SOURCE 2.0: A COMPUTER PROGRAM TO CALCULATE FISSION PRODUCT RELEASE FROM MULTIPLE FUEL ELEMENTS FOR ACCIDENT SCENARIOS

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ABSTRACT

SOURCE 2.0 is a computer code being jointly developed within the Canadian nuclear industry. It will model the necessary mechanisms required to calculate the fission product release for a variety of accident scenarios, including large break loss of coolant accidents with or without emergency coolant injection. This paper presents the origin of SOURCE 2.0, describes the code structure, the fission product mechanisms modelled, and the quality assurance procedures that are being followed during the code's life cycle.

1. INTRODUCTION

SOURCE 2.0 is being jointly developed within the Canadian nuclear industry for the assessment of the release of fission products in a variety of postulated accident scenarios in CANDU reactors: large break loss of coolant accidents with or without emergency coolant injection, stagnation feeder breaks, end fitting failures, and fuel handling accidents. During these accident scenarios, the fuel is assumed to be exposed to a wide range of temperatures and environments. The flexibility required to address this wide range of conditions has been a major goal in the design of the code structure and in the selection of the fission product release models. The fuel geometries modeled in SOURCE 2.0 vary from a complete reactor core to channels, bundles, fuel elements and fuel axial sections/fragments. SOURCE 2.0 is designed to provide best effort estimates of fission product releases.

The models presented in this paper fall into two separate categories: fission product release models and fuel thermal properties models. The fission product release models will be implemented into SOURCE 2.0, and the fuel thermal properties models will be implemented into fuel performance codes. The fuel thermal models affect fuel thermal properties, which in turn affect fuel temperatures and fission product releases. Therefore, for consistent fuel input parameters which are used by SOURCE 2.0, the fuel thermal models are implemented into fuel performance codes.

The basis of the SOURCE 2.0 code will be presented in this paper. First, the code's origin and development history will be discussed. Then, details of the code organization are summarized together with input and output requirements. The fuel thermal models which will be implemented into the fuel performance codes to provide SOURCE 2.0 with boundary conditions are also described. The details of the fission product release models are then given. Lastly, the quality assurance requirements for the code life cycle are also discussed.

2. ORIGIN AND DEVELOPMENT HISTORY

The reference codes for the development of SOURCE 2.0 are those in the SOURCE Version 1 series: SOURCE 1.0 (References 1 to 3) and SOURCE 1.1 (Reference 4). Both SOURCE 1.0 and 1.1 have been used in end fitting failure and large break loss of coolant accident analyses at Ontario Hydro.

SOURCE 1.0 was initially developed as an upgrade to CURIES-II (Reference 5), in support of the 1991 Generic End Fitting Failure analysis which required the calculation of fission product releases from fuel element clusters, single fuel elements, fuel element pieces, and fuel fragments exposed to air environments. SOURCE 1.0 models the releases of 24 fission products which are divided into three groups: (i) noble gases; (ii) halogens and alkali metals; and (iii) alkaline earth and transition metals. For each of these three groups, the pre-transient fission product inventory distribution between the grain matrix, grain boundaries and fuel-to-sheath gap is assessed.

The fission product release mechanisms and operating conditions modelled in SOURCE 1.0 are:

- diffusion from fuel grains during temperature transients;
- steam-enhanced grain growth and grain boundary sweeping;
- transient gap inventory release after sheath failure;
- releases associated with air oxidation of the fuel;
- alloying and releases due to UO_2 dissolution by molten Zircaloy;
- grain boundary separation (microcracking);
- reduction of steady-state free inventory of short-lived fission products based on sweep gas tests;
- grain boundary release due to rewet; and
- load following operation.

SOURCE 1.0 was upgraded to SOURCE 1.1 to include through-wall oxidation failure and associated releases, releases due to leaching, and the effect of bundle shift scheme on fission product releases (Reference 4). The fuel transient temperatures necessary for the release calculations in both SOURCE 1.0 and 1.1 were obtained from simulations performed by fuel computer codes such as CHAN (Reference 6) and HOTSPOT (Reference 7).

The fission product release models implemented in SOURCE 1.0 and SOURCE 1.1 were developed between 1984 and 1988. At that time, the experimental information generated by COG- (CANDU Owner's Group) funded research and internationally sponsored programs was sparse and the knowledge of the principal release mechanisms was growing rapidly. For this reason, the release mechanisms included in both SOURCE 1.0 and 1.1 are represented by phenomenological models or correlations designed to overestimate the fission product releases over their range of applicability.

Recently, the database of fission product release tests and understanding of the governing release phenomena have evolved dramatically. The quality of the new experimental information and the available models to simulate the fission product release mechanisms motivated the development of SOURCE 2.0.

The main upgrades planned for SOURCE 2.0 are:

- improvement of some of the existing models in SOURCE 1.1,
- extension of the range of applicability of existing models, and
- implementation of new models.

With these new models, SOURCE 2.0 will be suitable for the analysis of a wide range of accident scenarios with their range of environments (*i.e.*, steam, hydrogen-steam mixtures, pure hydrogen), including large break loss of coolant accidents with or without emergency coolant injection availability.

3. CODE ORGANIZATION

3.1 Design Basis

SOURCE 2.0 is an independent and self-contained production tool. It has been designed to calculate the initial fission product inventory distribution in, and transient releases from, fuel exposed to inert, oxidizing, or reducing environments during temperature transients. SOURCE 2.0 will be used with various fuel performance codes (*e.g.*, FACTAR 2.0, ELESIM/ELOCA), which provide the fuel conditions for the calculation of fission product releases.

The fission products modelled in SOURCE 2.0 are divided into groups based on similar release characteristics (Reference 8). SOURCE 2.0 will model 12 fission product groups with 3 sub-groups in each group (to represent long, intermediate and short half-lives).

Because SOURCE 2.0 has been designed to be applied to several accident scenarios, it must have the ability to represent a range of fuel configurations: channel groups for core analysis, bundles in a channel for single channel events, and bundles, fuel element groups and fuel elements for detailed accident analyses. To simulate validation experiments, SOURCE 2.0 must also be able to model fuel fragments (bare samples of UO_2) and mini-elements (short length test elements obtained by cutting a section of a fuel element and adding Zircaloy end caps at both ends). In summary, the fuel configurations which SOURCE 2.0 must be able to represent are:

- channel groups, consisting of groups of channels with the same input transients, geometry and boundary conditions in each group;
- a single fuel channel, consisting of 'n' fuel bundles where 'n' depends on the reactor type and/or the accident scenario;
- a 37- or 28-element fuel bundle;
- fuel element groups, consisting of groups of fuel elements with the same input transients, geometry and boundary conditions in each group;
- fuel segments, which consist of cladded fuel with or without end caps; and
- fuel fragments, which consist of bare fuel (*e.g.*, fuel pellets, or smaller fuel samples).

These requirements dictate the code structure and the development philosophy of SOURCE 2.0.

3.2 Overview of Code Structure

Figure 1 shows the primary logic of SOURCE 2.0. The fuel segment (or fragment) is the smallest independent geometric "accounting" unit. All fuel configurations can be represented in terms of fuel segments. For example, in the case of a 37-element fuel bundle simulation, the code will internally map each fuel element into a corresponding fuel segment and all calculations will be internally performed for 37 fuel segments.

Figure 1 also shows that the innermost loop controls the solution in time, *i.e.*, the entire transient will be calculated for each segment sequentially. The fission product inventory distribution for the fuel element groups, bundles, and channel groups will be calculated by accumulating the entire transient results from the separate fuel segment assessments. The code has been designed in this manner in order to avoid large memory requirements during core analyses and single channel events.

For each geometric unit type, the inventory distribution for the entire simulation represented as being the intra-granular, grain boundary, free and released inventory is stored in four arrays. Note that the sum of these four inventories must always be equal to the initial inventory.

3.3 Input and Output Requirements

To perform a SOURCE 2.0 simulation, four input files are required:

- Generic input file: consists of information related to the type of analysis being performed (*e.g.*, geometric configuration, reactor type, fission product release groups simulated, duration of the transient).
- Steady-state input file: contains the pre-transient fission product inventory and/or distribution. The user may select whether i) SOURCE 2.0 will internally calculate the initial inventory and distribution, ii) the initial inventory is input but the distribution is calculated, or iii) both the initial inventory and distribution are input.
- Transient input file: contains information on transient fuel conditions required for the release calculations (*e.g.*, UO_2 transient temperatures, coolant conditions, sheath failure times, volumetric fraction of fuel dissolved by molten Zircaloy, volumetric fraction of fuel volatilized).
- "Reference data set" (RDS): consists of three types of data: reactor specific data (*e.g.*, number of fuel elements in a fuel bundle, pellet length, fuel stack length), model specific data (*i.e.*, parameters used in the models, such as correlation parameters, diffusion coefficients), and general data (*e.g.*, universal gas constant, unit conversion factors). This reference data will be stored with the executable of the code and will be accessed at the beginning of a simulation (see Figure 1). Changes to the reference data set will be allowed only under the change control process.

The output from SOURCE 2.0 consists of three types of files:

- Summary file: consists of the following information for each fission product group and sub-group: (i) transient fractional release summary, (ii) initial and final inventory distribution among the gap inventory, grain boundary inventory, intra-granular inventory and released inventory, and (iii) transient activity release summary.
- Transient output file: consists of output tables for each geometric unit (*i.e.*, fuel fragments, segments, fuel elements, bundles or channels) and fission product group. The tables contain the transient fission product distribution among the gap, grain boundary, intra-granular and released inventories.
- Plot files: consist of columns of data for plotting.

4. NEW MODELS

Two components which must be accurately modelled and calculated in fission product release analysis are the fuel conditions used to calculate the fission product releases (*i.e.*, fuel temperatures, stoichiometry changes) and the fission product release models themselves. This requirement is highlighted by the relationship that changes in the stoichiometry of the fuel have a strong impact on fission product release. In order for the fuel thermal codes to provide appropriate fuel initial and transient conditions to SOURCE 2.0, modelling of the phenomena that modify the fuel stoichiometry is essential. Among these, the most important are UO_2 oxidation, UO_2 reduction, matrix stripping, and UO_2 reaction/dissolution by Zircaloy. In addition, changes in fuel stoichiometry have marked effects on fuel material properties, which in turn affect the fuel thermal calculations. These models are described in Section 4.1. The fission product models which are new to SOURCE 2.0 are mostly related to the changes in the stoichiometry of the fuel and are described in Section 4.2.

4.1 Modelling Stoichiometric Changes of the Fuel Matrix

SOURCE 2.0 will be executed using fuel transient conditions as input. Thus, the models which affect the stoichiometry of the fuel should be implemented in the fuel performance code(s) (*i.e.*, FACTAR 2.0, ELESIM/ELOCA) to provide self-consistent input conditions for the fission product release models. The most important mechanisms which affect fuel properties are discussed in the following subsections.

4.1.1 UO_2 Oxidation in Steam

When UO_2 is exposed to a steam environment, it oxidizes to an equilibrium stoichiometry which depends on the fuel temperature and the oxygen potential of steam. This equilibrium composition will be calculated by equating the oxygen potential in the steam to the oxygen potential in the UO_2. The kinetics of the fuel steam oxidation process will be modelled as an interfacially controlled process such as that described in Reference 9.

At elevated temperatures (*i.e.*, in excess of 1000°C), the Zircaloy sheath competes with the UO_2 for the available oxygen. Experimental evidence clearly demonstrates that UO_2 oxidation does not begin until most of the Zircaloy has been consumed (Reference 10). As a result, in SOURCE 2.0, it will be assumed that oxidation of the UO_2 occurs only if oxygen is available in the environment and 90% or more of the sheath has been oxidized (to allow for a 10% confidence margin).

4.1.2 UO_2 Oxidation in Air

In some of the postulated accidents (*e.g.*, end fitting failure and fuel handling scenarios) the fuel is assumed to be exposed to air. Air environments have a higher oxygen potential than steam and thus produce a higher equilibrium stoichiometry. The model of UO_2 oxidation in air will be divided into two temperature regimes according to the highest oxide formed. For temperatures above about 1500°C and at atmospheric pressures, UO_{2+x} is the highest oxide formed. In this regime the fuel oxidation kinetics will be modelled following the theoretical approach detailed in Reference 9. For temperatures below about 1500°C and at atmospheric pressures, the fuel oxidation limit is defined by U_3O_8. In this case, fuel oxidation is a very complex process and may involve the sequential formation of U_4O_9, U_3O_7 and U_3O_8. This regime will be modelled by adapting the methodology developed in Reference 11.

4.1.3 UO_2 Volatilization

UO_2 matrix stripping, *i.e.*, volatilization, is a process by which the fuel "vaporizes" due to the formation of volatile uranium-bearing compounds. This may occur in either air or steam environments. The volatilization process can be rapid at high temperatures, and as such represents a possible mechanism for the release of fission products. The theoretical model developed by Cox *et al.* (Reference 9), based on the formation of gaseous UO_3 at the fuel surface, will be implemented. The subsequent transport of UO_3 to the coolant is modelled by a forced convection mass formalism.

4.1.4 UO_2 Interaction/Dissolution by Zircaloy

UO_2/Zircaloy solid/solid interaction may occur at sheath surface temperatures below 1760°C. The result of this interaction is to slightly reduce the fuel to UO_{2-x} and form a liquid phase at the interface between the fuel and the Zircaloy. The model, which will calculate the stoichiometry deviation and the volume fraction converted to liquid, has not been selected yet. The two options being assessed are to use either the FROM.SFD code (Reference 12) directly, or to use a simplified algorithm based on a similar methodology.

Molten Zircaloy has the capacity to dissolve the UO_2 in very specific geometries and environments. Typically, tests have been conducted using samples of UO_2 containing a molten Zircaloy core. Therefore, these experiments do not provide geometry and correlations representative of in reactor fuel elements which have the UO_2 pellets surrounded by the Zircaloy sheath. In a reactor fuel element geometry, when the sheath melts, the liquid Zircaloy readily relocates (Reference 13). Only a small mass of Zircaloy may maintain contact with the UO_2, thus minimizing the importance of this phenomenon. The dissolution may occur at fuel temperatures above 1760°C. A phenomenological model has been developed to estimate the volumetric fraction of the fuel dissolved by the molten Zircaloy. The model is based on experimental information reported in References 14 to 16.

4.1.5 UO_2 Material Properties

The UO_2 specific heat capacity, melting temperature and thermal conductivity are sensitive to changes in the fuel stoichiometry. The modelling of these properties in the fuel performance code(s) is essential for accurate fuel thermal calculations. Based on an extensive literature review of measurements on irradiated $UO_{2\pm x}$ (Reference 17), unirradiated $UO_{2\pm x}$ (References 18 to 20) and SIMFUEL (References 21 to 24) of these properties, along with theoretical treatments (Reference 25), expressions for non-stoichiometric specific heat capacity, thermal conductivity and fuel melting temperature have been developed.

4.2 Modelling Fission Product Release

SOURCE 2.0 will include both new and more detailed models for fission product releases relative to those used in SOURCE 1.1. In this section, a brief description of the most important fission product release mechanisms is given.

In general, the release of volatile fission products will be treated as a single step process. The volatile fission products will be released by diffusion from the grains to grain boundary bubbles. When these bubbles are large enough that they interconnect, the excess fission products will be released to the free volume.

For the case of non-volatile fission products, releases will be considered to occur by a two step process. In the first step, the non-volatile fission products will diffuse to the open surfaces. Releases to the free volume from these surfaces (second step) will then depend on the volatility of each particular fission product.

As previously stated, stoichiometric changes in the UO_2 have a significant effect on the release of fission products. Small changes in fuel stoichiometry may produce very large changes in the release kinetics of some fission products. The fission product release phenomena which will be modelled in SOURCE 2.0 are discussed in this section.

4.2.1 Diffusion

The diffusion algorithm in SOURCE 1.1 will be replaced by a new approach. A generalized model which has been recently developed accounts for the half-life of the fission products, as well as the variation of the diffusion coefficients with time.

During certain postulated reactor accidents, fuel elements can be exposed to oxidizing environments such as steam. If the Zircaloy sheath is heavily oxidized, the UO_2 will be exposed to an oxidizing environment thus forming hyperstoichiometric fuel (see Section 4.1.1). Because hyperstoichiometric fuel has faster fission product release kinetics than stoichiometric UO_2 (Reference 26), it is necessary to include this effect in SOURCE 2.0. Enhanced fission product releases due to the formation of UO_{2+x} will be modelled using the new diffusion methodology. The diffusion coefficients will depend on the deviation from stoichiometry in a manner similar to that described by Turnbull (Reference 27).

4.2.2 Matrix Stripping

When the UO_2 is exposed to oxidizing conditions, the condensed phase is volatilized due to the vaporization of the UO_2 matrix (see Section 4.1.3). For the volatile fission products, 100% of the inventory in the affected volume will be released. The non-volatile fission products will be released according to their volatility.

4.2.3 Effect of Temperature Transients on Releases

In-pile power ramps and out-of pile temperature ramp experiments have demonstrated enhanced releases than expected from the pure diffusion mechanism (Reference 8). Since the theory of the controlling physical/chemical mechanism has not been established yet, the methodology described by Purdy (Reference 28) will be assessed for implementation.

4.2.4 UO_2 Interaction/Dissolution by Zircaloy

Zircaloy can interact with UO_2 at high temperatures to produce liquid phases and fuel stoichiometry reductions (see Section 4.1.4). Both the changes in stoichiometry and the formation of liquid phases may affect the release of certain fission products. The effect of the formation of UO_{2-x} on the release of fission products is not yet clear. The results of Miekeley and Felix (Reference 29) show lower diffusion coefficients for UO_{2-x} than for UO_2. This behaviour contradicts that reported by Lewis *et al.* (Reference 30). A review of the available information is in progress and a phenomenological model will be developed for SOURCE 2.0.

In addition to the UO_2/Zircaloy solid/solid interaction, liquid fuel can also be produced by the dissolution of UO_2 by molten Zircaloy, and by the fuel itself melting. In one modelling approach, the release of high volatility fission products can be modelled by treating them as bubbles in a liquid, as described in References 31 and 32. Alternatively, a simpler approach which captures the important features of the phenomenon but is not as extensive may be used. A review of the available models will determine the final selection.

5. QUALITY ASSURANCE FOR CODE DEVELOPMENT

The development and usage of a computer program can be broken down into a number of phases: development, verification and validation, and configuration management/change control. A configuration management and change control process has been adopted for the code life cycle of SOURCE 2.0. The quality assurance procedures applied during the development and the verification and validation phases of the computer code life cycle are discussed in the following sections.

5.1 Code Development

SOURCE 2.0 is being developed in compliance with the interim quality assurance standard CSA N286.7 (Reference 33) and the Interim Ontario Hydro Reactor Safety and Operational Analysis Department Nuclear Safety Analysis Quality Assurance procedures (Reference 34).

Prior to computer program development, three documents have been produced which outline the development plan, program requirements, and details of the models to be implemented. These documents are: Software Requirements Specification (Reference 35), Development Plan (Reference 36) and Software Design Specification (Reference 37). A Verification and Validation Plan (Reference 38) will be released during the development stage.

A model description document will be written for each model. This document will contain the specific requirements for the model, theory, implementation, assumptions and justifications, verification, validation, and source code listing. Thus, all the information related to a model will be contained in one document.

5.2 Verification and Validation

The SOURCE 2.0 Verification and Validation Plan (Reference 34) will cover the verification of the entire SOURCE 2.0 code, and validation of the dominant fission product release phenomena. Verification and validation of the independent modules will be performed first, followed by integral code verification and validation. The goal of the verification and validation effort is to ensure quality, in the form of reliability and accuracy, to the SOURCE 2.0 computer code before its formal release.

The verification process assures that the software conforms to design requirements. This process will be divided into two parts: module verification and integration verification. Module verification will ensure that modules perform the tasks for which they were designed within the specified range of input parameters, and that the output parameters map onto a continuous domain without non-physical discontinuities. Module verification includes both source code review and testing. Integration verification will verify inter-module interaction and communication, as well as iteration and time stepping logic, as modules are integrated. The person(s) responsible for the verification and testing of each subroutine will be independent of the code developer(s) of that subroutine.

The validation process assesses the accuracy of the simulation software predictions. In order to validate the code, a technical basis document and a validation matrix will be developed.

The technical basis document describes the different accident scenarios of interest and the associated safety concerns. The phenomena affecting fission product releases are described, along with the key parameters used to quantify the phenomena. For each phase of an accident scenario, the possible primary and secondary phenomena are identified.

The validation matrix document identifies those data sets which can be used to validate one or more phenomena and provides a cross-reference between the governing phenomena and the test database. The validation matrix is, therefore, independent of the code to be ultimately validated. Thus, an effort is in progress to produce a Canadian nuclear industry single validation matrix for fission product release from CANDU fuel.

The list of fission product release tests performed in Canada and abroad will be compiled into a fission product release database. This database will comprise two separate parts: data for model development, and data for validation. From quality assurance requirements, tests used for validation must be different from those used for model development.

Validation of SOURCE 2.0 modules will be performed against data from the fission product validation database. This database will provide information on the following parameters: geometry of the sample, environment conditions (*e.g.*, the partial pressure of oxygen), sample temperature, and activity releases for fission products.

6. SUMMARY

SOURCE 2.0 is a code being developed in a joint effort within the Canadian nuclear industry. An overview of SOURCE 2.0's development history, code idealization, model components, and the quality assurance procedures followed during the code's life cycle has been given. When released, SOURCE 2.0 will provide a verified and validated production tool which is designed to calculate best effort estimates of fission product release from CANDU fuel in a variety of geometries (*e.g.*, fragments, mini-elements, fuel elements, bundles or channels) for a broad range of applications. SOURCE 2.0 will represent state of the art modelling of the applicable physical behaviour.

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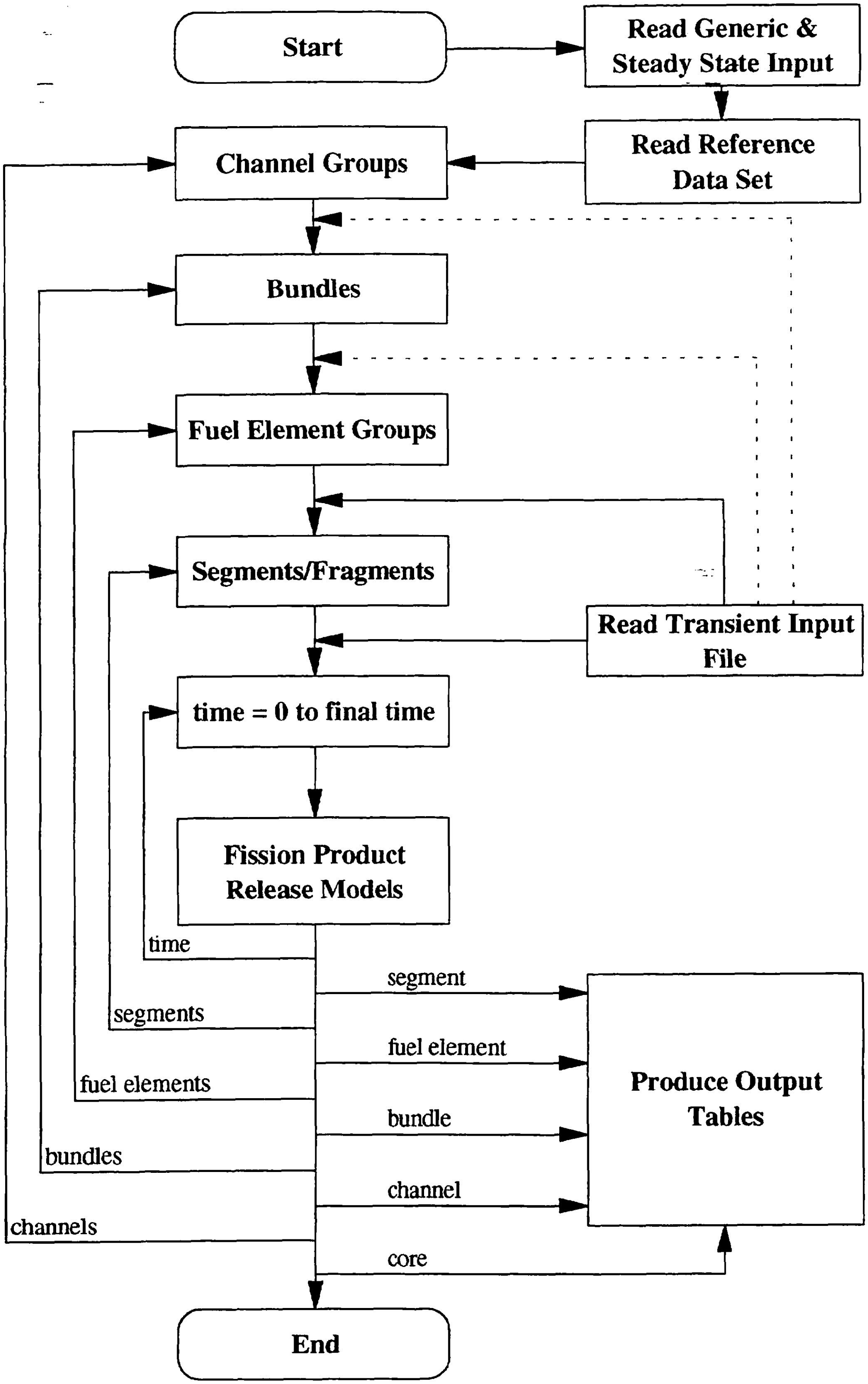

FIGURE 1
SOURCE 2.0 MAIN LOGIC