Development of a Fission Product Release Model and it's Application at PBMR

Jacobus Johannes van der Merwe

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Supervisor: Johan H Venter

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Opsomming

Lank-lewende klowingsproduk vrylatings van sferiese brandstof elemente word by PBMR deur middel van die Duitse sagteware produk GETTER bereken. GETTER is 'n nuttige stuk gereedskap vir berekeninge op brandstofsfere onder beheerde reaktor kondisies, insluitende bestralings toetse en na-bestralings verhittings toetse. Dit is veeldoelig bevind in reaktor analise, maar lomp wanneer ongelukke en sensitiwiteits analises ondersoek word. Ontwikkelinge in verlies van verkoelings-gas ongeluks analises met GETTER het gelei tot die ontwikkeling van FIPREX, en later FIPREX-GETTER. Die sagteware is ontwerp as 'n kode-hulsel om GETTER, sodat berekeninge uitgevoer kan word vir groot getalle brandstofsfere met ontwerps en operasionele parameters wat stochasties gevariëer kan word. Volle Monte Carlo analise is dus moontlik wat verteenwoordigende reaktore met groot getalle brandstofsfere kan modelleer.

Die ontwikkelingsproses en toepassing van FIPREX-GETTER in reaktor analise by PBMR word verduidelik en behoeftes vir toekomstige ontwikkelling word bespreek. Resultate vir 'n voorbeeldige PBMR reaktor ontwerp onder normale bedryfstoestande sowel as 'n reeks ontwerpbasis ongelukke word voorgelê ter illustrasie van FIPREX-GETTER se funksionaliteit. Monte Carlo sensitiwiteit analise beginsels word verduidelik vir elke berekeningstipe. Die verifikasie en validerings plan en huidige status word beskryf. Laastens word die effekte van hoë temperatuur gebeurtenisse op klowingsproduk vrylating ondersoek en bespreek.

Abstract

At PBMR, long-lived fission product release from spherical fuel spheres is calculated using the German legacy software product GETTER. GETTER is a good tool when performing calculations for fuel spheres under controlled operating conditions, including irradiation tests and post irradiation heat-up experiments. It has proved itself as a versatile reactor analysis tool, but is rather cumbersome when used for accident and sensitivity analysis. Developments in depressurized loss of forced cooling (DLOFC) accident analysis using GETTER led to the creation of FIPREX (FIssion Product REIease under accident (X) conditions), and later FIPREX-GETTER. FIPREX-GETTER is designed as a wrapper around GETTER so that calculations can be carried out for large numbers of fuel spheres with design and operating parameters that can be stochastically varied. This allows full Monte Carlo sensitivity analyses to be performed for representative cores containing many fuel spheres.

The development process and application of FIPREX-GETTER in reactor analysis at PBMR is explained and the requirements for future development of the code are discussed. Results are presented for a sample PBMR core design under normal operating conditions as well as a suite of design-base accident events, illustrating the functionality of FIPREX-GETTER. Monte Carlo sensitivity analysis principles are explained and presented for each calculation type. The plan and current status of verification and validation (V&V) is described. The effects high temperature events have on fission product transport are investigated and discussed.

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List of Acronyms and Terms

Acronyms

ACR	Accumulated Core Release
CCR	Cumulative Core Release
Cdf	Cumulative distribution function
CP	Coated Particle
DLOFC	Depressurized Loss of Forced Coolant
FIMA	Fission per Initial Metal Atom
FIPREX	Fission Product Release under Accident (X) Conditions
FPI	Fission Product Inventory
FS / FE	Fuel Sphere / Element
GE	Gas Expansion coefficient
HRB	Hochtemperatur-Reaktorbau
HTR	High Temperature Reactor
HTGR	High Temperature Gas-cooled Reactor
MPS	Main Power System
PBMR	Pebble Bed Modular Reactor
Pdf	Probability distribution function
PIE	Post Irradiation Examination
PLOFC	Pressurized Loss of Forced Coolant
PyC	Pyrocarbon
RDFM	Reactor Design and Fuel Management
SiC	Silicon Carbide

TCR	Time step total Core Release
TINTE	Time dependent neutronics and temperatures
TRISO	Triple coated - Isotropic
V&V	Verification and validation
VSOP	Very Superior Old Program

Terms

Legacy: Inherited. In the context of this dissertation it means that the calculation model, software product or parameter were not developed by the student or company presented, but was inherited or bought from an older program, company or developer.

Verification: Verification is the process of ensuring that the controlling physical equations have been correctly translated into computer code, or in case of hand calculations, correctly incorporated into the calculation procedure.

Validation: Validation is defined as the evidence that demonstrates that the analysis tool or analysis method is fit for its purpose. When calculating physical processes, it may mean showing that the calculation is bounded with a suitable degree of confidence rather than a best estimate.

Acknowledgement

I also wish to extend my deepest gratitude to the following people:

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Publication

This thesis has been condensed and published as a paper at the 3rd International Topical Meeting on High Temperature Reactor Technology, 1-4 October 2006 in Johannesburg, South Africa. The paper was selected by the conference organisers for publication in the Nuclear Engineering and Design's special issue on the HTR-2006.

1 Introduction

Nuclear power is a much debated and controversial issue. Accidents at Three Mile Island and Chernobyl have created public fears about the dangers of nuclear power. Assuring the safe and economical operation of nuclear power plants have therefore became significantly more difficult. In depth reactor and plant analyses are required, where all possible operational conditions and accident events are investigated [1]. Helium cooled and graphite moderated high temperature reactors (HTR's) has the intrinsic ability, if correctly designed, not to lose structural integrity of the reactor internals or fuel elements during all realistically anticipated accident events [2]. Core-melt down scenarios with accompanying mass release of fission products to the environment are therefore not possible for correctly designed reactors.

However, fission products are not completely retained in the fuel elements during normal operation and during accident events release from fuel elements may be accelerated [3]. Although the release of fission products from the fuel is only a small fraction of the total inventory, it still presents a radiological risk to operating personnel during operation and to the general public after accident events. When designing safe and economical reactors, the impact of fission product release from the reactor's fuel elements must be well understood. Release rates of the radiological important fission products from the fuel elements must be calculated to an acceptable accuracy, and transport and eventual deposition in the main power system (MPS) must be accounted for. Where fission products are deposited, whether directly plated out on cooler metallic surfaces, or carried by dust in the coolant gas stream, radiation fields result that limit personnel access and exposure times to perform required maintenance work.

Major accidents usually entail a pipe break in the MPS, followed by the rapid or slow depressurization (depending on the size of the pipe break) of coolant gas from the MPS and reactor cavity. This depressurization lifts fission products attached to dust and plated out in cooler regions, and transports them to the environment. Dust production and plate-out / lift-off are very difficult to mitigate, so that the only practical method to decrease the radiation fields in the plant and possible releases to the environment, is to limit releases from fuel elements.

Fuel development has come a long way since the conception of HTR's in the 1950's, and fuel performance has improved dramatically [4]. Modern reactors developers intend to utilize this good fuel performance to design highly economical and safe reactors. Reactors are therefore designed close to the fuel's operational limit. With current uncertainties in neutronic and thermo hydraulic analyses, and uncertainties in parameters that control fission product transport in fuel material, accurate calculation of fission product release from fuel during reactor operation is no easy task. More and more exact analyses are required to meet increasingly strict requirements set on safety analyses.

The complex interactions in the reactor core can only be calculated with software programs. Calculation models are continuously developed to supply answers to ever-changing questions that are asked about the safety and economics of nuclear reactors. Software programs were developed by various countries to estimate fuel performance and fission product release from nuclear reactors during operation and accident events during the previous century. With the increase in computing power of modern computers, the complexity and abilities of software programs and calculation models were enhanced as well. New generation reactor designers require calculation models that can analyze fission product release from reactors with complex layouts for all possible reactor scenarios. This often means that existing software programs are adapted or developed to perform a wide scope of calculations. There is however a limit to how far an existing software product can be developed before a new software model needs to be created.

At the Pebble Bed Modular Reactor company (PBMR) existing software products used to determine fission product release from fuel spheres and transport from the reactor to the MPS components were inherited from the German fuel and reactor development program [5]. These software products were further developed by PBMR to fulfill the analyses requirements for the PBMR safety case. Although they are excellent products, their development limit has been reached, and new software models that in conjunction with the inherited software could fulfill all PBMR's requirements, had to be developed. Specific new requirements were the ability to calculate the whole reactor core automatically, under all design base conditions.

There was a need for sensitivity analyses using Monte Carlo techniques that could not be met with existing software products. This dissertation describes the development of a calculation model with Monte Carlo sensitivity analyses abilities and its software product, that is currently applied at PBMR to determine fission product release from the PBMR core to the containment building during design base accident events.

1.1 Introduction of the problem

A 400 MW PBMR generates about 1.25×10^{19} nuclear fissions per second, which in turn produces about 2.5×10^{19} fission fragments per second. Most fission fragments, commonly known as fission products, are radioactive and dangerous to human life. HTR fuel elements are designed in principle to retain all fission products produced during operation. The spherical fuel elements (also known as fuel spheres) utilized by PBMR are shown in Figure 1.1. PBMR fuel is based on the specification for German fuel spheres produced for the High-Temperature Reactor (HTR) 500 and HTR-Modul Proof Tests [5]. This fuel type is generally regarded as state of the art for German pebble fuel production. It is designed for optimal performance under normal operating conditions, and to withstand all design base accident conditions.

Fuel spheres are manufactured from graphite matrix material, in which TRISO-coated particles are imbedded. The outer 5 mm layer consists of matrix material only. Graphite matrix material functions as a good heat transfer medium and stabilizes the coated particles in the sphere. Good thermal contact is achieved between coated particles and matrix material, so that low temperature gradients occur in the fuel sphere. The outer fuel free zone protects coated particles from damage from outside direct mechanical effects such as abrasion and shock. It further acts as a barrier layer against chemical corrosion in the case of water or air ingress into the core.

The TRISO-particle consists of a spherical UO_2-kernel, 500 micron in diameter, surrounded by four coating layers. UO_2 has a high melting point (~ 2 880 °C), therefore retaining its integrity under all reactor conditions. Oxygen released during fission in UO_2 binds with some fission products to form immobile oxides. The majority of fission products are retained in the kernel this way.

The kernel produces almost all the power of the reactor through nuclear fission. It also acts as a retention barrier of gaseous fission products, thereby reducing the internal pressure within the coated particle. Fission products that do not form stable oxides are released from the kernel through a diffusion process. Fission products are therefore retained to some extent by the UO_2 kernel.

The kernel is surrounded by a 95 micron thick low density pyrocarbon layer, known as the buffer layer. This layer acts as a sacrificial layer, allowing the kernel to swell under irradiation, and providing void volume for fission gases released from the kernel. The rest of the layers are therefore protected from recoiling fission products and excessive internal pressure by the buffer layer. Fission product retention in the buffer layer is negligible.

The next layer is made up of dense pyrocarbon, 40 micron thick known as the inner pyrocarbon (PyC) layer. It forms an impenetrable barrier to gaseous fission products, and slows down the transport of metallic fission products to the silicon carbide (SiC) layer. During manufacture it provides a smooth surface for the SiC to adhere to, and protects the kernel from chlorine in the form of hydrochloric acid during SiC deposition.

The SiC layer is the primary fission product barrier, being 35 micron thick. It retains all gaseous and metallic fission products, with the exception of silver and strontium to a very high extent. It provides the structural support required to contain the internal gas pressure in the coated particle.

The final layer is again dense pyrocarbon, 40 micron thick known as the outer pyrocarbon (PyC) layer. It is under compressive stress, putting positive pressure on the SiC, helping to contain internal gas pressures. It protects the SiC layer during manufacture from chemical and mechanical damage.

To prevent coated particles from touching each other in the matrix material, which may lead to failures during the pressing stage, each coated particle is overcoated with a layer of matrix material graphite before being mixed with the bulk matrix material. Fuel spheres are pressed and machined to form perfect spheres, 60 mm in diameter.

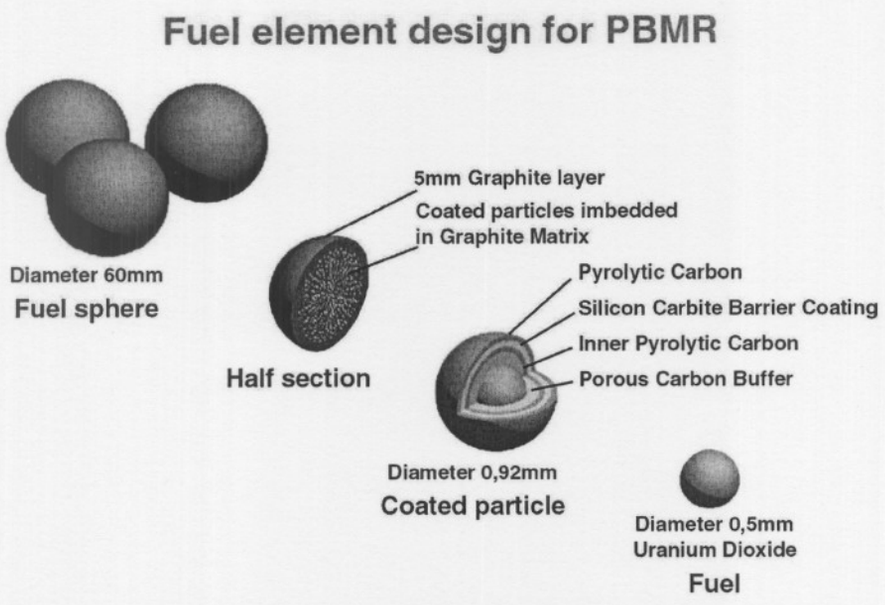

Figure 1.1 Fuel element design for PBMR

Fission products formed during the operation of a high-temperature gas-cooled reactor that are not retained in the uranium oxide kernel, may be released from the fuel spheres as a result of the failure of the TRISO-particle layers during extreme events. Long-lived fission products may also diffuse through intact TRISO-particle layers (albeit very slowly). Additional fission products are formed outside the TRISO-particle due to uranium and thorium contamination of the fuel sphere matrix material.

Fission products are transported (through i.e. diffusion or molecular vapor flow) from their origin, the fission sites, through the fuel materials to the surface of fuel spheres, where they are desorbed into the coolant gas. These released fission products either plate out on the cooler surfaces of the MPS (metallic and halogen fission products) or remain in the coolant gas (noble gases). This poses a risk to operating personnel who may need to access components for maintenance purposes, and increases the decontamination requirements for the plant. During accidents, where coolant gas escapes from the primary circuit into the containment building, fission products can be transported to operations personnel and the general public. Therefore it is imperative to estimate the fission product inventory available in, and released from, the fuel spheres.

At PBMR, fission product release calculations are performed by both legacy and newly developed models and software. Fission product transport through fuel materials is modelled using Fick's law of diffusion [6]. Fission products are divided into two groups, according to the nuclide's half-life. Certain approximations may be made for short-lived isotopes, resulting in the Booth equation [7]. For longer-lived nuclides, time-dependent numerical solutions to the diffusion equation are required. The parameters controlling transport processes were previously measured [8] and are used, along with physical models, in software that is verified and continuously validated [3].

Release calculations for long lived metallic nuclides and iodine-131 are performed under normal operational and accident conditions, primarily using the legacy code GETTER [9]. GETTER is used extensively in reactor analysis at PBMR, to assist in the design of planned irradiation tests, and to evaluate completed irradiation and heat-up experiments. Subroutines are provided for the calculation of fuel burn-up, fuel temperatures, fission and activation product inventories as well as transport and release from a fuel sphere [10]. The calculation considers the life-cycle of a single fuel sphere, given a user-defined irradiation and temperature history. Therefore, numerous reactor conditions can be analysed and particular phenomena can be investigated.

Earlier calculations approximated total core releases using a single representative fuel sphere. Accident analysis became very cumbersome as burn-up corrections had to be applied to specific irradiation histories used. The verification of each calculation was also problematic.

As the thermo-hydraulic and neutronic models improved, it became necessary to analyse fission product release from the reactor core in more detail. Analysis of a sufficiently large set of fuel spheres from the PBMR core was required, in such a way that the core was reliably represented under all expected operating and abnormal events. Furthermore, Monte Carlo-type sensitivity analyses were required to evaluate design limits. This was impossible to perform manually. New calculation models were called for, which could be used on all fuel and reactor parameters for all required fuel and core analyses, with Monte Carlo type sensitivity studies.

1.2 Required outcomes of the project

In order to perform accurate and reproducible fuel and reactor analyses a calculation model is required that will include an automated software product that will utilise the current verified and validated GETTER software. This will allow many different reactor conditions and abnormal operation scenario's to be evaluated [11]. Full Monte Carlo analyses will define ranges in which the calculation is verified for licensing and reactor analyses purposes.

The new software product must be able to perform all analysis requirements of the PBMR reactor design and fuel management (RDFM) group as well as the requirements of the National Nuclear Regulator licensing process. Calculations should be carried out for large numbers of fuel elements with design and operating parameters that can be stochastically varied. This will allow full Monte Carlo sensitivity analyses to be performed for representative cores containing many fuel elements.

Specific modern requirements that are outside the scope of existing software products and calculation models are described below:

- Full core analysis. Determination of fission product release from a representative set of fuel spheres and not only one fuel sphere at a time
- Monte Carlo uncertainty analysis on all uncertain parameters and input values
- Accident conditions, depressurized loss of forced coolant (DLOFC), pressurised loss of forced coolant (PLOFC)
- Fission product release from the reactor core to the containment building.

New theory must be developed to perform stochastic selection of fuel elements and input parameters for sensitivity analyses. Transport of fission products released from the fuel spheres to the containment building must be modelled.

1.3 Current level of knowledge on the problem

The current theories of fission product production and transport in and release from spherical fuel elements are well understood [8]. Applications of these theories in calculation models, especially under abnormal reactor conditions (accidents and operational occurrences are very limited [12]. Early attempts to create computer codes (FIPDIG [13] and later 2-DIFIP [14]) were hampered by computer speed and availability, rendering them with very simplified calculation models. Other reactor codes such as FRESCO [15] were developed that were more advanced but do not fulfil all the requirements necessary for PBMR core analyses.

Due to these inadequacies PBMR decided to acquire the GETTER calculation model. GETTER is currently one of the most advanced software products available to calculate fission product release from spherical fuel, and has the ability to perform almost all PBMR's original calculation requirements. This dissertation briefly describes the development of the original GETTER calculation model, the creation of the FIPREX software and later progression to the FIPREX-GETTER calculation model.

Outside PBMR's RDFM and fuel development groups, as well as a handful of researchers in Germany, China, Japan and the USA, there is very little interest in this field. Current level of knowledge worldwide is severely diminished after the shut down of the German HTR project. In fact, the only serious development program currently in the world is the development work being done at PBMR. This will soon change as the Chinese program is reaching a level of maturity that will require detailed analyses of fission product release from the core under normal and accident conditions [16]. Since 2000 there was also renewed interest in block-fuel reactors in Japan, France and the USA, which should see research and development in these areas expand in the next decade.

The development of FIPREX-GETTER is therefore crucial in advancing our understanding of reactor operation and safety. The publication of the basic theory employed and results of its application at PBMR is consequently very important as very little literature is available.

2 Development of the Calculation Models and Software

PBMR chose the German calculation model, as developed by HRB (HochTemperatur Reaktorbau), as the starting point for developing its own metallic fission product release calculation model. This calculation model was used primarily to evaluate irradiation experiments, to assess heat-up tests, and to determine fission product releases from HTR cores under various reactor conditions.

2.1 First calculation models

Analysis of depressurised loss of forced coolant (DLOFC) events led to the development of FIPREX, a spreadsheet-based utility, which was used to prepare input data for, and to post-process output data from GETTER calculations. Even though FIPREX generated the input data, the GETTER input files were still created by hand.

A typical PBMR core is modeled with several fuel sphere flow channels, each channel divided into axial layers, to yield 70 to 120 core regions. These core regions are used by core neutronics, thermo-hydraulic and fission product release codes to model the core parameters. For a typical PBMR core design containing six flow channels and 90 core regions, 15 to 20 core regions are selected in order to simplify the calculation. The resulting release rates refer to fuel spheres after 6 passes through the core under normal conditions and subsequent DLOFC. Therefore, the inventory of long-lived nuclides is higher than the average fuel sphere inventory in the selected core region. To account for this excess inventory the release rates are multiplied with the ratio of the average inventory divided by the inventory after each of the 6 passes of the spheres in the selected core region. For the shorter-lived halogen fission product ^{131}I the correction factor equals the ratio of the average power density to the power density of the selected core region entirely filled with fuel spheres after a 6-pass history.

The corrected DLOFC release rates per fuel sphere are weighted with the number (3 to 10) of core regions, which are represented by the 15 to 20 selected core regions. The sum of the weighted release rates multiplied with the number of fuel spheres per core region equals the total release rate from all fuel spheres into the gas volume of the core cavern.

It is assumed that the released fission products are homogenously distributed in the gas volume of the core cavern (pebble bed porosity + upper plenum) and that the release out of the core cavern (core release) is driven by the thermal expansion of the remaining helium in the core cavern under ambient pressure. Thus, the core release rate is determined by the inventory of released gaseous fission products in the core cavern multiplied by the fractional expansion rate of the remaining helium mass.

This utility simplified accident calculations, but sensitivity analyses were impractical and analysis was restricted to relatively simple reactor models. A set of requirements for an advanced software product was developed. The result was FIPREX-GETTER, a software product that uses stochastic methods to calculate representative core releases. FIPREX-GETTER is essentially a Monte Carlo driver for the software product GETTER. The methods employed by the code are described in the following sections.

2.2 Automated full core analyses

The PBMR core consists of a bed of spherical fuel elements, simply known as fuel spheres. The fuel spheres are introduced at the top of the core, flow downwards and exit from the base of the core. This flow pattern is modelled using a number of vertical flow channels, each flow channel being axially subdivided into core regions. A typical PBMR core is modelled as 4 to 6 flow channels, each channel consisting of between 10 and 20 axial subdivisions, resulting in 70 to 120 core regions. The axial subdivisions are chosen so that the residence times for fuel spheres in all core regions are equal, typically 8 to 12 days. These core regions, not necessarily of equal volume, are used by the core neutronics, thermo-hydraulic and fission product release codes to model the entire core. Sample core geometry is presented in figure 2.1.

Depending on the chosen fuel-loading scheme, fuel may pass through the core up to 16 times before finally being discarded. The core therefore consists of a random mixture of fuel spheres with different irradiation histories.

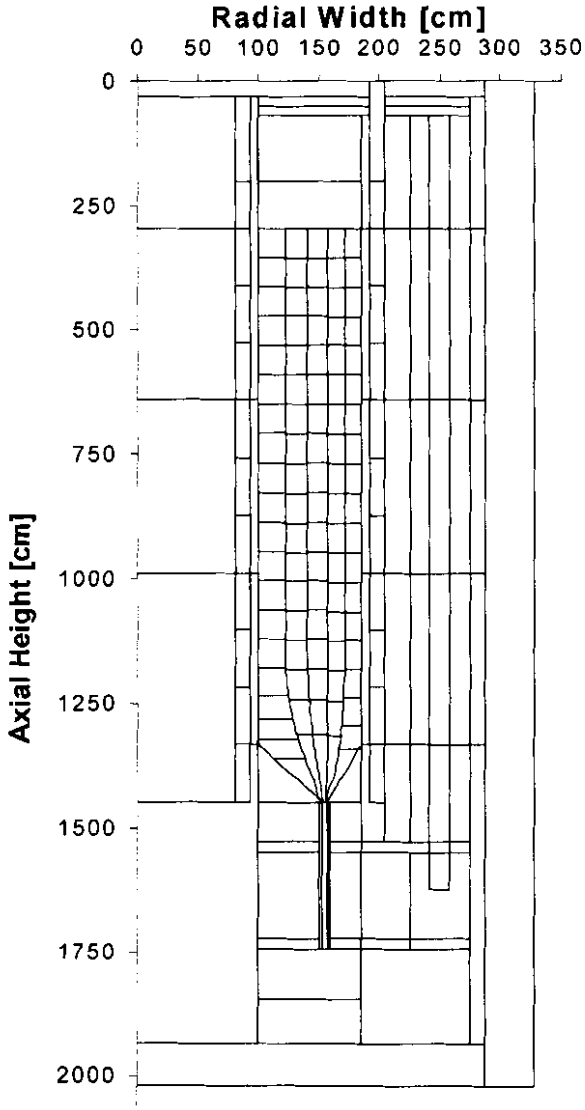

Figure 2.1 Sample PBMR VSOP calculation model layouts

GETTER calculates the fission product release rate for a single fuel sphere for each time-step throughout its residence history in the core. In order to accurately represent the entire core (approximately 450 000 fuel spheres), individual fuel-sphere histories are stochastically sampled and a GETTER calculation performed for each. The results may then be combined using arithmetic averaging and normalization to determine total core release rates.

This implies that GETTER must calculate all the fuel sphere release histories in the core for all the possible irradiation histories, given that the irradiation and temperature conditions in each flow channel of the core are unique. GETTER calculations for each of the 450 000 fuel spheres in the reactor core are not feasible. Furthermore, exact calculation of DLOFC-type accidents would be virtually impossible because the accident can occur at any time-step in a specific fuel sphere's irradiation history. The exact calculation of such an accident would then require that in the order of 35 million GETTER calculations to be performed.

The associated computational requirements initially seemed to make this method of calculation unfeasible. However, it was found that significantly smaller sample sizes give satisfactory statistical convergence. Multiple independent calculations using sample sizes of 10 000 fuel spheres, for example, showed a variance in calculated release rates of less than 1%.

For the simple case of steady-state analysis (nominal operating conditions), a fresh fuel sphere with a known initial TRISO-particle failure fraction is introduced at the top of the core and its movement tracked. With each changing position in the core the temperatures and neutron fluxes are updated and, subsequently, the updated TRISO-particle failure fraction is calculated. Steady-state spatial temperature and flux values are obtained using results from a diffusion code (VSOP [17] or TINTE [18]) calculation, mapped to the predefined flow regions. The randomly sampled history is then passed to GETTER, which calculates the expected release rates. The model is shown diagrammatically in figure 2.2. This process is repeated for a user-defined number of fuel spheres (N_S) until such time as the core has been adequately represented.

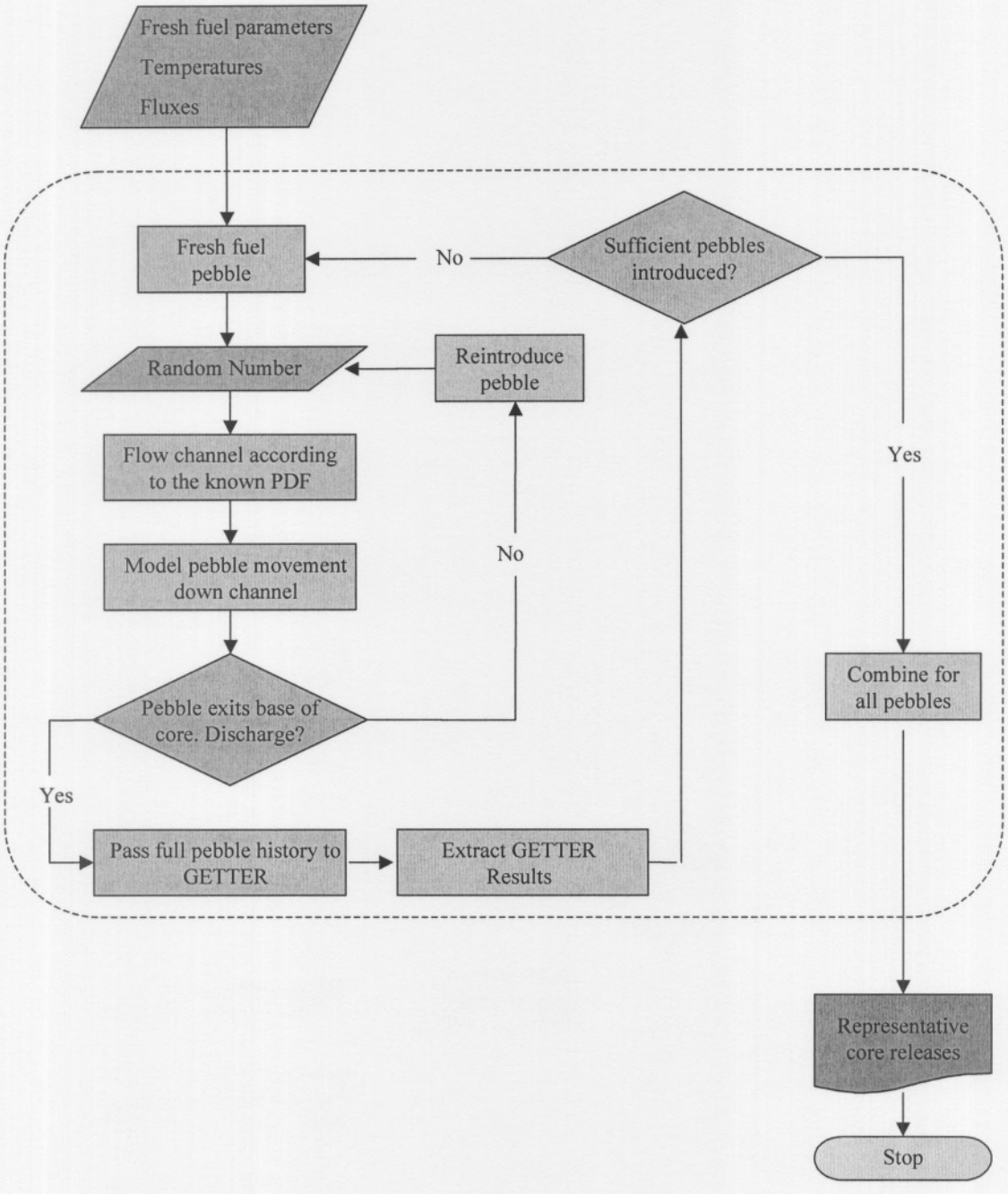

Figure 2.2 Flow diagram of FIPREX-GETTER for nominal steady state analysis

The expected core release rate is then calculated as the arithmetic average of all samples, normalized to the total fuel sphere inventory (N_C) of the core.

$$\left(\frac{dn}{dt}\right)_{core} = \frac{N_C}{N_S}\sum_{i=1}^{N_S}\left(\frac{dn}{dt}\right)_i \tag{1}$$

The random fuel sphere history is selected by assigning a random core pass history based on the probability of a fuel sphere passing through each flow channel. This probability is dependent on the volume of the core channel and the speed at which fuel spheres flow downwards. All core regions have an equal residence time; this probability is therefore directly related to the volume of the uppermost region of each flow channel.

For transient accident analysis, a time-of-accident is chosen randomly upon initial introduction of the fuel sphere. As with the steady-state case, the fuel sphere is repeatedly passed through the core until the chosen time-of-accident is reached. Thereafter the flow of fuel through the core is assumed to cease. For the duration of the accident, the time-dependent temperature and neutron flux value experienced by the fuel sphere in its region of residence are calculated using time-dependent spatial data obtained from a diffusion calculation (e.g. TINTE). Fuel temperatures for each time interval in the accident event are used to calculate a time dependent TRISO-particle failure fraction. GETTER is executed using the generated history data, and the expected release rates calculated. This calculation is repeated for multiple fuel spheres until such time as the core has been adequately represented. The model is shown diagrammatically in figure 2.3. As in the steady-state case, the results for all samples are combined to give time-dependent release rates for the full core, for the duration of the accident.

$$n_{core}(t) = \frac{N_C}{N_S}\sum_{i=1}^{N_S} n_i(t) \tag{2}$$

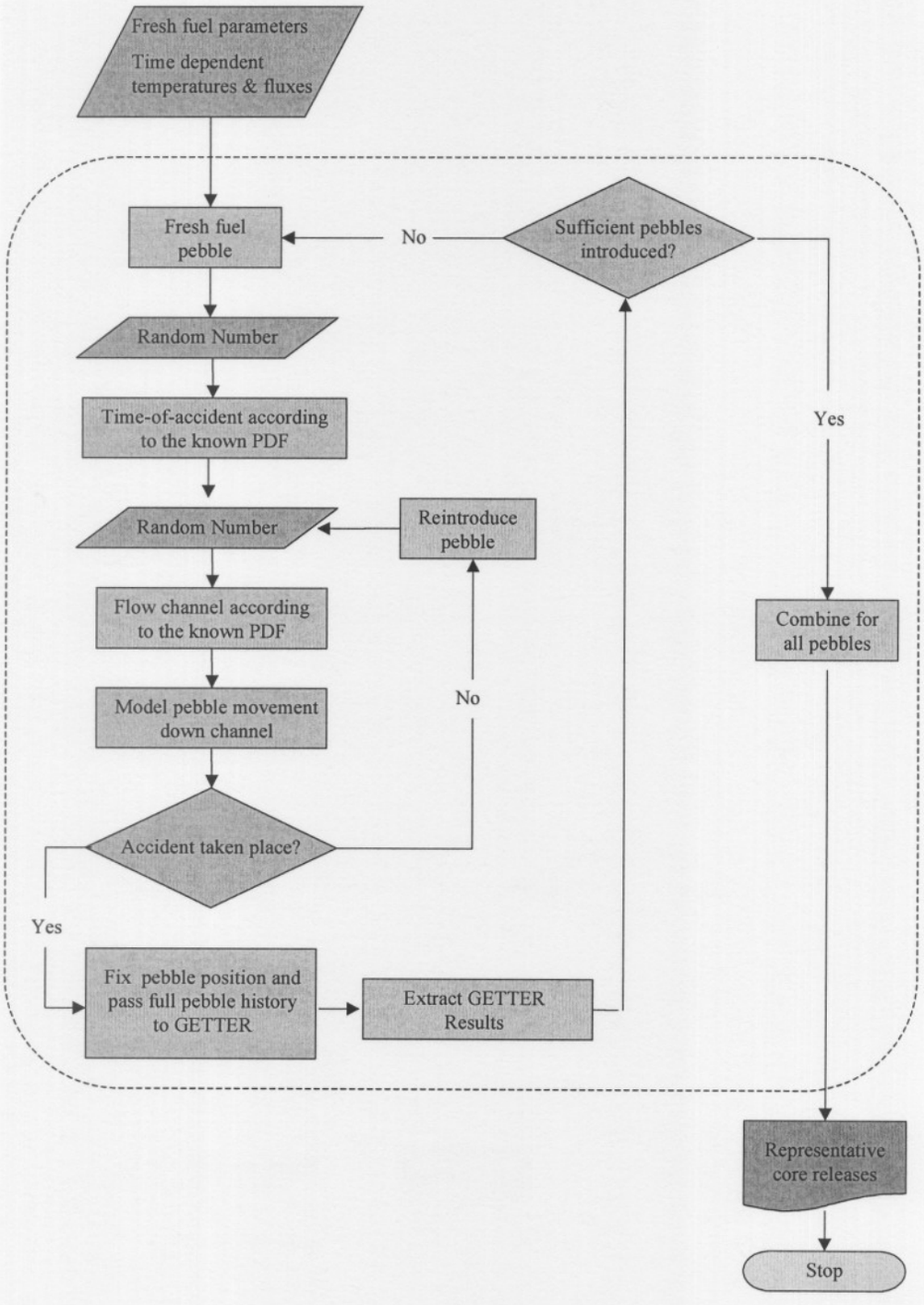

Figure 2.3 Flow diagram of FIPREX-GETTER for nominal accident analysis

2.3 Uncertainty analyses

Input parameters, values and data sets that include uncertainty in their derivation are investigated to determine a design value for fission product release under the specified operating conditions. Uncertain parameters and values can be categorized and described as follows:

- The diffusion coefficients describing metallic fission product transport through the fuel materials were derived from irradiation experiments conducted on TRISO-particles, fuel compacts and complete fuel spheres. Due to uncertainties in the measurements taken during irradiation and in irradiation conditions, uncertainty factors of between two and eight were suggested for metallic diffusion constants.

- The fuel specification allows maximum values for the uncontained uranium fraction of 6×10^{-5} and the thorium contamination of 0.4 mg Th/FS (thorium per fuel sphere). This defines upper limits for the failed particle fraction, the uranium contamination and the thorium contamination of 5.6×10^{-5}, 4.0×10^{-6} and 6.0×10^{-6} (effective) respectively.

- The uncertainty in the sorption isotherm was calculated by assuming a variation in the partial pressures by a factor of four.

- For accident analysis full neutronic and thermo hydraulic Monte Carlo sensitivity studies were carried out using the neutron diffusion code, TINTE [18]. Monte Carlo samples from these studies are used directly in FIPREX-GETTER. At present, full Monte Carlo analyses have not been performed for steady state analyses, and therefore only TINTE results are used. For steady-state operation, temperatures passed to FIPREX-GETTER from VSOP are conservatively assumed to be 50°C above the calculated values.

- The statistical evaluation of German irradiation experiments with TRISO UO_2 particles showed that due to the restricted sample size (Poisson distribution), growing failure fractions cannot be excluded at burn-ups above 5% Fissions per Initial Metal Atoms (FIMA). The uncertainty in the failure rate under excessive temperature is derived from statistical evaluations of experimentally measured failure fractions. These expected curves and their uncertainty ranges were modelled and are used in design calculations [19].

- GETTER, using temperature and neutron flux data from the neutron diffusion codes TINTE and VSOP, calculates the fuel sphere power distribution. No additional uncertainties are employed other than that inherent in the sampled input data.

The uncertainties can be divided into two groups. Firstly, thermo-hydraulic and neutronic uncertainties are accounted for by using sampled temperature and neutron flux data. This sampled data is obtained from separate Monte Carlo analyses using the neutron diffusion code TINTE. The second group consists of material parameters and diffusion model uncertainties. For each parameter, a suitable probability distribution is chosen and values are randomly sampled. In most cases the distributions are highly skewed and have a known minimum value. For these parameters, the Weibull distribution was chosen. Figure 2.4 shows the approximated uncertainty distribution for strontium's diffusion coefficient in pyrocarbon (PyC). Both the probability distribution function (pdf) and the cumulative distribution function (cdf) are shown.

After the Monte Carlo calculations are done, the sampled output data from the FIPREX-GETTER calculations are plotted on a histogram and, using this, the upper 95% confidence limit is determined. The result is used for comparisons with design limits.

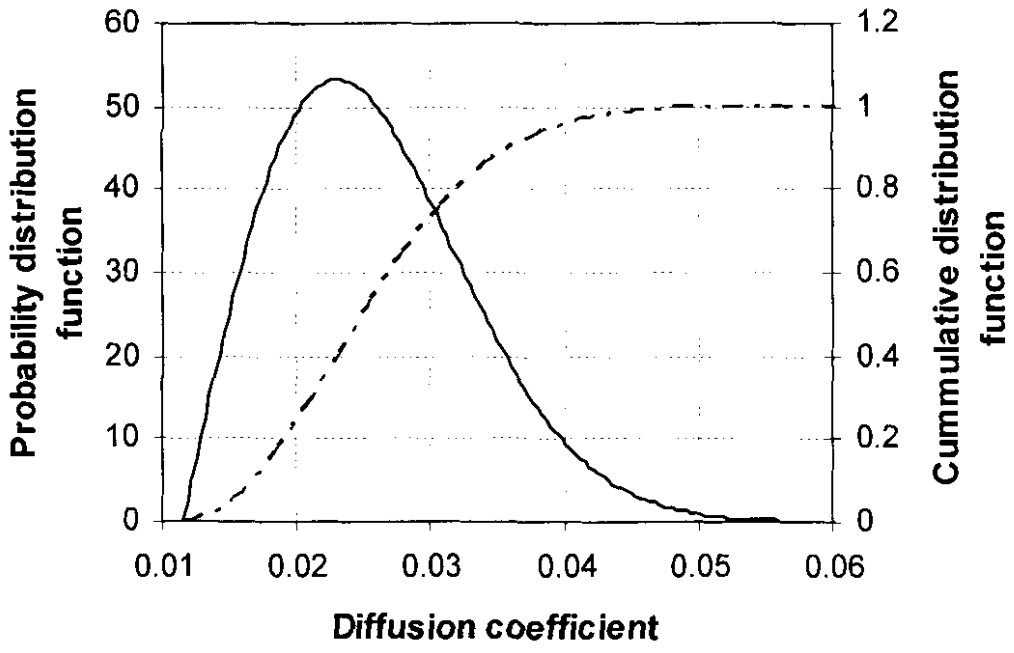

Figure 2.4 Probability distribution for Strontium's PyC diffusion coefficient

Figure 2.5 shows diagrammatically the sequence of operation of FIPREX-GETTER for a full Monte Carlo sensitivity analysis. A further approximation is made for Monte Carlo type sensitivity analyses. In this case, the large variance in single fuel sphere release rates makes it difficult to extract meaningful relationships from the data. It is therefore necessary to calculate representative core releases for each Monte Carlo sample. This would require the sampling of 10 000 fuel spheres per Monte Carlo sample, which amounts to in excess of a million samples for a single Monte Carlo study. This requirement is currently overcome by selecting a relatively small subset (~ 100) of fuel spheres. This subset is chosen so that it closely reproduces the nominal results for the full core calculation. While this method introduces some error in the nominal core release, the resulting probability distribution shape is preserved and accurate sensitivity studies may still be carried out using this method.

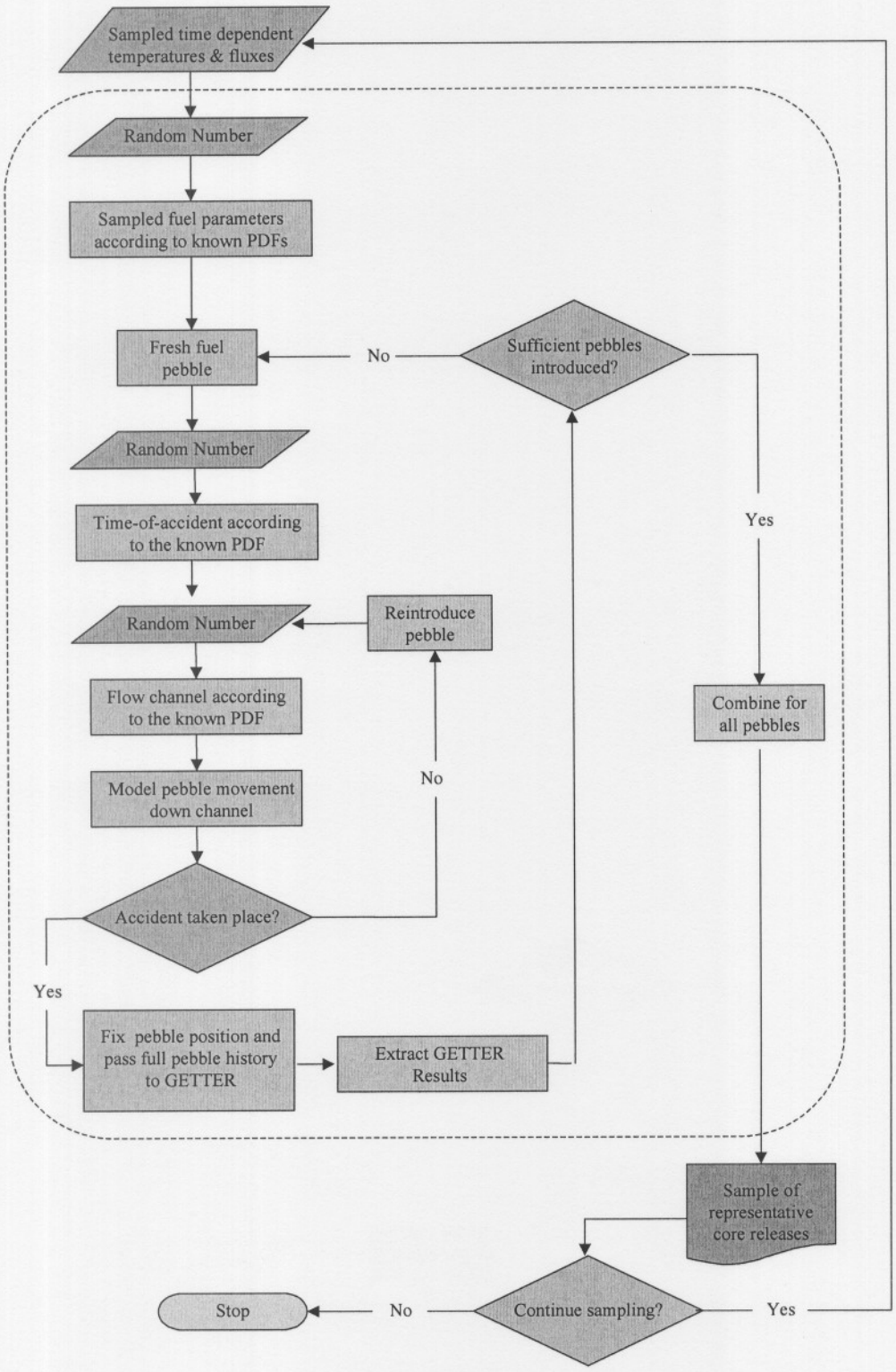

Figure 2.5 Flow Diagram of FIPREX-GETTER for Monte Carlo Accident Analysis

2.4 Fission product transport from the reactor core

GETTER calculates the fission product release from fuel spheres into the coolant stream, which subsequently transports the fission products from the core. Under DLOFC conditions, when depressurisation is complete, there is no forced coolant flow to remove released fission products from the core. Transport mechanisms are therefore limited to stationary gas expansion, diffusion and temperature-induced convective flows. Preliminary calculations have shown that, given the expected types and sizes of breaks occurring near the reactor pressure vessel, fission product transport from the core is dominated by gas expansion only.

2.4.1 Gas expansion coefficient (GE)

During a DLOFC event, the increased temperature of the fuel spheres and, subsequently, the surrounding coolant gas results in an expansion of the gases within the core. The sudden drop in coolant mass flow rate causes this increase in fuel temperatures, while the radioactive decay of fission products continues to produce significant heat in the fuel spheres. At constant pressure the coolant gas expands and flows from the reactor vessel to the containment building through the break opening. Fission products are transported from the fuel spheres into the coolant and from there through the break opening to the containment building by the expanding coolant gas. In calculating this transport mechanism the following assumptions are made:

- The gas expands according to the ideal gas law.
- The pressure in the core immediately reverts to and remains constant at atmospheric pressure after the initial pipe breakage. This assumption is applicable only to large and medium break events.
- Fission products are assumed to be evenly distributed in the coolant gas.
- Expansion within the above-core plenum has a minimal effect on fission product transport in the current calculation model and is therefore currently ignored.

From the ideal gas law:

$$P = \rho RT \tag{3}$$

Or alternatively using specific volume v:

$$v = \frac{RT}{P} \tag{4}$$

Given an initial mass of helium m_0 within a closed volume, the time-dependent volume occupied by the gas is:

$$V(t) = m_0 v(t) \tag{5}$$

We now define the gas expansion coefficient as:

$$GE(t) = \frac{V(t)}{V_0} = \frac{m_0 v(t)}{m_0 v_0} = \frac{\frac{RT(t)}{P}}{\frac{RT_0}{P}} = \frac{T(t)}{T_0} \tag{6}$$

We now define the average/mean gas expansion coefficient as the volume weighted average gas expansion coefficient of all core and plenum regions.

$$\bar{GE} = \frac{\int GE dV}{\int dV} \tag{7}$$

The core is discretized into regions, including the plenum region. The integral may now be written as a sum.

$$\begin{aligned} \bar{GE}(t) &= \frac{GE_{plenum}(t)V_{plenum} + GE_{rel}(t)V_{rel} + \sum_{i=1}^{nRegions} GE_i(t)V_i}{V_{core} + V_{rel} + V_{plenum}} \\ &= \frac{\frac{T_{plenum}(t)}{T_{plenum,0}}V_{plenum} + \frac{T_{rel}(t)}{T_{rel,0}}V_{rel} + \sum_{i=1}^{nRegions} \frac{T_i}{T_{i,0}}(t)V_i}{V_{core} + V_{rel} + V_{plenum}} \end{aligned} \tag{8}$$

Where

$$T_{plenum}(t) = T_{plenum,0} \tag{9}$$

Using discrete time intervals 0 through τ, the volume weighted average gas expansion coefficient reduces to:

$$\bar{GE}_{\tau} = \frac{\sum_{i=1}^{nRegions} \frac{V_i T_{\tau,i}}{T_{0,i}} + V_{plenum}}{V_{core} + V_{plenum}} \tag{10}$$

A typical gas expansion curve following DLOFC is shown in figure 2.6. From this figure it may be seen that the gas expansion reaches a maximum after ~36 hours, corresponding to the maximum fuel temperature for the event. This point represents the final gas expansion release to the containment building. Following this, the core begins to cool and the gas expansion reverses.

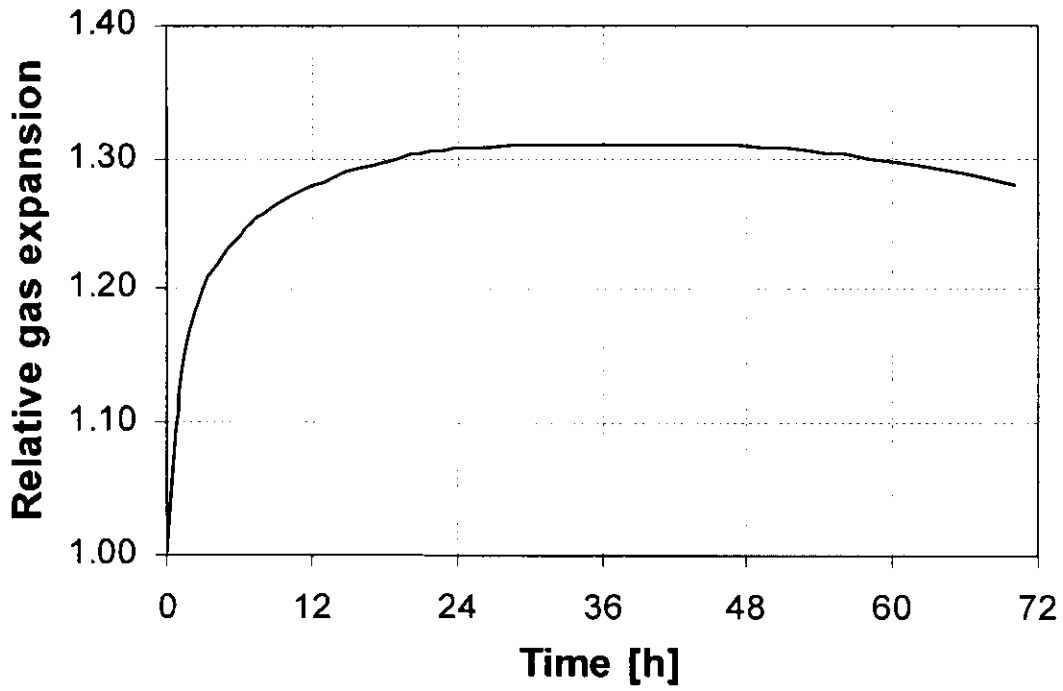

Figure 2.6 Relative gas expansion in the core cavern after a DLOFC event

2.4.2 Time step total core release (TCR)

We define the time step total core release as the total number of atoms of fission product released from the core structure over a set time interval. This is dependent on the gas expansion during the time interval.

$$TCR = \frac{V - V_0}{V_0} N \tag{11}$$

where N is the number of atoms of a given fission product originally in volume V_0. We introduce the fission product inventory (See 2.4.3) and gas expansion definition.

$$TCR = \left(\frac{GE}{GE_0} - 1 \right) FPI \tag{12}$$

Using discrete time intervals.

$$TCR_\tau = \left(\frac{GE_\tau}{GE_{\tau-1}} - 1 \right) \frac{FPI_\tau + FPI_{\tau-1}}{2} \tag{13}$$

2.4.3 Fission product inventories (FPI)

The fission product inventory is the total number of free fission product atoms in the coolant gas already released from the fuel elements, not yet decayed nor released from the core structure, and available to be transported from the core region by expanding coolant gas. Fission products are released from fuel elements at a rate R atoms/s. At the same time fission products undergo radioactive decay, and are released from the core region at TCR atoms per time step (See 2.4.2). Radioactive decay of the fission product inventory and newly released atoms can be described as follows:

$$FPI = FPI_0 e^{-\lambda (t - t_0)} + \frac{R}{\lambda} \left(1 - e^{-\lambda (t - t_0)} \right) \tag{14}$$

Including the release of fission products to the containment building through the break opening FPI becomes:

$$FPI = FPI_0 e^{-\lambda (t-t_0)} + \frac{R}{\lambda}\left(1 - e^{-\lambda (t-t_0)}\right) - TCR \tag{15}$$

Using discrete time intervals and release rates over the entire core of N_C fuel elements

$$FPI_\tau = \frac{R_\tau + R_{\tau-1}}{2\lambda} N_C \left(1 - e^{-\lambda (t_\tau - t_{\tau-1})}\right) + FPI_{\tau-1} \quad e^{-\lambda (t_\tau - t_{\tau-1})} - TCR_{\tau-1} \quad [atoms] \tag{16}$$

2.4.4 Accumulated core release (ACR)

The accumulated core release is defined as the total number of atoms of a fission product released to the surrounding. If assumed constant over a time period, fission products escape from the core at a rate of CCR (core cavern release rate) atoms/s.

$$CCR = \frac{TCR}{t - t_0} \tag{17}$$

Using discrete time intervals,

$$ACR_\tau = \frac{CCR_\tau}{\lambda}\left(1 - e^{-\lambda t}\right) + ACR_{\tau-1} \quad e^{-\lambda t} \tag{18}$$

3 Verification and Validation

As with all new software products and calculation models outstanding issues always exist. Outstanding issues have been identified and these are listed in the respective verification and validation (V&V) plans for FIPREX-GETTER and for the calculation model. These outstanding issues are for the probability distributions of input parameters, the relatively small sample size currently used for Monte Carlo analyses, and the validity of the simple gas expansion approximation currently used for transport from the core.

Uncertainties in the thermo-hydraulic and neutron flux input data are calculated by Monte Carlo analyses of the core. These analyses require the development of Monte Carlo analysis techniques for legacy software products such as VSOP and TINTE, which are substantial projects in themselves. TINTE uncertainty analyses are currently at an advanced stage, with the development of the FIPREX-TINTE calculation model. However, VSOP analyses are currently limited to single analyses of specific parameters and phenomena. Therefore, uncertainties in core temperatures during normal operation are conservatively estimated for FIPREX-GETTER analyses.

Fuel parameter uncertainties are based on experimental results and measurements obtained during the German fuel development program. It is assumed that the PBMR fuel will be equivalent to or better than German proof test fuel [5]. Actual PBMR fuel performance data will only be available once fuel irradiation testing and post irradiation examination (PIE) is completed.

At present little attention has been paid to the optimal choice of samples. More specifically, advanced random sampling techniques have not been implemented, even though they could improve convergence significantly. Relatively large sample sets are therefore currently required for all nominal release calculations.

Coolant gas expansion during post depressurization core heat-up is currently calculated using a simplified model. Validation of this model will only be completed when detailed results are available, using more advanced thermo-hydraulic software to calculate the heat and mass transfer behaviour of the coolant gas under such conditions. FIPREX-GETTER currently has the added functionality of being able to read gas expansion data from other sources and being able to apply this to the calculation, if so required, and is therefore not limited to this simplified model.

All other models and equations used by FIPREX-GETTER have been verified in detail. Development of the software and calculation model is ongoing and more issues and questions will arise. All future issues will be dealt with in the current quality control framework.

4 Application in PBMR Reactor Analyses

The FIPREX-GETTER calculation model has been applied to various reactor conditions for selected fission products. Based on their radiological impact during normal operation cesium isotopes ^{137}Cs and ^{134}Cs, silver isotopes ^{110m}Ag and ^{111}Ag, ^{90}Sr and the halogen isotope ^{131}I were selected for in-depth analyses. Short-lived gaseous fission products are well calculated by the NOBLEG calculation model [3], with the exception of ^{85}Kr that is also calculated with the FIPREX-GETTER calculation model specifically for the used and spent fuel tank cases.

Several examples of FIPREX-GETTER applications are discussed in this section.

4.1 ^{110m}Ag-110m release during reactor start-up with fresh fuel

One of the important aspects to take into account in the design and maintenance of high temperature reactors with high outlet gas temperatures is the release rates of silver fission and activation products from fuel spheres. ^{110m}Ag, which tends to plate out on the cooler surfaces within the turbine and recuperator, can be a radiation hazard during planned maintenance. It is thus important to model silver releases and plate out distributions in detail. Because of the relatively large uncertainties in fuel performance and fission product release rates, conservative values are used to estimate radiation doses in the power conversion unit (PCU). The first PBMR module will be a demonstration unit, and it will be necessary to evaluate component performances regularly during the first years of operation.

The start-up ^{110m}Ag release and eventual accumulation in the PCU was investigated with FIPREX-GETTER. The 95% design results from FIPREX-GETTER analyses on a sample PBMR core are presented in figure 4.1.

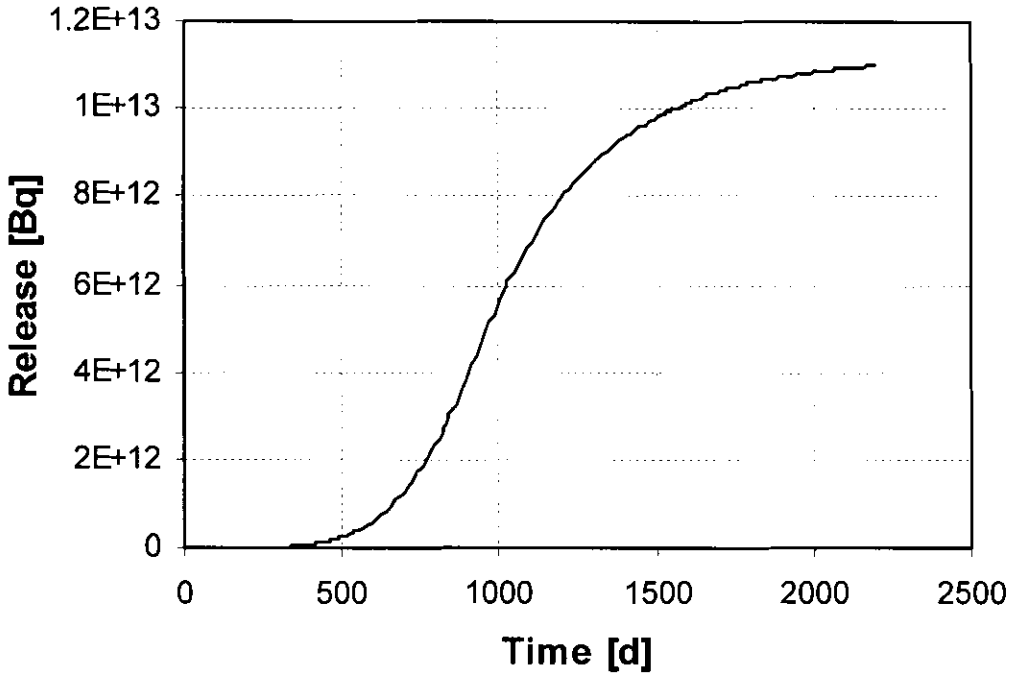

Figure 4.1 ^{110m}Ag release inventory in the PCU

The ^{110m}Ag inventory climbs almost exponentially at the beginning of reactor operation until the core fuel inventory matures, after about 1 000 d. Release and decay of ^{110m}Ag grows slowly into equilibrium, and after 2 500 d more than 99% of the 36-year inventory is reached. Release at the beginning of plant operation is very slow as only fresh fuel will be used at start-up. Fission product inventories of long-lived fission products are very small, plutonium breeding has just begun (^{239}Pu is the main source of ^{109}Ag, the precursor to ^{110m}Ag), and fission products have just started their long diffusion journey through the fuel layers. After one year in operation at full power, the released ^{110m}Ag inventory plated out on the turbine is more than 200 times lower than 36-year levels. After 2 y the inventory is still ten times lower. Requirements for the handling and maintenance of components during early inspection are therefore easily evaluated by FIPREX-GETTER.

The Monte Carlo release uncertainty distribution is shown in Figure 4.2. This analysis is conservative in that the temperature is not sampled, but rather increased by a maximum of 50 °C for the calculation. The resulting distribution is approximately a Weibull distribution - a result of the choice of uncertainty distributions for input parameters. The upper 95th-percentile result is accepted as the design value. For this specific design and parameter uncertainties, the design value exceeds the best estimate by a factor of 16. This large design factor is due to a high sensitivity of the silver transport mechanism through SiC. Similar analyses of other nuclides yielded design factors of 4, 5 and 8 for caesium, strontium and iodine respectively.

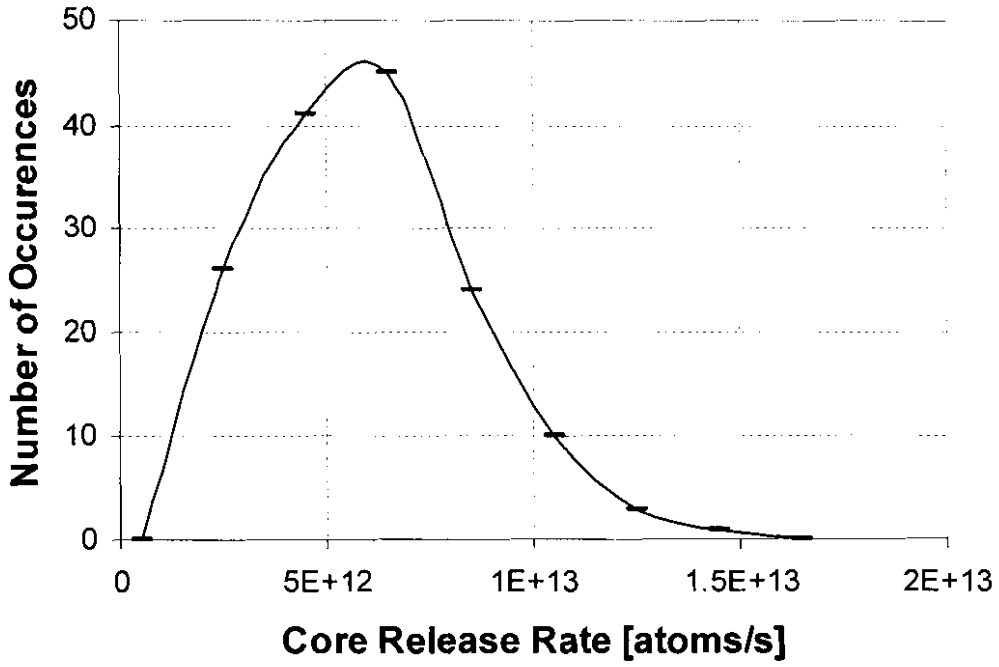

Figure 4.2 ^{110m}Ag release rate uncertainty distribution

4.2 Application in accident event analyses

FIPREX-GETTER has been used for a number of accident and transient analyses, including:

- Depressurized loss of forced cooling (DLOFC) accident [18].
- Pressurized loss of forced cooling (PLOFC) accident [18].
- Seismic events [20].

These events were modelled in detail with TINTE where all feedback effects are taken into account. In each event the core is sub-critical soon after the event has started (due to inherent feedback effects). Therefore, no contributions from additional fission events are assumed in the FIPREX-GETTER analyses. For the case of loss-of-forced-cooling accidents, there is significantly reduced coolant flow, and the decay heat within the core causes fuel temperatures to rise. After some time, the decay heat is sufficiently reduced for fuel temperatures to begin to drop. The main modes of heat transport for such calculation types are conduction and radiation to the environment.

4.3 Fission product release during a medium break DLOFC event

A typical 400 MW PBMR core design has been analyzed for a medium break DLOFC event, to present the FIPREX-GETTER calculation model's abilities.

Three key nuclides have been identified [21]:

1) ^{131}I

2) ^{111}Ag

3) ^{137}Cs

The three selected fission products present more than 80 % of the expected radiological impact of a DLOFC event.

4.3.1 ^{131}I release during a medium break DLOFC event

For the first few weeks of a DLOFC type accident event, airborne radiological risk is dominated by the halogen fission products ^{131}I and ^{133}I. Releases for relatively short-lived iodine during normal operation are normally calculated with NOBLEG [3]. NOBLEG however lacks the ability to calculate the transient behaviour of fission products. Therefore the GETTER calculation model had to be adapted to allow evaluations of ^{131}I release and transport from the fuel spheres to the containment building to be carried out using FIPREX-GETTER. Kernel and matrix diffusion constants of iodine at temperatures below 1150 °C were adjusted so that the release rate under normal operation conditions agrees with the reference result of the NOBLEG calculation with the same temperature dependence (equal activation energy of diffusion constants).

The diffusion constants in pyrocarbon and SiC were set sufficiently low so that these layers act as impermeable barriers for iodine (factor 100 and 1000 below standard cesium values). For iodine at temperatures above 1150 °C, 2-branch UO2 kernel diffusion constants are used [8]. For the matrix diffusion constant a relatively high activation energy was chosen so that above 1150 °C the contamination induced ^{131}I-atoms are rapidly degassed from the matrix material. Similarly, for the metal fission products standard sorption isotherms of the A3 matrix material are used. For iodine the sorption isotherm was set so high that the evaporation from the fuel sphere surface does not control the release (factor 100 higher than the cesium isotherm).

The maximum total release rate from all fuel spheres in the core is attained after 36 hours DLOFC duration. This value exceeds the normal operation release rate by a factor of 300. This factor is reduced to 3.5 for the release rates from the core cavern due to the limited thermal expansion fraction of the remaining gas in the core. Calculated ^{131}I releases from the fuel are presented in figure 4.3. Less than 1% of the ^{131}I released from the fuel spheres is released from the core cavern. Of the available ^{131}I inventory in the fuel spheres, less than a factor of 1.2×10^{-7} is released during a DLOFC event.

These factors demonstrate the high retention capability of the fuel spheres up to temperatures of 1 600 °C, and the effective barrier of the core structure under DLOFC conditions. It can be seen that after 36 h, no more atoms are released from the core cavern due to the reverse gas flow into the core, and the decline in the number of iodine atoms over time due to radioactive decay. Breathing effects of the reactor building and other variations in core pressure after gas pressure reached equilibrium after 36 hours must still be evaluated.

^{131}I release rates from the fuel spheres of channel 1 are shown in figure 4.4. For region 1/7 (the hottest region in the whole core), two local maxima are observed. The first maximum (15 hrs) is due to outgassing of ^{131}I, which was bound in the matrix material. The second maximum (36 hours) is due to release from failed coated particles. For region 1/4 another small initial maximum is noticed at 5 hours, which is caused by the ^{131}I atoms produced by uranium contamination of the fuel sphere shell near to the sphere surface.

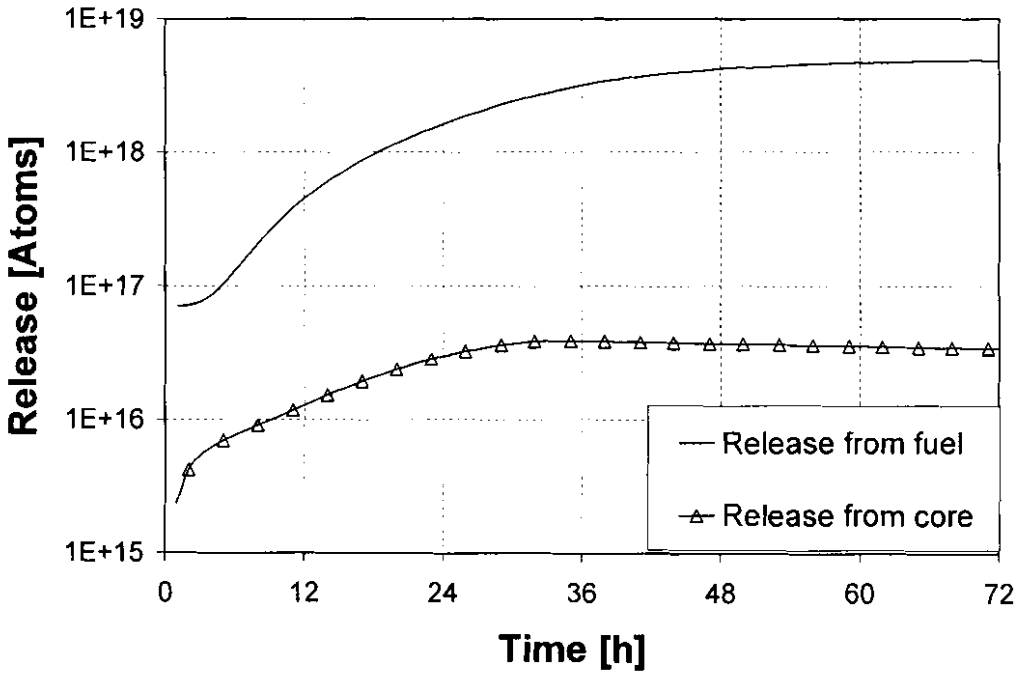

Figure 4.3 ^{131}I release from fuel and core structure

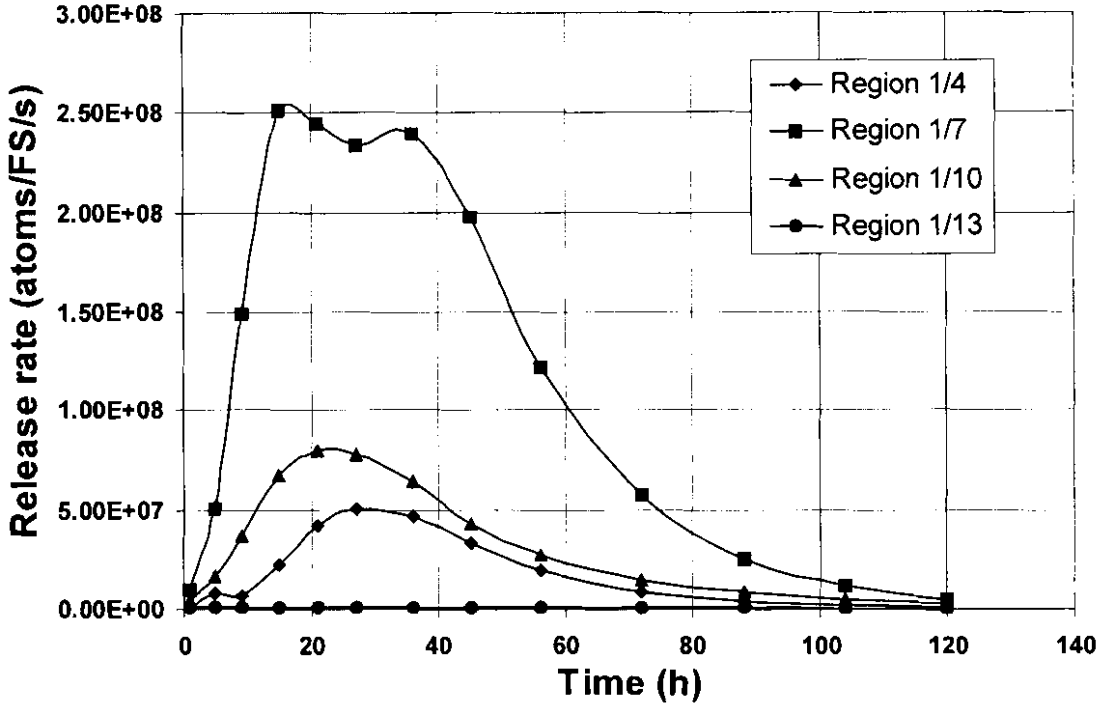

Figure 4.4 ^{131}I Release rate from fuel spheres of channel 1

4.3.2 ^{111}Ag release during a medium break DLOFC event

Interestingly, the ^{111}Ag release rate curve for channel 1, displayed in figure 4.5, looks quite different. The first smaller maximum observed in figure 4.5 is due to uranium and thorium contamination in the matrix material and the outer pyrocarbon layer. Silver fission products formed in these layers are released first. Silver fission products formed in the fuel kernel are delayed for about thirty hours as it diffuses through the SiC layer. This 'delayed release' of silver limits the release from the core structure significantly, as the bulk of the silver is only released once the core gas expansion has reversed (figure 2.6).

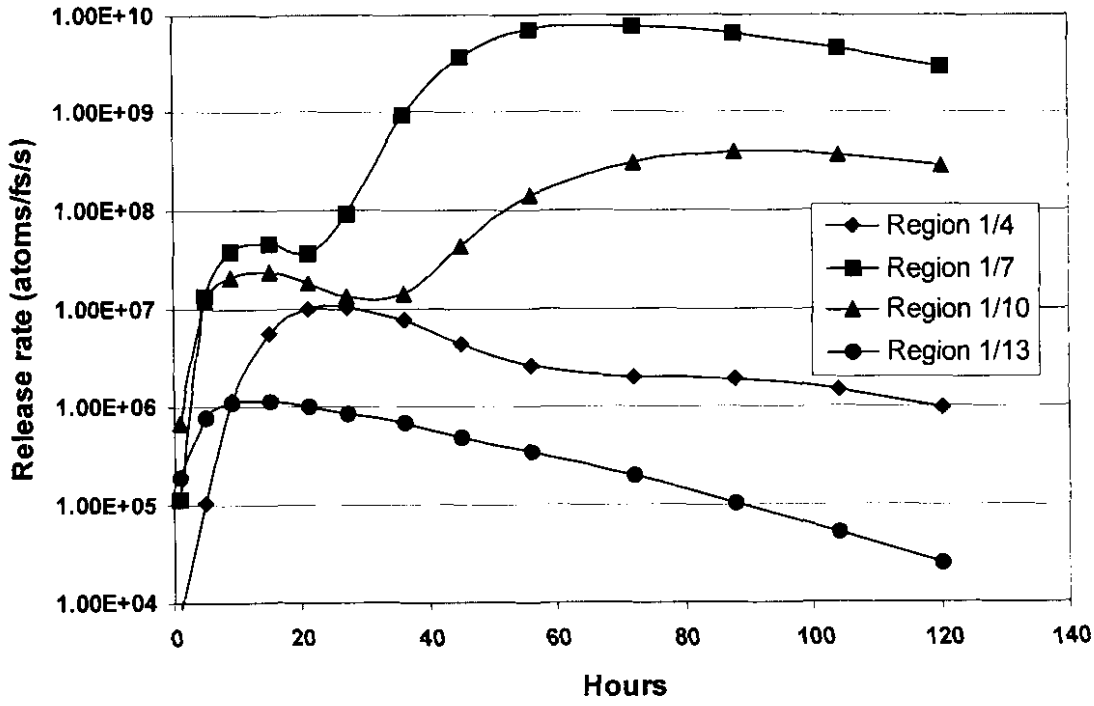

Figure 4.5 ^{111}Ag Release rate from fuel spheres of channel 1

4.3.3 ^{137}Cs release during a medium break DLOFC event

Calculated ^{137}Cs release rates from fuel spheres in four selected core regions of channel 1 are depicted versus time in figure 4.6. The highest release rate in the core occurs after 36 hours in core region 1/7 with its maximum temperature of 1506 °C. This maximum release rate (1.8 x10^{10} atoms/FS/s) exceeds the maxima in channels 2; 3; 4; 5 and 6 by factors 1.2; 1.8; 3.2; 8.1 and 32, respectively. About 50% of the release from core region 1/7 is caused by the transient induced particle failure. Because this fraction is so large we see very smooth curves in figure 4.6. The maxima observed in ^{131}I and ^{111}Ag release rate curves are absent.

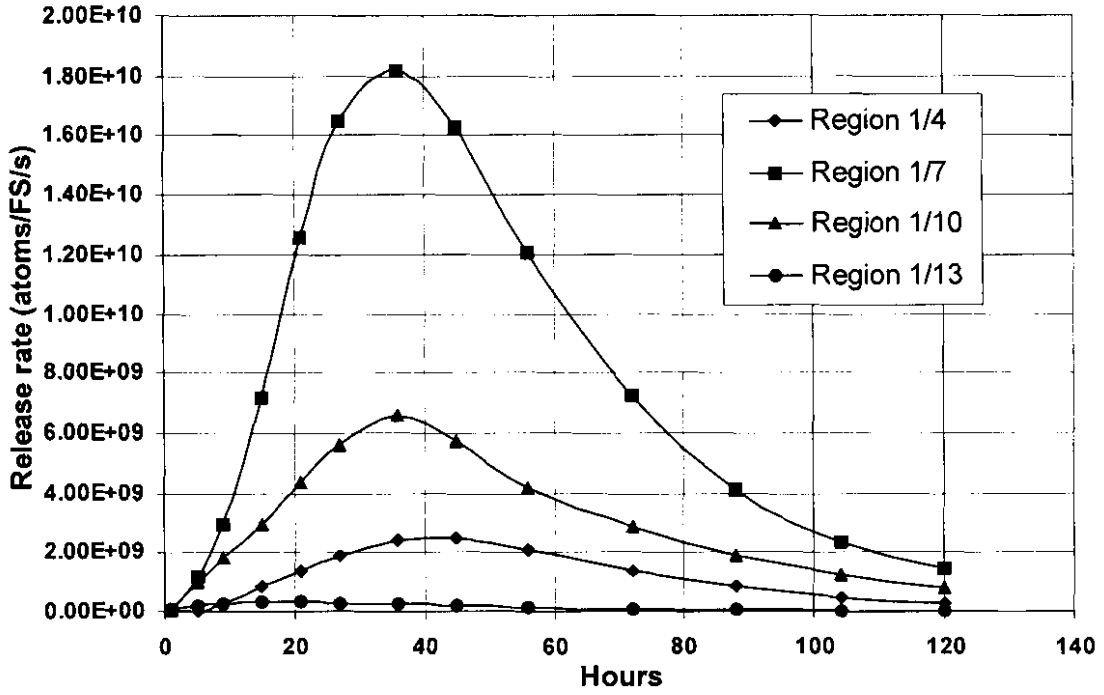

Figure 4.6 ^{137}Cs Release rate from fuel spheres of channel 1

4.4 Ag-111 release during small break DLOFC events

For cases where small breaks cause longer depressurization times, analyses with FIPREX-GETTER were performed for three depressurization times, namely 24, 48 and 72 h. In these cases coolant gas transports fission products from the core cavern to the containment building during depressurization. Per hour, approximately 18.1%, 8.7% and 5.7% of the available core coolant gas inventory is released to the containment during the blow-down phase of the 24, 48 and 72 h events respectively. Figure 4.7 shows the cumulative fraction of gas released from the core, expressed in terms of a "gas expansion factor" for the cases.The gas expansion factor is simply the inverse of the fractional amount of coolant gas remaining of the coolant gas available at the beginning of the event.

Also shown on this graph, for comparison purposes, is the gas expansion factor for the medium-break calculation (exactly the same as in the small break cases, a significantly greater flow of gas exists to transport fission products out of the core due to the slow depressurization. For this reason, releases to the containment building are significantly greater than for the medium break case, despite lower fuel temperatures and fuel sphere release rates.

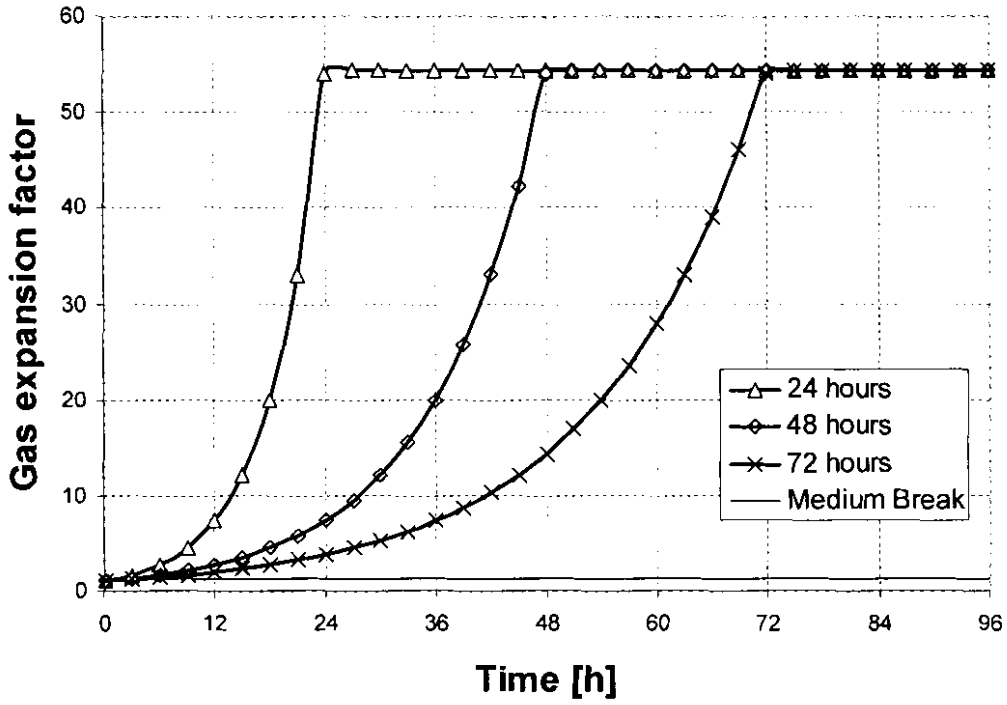

Figure 4.7 Gas expansion during small and medium break events

Silver releases are highly dependent on temperature and depressurization time. The total Ag-111 release from fuel spheres for the small and medium break cases is shown in figure 4.8. This shows that the fission product inventory released from the fuel spheres during small break events is significantly lower than for medium break conditions. A sharp secondary increase in releases is seen for all cases after 24 h. This represents delayed Ag-111 release from intact TRISO-particles. Elevated fuel temperatures during the DLOFC allow substantial diffusion of Ag-111 fission products, initially retained in the fuel kernel, through the SiC layers.

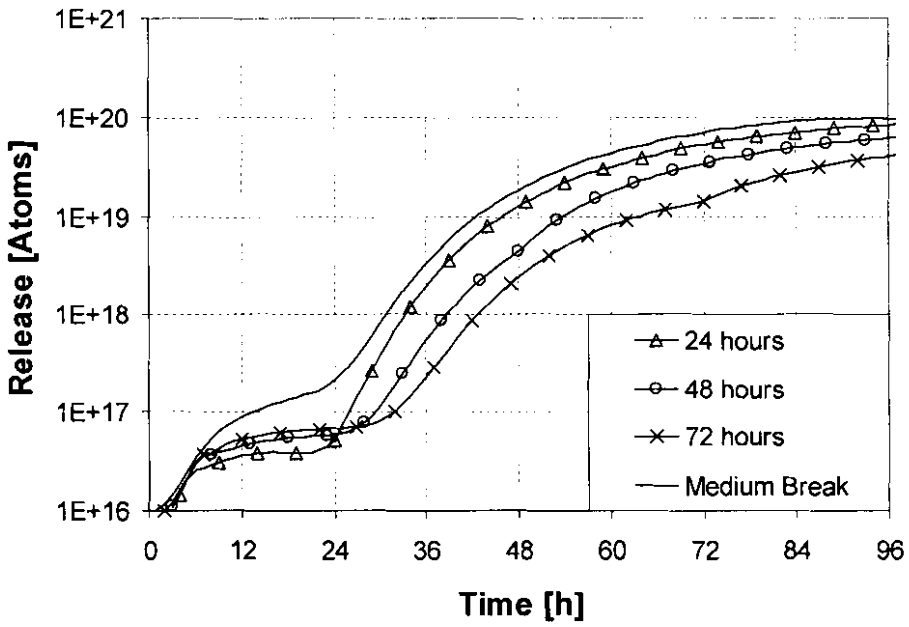

Figure 4.8 Ag-111 releases from fuel spheres during small and medium break events

Figure 4.9 shows Ag-111 release to the containment building. The small break releases are factors of 14, 240 and 1200 greater than for the medium break case. After 24 h, gas expansion factors for the 48 and 72 h cases are still increasing and, as a result, significant delayed releases from intact TRISO-particles are released into the containment building. Of the total fuel-released core inventory, 0.21%, 5.2% and 43.2% are released to the containment for the three small break cases respectively, compared to 0.01% for the medium break event. This represents release fractions from the total fuel sphere inventory of 9.25×10^{-6}, 1.61×10^{-4} and 8.23×10^{-4} for the three small break cases, compared to 6.65×10^{-7} for the medium break event.

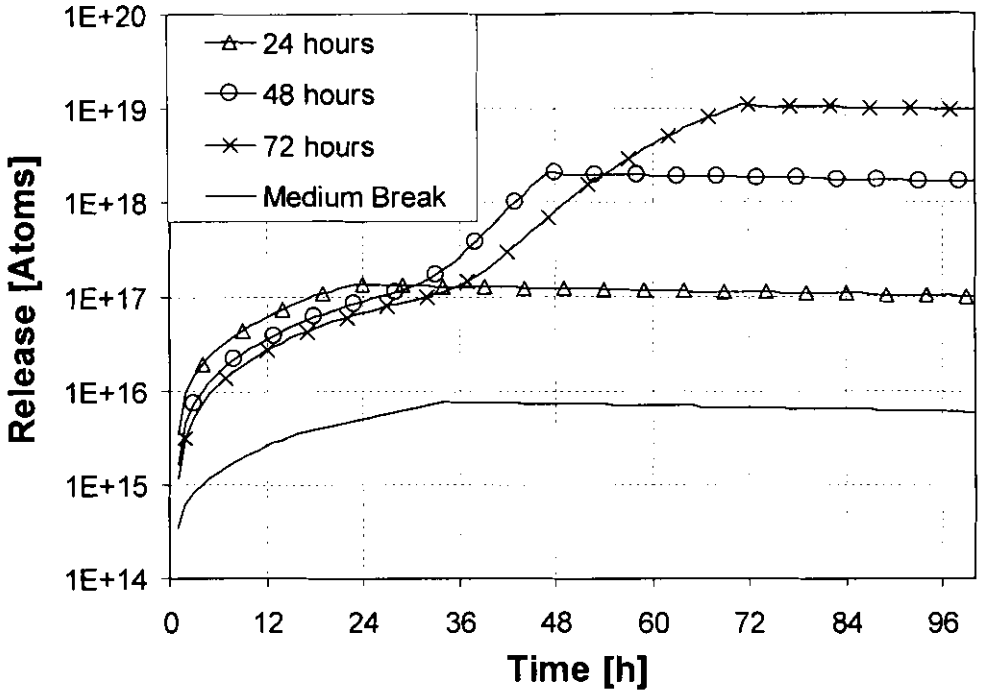

Figure 4.9 Ag-111 releases from the core structure during small and medium break events

These values are used as input into analysis methods to determine public dose rates through the various radiological delivery paths. These models consider building retention and plate out, as well as environmental distribution mechanisms such as wind and rain.

5 High accident temperature investigation

The first estimates for maximum temperatures during a DLOFC accident for the PBMR were in the 1500 °C to 1550 °C region. Now that the core design has matured and thermo hydraulic uncertainties are better understood, the expected maximum fuel temperatures have increased to 1650 °C. With increases in reactor power and higher outlet temperatures, the maximum expected fuel temperature might even increase to higher values. The effect of increasing maximum fuel temperatures reached in the PBMR core during a DLOFC event on fission product releases was investigated. The maximum expected fuel temperature (1506 °C for this study) was increased stepwise by ~50 °C to 1750 °C. The release of the principal DLOFC nuclides was calculated for each DLOFC maximum fuel temperature. The results were plotted and curves were created to guide future investigations to increase the maximum fuel temperatures during a DLOFC event.

5.1 Input parameters

All input parameters were taken from the expected DLOFC event calculations [22]. The core geometry, transport parameters, and fuel sphere inventories were used as for a typical 400 MW PBMR reactor design. The temperature-heating span was increased according to

$$T = T_i + \frac{(T_i - T_o)}{(T_m - T_o)}(44 + 50a), \quad a = 0,1,2,3... \tag{19}$$

with T new temperature for each region, T_i the original DLOFC VSOP temperature, and T_o the temperature at $t = 0$. The maximum original VSOP fuel temperature is T_m.

This means that initial temperatures stay the same but that maximum fuel temperatures increase with 50 °C, except the first temperature step, which increases by 44 °C (1506 - 1550). Fission product release code GETTER was used to calculate releases from selected core regions, and FIPREX was used for post calculation data manipulation. The only assumptions were that transport parameters did not change with increased temperature and that backpressure effects are insignificant.

5.2 Fission product Cesium-137

^{137}Cs is considered the third most important nuclide identified for DLOFC analysis. Figure 5.1 displays the curve derived from seven DLOFC calculations with increasing maximum fuel temperatures reached during the DLOFC event. There is a 7-fold increase of ^{137}Cs atoms released from 1506 °C to 1750 °C. The increase of fission products released versus maximum temperature achieved follows an exponential curve as shown in Figure 5.1. This modest increase agrees with the temperature sensitivity analyses performed before [23], where a 25°C increase in average fuel temperature under normal conditions increased the core release rate by 40%. Table 5.1 lists ^{137}Cs activity released from the core in Becquerel.

Table 5.1 Total ^{137}Cs activity released for each max fuel temperature-heating span

Temperature	1506 °C	1525 °C	1550 °C	1600 °C	1650 °C	1700 °C	1750 °C
1 hour	1.79E+06	1.90E+06	2.08E+06	2.67E+06	3.59E+06	4.78E+06	8.33E+06
5 hours	4.03E+07	4.65E+07	5.51E+07	8.13E+07	1.17E+08	1.68E+08	2.60E+08
9 hours	1.13E+08	1.31E+08	1.57E+08	2.39E+08	3.48E+08	5.12E+08	7.82E+08
15 hours	3.18E+08	3.75E+08	4.56E+08	7.17E+08	1.06E+09	1.58E+09	2.39E+09
21 hours	5.65E+08	6.70E+08	8.22E+08	1.30E+09	1.93E+09	2.89E+09	4.26E+09
27 hours	8.12E+08	9.65E+08	1.19E+09	1.88E+09	2.79E+09	4.16E+09	5.97E+09
36 hours	1.05E+09	1.25E+09	1.54E+09	2.43E+09	3.59E+09	5.31E+09	7.50E+09

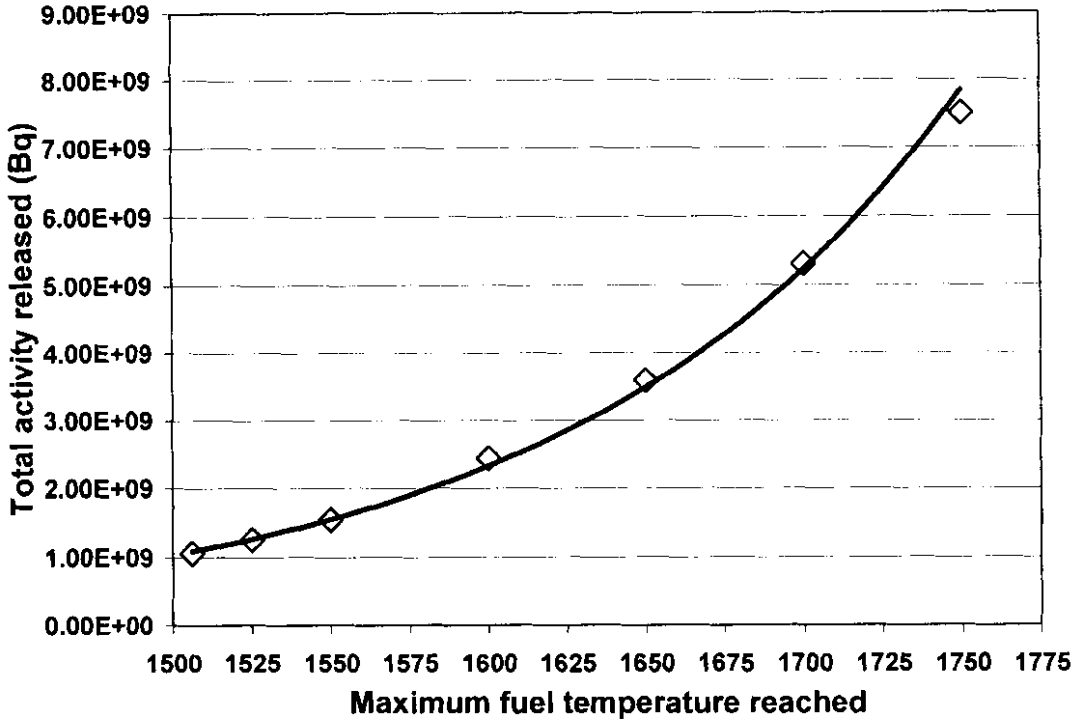

Figure 5.1 ^{137}Cs activity release vs maximum fuel temperature reached

5.3 Fission product iodine-131

The most important nuclide for DLOFC event analysis shows similar modest increases as ^{137}Cs. The ^{131}I release increases 6 fold from 1506°C to 1750°C, which is higher than expected when compared with previous calculated temperature sensitivities[5]. This is due to the different measured iodine transport parameters used above 1150 °C, compared with the normal operating conditions parameters that are valid up to 1150 °C. There exists however, some uncertainty about the transport parameters of iodine above 1600°C. The increase of fission products released versus maximum temperature achieved, follows an exponential curve as shown in figure 5.2. Table 5.2 lists the ^{131}I activity released from the core in Becquerel.

Table 5.2 Total ^{131}I activity released for each max fuel temperature heating-span

Temperature	1506 °C	1550 °C	1600 °C	1650 °C	1700 °C	1750 °C
1 hour	3.21E+08	3.15E+08	3.53E+08	3.95E+08	4.73E+08	5.62E+08
5 hours	3.17E+09	4.00E+09	5.51E+09	7.62E+09	1.12E+10	1.53E+10
9 hours	4.71E+09	6.36E+09	8.97E+09	1.26E+10	1.87E+10	2.57E+10
15 hours	1.06E+10	1.46E+10	2.06E+10	2.91E+10	4.45E+10	6.27E+10
21 hours	1.03E+10	1.43E+10	2.02E+10	2.91E+10	4.54E+10	6.45E+10
27 hours	8.44E+09	1.18E+10	1.69E+10	2.49E+10	3.90E+10	5.45E+10
36 hours	6.71E+09	9.56E+09	1.39E+10	2.04E+10	3.15E+10	4.31E+10

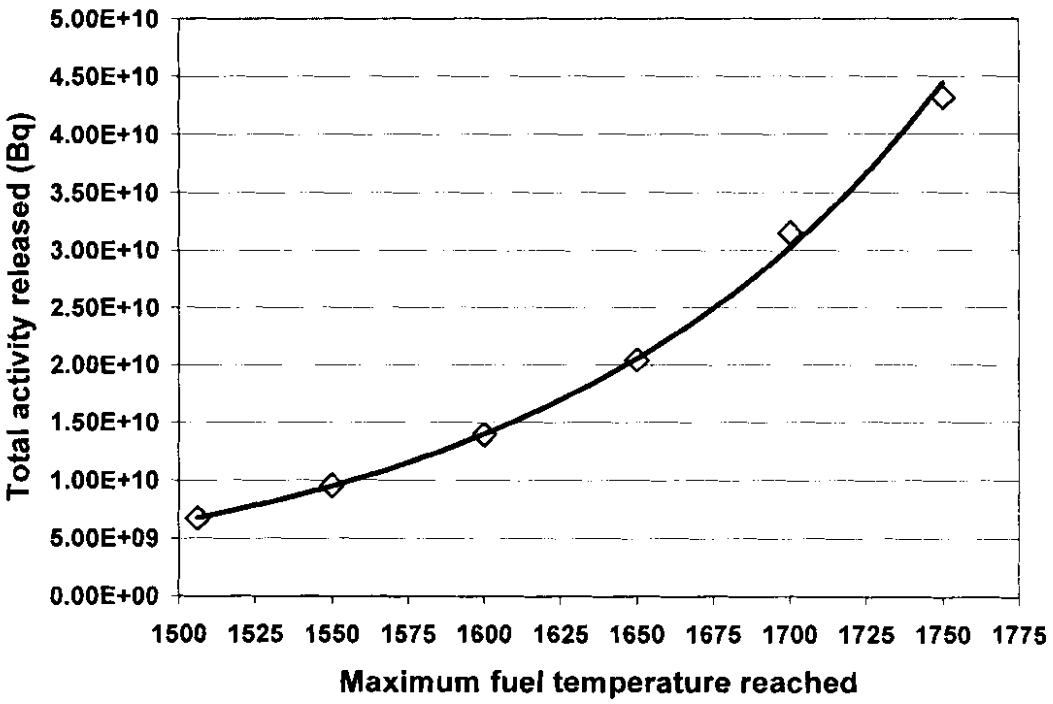

Figure 5.2 ^{131}I activity release vs maximum fuel temperature reached

5.4 Fission product Silver-111

The second most important for analyses of the DLOFC event, ^{111}Ag is the most temperature sensitive in accordance with previous temperature sensitivity analysis. The fission product release increases with a factor 90 from 1506°C to 1750°C for maximum fuel temperatures achieved. Table 5.3 lists the ^{111}Ag activity released from the core in Becquerel and figure 5.3 shows it graphically.

Table 5.3 Total ^{111}Ag activity released for each max fuel temperature

Temperature	1506 °C	1550 °C	1600 °C	1650 °C	1700 °C	1750 °C
1 hour	1.28E+07	2.51E+07	2.88E+07	3.37E+07	6.37E+07	7.49E+07
5 hours	6.06E+08	9.25E+08	1.44E+09	1.89E+09	3.03E+09	3.75E+09
9 hours	1.41E+09	2.12E+09	3.07E+09	4.08E+09	6.36E+09	7.82E+09
15 hours	3.07E+09	4.55E+09	6.01E+09	8.23E+09	1.36E+10	2.32E+10
21 hours	4.83E+09	7.08E+09	9.62E+09	1.67E+10	4.02E+10	1.01E+11
27 hours	6.37E+09	9.60E+09	1.73E+10	4.39E+10	1.25E+11	3.21E+11
36 hours	8.39E+09	1.60E+10	4.35E+10	1.25E+11	3.32E+11	7.58E+11

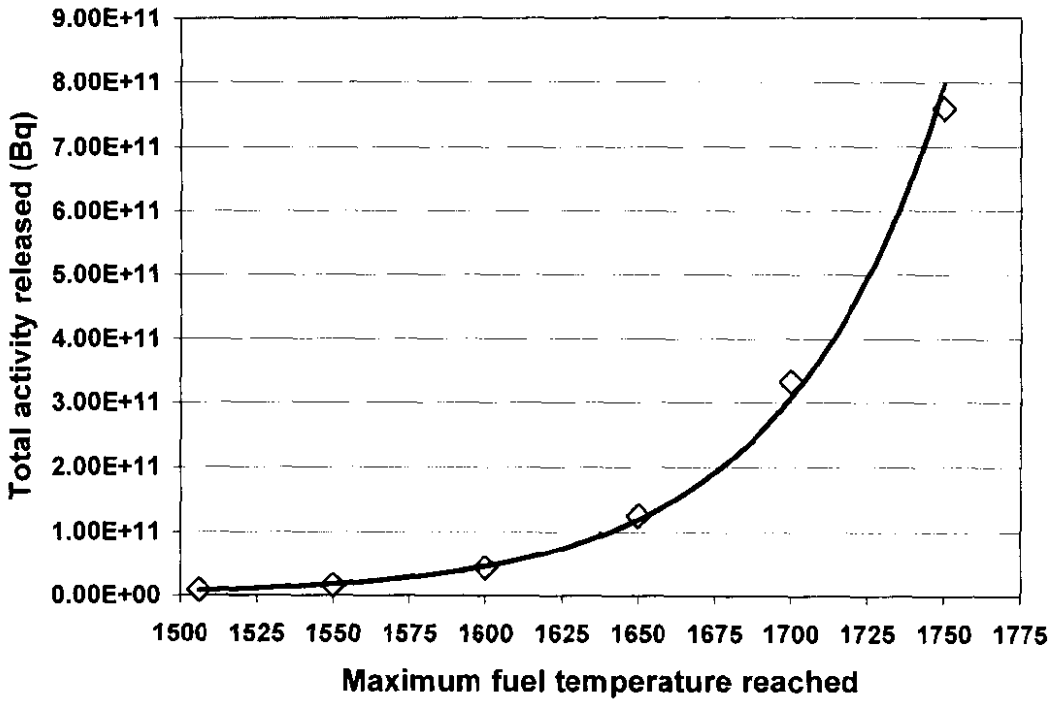

Figure 5.3 ^{111}Ag activity release vs maximum fuel temperature reached

5.5 Discussion

A physical relation can model the curves generated by the extrapolation of the fission product release for higher temperatures. Considering the Arrhenius equation for rate constants

$$k = Ae^{\frac{E_a}{RT}} \tag{20}$$

used to determine diffusion rates of fission products at specific temperatures through the layers of the fuel element and particle. The release from the core (CR) can be modeled as follows:

Caesium-137: $CR = 1.29x10^{16} e^{\frac{-212kJ/mol}{RT}}$ Bq (21)

Iodine-131: $CR = 3.33x10^{16} e^{\frac{-228kJ/mol}{RT}}$ Bq (22)

Silver-111: $CR = 1.38x10^{26} e^{\frac{-552kJ/mol}{RT}}$ Bq (23)

Where R is the gas constant, 8.3145 J/mol/K, and T is the absolute maximum temperature reached in the core. With these simple relations fission product release for any maximum temperature during a DLOFC event for this core design can be calculated as a first estimate.

6 Conclusion

Reactor analysis and fuel performance software and calculation models are continuously being developed as part of reactor design and fuel management in nuclear engineering analysis at PBMR. New safety and design optimization requirements demand the development of state-of-the-art analysis techniques. Quality control and delivery requirements demand in-depth verification and validation of models, calculations, parameters and software used. These requirements are met by developing calculation models and software using modern analysis techniques in a quality control system. The FIPREX-GETTER calculation model was developed in such a quality environment and delivers all current requirements:

- Full core analyses
- Analysis of all relevant fission and activation products
- Analysis of all relevant operational modes and occurrences as well as all postulated accident events
- Monte Carlo uncertainty analyses
- Integrated calculation

The development of FIPREX-GETTER is by no means complete. New requirements and abilities are continuously being developed. The ultimate goal of software and model progress is the development of an integrated reactor analysis software structure, which can perform complete reactor analysis in one system. This would consist of several interlinking modules, allowing the power plant operator to calculate the effects of changes in fuel specifications or in reactor conditions quickly and efficiently.

The high accident temperature investigation had interesting results. All three investigated nuclides show exponential release increases against temperature. The ^{137}Cs and ^{131}I releases show modest increases from 1506 to 1750 °C of just factors 6 and 7 respectively. ^{111}Ag showed a more pronounced increase of 90 times the release from 1500 to 1750°C. The relatively low increases can be attributed to the fact that although the maximum fuel temperature increased to 1750 °C by 244 °C or 16.2%, the average pebble-bed temperature only increased by 135 °C or 11.3%. The increase factors however agree well with previously calculated temperature sensitivity factors.

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