by the CSAS module of the SCALE-4 code system. Heterogeneity of the fuel pin configuration can be handled and the self shielding factor are treated by the Bondarenko method to generate the effective cross section files. A utility program MKISO is prepared to convert the effective microscopic cross section file

from the SCALE standard AMPX format to the CCCC format[12]

2.8 Pre-processing module -ATRAS Driver-

To obtain the neutronics and burnup characteristics of accelerator-driven system, several calculation codes in ATRAS are often used. We developed a pre-processing program named "ATRAS Driver". The user specifies the calculation model, material composition and source specification in the input data file of the ATRAS Driver. The ATRAS Driver creates input data files for spallation analysis, fixed source data calculation, effective cross section formation, neutron transport calculation and burnup analysis. Those parameters should be changed according to the analysis condition such as the heterogeneous cell calculation and neutron transport calculation are also specified in the input data file of the ATRAS Driver. Figure 2.2 shows the process flow of the ATRAS Driver.

2.9 Post-processing module -ATRAS Utility-

The ATRAS code system adopts the CCCC format binary files to save the disk space and access time. These files are, however, unreadable for the user. Furthermore, some calculation results like the neutron energy spectra are listed in separate files from the spallation analysis code and the neutron transport code. A post-processing program "ATRAS Utility" is created to read the binary files and the code calculates the quantities such as a particle energy spectrum from high-energy region to low energy region, reaction rates and actinide inventories at each burnup step. The decay heat[13] and the radiotoxicity of residual MA in the spent fuel can also be analyzed by the ATRAS Utility. The decay heat and the radiotoxicity of the nuclides are listed together with some physical values such as the decay constant, the atomic number and the mass number in the ASCII text file. The user can modify or revise these values according to the user requirement.

The ATRAS Utility calculates the following quantities and then creates output in ASCII text format:

1) Neutron flux distribution at specific fine mesh points
2) Zone averaged neutron energy spectrum (includes high-energy regions)
3) Nuclide number densities in each burnup step
4) Effective microscopic cross section
5) Effective macroscopic cross section
6) One group cross section (Zone averaged and/or at specific mesh point)
7) Reaction rate at specific fine mesh point
8) Power distribution
9) Radiotoxicity of the spent fuel immediately after the burnup
10) Decay heat of the spent fuel immediately after the burnup
11) Required proton beam intensity for rated thermal power of the core.

3. Formation of multi-group cross section set for ATRAS

The group cross section set for ATRAS was prepared based on the JENDL-3.2[14] cross section library. The ATRAS cross section set was created as an extended version of the JFS-3-J2[15] cross section set which has been used for fast reactor analysis. The structure of the ATRAS group cross section set is the same as that of JFS-3-J2 except for the number of the energy groups. The JFS-3-J2 cross section set is formed in 70 energy groups from 10^5 eV to 10 MeV. Three groups were added in the energy range from 10 MeV to 20 MeV to simulate threshold reactions of actinides more accurately than the spallation analysis code. The energy group structure below 10 MeV is exactly the same as that of JFS-3-J2. The energy boundary and the lethargy width of the ATRAS 73 group cross section are shown in Table 3.1. Other parameters to create the self shielded effective cross section are listed in Table 3.2. About 150 nuclides are selected from the JENDL-3.2 pointwise library. Higher actinides such as berkelium and californium, long-lived fission products and lanthanides are included into the ATRAS cross section set. Seven isotopes of mercury[16] were also included. Average cross sections of fission products are prepared for burnup analysis. These lumped fission products cross sections were prepared to consider the nuclides which are not explicitly considered in the burnup and decay chain. Nuclides required for the analysis of systems using Th/U-233 fuel are assembled and stored into the ATRAS cross section set. Tables 3.3.1 and 3.3.2 indicate the nuclides in the ATRAS group cross section set.

To create the ATRAS group cross section set, the NJOY[17] code system is used for the Doppler broadening, unresolved resonance calculation and scattering matrix formation. The following modules in NJOY are used:

MODER	File format conversion,
RECONR	Resolved resonance calculation,
BROADR	Doppler broadening calculation,
UNRESR	Unresolved resonance calculation,
THERMR	Scattering matrix formation and
GROUPR	Groupwise cross section formation.

To make multigroup cross section, following weighting spectrum is assumed:

20 MeV to 1.4 MeV	Fission neutron spectrum of Pu-239,
1.4 MeV to 0.8203 eV	1 / E spectrum and
0.8023 eV to 1.0×10^{-5} eV	Maxwellian distribution at 20 ℃.

After the NJOY calculation, the AJAX code in the SCALE-4 code system is used to build a cross section set in AMPX format that is based on the group cross sections for individual nuclide. Detail procedure of the cross section formation is shown in Fig. 3.1.

4. Input Instruction

This section mainly describes the instruction of input data of the ATRAS Driver and the ATRAS Utility. Brief input instruction for the NMTC/JAERI, FSOURCE, SCALE-4, MKISO, TWODANT and BURNER are also summarized. For more detail of the input, see the original manuals[5-10] .

4.1 ATRAS Driver

The input data for the ATRAS Driver is described. All the input data are in free format except card 1-1, 2-1, 2-2 and 2-3. Card 1-1 for the case title is in fixed format (A80). Card 2-1 is also in fixed format (A12). Cards 2-2 and 2-3 are the free format similar to the standard composition input of SCALE-4 code system.

(1) Case Title

Card 1-1 Title of the analysis (A80)

(2) Material Composition

Card 2-1 Cell calculation model (A12)

INFHOMMEDIUM Homogeneous model

LATTICECELL Heterogeneous model

Note: By the homogeneous model specified by the keyword "INFHOMMEDIUM", the effective microscopic cross sections for the infinite homogeneous media are calculated by the CSASN module of the SCALE-4 code system and used directly to the burnup calculation by the TWODANT and the BURNER.

By the heterogeneous model specified by the keyword "LATTICECELL", the microscopic effective cross sections (so called "cell-weighted cross-section") are calculated by using the pin-cell model specified by Cards 2-3, and the one-dimensional cell calculation is performed by the XSDRNPM code (the CSAS1X module of the SCALE-4). In this case, the cell averaged cross section is formed

in the macroscopic cross section file with the material number of 500. See the SCALE-4 manual[1] for more detail.

Card(s) 2-2 SCALE-like standard compositions specification data (Free Format)

1	SC	Standard composition name
2	MX	Mixture ID number
3	ADEN	Number density for the nuclide (atoms/barn-cm)
4	TEMP	Material temperature in Kelvin
5	END	Terminate a standard composition.

Note: Enter once for each standard composition component. Enter END to terminate the component. Repeat entries 1 through 5 until all the mixtures have been defined.

Standard composition names of the nuclides are summarized in Tables 3.3.1 and 3.3.2.

END COMP Terminate the material composition data block.

Note: Enter the keyword "END COMP" once in the input data file at the end of standard composition specification.

Card(s) 2-3 Unit cell specification for LATTICECELL problems (Free Format)

(Required only for the Card 2-1 is "LATTICECELL".)

1 CTP Type of lattice

SQUAREPTCH	Cylindrical rods in a square pitch
TRIANGPITCH	Cylindrical rods in a triangular pitch
SPHSQUAREP	Spherical pellets in a cubic lattice
SYMMSLABCELL	A symmetric array of slabs

(Above four geometries are available in the ATRAS Driver.)

2 PITCH Array pitch (cm)

3	FUELOD	Outside diameter of the fuel (cm), or the thickness of the fuel in a slab geometry (cm)
4	MFUEL	Mixture number of the fuel
5	MMOD	Mixture number of the moderator
6	CLADOD	Outside diameter of the clad (cm)
7	MCLAD	Mixture number of the clad
8	CLADID	Inside diameter of the clad (cm)
9	MGAP	Mixture number of the gap between clad and fuel (0 means void.)
	END	Terminate LATTICECELL data

(3) Geometry for two-dimensional calculation (list indicated format)

Card 3-1 The number of mesh intervals

1	IM	Number of coarse mesh intervals in radial (R-) direction
2	JM	Number of coarse mesh intervals in axial (Z-) direction

Card(s) 3-2 Radial coordinates of coarse mesh edges

(R(I), I=1, IM+1)

Radius of the coarse mesh boundaries (cm)

Card(s) 3-3 Number of fine mesh intervals in R-direction

(ID(I), I=1, IM) Number of fine meshes for each radial coarse mesh interval

Card(s) 3-4 Axial coordinates of the coarse mesh edges

(Z(I), J=1, JM+1)

Height of the coarse mesh boundaries (cm)

Card(s) 3-5 Number of fine mesh intervals in Z-direction

(JD(J), J=1, JM) Number of fine meshes for each axial coarse mesh interval

Card(s) 3-6 Material specification for the coarse mesh regions

((M0(I, J), I=1, IM), J=1, JM)

Material number (MX in Card 2-2) for each coarse mesh regions

(4) Burnup specification of the subcritical core (Free format)

Card 4-1 Number of burnup steps

1 NSTEP Number of burnup steps

Card(s) 4-2 Period and power of each burnup steps (repeated NSTEP times)

1 PERIOD Operation time (days)

2 POWER Thermal output of the core (MW)

(5) Parameters for Spallation Calculation (Free format)

Card 5-1 Proton beam profile

1 E0 Incident particle energy (MeV)

2 TIPO Incident particle type

=0 Proton

=1 Neutron

3 R0 Source beam radius (cm)

4 Z0 Z-coordinate for the top of cylindrical beam (cm)

5 Z1 Z-coordinate for the bottom of cylindrical beam (cm)

6 DIREC Z-component of beam direction cosine

Note: In ATRAS Driver, source beam profile is fixed to uniform distribution. Beam energy is monochromatic value of E0. Shape of the source is cylinder. If Z0=Z1, surface source is assumed. See the manual of NMTC/JAERI97 for more detail source specification.

Card 5-2 Histories for spallation analysis (Free Format)

1 MAXCAS Number of histories per one batch

2 MAXBCH Number of batches

(6) Optional data

Card 6-0 Optional control data (Free Format)

(All the data in this card is set to zero if the end-of-file is found in this line.)

1 ICHI Fission spectrum (χ vector) for the TWODANT calculation

=0 Use χ vector in an effective cross section library

=1 User input χ vector (Card 6-1 required)

=2 Calculated by Maxwellian formula (Card 6-2 required.)

=3 Calculated by Watt formula (Card 6-3 required)

=-ID Use χ vector of nuclide ID (to be supported)

2 ITWO Special parameters for TWODANT calculation

=0 Use the default value of TWODANT

=1 input conversion criteria

=2 input other TWODANT optional data

3 NEH Number of high-energy neutron groups tallied by NMTC/JAERI

=0 use default group structure shown in Table 4.1.

Card 6-1 Fission spectrum (Required for ICHI=1 in Card 6-0)

(CHI(IG), IG=1, 73) 73-group fission spectrum averaged in the whole core

Card 6-2 Maxwellian parameter (Required for ICHI=2 in Card 6-0)

1 T Parameter T in Formula 2-1 (Nuclear temperature). (MeV)

$$f(E)=CE^{1/2}e(-E/T) \quad \text{2-1}$$

Card 6-3 Watt parameter (Required for ICHI=3 in Card 6-0)

1	A	Parameter *a* in Formula 2-2.
2	B	Parameter *b* in Formula 2-2.

$$f(E)=Ce(-E/a)\sinh(bE)^{1/2} \quad \text{2-2}$$

Card 6-4 TWODANT optional parameter (Required for ITWO≧1 in Card 6-0)

1	EPSI	Convergence criteria. Default value is 0.0001 (10^{-4}).

Card 6-5 TWODANT optional parameter (Required for ITWO≧2 in Card 6-0)

1	ISN	The number of angular quadrature sets. Default is 8.
2	IITM	Maximum number of inner iterations summed over all the outer iterations. Default is 30,000.
3	IITL	Maximum number of initial inner iterations. Default is 1.
4	OITM	Maximum number of outer iterations. Default is 20.

Card 6-6 high-energy neutron group structure (required for NEH>0 in Card 6-0)

(EBINH(IG), IG=1, NEH) Upper energy boundaries for high-energy neutron spectrum calculated by NMTC/JAERI.

4.2 ATRAS Utility

Card 1 Output unit (Free Format)

1	IOPFLX	Output unit for neutron flux at each fine mesh point
2	IOZFLX	Output unit for zone averaged neutron spectrum
3	IOXEFF	Output unit for effective microscopic cross sections
4	IOSEFF	Output unit for effective macroscopic cross sections
5	IOXS1G	Output unit for region averaged one group cross sections
6	IORR	Output unit for region averaged reaction rates
7	IOPOW	Output unit for power density distribution

8	IOTOX	Output unit for radiotoxicity
9	IOHEAT	Output unit for decay heat
10	IOXS1D	Output unit for one group cross sections at specific mesh points
11	IORRD	Output unit for reaction rates at specific mesh points

Note: No output files are created when the unit number is zero. If this card is omitted, number 51 to 61 are automatically assigned for each input and all files are created.

Card 2 Edit options (Free Format)

1	NZONE	Number of interested regions
	=0	All regions in TWODANT calculation model
2	NPOINT	Number of specific mesh points
3	NREAC	Number of interested reactions
	=0	All reactions in ISOTXS file
4	NMTC	Write high-energy neutron spectrum in IOZFLX file
	=0	No
	=1	Yes
5	NEXRR	Number of user specified response function

Card 3 Region of interest

(IZP(IZ), IZ=1, NZONEP)

Region number of interest

Card 4 Output mesh point

(RP(I), I=1, NPOINT), (ZP(J), J=1, NPOINT)

Radial and axial coordinates of specific mesh points

Card 5 Nuclides and reactions of interest

(IDRR(K), IREAC(K), K=1, NREAC)

Nuclide ID and reaction number to be output

Note: Nuclide ID is indicated by seven numbers (rrZZAAA) with following manner:

rr	Region number of interested nuclide
ZZ	Atomic number of interested nuclide
AAA	Mass number of interested nuclide.

Correspondence of reaction number and reaction is as follows:

1	Fission
2	Capture
3	(n, α)
4	(n, p)
5	(n, 2n)
6	(n, d)
7	(n, t).

4.3 NMTC/JAERI

4.3.1 Input data file

This file specifies the calculation geometry and parameters using the analysis. All data must be written in fixed format as indicated in parentheses. Parameters which start with character "I", "J", "K", "L", "M", "N" and "O" must be expressed by integer, others are real values.

Card 1 (8A10) Title

Card 2 (8A10) Title

Card 3 (I10)

IRAND Final random number of previous analysis

Note: Blank card must be given for initial run.

Card 4 (3E10.4 , 4I10)

1 EMAX Incident particle energy (MeV)
(<3500 for nucleon, <2500 for pion)

2 ELOP Cut-off energy for proton (MeV)

3 ELON Cut-off energy for neutron (MeV)

4 MXMAT Number of materials excluding voids (<16)

5 MAXCAS Number of source particles per one batch

6 MAXBCH Number of batches in a run

7 N1COL =0 (Not used but required)

Card 5 (6I10)

1 NQUIT Number of calculation repetitions (Usually it should be unity.)

2 NEUTP =23 (Not used but required)

3 NBERTP =21 (Logical unit number of nuclear structure data)

4 NPOWR =11 (Not used but required)

5 NPIDK Option for the treatment of π^- particle

= 0 Consider π^- reaction

= 1 π^- decays immediately

6 NHSTP =22 (Not used but required)

Card 6 (2E10.4, 4I10)

1 ANDIT Angular distribution of an isobar

= 0 50% isotropic, 50% forward

= 1 100% isotropic

= 2 100% forward

2 CTOFE =0 (not used but required)

3	NBOGUS	Option for the evaporation calculation
	< 0	Evaporation calculation is not executed
	> 0	Consider recoil energy of a residual nucleus
	= 0	Recoil energy of a residual nucleus is not taken in account
4	NSPRED	Repulsive enlargement of incident proton beam due to the Coulomb force
	≤ 0	No effect
	> 0	This effect is taken into account
5	NWSPRD	Option for recording tracks of incident protons
	> 0	Yes
	≤ 0	No
6	NSEUDO	Option of recording the information of pseudo event
	> 0	Yes
	≤ 0	No

Card 7 (4I10)

1	IELAS	Selection of cross section for nucleon-nucleus elastic evaporation
	= 0	Geometrical cross section (Not recommended)
	= 1	Cross sections given by Pearlstein's systematics are employed only for neutron below 1 GeV
	= 2	Cross sections given by Pearlstein's systematics are employed for proton and neutron below 1 GeV
2	ICASC	Option for the intranuclear cascade calculation
	= 1	BERTINI model
	= 2	ISOBAR model
3	IQSTEP	Option for preequilibrium calculation
	= 2	No (Only intranuclear cascade and evaporation are considered)
	= 3	Yes (Considered above two and preequilibrium)
4	LVLOPT	Option for level density parameter
	= 1	8 / A

= 2 Parameters derived by Baba

= 3 Parameters given by Ignatyuk

Card 8 (E10.4, I10) The set of Cards 8 and 9 must be repeated MXMAT times.

1 DENH(M) Hydrogen(^{1}H) number density in M-th medium (atoms/barn-cm)

2 NEL(M) Number of nuclides in M-th material excluding Hydrogen (≤30)

Card 9 (3E10.4) Repeat NEL times

1 ZZ(L, M) Atomic number of L-th nuclide in M-th medium

2 AA(L, M) Mass number of L-th nuclide in M-th medium

3 DEN(L, M) Number density of L-th nuclide in M-th medium (atoms/barn-cm)

Note: NMTC/JAERI does not accept the elemental material specification. Thus, when input data of the ATRAS Driver includes the elemental specification, ATRAS Driver refers the "natural.elm" file in "lib/database" directory. Then the ATRAS Driver divides the material composition of element into that of isotopes according to the natural abundance specified in "natural.elm".

Card 10 (I5, I2, I2, A) Cell specification (This block ends with blank card)

1 IDF1 Cell number

2 IDF2 Material number of the cell

3 IDF3 = 1. (Fixed)

4 IBF Cell specification

Note: If the cell is void, both IDF2 and IDF3 must be expressed by "66".

Card 11 (I5, A5, A) Surface specification (This block ends with blank card)

1 IDF1 Surface number

2 IDF2 Mnemonic of the surface

3	IBF	Parameters of the surface

Card 12 (3X, I2, A) Cell importance (This block ends with blank card)

1	IDF	"I0" (Fixed)
2	IBF(I)	Importance of the cell
	= 0	The cell is at outside the calculation model
	= 1	The cell is at inside the calculation model

Card 13 (I5)

1	J	Option for source particle distribution
	= 1	Cylinder (Includes pencil beam)
	= 2	Rectangular

Card 14-1 (8F10.3) Required only for J=1 in Card 13

1	R0	Radius of cylinder (cm)
	= 0	Pencil beam
2	Z0	Lower limit of axial position (cm)
3	Z1	Upper limit of axial position (cm)
	= Z0	Surface source
4	E0	Incident particle energy (MeV)
5	TIP0	Type of incident particle
	= 0	Proton
	= 1	Neutron
6	TL	Time limit (Not used, Zero must be specified)
7	DIREC	Directional cosine about Axial (Z) direction
	= 1.0	+ Z direction
	= -1.0	- Z direction

Card 14-2 (8F10.3) Required only for J=2 in Card 13

1	X0	Lower limit of X-axis of a rectangular (cm)

2	X1	Upper limit of X-axis of a rectangular (cm)
3	Y0	Lower limit of Y-axis of a rectangular (cm)
4	Y1	Upper limit of Y-axis of a rectangular (cm)
5	Z0	Lower limit of Z-axis of a rectangular (cm)
6	Z1	Upper limit of Z-axis of a rectangular (cm)
7	E0	Incident particle energy (MeV)
8	TIP0	Type of incident particle
	= 0	Proton
	= 1	Neutron
9	TL	Time limit (Not used, Zero must be specified)
10	DIREC	Directional cosine about Axial (Z) direction
	= 1.0	+ Z direction
	= -1.0	- Z direction

4.3.2 Statistical input data

Card 1 (Free Format)

NANAL	Number of intermediate files to be processed

Card 2 (Free Format)

1	PIN	Incident particle type
2	EIN	Incident particle energy (MeV)
3	DIR	Directional cosine of incident particle
4	NP	Number of source particles (=MAXCAS×MAXBCH)

Card 3 (Free Format)

1	NR	Number of radial meshes (≤30)
2	NZ	Number of axial mesh boundaries (≤99)
3	NREG	Number of regions (≤450)
4	NE	Number of energy meshes (≤40)

5 NA Number of angular meshes (≤19)

Card 4 (7F10.2)

(BR(I), I=1, NR+1) Radial mesh boundary (cm)

Card 5 (7F10.2)

(BZ(I), I=1, NZ+1) Axial mesh boundary (cm)

Card 6 (7F10.2)

(EB(I), I=1, NE+1) Energy boundary (MeV)

Card 7 (10X, 5(F10.0))

(ANG1(I), I=1, NA+1) Angular boundary

Card 8 (7F10.0)

(VO(I), I=1, NR*(NZ-1)) Volume of the mesh (≤ 450)

Card 9 (14I5)

((IAMED(I, J), J=1, NR), I=1, NZ-1)

Importance of the mesh

Card 10 (3I5) This card is not used but should be exist.

1 ICOUNTI = 0

2 IZSTART = 0

3 IFILMX = 40

Card 11 (Free Format)

1 NRP Number of radial meshes to be printed

2 NZP Number of axial boundaries to be printed

3 LOP Normalization unit

= 1 Normalized per MeV

= 2 Normalized per lethargy

Card 12 (14I5)

(NBR(I), I=1,NRP)

Radial mesh number to be printed

Card 13 (14I5)

(NBZ(I), I=1,NZP)

Axial mesh boundary to be printed

Card 14 (Free Format)

MREG Number of regions to print residual nuclides yield (<25)

Card 15 (I5, A) Repeat MREG times

1 NREG Region number to be prints residual nuclides yield

2 TITLE Comment of the region

Card 16 (Free Format)

MZONE Number of axial mesh to print leakage particle distribution

Card 17 (10X, 5(F10.0))

(BNDZ(I), I=1, MZONE+1)

Mesh boundaries to be print leakage particle distribution

4.4 FSOURCE

Card 1 (Free Format) Control data

1 IM Number of coarse meshes for transport calculation

2 JM Number of coarse meshes

3	IGM	Number of energy groups
4	NHIST	Number of histories in spallation calculation
5	CURR	Normalization factor
	=0	Normalize by one source particle
	=n	Normalize by n mA of proton beam
6	MPL	Order of the Legendre polynomial (0 to 3)
7	ITYP	Input intermediate file format
	=0	NMTC/JAERI
	=1	LCS-2.70
	=2	NMTC/JAERI97

Card 2 (Free Format) Energy boundaries

(EE(I), I=1, IGM)

Energy group boundary (Descending order)

Card 3 (Free Format) Coarse mesh interval in radial direction

(RR(I), I=1, IM+1)

Radial coarse mesh boundary

Card 4 (Free Format) Fine mesh numbers for radial direction

(IX(I), I=1, IM) Number of fine meshes in each coarse mesh intervals

Card 5 (Free Format) Coarse mesh interval in axial direction

(RR(J), J=1, JM+1)

Axial coarse mesh boundary

Card 6 (Free Format) Fine mesh numbers for axial direction

(JX(J), J=1, JM) Number of fine meshes in each coarse mesh intervals

4.5 SCALE-4

Card 1 (Free Format) Analysis sequence specification

=CSASN Homogeneous cell model

=CSAS1X Heterogeneous cell model

Card 2 (Free Format) Title card

Card 3 (Free Format) Cross section and lattice specification

1 LIB Cross section library name

=73GROUPJFSJ3 ATRAS original library

2 LATICE Type of calculation lattice

=INFHOMMEDIUM Infinite homogeneous medium

=LATTICECELL Lattice type cell

Card 4 (Free Format) Material composition specification block

1 SC Name of standard composition

2 MX Medium number of the material

3 VF Volume fraction (Ordinary =1.)

4 ADEN Atomic number density (atoms/barn-cm)

5 TEMP Temperature of the material (K)

6 END End of this data line

Card 5 (Free Format) End of the material composition specification

= END COMP

Card 6 (Free Format) Unit cell specification for LATTICECELL problem

(Required only for the heterogeneous cell calculation)

1 CTP Type of lattice

= SQUAREPITCH Cylindrical rods in a square pitch

= TRIANGPITCH Cylindrical rods in a triangular pitch

= SPHSQUAREP Spherical pellets in a cubic lattice

= SYMMSLABCELL A symmetric array of slabs

2 PITCH Pin pitch or array pitch (cm)

3 FUELOD Outside diameter of fuel (cm)
or the thickness of the fuel in a slab (cm)

4 MFUEL Mixture number representing the fuel

5 MMOD Mixture number representing the moderator

6 CLADOD Outside diameter of clad (cm)

7 MCLAD Clad mixture number

8 CLADID Inside diameter of clad (cm)

9 MGAP Gap mixture number (0 denotes void.)

Card 7 (Free Format) End of the lattice cell specification
(Required only for the heterogeneous cell calculation)

= END Terminate LATTICECELL data

Card 8 (Free Format) End of the dataset

= END Terminate SCALE-4 input data

4.6 MKISO

Card 1 (A80) Input data file name

1 FILAMP Input data file name (AMPX format)

Card 2 (A80) Output file name

1 FILISO Output data file name (ISOTXS format)

Card 3 (I4) Cross section dump flag

1 IDUMP Selection of dump data

=0	Card input only
=1	All data excluding cross sections
=2	All data including cross sections

Card 4 (I4) Fission spectrum specification

1 NUCX File-wide fission spectrum specification

=n	χ -vector of nuclide n is taken as file-wide chi-vector
=0	Use χ -vector of Pu-239
<0	Card input (Card 5 required.)

Card 5 (Free Format) User specified fission spectrum

1 (CHII(I),I=1,73)

User specified χ -vector

4.7 TWODANT

Cards 1 and 2 are always required. Part or all blocks from 1 to 6 are followed after two cards. Here describes a part of original TWODANT input. See the manual[8] for more details.

Card 1 (3I6) Title card control

1 NHEAD Number of title cards to follow

2 NOTTY Output to on-line terminal

= 0	No
= 1	Yes

3 NOLIST Print card image input

= 0	No
= 1	Yes

Card 2 (12A6) Title cards (Repeat NHEAD times)

Block 1 Controls and dimensions (Free format and free order)

IGEOM	Calculation geometry
= 6	X-Y
= 7	R-Z
= 11	R-THETA
NGROUP	Number of energy groups
ISN	S_n order to be used
NISO	Number of isotopes stored in the cross section file
MT	Number of materials to be created
IM	Number of mesh intervals in the R (or X) direction
IT	Total number of fine mesh intervals in the R (or X) direction
JM	Number of mesh intervals in the Z (or Y) direction
JT	Total number of fine mesh intervals in the Z (or Y) direction

Block 2 Geometry specification

XMESH (IM+1)	R (or X) coordinates of coarse mesh edges
YMESH (JM+1)	Z (or Y) coordinates of coarse mesh edges
XINTS (IM)	Number of fine meshes in each coarse R mesh
YINTS (JM)	Number of fine meshes in each coarse Z mesh
ZONES (IM, JM)	Zone number for each coarse mesh

Block 3 Nuclear data specifications

LIB	Source of the cross section data
= ISOTXS	CCCC standard cross section file
= XSLIB	Card image BCD library
= MACRXS	Use MACRXS file created at previous run
CHIVEC (NGROUP)	χ vector

Block 4 Material composition specifications

MATLS

= mat1 comp1 den1, comp2 den2, ...etc.... ;

Note: mat1 is the desired Hollerith name of the first material and comp1, comp2, and so on are the Hollerith names of its components which have densities of, respectively, den1, den2, and so on. Additional materials (i.e. mat2, mat3, and so on up to the required MT) are defined in subsequent strings.

ASSIGN

= MATLS Assigns the material no. N to zone no. N.

Block 5 Solver specifications

IEVT Calculation type

= 0 Fixed source calculation

= 1 k_{eff}

ISCT Legendre order of scattering

ITH

= 0 Forward calculation

= 1 Adjoint calculation

IBL Left boundary condition

= 0 Vacuum

= 1 Reflective

= 3 White

IBR Right boundary condition

Parameters are the same as IBL

IBT Top boundary condition

Parameters are the same as IBL

IBB Bottom boundary condition

Parameters are the same as IBL

EPSI Convergence precision

IITM Maximum number of inner iterations summed over all outer

iterations.

IITL Maximum number of initial inner iterations.

OITM Maximum number of outer iterations.

INFLUX Read the initial flux guess from RTFLUX file

= 0 No

= 1 Yes

INSORS Read the fixed neutron source from FIXSRC file

= 0 No

= 1 Yes

FLUXP Final flux print

= 0 No

= 1 Isotropic

= 2 All moments

BALP Coarse mesh interval print

= 0 No

= 1 Print coarse mesh balance table only

= 2 Print coarse mesh negative flux fixup monitor only

= 3 Print both balance tables and flux fixup monitor

TRCOR Apply transport correction to cross section on MACRXS

= DIAG Diagonal transport correction

= BHS Bell-Hansen-Sandmeier correction

= CESARO Cesaro "correction"

= NO Not apply correction

Block 6 Edit input specifications

POWER Normalize the thermal output to POWER (MW)

RZFLUX Write the zone averaged flux into RZFLUX file

= 0 No

= 1 Yes

4.8 BURNER

Two files are required to run BURNER: one is the file containing BURN block and the other file consists of NUCLIDE, CHAIN and YIELD blocks. In section 4.8.1, first one which contains BURN block are described and latter one describes in section 4.8.2.

4.8.1 Standard input file

Card 1 (A72) Title card

Card 2 (Free Format) BURN block

=BURN Beginning of BURN block

Card 3 (Free Format)

POWER Thermal output (MW)

PERIOD Burnup period (day)

Card 4 (Free Format) End of input

= EOI End of input

4.8.2 Nuclide information and chain data file

Card 1 (A72) Title card

Card 2 (Free Format) NUCLIDE block

=NUCLIDE Beginning of NUCLIDE block

Card 3 (Free Format) NUCLIDE block data

1 IDNUC ID number of nuclide

2 NAMNUM Name of nuclide

3	IFIS	Fission option	
	=1		Fissile nuclide (uranium series)
	=2		Fissile nuclide (plutonium series)
	=-1		FP nuclide
	=0		Others
4	NBURN		
	=1		Fissile nuclide
	=2		Fertile nuclide
	=3		Other fuel nuclide
	=4		FP nuclide
	=5		Other burnup nuclide
	>5		Non burnup nuclide
5	KLIB	Reference option of ATW, EFISS and ECAPT	
	=0		Use following input data
	=1		Use the data in ISOTXS
6	ATW	Nuclide mass	
7	EFISS	Fission release energy (J/fission)	
8	ECAPT	Capture release energy (J/capture)	
9	DECAY	Decay constant (sec^{-1})	

Card 4 (Free Format) CHAIN block

=CHAIN Beginning of CHAIN block

Card 5 (Free Format) CHAIN block data

1	IDPAR	ID number of parent nuclide	
2	IDDAU	ID number of daughter nuclide	
3	ITYPE	Type of reaction	
	=1		Decay
	=2		(n, γ) reaction
	=3		(n, α) reaction

	=4	(n,p) reaction
	=5	(n,2n) reaction
	=6	(n,d) reaction
	=7	(n,t) reaction
	=8	Fission
4	RATE	Branching ratio

Card 6 (Free Format) YIELD block

=YIELD	Beginning of YIELD block

Card 7 (Free Format) YIELD block data

1	IFPR	Nuclide ID of yielded FP nuclide
2	IFSLR	ID number of fissile nuclide
3	YFFP	Fission product yield

Card 8 (Free Format)

= EOI	End of input

4.9 CHFUEL

Card 1 (Free Format)

1	IZONE	Zone number to be processed
2	NUMSUB	Number of nuclides to be removed
3	NUMADD	Number of nuclides to be added

Card 2 (Free Format)

(SUBNUC(I),I=1,NUMSUB)

Nuclide ID numbers to be removed

Card 3 (Free Format)

(ADDNUC(I),VALUE(I),I=1,NUMADD)

Nuclide ID number to be added and its fraction

5. Installation and Input / Output file specification

5.1 Installation of ATRAS code system

ATRAS code system is distributed as a compressed archive. After extraction of compressed archive, several directories are created in the directory "ATRAS" which is also newly created. The latest information is written in the file named "README" in directory "ATRAS". Detail information and limitation of installation are also described in "README". A procedure to install the ATRAS executable modules was tested at the SUN Ultra-1 workstation operated on Solaris 2.5.1. All executable modules can be created by the Sun SPARComplier FORTRAN 4.0. Several problems may occur by user defined (or system administrator suggested) shell environmental valuables. The authors recommend to install ATRAS by system default setting of environmental valuables.

After the necessary modification of makefile, the control script for creation and location of ATRAS execution modules, a directory is created and all files are stored in the directory. Directory structure and information for the files stored in the directory are summarized in Appendix B.

5.2 ATRAS Driver

5.2.1 Components

Components of the ATRAS Driver are listed in Table 5.1.

The ATRAS Driver is consists of the Driver program and AUTO_DCHAIN, the decay chain generator that is automatically called by control shell script of the ATRAS Driver.

Several data files are required to create input data files for analysis. These files are stored in the same directory "lib/database". As mentioned before, data stored in the directory "lib/database" is written in text format. The user can modify or revise the data and then can apply the latest values to the analysis.

5.2.2 Execution

Execution procedure of the ATRAS Driver is as follows:

1) Create input data. File name is specified by "*filename*.dat".

2) Execute shell script ATRAS. Format of the command is

   ATRAS *filename*

3) After execution, following message appears on the terminal.

```
 ATRAS --- starts ------------------------------------------
 ATRAS :i: working directory (Nitride) will be made
*****************************************************************
*                                                               *
*  ATRAS Execution                                              *
*                                                               *
*   Option                                                      *
*   ------                                                      *
*   =0   :   exit now ( input data creation only)               *
*   =+-1 :   NMTC-JAERI94    for intra-nuclear cascade calc.    *
*   =+-2 :   FSOURCE         to make fixed source for TWODANT   *
*   =+-3 :   SCALE+MKISO     for cross section processing       *
*   =+-4 :   TWODANT-BURNER  for 2D Sn burnup analysis          *
*                                                               *
*                                                               *
*   Positive sign means the steps following the step specified  *
*   by the option will be executed, and negative means that     *
*   only specified step will be executed then job terminated.   *
*                                                               *
*****************************************************************
 Option ?
```

4) If user wants to check or modify input data, input 0 to the terminal. Then, command is terminated. Following directories are created by ATRAS command.

filename/	directory for specific problem
filename.GO	restart shell script
NMTC/	for NMTC/JAERI
filename.nin	input for NMTC/JAERI
filename.stat	input for NMTC/JAERI

FSOURCE/	for FSOURCE
filename.hin	input for FSOURCE
SCALE/	for SCALE-4
filename.sin	input for SCALE-4
TWODANT-BURN/	for TWODANT and BURNER
filename.tin	for TWODANT eigenvalue calculation
filename.t1i	for TWODANT initial fixed source calculation
filename.t2i	for TWODANT fixed source calculation
burner-*n*.inp	for *n*-th cycle burnup calculation by BURNER

5) If user entered the values except 0, calculation is performed. When user wants to perform analysis after the modification of input file or by the background process, the shell script *filename*.GO can be used. The user can specify the options that previously indicated in terminal.

5.3 ATRAS Utility

Following analysis products are required to run ATRAS Utility.

a) ISOTXS file (Effective microscopic cross section)
b) GEODST file (Geometry specification information)
c) ZNATDN files (Material composition information for each burnup step)
d) RTFLUX files (Neutron flux distribution for each burnup step)
e) Burnup chain data
f) high-energy neutron spectrum
g) Output thermal power in each burnup step
h) Table of decay heat and radiotoxicity

Items a) to d) are recorded in CCCC format and automatically created by the ATRAS Driver and TWODANT. Item c) and d) are required for the number of burnup steps that user

analyzed. Item e) and g) are automatically created by the ATRAS Driver. Item f) is created by NMTC/JAERI with suffix of ".erg". Item h) is a tabulated data which stored in the "lib/database" directory. User can change and/or add the data according to the user requirements. Format of the file is described below:

NAME(1), ID(1), TL2(1), UNIT(1), SACT(1), DHEAT(1), ALI(1), AAA(1)
NAME(2), ID(2), TL2(2), UNIT(2), SACT(2), DHEAT(2), ALI(2), AAA(2)
⋮
NAME(i), ID(i), TL2(i), UNIT(i), SACT(i), DHEAT(i), ALI(i), AAA(i)
⋮

where:

NAME(i)	Name of nuclide (A8),
ID(i)	Nuclide ID in Tables 3.3.1 and 3.3.2 (I6),
TL2(i)	Half life (E11.3),
UNIT(i)	Unit of half life (A7),
SACT(i)	Specific activity in unit of Bq/g (E11.3),
DHEAT(i)	Decay heat in unit of W/g (E13.3),
ALI(i)	Annual limits of intake in unit of Bq (E9.1), and
AAA(i)	Atomic mass number (F10.4).

6. Summary

The code system named "ATRAS" (Accelerator-driven Transmutation Reactor Analysis Code System) has been developed to perform the neutronics and burnup analysis of the accelerator-driven system. ATRAS is the integrated code system containing the spallation analysis code, fixed neutron source calculation code, neutron transport code and burnup analysis code. We also developed important utility codes to perform pre-processing, post-processing and simulation of fuel exchange procedure. This code system is applicable for the accelerator-driven transmutation system studied under the national OMEGA program and accelerator-driven experimental facilities in the JAERI Neutron Science Project.

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Table 3.1 Groups structure of the ATRAS 73 Cross Section Set

Group No.	Upper Bnd. (eV)	Lower Bnd. (eV)	Leth. Width	Group No.	Upper Bnd. (eV)	Lower Bnd. (eV)	Leth. Width
1	2.000E+7	1.649E+7	0.19	38	2.035E+3	1.585E+3	0.25
2	1.649E+7	1.284E+7	0.25	39	1.585E+3	1.234E+3	0.25
3	1.284E+7	1.000E+7	0.25	40	1.234E+3	9.611E+2	0.25
4	1.000E+7	7.788E+6	0.25	41	9.611E+2	7.485E+2	0.25
5	7.788E+6	6.065E+6	0.25	42	7.485E+2	5.830E+2	0.25
6	6.065E+6	4.724E+6	0.25	43	5.830E+2	4.540E+2	0.25
7	4.724E+6	3.679E+6	0.25	44	4.540E+2	3.536E+2	0.25
8	3.679E+6	2.865E+6	0.25	45	3.536E+2	2.754E+2	0.25
9	2.865E+6	2.231E+6	0.25	46	2.754E+2	2.145E+2	0.25
10	2.231E+6	1.738E+6	0.25	47	2.145E+2	1.670E+2	0.25
11	1.738E+6	1.353E+6	0.25	48	1.670E+2	1.301E+2	0.25
12	1.353E+6	1.054E+6	0.25	49	1.301E+2	1.013E+2	0.25
13	1.054E+6	8.209E+5	0.25	50	1.013E+2	7.889E+1	0.25
14	8.209E+5	6.393E+5	0.25	51	7.889E+1	6.144E+1	0.25
15	6.393E+5	4.979E+5	0.25	52	6.144E+1	4.785E+1	0.25
16	4.979E+5	3.877E+5	0.25	53	4.785E+1	3.727E+1	0.25
17	3.877E+5	3.020E+5	0.25	54	3.727E+1	2.902E+1	0.25
18	3.020E+5	2.352E+5	0.25	55	2.902E+1	2.260E+1	0.25
19	2.352E+5	1.832E+5	0.25	56	2.260E+1	1.760E+1	0.25
20	1.832E+5	1.426E+5	0.25	57	1.760E+1	1.371E+1	0.25
21	1.426E+5	1.111E+5	0.25	58	1.371E+1	1.068E+1	0.25
22	1.111E+5	8.652E+4	0.25	59	1.068E+1	8.315E+0	0.25
23	8.652E+4	6.738E+4	0.25	60	8.315E+0	6.476E+0	0.25
24	6.738E+4	5.248E+4	0.25	61	6.476E+0	5.044E+0	0.25
25	5.248E+4	4.087E+4	0.25	62	5.044E+0	3.928E+0	0.25
26	4.087E+4	3.183E+4	0.25	63	3.928E+0	3.059E+0	0.25
27	3.183E+4	2.479E+4	0.25	64	3.059E+0	2.382E+0	0.25
28	2.479E+4	1.931E+4	0.25	65	2.382E+0	1.855E+0	0.25
29	1.931E+4	1.503E+4	0.25	66	1.855E+0	1.445E+0	0.25
30	1.503E+4	1.171E+4	0.25	67	1.445E+0	1.125E+0	0.25
31	1.171E+4	9.119E+3	0.25	68	1.125E+0	8.764E-1	0.25
32	9.119E+3	7.102E+3	0.25	69	8.764E-1	6.826E-1	0.25
33	7.102E+3	5.531E+3	0.25	70	6.826E-1	5.316E-1	0.25
34	5.531E+3	4.307E+3	0.25	71	5.316E-1	4.140E-1	0.25
35	4.307E+3	3.355E+3	0.25	72	4.140E-1	3.224E-1	0.25
36	3.355E+3	2.613E+3	0.25	73	3.224E-1	1.000E-5	10.38
37	2.613E+3	2.035E+3	0.25				

Table 3.2 Self Shilded parameters of ATRAS 73 Group Cross Section Set

Background Cross Section

Number	σ_0
1	1.0×10^{10} (Infinit Dilution)
2	1.0×10^{6}
3	1.0×10^{5}
4	1.0×10^{4}
5	1.0×10^{3}
6	1.0×10^{2}
7	1.0×10^{1}
8	1.0
9	0.1

Temperature

Number	Temperature (Kelvin)
1	300
2	800
3	2100
4	4500

Table 3.3.1 Contents of ATRAS 73 Group Cross Section Set (Straucutral Material, FP)

SCALE	ID	Nuclide	SCALE	ID	Nuclide
H	1001	HYDROGEN-1	CE-142	58142	CERIUM-142
HE	2004	HELIUM-4	CE-144	58144	CERIUM-144
LI-6	3006	LITHIUM-6	PR-141	59141	PRASEODYMIUM-141
LI-7	3007	LITHIUM-7	PR-143	59143	PRASEODYMIUM-143
BE-9	4009	BERYLLIUM-9	ND-142	60142	NEODYMIUM-142
B-10	5010	BORON-10	ND-143	60143	NEODYMIUM-143
B-11	5011	BORON-11	ND-144	60144	NEODYMIUM-144
C	6012	CARBON-12	ND-145	60145	NEODYMIUM-145
N-14	7014	NITROGEN-14	ND-146	60146	NEODYMIUM-146
N-15	7015	NITROGEN-15	ND-147	60147	NEODYMIUM-147
O	8016	OXYGEN-16	ND-148	60148	NEODYMIUM-148
F	9019	FLUORINE-19	ND-149	60150	NEODYMIUM-150
NA	11023	SODIUM-23	PM-147	61147	PROMETHIUM-147
MG	12000	MAGNESIUM (Nat.)	PM-148	61148	PROMETHIUM-148
AL	13027	ALUMINUM-27	PM-149	61149	PROMETHIUM-149
SI	14000	SILICON (Nat.)	SM-144	62144	SAMARIUM-144
P	15031	PHOSPHORUS-31	SM-147	62147	SAMARIUM-147
S	16000	SULFUR (Nat.)	SM-148	62148	SAMARIUM-148
CL-35	17035	CHLORINE-35	SM-149	62149	SAMARIUM-149
CL-37	17037	CHLORINE-37	SM-150	62150	SAMARIUM-150
CL	17000	CHLORINE (Nat.)	SM-151	62151	SAMARIUM-151
TI	22000	TITANIUM (Nat.)	SM-152	62152	SAMARIUM-152
V	23051	VANADIUM-51	SM-153	62153	SAMARIUM-153
CR	24000	CHROMIUM (Nat.)	SM-154	62154	SAMARIUM-154
MN	25055	MANGANESE-55	EU-151	63151	EUROPIUM-151
FE	26000	NATURAL IRON	EU-152	63152	EUROPIUM-152
CO-59	27059	COBALT-59	EU-153	63153	EUROPIUM-153
NI	28000	NICKEL (Nat.)	EU-154	63154	EUROPIUM-154
CU	29000	COPPER (Nat.)	EU-155	63155	EUROPIUM-155
SE-79	34079	SELENIUM-79	TA-181	73181	TANTALUM-181
KR-85	36085	KRYPTON-85	W-182	74182	TUNGSTEN-182
RB-87	37087	RUBIDIUM-87	W-183	74183	TUNGSTEN-183
SR-90	38090	STRONTIUM-90	W-184	74184	TUNGSTEN-184
Y-89	39089	YTTRIUM-89	W-186	74186	TUNGSTEN-186
ZR	40000	ZIRCONIUM (Nat.)	W	74000	TUNGSTEN (Nat.)
ZR-93	40093	ZIRCONIUM-93	HG-196	80196	MERCURY-196
NB-93	41093	NIOBIUM-93	HG-198	80198	MERCURY-198
NB-94	41094	NIOBIUM-94	HG-199	80199	MERCURY-199
NB-95	41095	NIOBIUM-95	HG-200	80200	MERCURY-200
MO	42000	MOLYBDENUM (Nat.)	HG-201	80201	MERCURY-201
TC-99	43099	TECHNETIUM-9	HG-202	80202	MERCURY-202
PA-107	46107	PALLADIUM-107	HG-204	80204	MERCURY-204
IN-115	49115	INDIUM-115	PB-204	82204	LEAD-204
SN-126	50126	TIN-126	PB-206	82206	LEAD-206
I-129	53129	IODINE-129	PB-207	82207	LEAD-207
CS-135	55135	CESIUM-135	PB-208	82208	LEAD-208
CS-137	55137	CESIUM-137	PB	82000	LEAD (Nat.)
CE-140	58140	CERIUM-140	BI-209	83209	BISMUTH-209
CE-141	58141	CERIUM-141			

Table 3.3.2 Contents of ATRAS 73 Group Cross Section Set (Actinides, Lumped FPs)

SCALE	ID	Nuclide
TH-232	90232	THORIUM-232
PA-231	91231	PROTACTINIUM-231
PA-233	91233	PROTACTINIUM-233
U-232	92232	URANIUM-232
U-233	92233	URANIUM-233
U-234	92234	URANIUM-234
U-235	92235	URANIUM-235
U-236	92236	URANIUM-236
U-237	92237	URANIUM-237
U-238	92238	URANIUM-238
NP-236	93236	NEPTUNIUM-236
NP-237	93237	NEPTUNIUM-237
NP-238	93238	NEPTUNIUM-238
NP-239	93239	NEPTUNIUM-239
PU-238	94238	PLUTONIUM-238
PU-239	94239	PLUTONIUM-239
PU-240	94240	PLUTONIUM-240
PU-241	94241	PLUTONIUM-241
PU-242	94242	PLUTONIUM-242
AM-241	95241	AMERICIUM-241
AM-242	95242	AMERICIUM-242
AM-242M	95601	AMERICIUM-242M
AM-243	95243	AMERICIUM-243
AM-244	95244	AMERICIUM-244
AM-244M	95602	AMERICIUM-244M
CM-242	96242	CURIUM-242
CM-243	96243	CURIUM-243
CM-244	96244	CURIUM-244
CM-245	96245	CURIUM-245
CM-246	96246	CURIUM-246
CM-247	96247	CURIUM-247
CM-248	96248	CURIUM-248
CM-249	96249	CURIUM-249
BK-249	97249	BERKELIUM-249
BK-250	97250	BERKELIUM-250
CF-249	98249	CALIFORNIUM-249
CF-250	98250	CALIFORNIUM-250
CF-251	98251	CALIFORNIUM-251
CF-252	98252	CALIFORNIUM-252

SCALE	ID	Nuclide
FP-232	92920	FP(Th-232
FP-233	93930	FP(U-233)
FP-235	93951	FP(U-235-180d)
FP-235-2	93952	FP(U-235-1080d)
FP-235-3	93953	FP(U-235-1800d)
FP-238	93981	FP(U-238-180d)
FP-238-2	93982	FP(U-238-1080d)
FP-238-3	93983	FP(U-238-1800d)
FP-239	94991	FP(Pu-239-180d)
FP-239-2	94992	FP(Pu-239-1080d)
FP-239-3	94993	FP(Pu-239-1800d)
FP-241	94911	FP(Pu-241-180d)
FP-241-2	94912	FP(Pu-241-1080d)
FP-241-3	94913	FP(Pu-241-1800d)

Table 4.1 Default high-energy group structure

Group	Upper Energy
1	3500.0
2	400.0
3	375.0
4	350.0
5	325.0
6	300.0
7	275.0
8	250.0
9	225.0
10	200.0
11	180.0
12	160.0
13	140.0
14	120.0
15	110.0
16	100.0
17	90.0
18	80.0
19	70.0
20	65.0
21	60.0
22	55.0
23	50.0
24	45.0
25	40.0
26	35.0
27	30.0
28	27.5
29	25.0
30	22.5
31	20.0

Table 5.1 Components of the ATRAS Driver

File name	Category	Function
ATRAS Driver	Program	Input and shell script generator
AUTO_DCHAIN	Program	Generate problem dependent decay chain
Chain.base	Data	Master decay chain data
energy.dat	Data	Energy boundary of ATRAS 73 Group XS
natural.elm	Data	Natural abandance of isotopes
scale-comp-pre.dat	Data	Standard compositions (Used by SCALE-4)
BURNER	Shell script	Shell script to run BURNER
TWODANTI	Shell script	Initial fixed source analysis by TWODANT
TWODANTF	Shell script	Fixed source analysis after 2nd cycle by TWODANT
TWODANTE	Shell script	Last fixed source analysis by TWODANT
TWODANTK	Shell script	Eigenvalue analysis by TWODANT
GO_BASE	Shell script	Pattern shell script to execute ATRAS

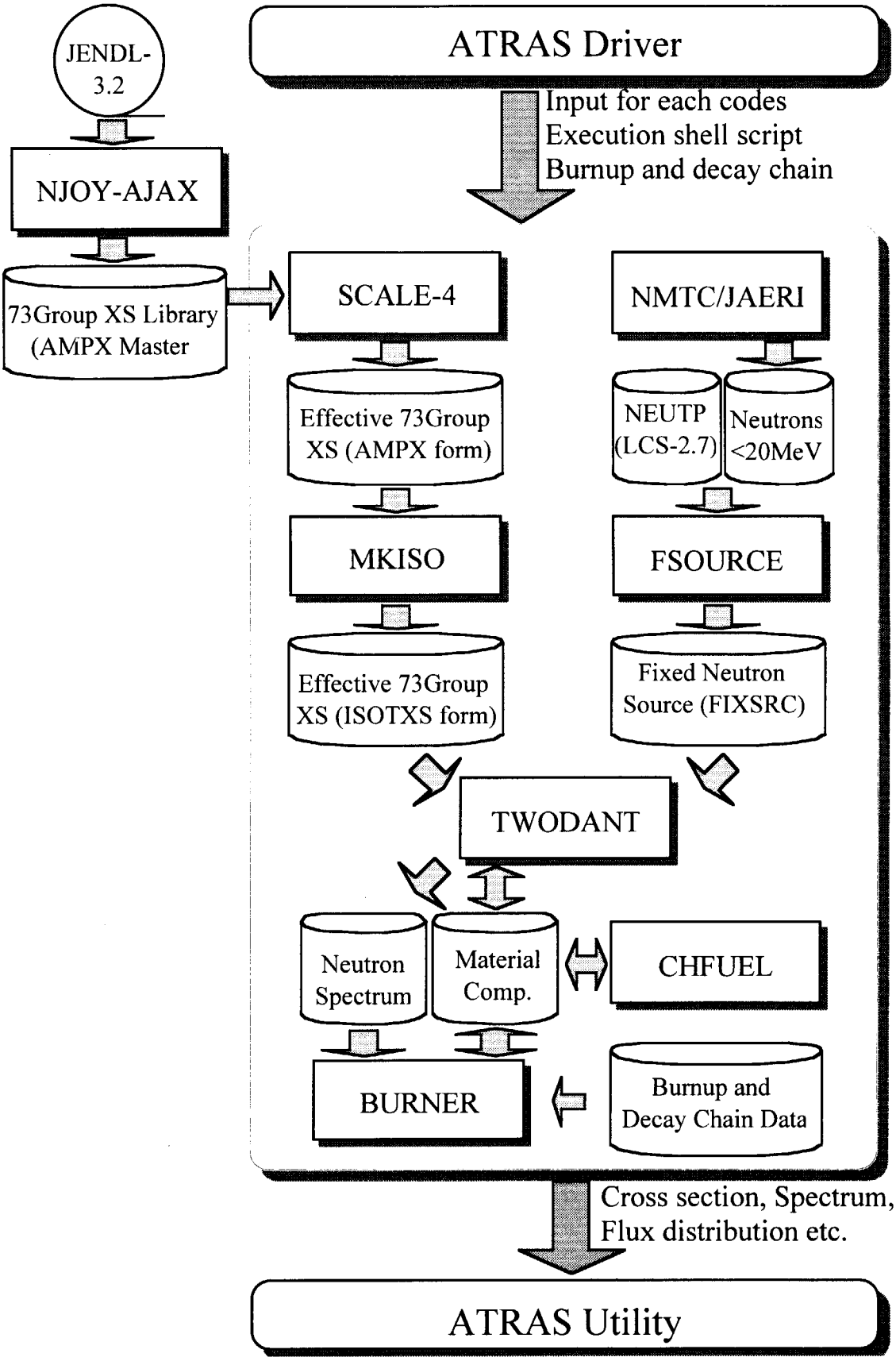

Fig. 2.1 Structure of the ATRAS Code System

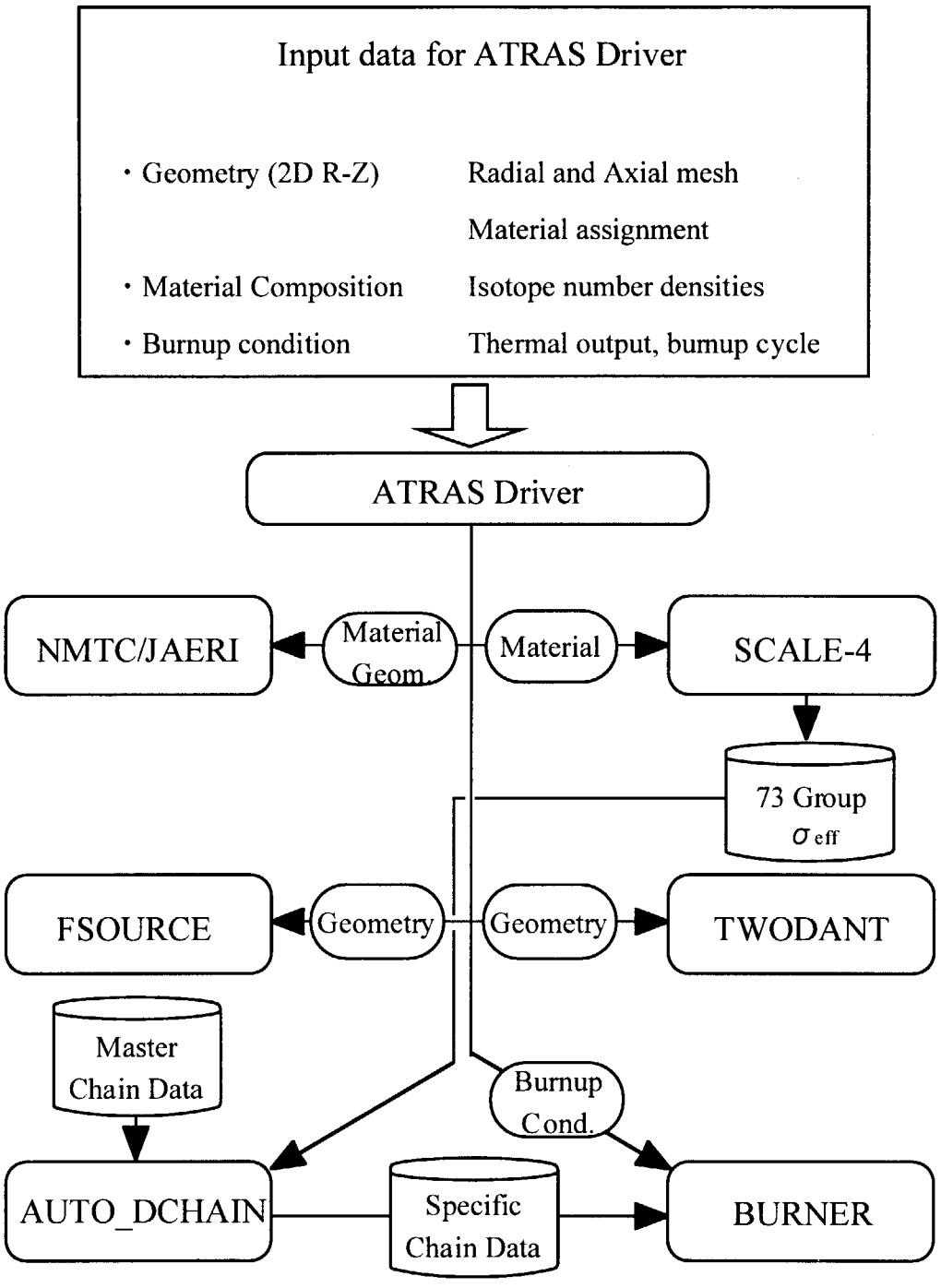

Fig.2.2 Process flow of the ATRAS Driver

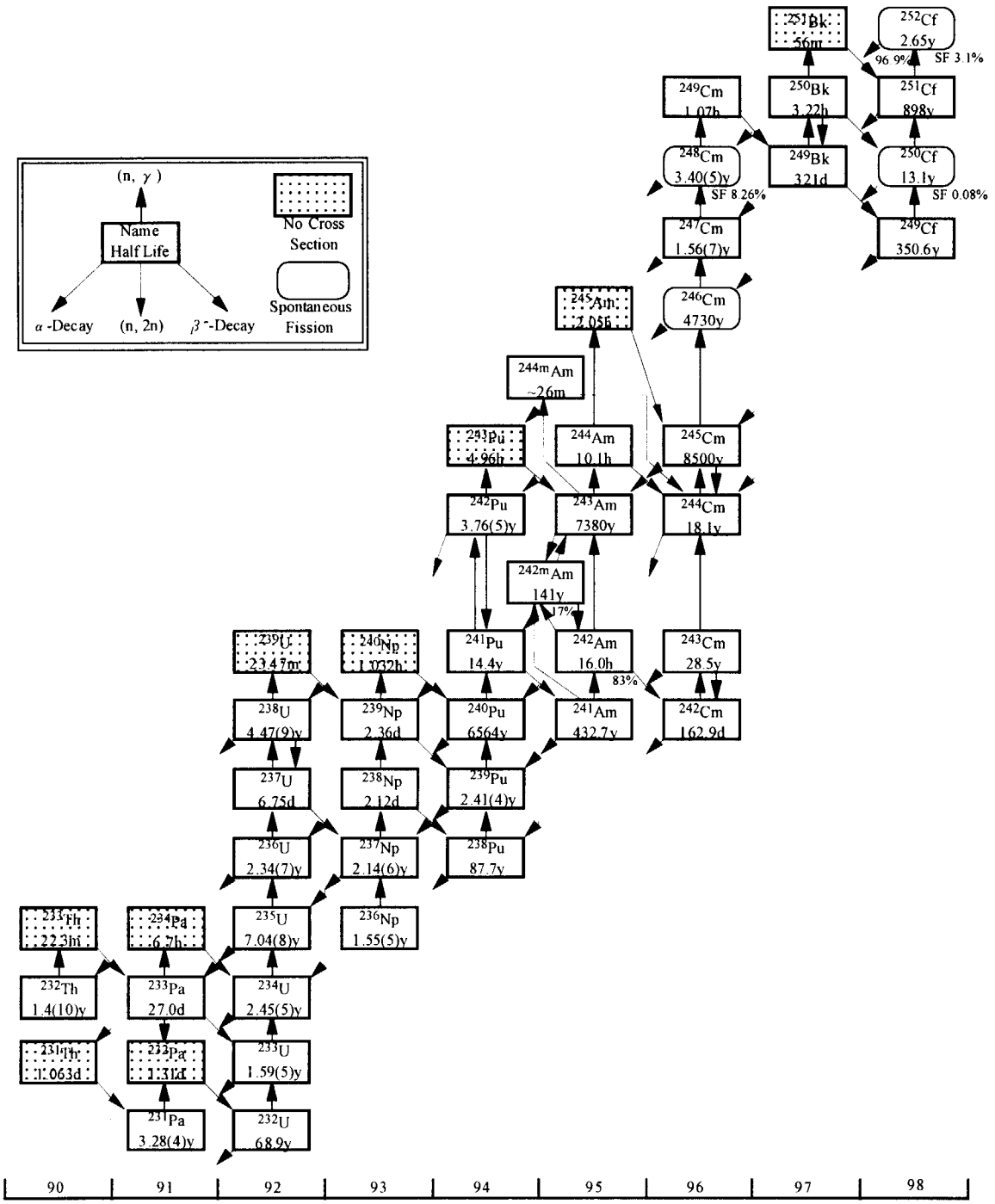

Fig. 2.3 Master burnup chain

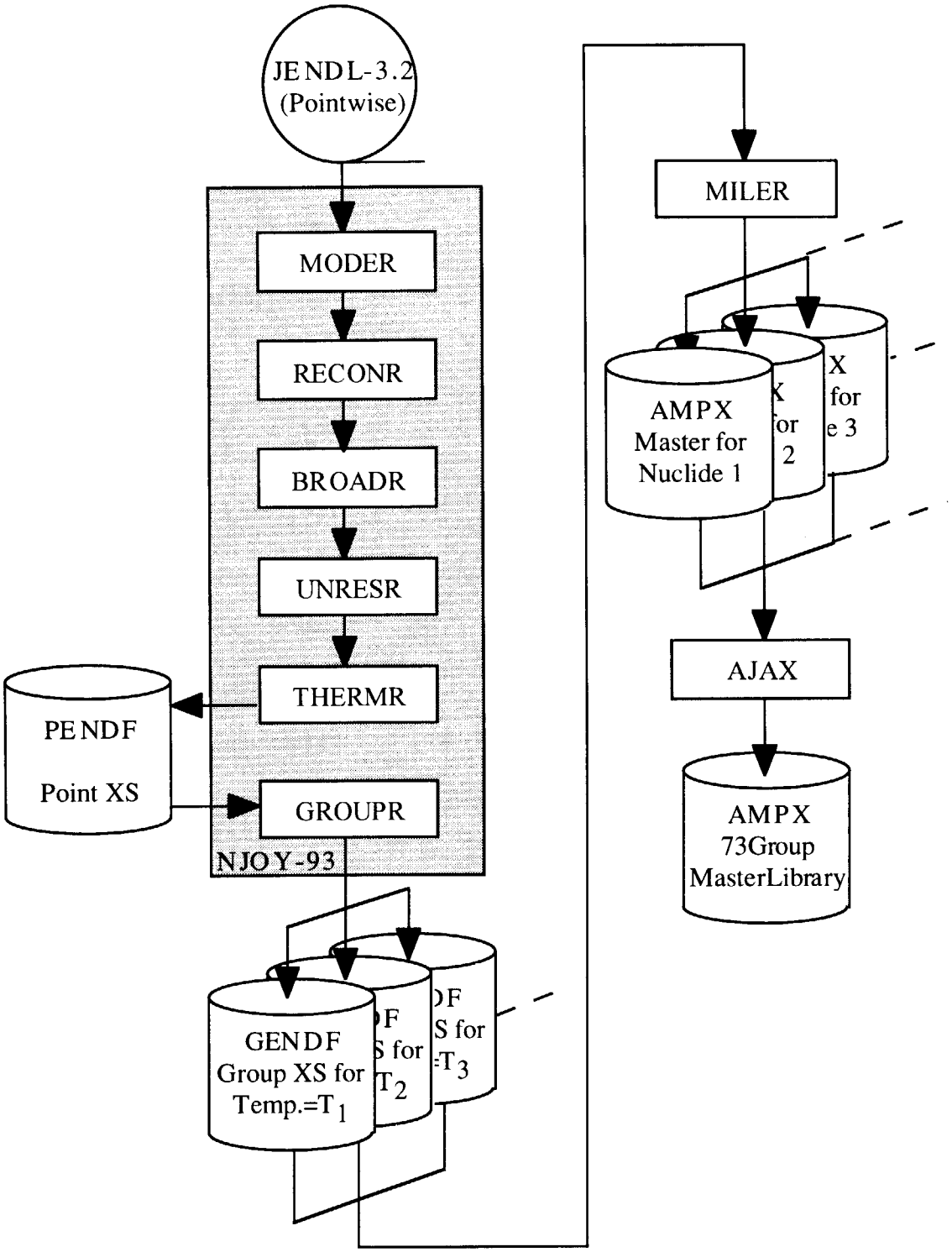

Fig. 3.1 Flow of ATRAS 73 group cross section formation

Appendix A. Sample Input

A sample input attached with the ATRAS code system is based on the benchmark problem of the OECD NEA/NSC Benchmark on Physics Aspects of Different Transmutation Concepts. The calculation model of two-dimensional R-Z geometry is mainly consist of two target regions, fuel region, reflector region and vacuum region simulating beam duct. Figure A.1 shows the calculation model. Material composition for each region is shown in Table A.1. To simplify the problem, reflector and core structual material are substituted from stainless steel to Iron. Input beam specification and other parameters are listed in Table A.2.

Input data of the ATRAS driver is shown in Fig. A.2. Figure A.3 shows the input data to run the ATRAS Utility. Input data files for NMTC/JAERI, FSOURCE, SCALE-4, TWODANT and BURNER, these are automatically created by the ATRAS Driver, are also shown in Fig. A.4 to A.8.

Table A.1 Material composition for each region

Unit: Atoms / barn-cm

	Thin Target	Thick Target	Fuel	Reflector	Beam Duct
W	1.0104E-2	4.0417E-2	1.0250E-5		
Na	1.8214E-2	7.8059E-3	1.2958E-2	8.6731E-3	
Fe			5.3909E-3	3.4242E-2	
Np-237			3.8455E-3		
Pu-238			1.3431E-5		
Pu-239			4.8244E-4		
Pu-240			1.9988E-4		
Pu-241			9.3743E-5		
Pu-242			4.4623E-5		
Am-241			2.6953E-3		
Am-243			7.7047E-4		
Cm-243			2.2225E-6		
Cm-244			1.9483E-4		
Cm-245			9.5568E-6		
N-15			8.3520E-3		
He					1.0000E-20

Table A.2 Problem Specification

Proton Beam	1.0 GeV, 10mA
Beam Radius	15 cm
Beam Profile	Uniform
Beam Duct Radius	15 cm
Target/Core	Concentric cylinders with height of 1 m
Radii	15 cm / 40 cm
Target	Tungsten (Disk layer type)
Thin Target Region	Height 26 cm, Disk Thickness 1.5 cm
Thick Target Region	Height 54 cm, Disk Thickness 13 cm
Fuel	Pin-bundle type
Composition	(90MA-10Pu)N
N-15 Enrichment	100 %
Fuel Pin Outside Diameter	7.3 mm
Fuel Pin Pitch	9.9 mm
Fuel effective height	80 cm
Fuel Pellet Diameter	6 mm
Na bond thickness	0.35 mm
Cladding Material	HT-9
Cladding Thickness	0.3 mm
Reflector	Stainless Steel
Inner / Outer Radii	40 cm / 90 cm
Top Thickness	30 cm
Bottom Thickness	40 cm

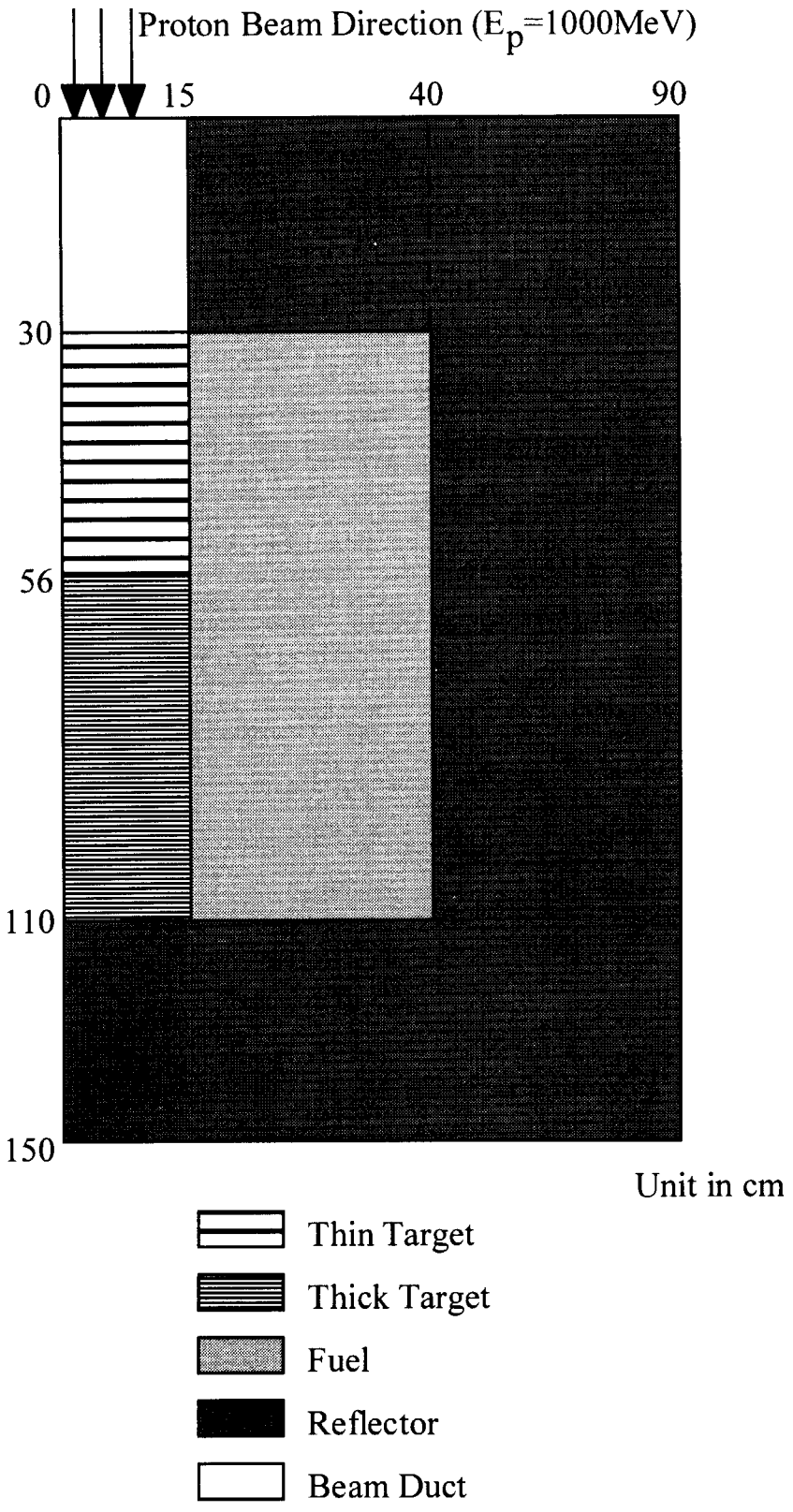

Fig. A.1 Calculation model

```
Sample 1 : MA-Nitride System Calculation by ATRAS          Card 1-1
INFHOMEDIUM                                                Card 2-1
W        1    1.0104E-02  823  END                        Card 2-2
NA       1    1.8214E-02  823  END
W        2    4.0417E-02  823  END
NA       2    7.8059E-03  823  END
NP-237   3    3.8455E-03  823  END
PU-238   3    1.3431E-05  823  END
PU-239   3    4.8244E-04  823  END
PU-240   3    1.9988E-04  823  END
PU-241   3    9.3743E-05  823  END
PU-242   3    4.4623E-05  823  END
AM-241   3    2.6953E-03  823  END
AM-243   3    7.7047E-04  823  END
CM-243   3    2.2225E-06  823  END
CM-244   3    1.9483E-04  823  END
CM-245   3    9.5568E-06  823  END
N-15     3    8.3520E-03  823  END
NA       3    1.2958E-02  823  END
W        3    1.0250E-05  823  END
FE       3    5.3909E-03  823  END
NA       4    8.6731E-03  823  END
FE       4    3.4242E-02  823  END
HE       5    1.0000E-20  823  END
NP-238   6    1.0000E-20  823  END
AM-242   6    1.0000E-20  823  END
AM-242M  6    1.0000E-20  823  END
AM-244   6    1.0000E-20  823  END
AM-244M  6    1.0000E-20  823  END
CM-242   6    1.0000E-20  823  END
CM-246   6    1.0000E-20  823  END
CM-247   6    1.0000E-20  823  END
FP-238   6    1.0000E-20  823  END
FP-239   6    1.0000E-20  823  END
FP-241   6    1.0000E-20  823  END
END COMP
```

Fig A.2 Sample input data for ATRAS Driver

```
3 4                                                    Card 3-1
 0.0  15.0  40.0  90.0                                Card 3-2
    3     5     10                                    Card 3-3
 0.0  30.0  56.0  110.0  150.0                        Card 3-4
    6     5     11     9                             Card 3-5
  5    4    4                                        Card 3-6
  1    3    4                                          |
  2    3    4                                          |
  4    4    4                                          |
 2                                                     Card 4-1
  30. 800.                                             Card 4-2
  30. 800.                                               |
1000.  0  10. 0. 0. 1.                                 Card 5-1
2500  20                                               Card 5-2
  3   1                                                Card 6-1
  0.966  2.842                                         Card 6-3
  0.0001                                               Card 6-4
```

Fig A.2 Sample input data for ATRAS Driver (Continued)

```
 51 52  0  0 55 56 57 58 59 60 61                      Card 1
  8   8   4   1   0                                   Card 2
  1   2   3   4   5   6   7   8                       Card 3
   70. 70. 70. 70. 70. 70. 70. 70.                    Card 4
   10. 20. 30. 40. 50. 60. 70. 80.                      |
  92235      1                                        Card 5
  92235      2                                          |
  92238      1                                          |
  92238      2                                          |
```

Fig. A.3 Sample input data for ATRAS Utility

```
Sample 1 : MA-Nitride System calculation by ATRAS
THIS DATA WAS MADE BY ATRAS_DRIVER

1.0000E+03      20.0      20.0         5         2        10         0
         1        23        21        11         0        22
       0.0       0.0         1         0         0         0
         1         1         2         3
0.0000E+00         6
       74.      180.1.3135E-05
       74.      182.2.6574E-03
       74.      183.1.4449E-03
       74.      184.3.0989E-03
       74.      186.2.8897E-03
       11.       23.1.8214E-02
0.0000E+00         6
       74.      180.5.2542E-05
       74.      182.1.0630E-02
       74.      183.5.7796E-03
       74.      184.1.2396E-02
       74.      186.1.1559E-02
       11.       23.7.8059E-03
0.0000E+00        22
       93.      237.3.8455E-03
       94.      238.1.3431E-05
       94.      239.4.8244E-04
       94.      240.1.9988E-04
       94.      241.9.3743E-05
       94.      242.4.4623E-05
       95.      241.2.6953E-03
       95.      243.7.7047E-04
       96.      243.2.2225E-06
       96.      244.1.9483E-04
       96.      245.9.5568E-06
        7.       15.8.3520E-03
       11.       23.1.2958E-02
       74.      180.1.3325E-08
       74.      182.2.6957E-06
       74.      183.1.4658E-06
       74.      184.3.1437E-06
       74.      186.2.9315E-06
       26.       54.3.1267E-04
       26.       56.4.9445E-03
       26.       57.1.1860E-04
       26.       58.1.5095E-05
```

Fig.A.4.1 Sample input data for NMTC/JAERI (Geometrical data)

```
0.0000E+00          5
       11.        23.8.6731E-03
       26.        54.1.9860E-03
       26.        56.3.1407E-02
       26.        57.7.5332E-04
       26.        58.9.5878E-05
0.0000E+00          1
        2.         4.1.0000E-20
    1 5 1.           -1,  2   4, 13  -5,  4
    2 4 1.    1,  1  -2,  3   4, 13  -5,  5
    3 4 1.    2,  2  -3, 14   4, 13  -5,  6
    4 1 1.           -1,  5   5,  1  -6,  7
    5 3 1.    1,  4  -2,  6   5,  2  -6,  8
    6 4 1.    2,  5  -3, 14   5,  3  -6,  9
    7 2 1.           -1,  8   6,  4  -7, 10
    8 3 1.    1,  7  -2,  9   6,  5  -7, 11
    9 4 1.    2,  8  -3, 14   6,  6  -7, 12
   10 4 1.           -1, 11   7,  7  -8, 15
   11 4 1.    1, 10  -2, 12   7,  8  -8, 15
   12 4 1.    2, 11  -3, 14   7,  9  -8, 15
   13 6666  -4,  1,  2,  3,
   14 6666   3,  3,  6,  9, 12,
   15 6666   8, 10, 11, 12,

    1 CZ  15.000
    2 CZ  40.000
    3 CZ  90.000
    4 PZ   0.000
    5 PZ  30.000
    6 PZ  56.000
    7 PZ 110.000
    8 PZ 150.000

   IO 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 0. 0. 0.

    1
    10.000     0.000     0.000  1000.000     0.000     0.000     1.000
```

Fig.A.4.1 Sample input data for NMTC/JAERI (Continued)

```
   1
    0.000  1000.000     1.000        20
   3    5   12    9    1
    0.000    15.000    40.000    90.000
    0.000    30.000    56.000   110.000   150.000
0.000E+00 2.000E+01 3.000E+01 5.000E+01 1.000E+02 3.000E+02 5.000E+02
1.000E+03 1.500E+03 3.000E+03
                0.      180.
2.121E+04 1.296E+05 6.126E+05 1.838E+04 1.123E+05 5.309E+05 3.817E+04
2.333E+05 1.103E+06 2.827E+04 1.728E+05 8.168E+05
   1    1    1
   1    1    1
   1    1    1
   1    1    1
   0    0   40
   3    5    1
   1    2    3
   1    2    3    4    5
   1
   1     REGION NO.  1
   4
            0.000    30.000    56.000   110.000   150.000
```

Fig. A.4.2 Sample input data for NMTC/JAERI (Statistical input data)

```
        3         4        73        20 0.00000E+00   3   0
 2.00000E+01 1.64872E+01 1.28403E+01 1.00000E+01 7.78801E+00
 6.06530E+00 4.72366E+00 3.67879E+00 2.86505E+00 2.23130E+00
 1.73774E+00 1.35335E+00 1.05399E+00 8.20848E-01 6.39277E-01
 4.97870E-01 3.87741E-01 3.01973E-01 2.35177E-01 1.83156E-01
 1.42642E-01 1.11090E-01 8.65166E-02 6.73792E-02 5.24750E-02
 4.08675E-02 3.18277E-02 2.47874E-02 1.93044E-02 1.50343E-02
 1.17087E-02 9.11877E-03 7.10171E-03 5.53081E-03 4.30740E-03
 3.35460E-03 2.61257E-03 2.03467E-03 1.58460E-03 1.23409E-03
 9.61110E-04 7.48513E-04 5.82943E-04 4.53996E-04 3.53573E-04
 2.75362E-04 2.14452E-04 1.67016E-04 1.30072E-04 1.01300E-04
 7.88926E-05 6.14416E-05 4.78508E-05 3.72662E-05 2.90229E-05
 2.26031E-05 1.76033E-05 1.37095E-05 1.06769E-05 8.31521E-06
 6.47589E-06 5.04343E-06 3.92783E-06 3.05899E-06 2.38235E-06
 1.85537E-06 1.44497E-06 1.12534E-06 8.76415E-07 6.82553E-07
 5.31573E-07 4.13989E-07 3.22415E-07 1.00000E-11
     0.00000    15.00000    40.00000    90.00000
           3           5          10
     0.00000    30.00000    56.00000   110.00000   150.00000
           6           5          11           9
```

Fig. A.5 Sample input data for FSOURCE

```
=CSASN
Sample 1 : MA-Nitride System calculation by ATRAS
73GROUPJFSJ3   INFHOMMEDIUM
W                    1       0     1.01040E-02   823.0  END
NA                   1       0     1.82140E-02   823.0  END
W                    2       0     4.04170E-02   823.0  END
NA                   2       0     7.80590E-03   823.0  END
NP-237               3       0     3.84550E-03   823.0  END
PU-238               3       0     1.34310E-05   823.0  END
PU-239               3       0     4.82440E-04   823.0  END
PU-240               3       0     1.99880E-04   823.0  END
PU-241               3       0     9.37430E-05   823.0  END
PU-242               3       0     4.46230E-05   823.0  END
AM-241               3       0     2.69530E-03   823.0  END
AM-243               3       0     7.70470E-04   823.0  END
CM-243               3       0     2.22250E-06   823.0  END
CM-244               3       0     1.94830E-04   823.0  END
CM-245               3       0     9.55680E-06   823.0  END
N-15                 3       0     8.35200E-03   823.0  END
NA                   3       0     1.29580E-02   823.0  END
W                    3       0     1.02500E-05   823.0  END
FE                   3       0     5.39090E-03   823.0  END
NA                   4       0     8.67310E-03   823.0  END
FE                   4       0     3.42420E-02   823.0  END
HE                   5       0     1.00000E-20   823.0  END
NP-238               6       0     1.00000E-20   823.0  END
AM-242               6       0     1.00000E-20   823.0  END
AM-242M              6       0     1.00000E-20   823.0  END
AM-244               6       0     1.00000E-20   823.0  END
AM-244M              6       0     1.00000E-20   823.0  END
CM-242               6       0     1.00000E-20   823.0  END
CM-246               6       0     1.00000E-20   823.0  END
CM-247               6       0     1.00000E-20   823.0  END
FP-238               6       0     1.00000E-20   823.0  END
FP-239               6       0     1.00000E-20   823.0  END
FP-241               6       0     1.00000E-20   823.0  END
END COMP
END
```

Fig. A.6 Sample input data for SCALE-4

```
2     0     0
Sample 1 : MA-Nitride System calculation by ATRAS
Eigen-value calculation
/
/**** block i ( control ) ****
/
    igeom=r-z
    ngroup=73
    isn=8
    niso=33
    mt=5
    nzone=5
    im=3
    jm=4
    it=18
    jt=31
    maxscm=100000
    maxlcm=2000000
  t
/
/**** block ii ( geometory ) ****
/
    xmesh=    0.000   15.000   40.000   90.000
    xints=        3        5       10
    ymesh=    0.000   30.000   56.000  110.000  150.000
    yints=        6        5       11        9
    zones=        5        4        4;
                  1        3        4;
                  2        3        4;
                  4        4        4;
  t
/
/**** block iii ( cross sections ) ****
/
    lib=isotxs
    chivec=
   7.3315E-06  1.4767E-04  1.3400E-03  6.7018E-03  2.1077E-02  4.6262E-02
   7.6952E-02  1.0349E-01  1.1834E-01  1.1964E-01  1.1020E-01  9.4606E-02
   7.7015E-02  6.0228E-02  4.5692E-02  3.3875E-02  2.4677E-02  1.7739E-02
   1.2621E-02  8.9098E-03  6.2518E-03  4.3666E-03  3.0387E-03  2.1088E-03
   1.4603E-03  1.0095E-03  6.9701E-04  4.8074E-04  3.3132E-04  2.2820E-04
   1.5710E-04  1.0811E-04  7.4382E-05  5.1162E-05  3.5185E-05  2.4193E-05
   1.6634E-05  1.1436E-05  7.8613E-06  5.4040E-06  3.7146E-06  2.5533E-06
   1.7550E-06  1.2063E-06  8.2911E-07  5.6985E-07  3.9166E-07  2.6919E-07
   1.8502E-07  1.2716E-07  8.7398E-08  6.0068E-08  4.1285E-08  2.8375E-08
   1.9501E-08  1.3403E-08  9.2119E-09  6.3314E-09  4.3513E-09  2.9907E-09
   2.0555E-09  1.4127E-09  9.7095E-10  6.6731E-10  4.5864E-10  3.1521E-10
   2.1665E-10  1.4890E-10  1.0234E-10  7.0334E-11  4.8340E-11  3.3224E-11
   7.3018E-11
  t
```

Fig. A.7 Sample input data for TWODANT

```
/
/**** block iv ( mixing ) ****
/
    assign=matls
  t
/
/**** block v ( solver ) ****
/
    influx=0
    ievt=1
    isct=3
    ith=0
    ibl=1
    ibr=0
    ibt=0
    ibb=0
    ibb=0
    epsi=1.00000E-04
    oitm=20
    iitm=30000
    iitl=1
    norm=1
    insors=0
    xsectp=0
    fluxp=0
    fissrp=1
    balp=3
  t
/
/**** block vi ( edits ) ****
/
    rzflux=1
  t
!eof
```

Fig. A.7 Sample input data for TWODANT (Continued)

```
Sample 1 : MA-Nitride System calculation by ATRAS
BURN
POWER=8.00000E+02       PERIOD=3.00000E+01
EOI
```

Fig. A.8 Sample input data for BURNER

Appendix B. Directory structure of the ATRAS code system

atras	exec	Executable modules of ATRAS
	ATCHN.exe	AUTO_DCHAIN
	ATDRV.exe	ATRAS Driver
	atutil.exe	ATRAS Utility
	BURNER	BURNER
	CSAS, SCALE	SCALE-4 executable module
	BONAMC, BONAMI,	Modules called by SCALE-4
	ICE, ICEC,	Same as above
	KENOVA, KENOVB,	Same as above
	NITAWC, NITAWL,	Same as above
	XSDRNC, XSDRNP	Same as above
	FSOURCE	FSOURCE
	MKISO	MKISO
	NMTC95	NMTC/JAERI
	TWODANT	TWODANT
	ALPO, compoz, dial	Auxilialy utilities for AMPX library maintenance
	lib	database
		ALI
		ATRAS
		ATUTIL
		BURNER
		Chain.base
		energy.dat
		GO_BASE
		README
		TWODANTE
		TWODANTF
		TWODANTI
		TWODANTK
		natural.elm
		nuclide.info
		scale-comp-pre.dat
		leveld.dat
		mkiso.inp
		nmtclb25.dat
		scale73.lib
		sclib.lib

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国際単位系（SI）と換算表

表1　SI基本単位および補助単位

量	名称	記号
長さ	メートル	m
質量	キログラム	kg
時間	秒	s
電流	アンペア	A
熱力学温度	ケルビン	K
物質量	モル	mol
光度	カンデラ	cd
平面角	ラジアン	rad
立体角	ステラジアン	sr

表2　SIと併用される単位

名称	記号
分，時，日	min，h，d
度，分，秒	°，′，″
リットル	l，L
トン	t
電子ボルト	eV
原子質量単位	u

1 eV=1.60218×10^{-19}J

1 u=1.66054×10^{-27}kg

表3　固有の名称をもつSI組立単位

量	名称	記号	他のSI単位による表現
周波数	ヘルツ	Hz	s^{-1}
力	ニュートン	N	m·kg/s^2
圧力，応力	パスカル	Pa	N/m^2
エネルギー,仕事,熱量	ジュール	J	N·m
工率，放射束	ワット	W	J/s
電気量，電荷	クーロン	C	A·s
電位，電圧，起電力	ボルト	V	W/A
静電容量	ファラド	F	C/V
電気抵抗	オーム	Ω	V/A
コンダクタンス	ジーメンス	S	A/V
磁束	ウェーバ	Wb	V·s
磁束密度	テスラ	T	Wb/m^2
インダクタンス	ヘンリー	H	Wb/A
セルシウス温度	セルシウス度	℃	
光束	ルーメン	lm	cd·sr
照度	ルクス	lx	lm/m^2
放射能	ベクレル	Bq	s^{-1}
吸収線量	グレイ	Gy	J/kg
線量等量	シーベルト	Sv	J/kg

表4　SIと共に暫定的に維持される単位

名称	記号
オングストローム	Å
バーン	b
バール	bar
ガル	Gal
キュリー	Ci
レントゲン	R
ラド	rad
レム	rem

1 Å=0.1nm=10^{-10}m

1 b=100fm^2=10^{-28}m^2

1 bar=0.1MPa=10^5Pa

1 Gal=1cm/s^2=10^{-2}m/s^2

1 Ci=3.7×10^{10}Bq

1 R=2.58×10^{-4}C/kg

1 rad=1cGy=10^{-2}Gy

1 rem=1cSv=10^{-2}Sv

表5　SI接頭語

倍数	接頭語	記号
10^{18}	エクサ	E
10^{15}	ペタ	P
10^{12}	テラ	T
10^{9}	ギガ	G
10^{6}	メガ	M
10^{3}	キロ	k
10^{2}	ヘクト	h
10^{1}	デカ	da
10^{-1}	デシ	d
10^{-2}	センチ	c
10^{-3}	ミリ	m
10^{-6}	マイクロ	μ
10^{-9}	ナノ	n
10^{-12}	ピコ	p
10^{-15}	フェムト	f
10^{-18}	アト	a

（注）

1．表1－5は「国際単位系」第5版，国際度量衡局1985年刊行による。ただし，1 eVおよび1 uの値はCODATAの1986年推奨値によった。

2．表4には海里，ノット，アール，ヘクタールも含まれているが日常の単位なのでここでは省略した。

3．barは，JISでは流体の圧力を表わす場合に限り表2のカテゴリーに分類されている。

4．EC閣僚理事会指令ではbar，barnおよび「血圧の単位」mmHgを表2のカテゴリーに入れている。

換算表

力	N(=10^5dyn)	kgf	lbf
	1	0.101972	0.224809
	9.80665	1	2.20462
	4.44822	0.453592	1

粘度　1 Pa·s(N·s/m^2)=10 P(ポアズ)(g/(cm·s))

動粘度　1m^2/s=10^4St(ストークス)(cm^2/s)

圧力	MPa(=10bar)	kgf/cm^2	atm	mmHg(Torr)	lbf/in^2(psi)
	1	10.1972	9.86923	7.50062×10^3	145.038
	0.0980665	1	0.967841	735.559	14.2233
	0.101325	1.03323	1	760	14.6959
	1.33322×10^{-4}	1.35951×10^{-3}	1.31579×10^{-3}	1	1.93368×10^{-2}
	6.89476×10^{-3}	7.03070×10^{-2}	6.80460×10^{-2}	51.7149	1

エネルギー・仕事・熱量	J(=10^7 erg)	kgf·m	kW·h	cal(計量法)	Btu	ft·lbf	eV
	1	0.101972	2.77778×10^{-7}	0.238889	9.47813×10^{-4}	0.737562	6.24150×10^{18}
	9.80665	1	2.72407×10^{-6}	2.34270	9.29487×10^{-3}	7.23301	6.12082×10^{19}
	3.6×10^6	3.67098×10^5	1	8.59999×10^5	3412.13	2.65522×10^6	2.24694×10^{25}
	4.18605	0.426858	1.16279×10^{-6}	1	3.96759×10^{-3}	3.08747	2.61272×10^{19}
	1055.06	107.586	2.93072×10^{-4}	252.042	1	778.172	6.58515×10^{21}
	1.35582	0.138255	3.76616×10^{-7}	0.323890	1.28506×10^{-3}	1	8.46233×10^{18}
	1.60218×10^{-19}	1.63377×10^{-20}	4.45050×10^{-26}	3.82743×10^{-20}	1.51857×10^{-22}	1.18171×10^{-19}	1

1 cal= 4.18605J（計量法）

= 4.184J（熱化学）

= 4.1855J（15℃）

= 4.1868J（国際蒸気表）

仕事率　1 PS(仏馬力)

= 75 kgf·m/s

= 735.499W

放射能	Bq	Ci
	1	2.70270×10^{-11}
	3.7×10^{10}	1

吸収線量	Gy	rad
	1	100
	0.01	1

照射線量	C/kg	R
	1	3876
	2.58×10^{-4}	1

線量当量	Sv	rem
	1	100
	0.01	1

（86年12月26日現在）

ACCELERATOR-DRIVEN TRANSMUTATION REACTOR ANALYSIS CODE SYSTEM — ATRAS —