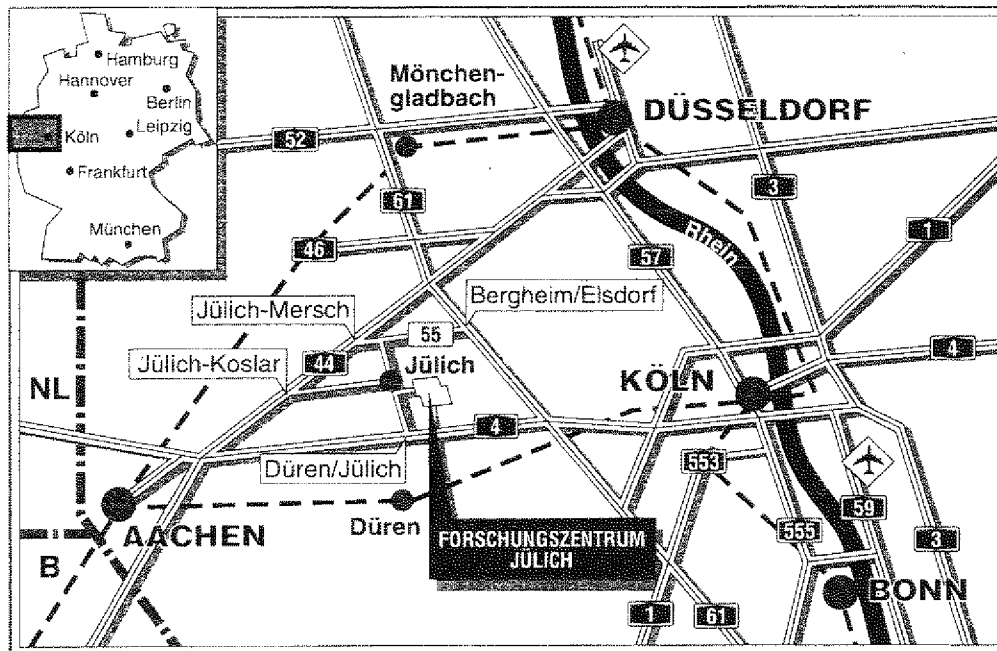


*Institut für Sicherheitsforschung
und Reaktortechnik*

Comparison of US/FRG Accident Condition Models for HTGR Fuel Failure and Radionuclide Release

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COMPARISON OF US/FRG ACCIDENT CONDITION MODELS FOR HTGR FUEL FAILURE AND RADIONUCLIDE RELEASE

by

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ABSTRACT

This report describes cooperative work on HTGR safety research as agreed to in the "US/FRG Umbrella Agreement for Cooperation in GCR Development: Safety Research Subprogram Plan". The objective was to compare calculation models used in safety analyses in the US and FRG which describe fission product release behavior from TRISO coated fuel particles under core heatup accident conditions.

The first step performed is the qualitative comparison of both sides' fuel failure and release models in order to identify differences and similarities in modeling assumptions and inputs. Assumptions of possible particle failure mechanisms under accident conditions (SiC degradation, pressure vessel) are principally the same on both sides though they are used in different modeling approaches. The characterization of a standard (= intact) coated particle to be

of non-releasing (GA) or possibly releasing (KFA/ISF) type is one of the major qualitative differences referring to the philosophy which the recently developed statistical model (Integrated Failure and Release Model for Standard Particles) and the classical diffusion model, respectively, are based upon. Similar models are used regarding radionuclide release from exposed particle kernels.

In a second step, a quantitative comparison of the calculation models was made by assessing a benchmark problem predicting particle failure and radionuclide release under MHTGR conduction cooldown accident conditions. Calculations with each side's reference method have come to almost the same failure fractions after 250 hours for the core region with maximum core heatup temperature despite the different modeling approaches of SORS and PANAMA-I. The comparison of the results of particle failure obtained with the Integrated Failure and Release Model for Standard Particles and its revision which are used on both sides provides a "verification" of these models in this sense that the codes (SORS and PANAMA-II, and -III, respectively) which were independently developed lead to very good agreement in the predictions. Differences in radionuclide release fractions are basically related to a different degree of simplification in the description of certain phenomena in the models by empirical approach and to different input data whose derivation could be based upon different experiments. These differences would need further study in order to be resolved.

VERGLEICH US-AMERIKANISCHER UND DEUTSCHER RECHENMODELLE ZUM PARTIKELBRUCH UND ZUR SPALTPRODUKTFREISETZUNG UNTER STÖRFALLBEDINGUNGEN

von

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KURZFASSUNG

Dieser Bericht umfaßt eine gemeinschaftliche Arbeit im Bereich der HTR-Sicherheitsforschung, wie sie im "US/FRG Umbrella Agreement for Cooperation in GCR Development: Safety Research Subprogram Plan" vereinbart worden ist. Ziel war es, Rechenmodelle zur Beschreibung der Spaltproduktfreisetzung aus TRISO beschichteten Brennstoffpartikeln im Kernaufheizstörfall miteinander zu vergleichen.

Der erste Schritt enthält den qualitativen Vergleich der Modelle beider Seiten zum Partikelversagen und zur Freisetzung, um die Unterschiede und Gemeinsamkeiten in den Modellannahmen und Eingangsdaten herauszufinden. Die angesetzten Versagensmechanismen unter Störfallbedingungen (SiC-Zersetzung, Druckkesselversagen) sind im Prinzip auf beiden Seiten

dieselben; sie werden jedoch unterschiedlich modelliert. Die Charakterisierung eines Standard (= intakten) -Brennstoffpartikels als nicht-freisetzend (GA) oder eventuell freisetzend (KFA/ISF) ist einer der größeren qualitativen Unterschiede, der auf die Philosophie zurückgeht, auf der das kürzlich entwickelte statistische Modell ("Integriertes Bruch- und Freisetzungsmodell für Standardpartikel) bzw. das Diffusionsmodell basieren. Im Hinblick auf die Spaltproduktfreisetzung aus Partikelkernen werden von beiden Seiten ähnliche Modelle benutzt.

In einem zweiten Schritt wurde ein quantitativer Vergleich der Rechenmodelle angestellt. Dazu wurde ein Benchmark-Fall definiert, für den das Partikelversagen und die Spaltproduktfreisetzung unter Bedingungen der Kernaufheizung im druckentlasteten MHTGR vorhergesagt wurde. Rechnungen mit der Referenzmethode jeder Seite haben fast denselben Partikelbruchanteil nach 250 h an der Stelle im Core ergeben, die die maximale Brennstofftemperatur aufweist, trotz der unterschiedlichen Modellierungsverfahren von SORS und PANAMA-I. Der Vergleich der Ergebnisse, die mit dem auf beiden Seiten benutzten "Integrierten Bruch- und Freisetzungsmodell für Standardpartikel" sowie dessen revidierter Fassung gewonnen wurden, erlaubt die Feststellung einer "Verifikation" dieser Modelle in dem Sinne, daß diese Codes (SORS bzw. PANAMA-II, und -III), die unabhängig voneinander entwickelt worden sind, zu einer sehr guten Übereinstimmung bei den Vorhersagen führen. Unterschiede in den Spaltproduktfreisetzunganteilen sind prinzipiell zurückzuführen auf ein unterschiedliches Maß an Vereinfachungen bei der Beschreibung bestimmter Phänomene in den Modellen sowie durch verschiedene Eingabedaten, deren Ableitung möglicherweise auf unterschiedlichen Interpretationen von Experimenten beruht hat. Die Klärung dieser Unterschiede bedarf weiterer Untersuchungen.

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1. INTRODUCTION

Although there are many differences between the High-Temperature Gas-Cooled Reactor (HTGR) concepts being developed in the US and the High-Temperature Reactor (HTR) concepts in the Federal Republik of Germany (FRG), the coated fuel particles are very similar. Significant benefits are achievable through cooperative research and exchange of information and data on the fuel performance and radionuclide retention in the coated fuel particle.

This report describes cooperative work on HTGR safety research as agreed to in the "US/FRG Umbrella Agreement for Cooperation in GCR Development: Safety Research Subprogram Plan". Specifically, this work was conducted under Project Work Statement (PWS) S-6 titled "Fission Product Retention in Fuel". It was accomplished at General Atomics, San Diego (USA) from October through December 1988.

The objectives of PWS S-6 are to confirm the fission product release models used in safety analysis in the US and FRG and to compare the fission product release models by assessing a benchmark problem. The planned approach to achieve these objectives is to exchange and review the data and methods used in the US and FRG for assessment of radionuclide retention in the fuel in order to assure a common and comparable basis. From this basis, consistent fission product transport models would be developed and compared with the goal of specifying or acquiring data to validate these computer models.

The scope of this study is limited to qualitative and quantitative comparisons of the US and FRG models for fuel particle failure and fission product release under core heatup accident conditions. The study includes the identification of key modeling assumptions, inputs and approaches in order to find out the differences and similarities in the release models.

The numerical models examined in this study are those used by General Atomics (GA) in the US and by the Nuclear Research Center's Institute for

1. INTRODUCTION

Nuclear Safety Research (KFA/ISF)¹ at Jülich in the FRG. All codes were independently developed although some tend to have similar approaches due to the international database and cooperation used as the basis for the model development. Benchmark calculations were performed to quantify their consistency by comparing results from each country's models. Such a comparison of calculated particle failure and radionuclide release provides valuable input to each country's code verification effort.

The qualitative comparison of US and FRG methods are presented in Sections 2 and 3. Section 2 describes the TRISO coated fuel particle and each country's assumptions related to fuel quality after manufacture and irradiation. In Section 3, each country's models for fuel particle failure and radionuclide release are described and compared as applied to accident conditions. Conclusions from the qualitative comparison are presented in Section 7.1.

The selection of a benchmark problem and the results of the quantitative comparison are presented in Sections 4, 5, and 6. Section 4 defines the benchmark problem and input parameters selected for the quantitative comparison. Section 5 presents the results from the benchmark comparison of fuel particle failure models. Section 6 presents the results from the benchmark comparison of radionuclide release models. Conclusions from the quantitative comparison are presented in Section 7.2.

¹ Names have changed in the meantime into: Institute for Safety Research and Reactor Technology (ISR) at the Research Center Jülich (KFA)

1. INTRODUCTION

2. US AND FRG FUEL DESIGN

2.1 Fuel Element Design

The fuel elements used in the US HTGR and in the FRG HTR designs have quite different geometries. Both designs, however, use TRISO coated fuel particles with graphite acting as both moderator and structure for the fuel element. Because of the ceramic composition of the fuel element designs, they are able to withstand very high temperatures without disrupting the core geometry.

The US fuel element design (Fig. 2-1, top) is a hexagonal graphite block containing 102 coolant channels with a diameter of 15.9 mm and 210 blind fuel holes. Each block is 793 mm tall and 360 mm wide across the flats. Each fuel hole is filled with fuel rods and sealed. The fuel rods are a mixture of TRISO coated fissile and fertile particles, and graphite shim particles bonded by a carbonaceous matrix. A nominal radial gap of 0.13 mm exists between the fuel rod and the fuel hole. The active core of the 350 MW(th) Modular High Temperature Gas Cooled Reactor (MHTGR) consists of 660 of these graphite fuel elements.

The FRG fuel element design (Fig. 2-1, bottom) is a graphite sphere with a diameter of 60 mm. Each fuel sphere contains approximately 11,000 TRISO coated fissile particles. Every particle is surrounded by matrix graphite. The outermost 5 mm of the fuel sphere is a shell of matrix graphite only without any particles. The active core of the 200 MW(th) HTR-Module consists of about 360,000 spherical fuel elements.

2.2 Fuel Particle Design

Both the US and FRG small modular HTGR concepts rely on the ability of the TRISO coated fuel particles to retain radionuclides during normal operations and in design basis accident sequences. The analysis described in this re-

port is focussed primarily on the radionuclide release barriers provided by the coated fuel particle during core heatup accident conditions.

The principal barrier against radionuclide release from an HTGR represents the fuel particle coating with its four ceramic layers around the fuel kernel. A typical TRISO coated fuel particle is shown in Fig. 2-2. The nominal specifications for the US and FRG fuel particles are presented in Table 2-1.

The fissile particle consists of a spherical fuel kernel containing 19.8 % enriched uranium oxycarbide (UCO) in the US fuel design and 10.6 % enriched uranium dioxide (UO_2) in the FRG fuel design. The purpose of the fuel kernel is to provide a source of fission energy and to retain radionuclides. The fuel kernel is surrounded by a porous buffer layer which is designed to provide a reservoir for fission gases released from the fuel kernel, to attenuate fission product recoil, and to accomodate fuel kernel swelling. The inner pyrocarbon coating (IPyC) is a high density coating which seals the buffer layer. The IPyC coating provides a substrate for silicon carbide (SiC) deposition during manufacturing in addition to attenuating migration of radionuclides which could chemically interact with the SiC layer. The SiC layer is a strong, high temperature coating which primarily acts like a pressure vessel and is the principal barrier to the release of both gaseous and metallic radionuclides. The final coating is the outer pyrocarbon (OPyC) layer which provides an effective barrier to fission gas release in fuel particles with a defective or failed SiC layer. Both pyrocarbon layers reduce tensile stresses in the SiC layer. The OPyC layer provides bonding surface with the surrounding graphite matrix material.

2.3 Fuel Manufacturing Defects

During the manufacture of the fuel particles, a certain level of unavoidable defects is introduced in the fuel product. Manufacturing target specifications define acceptable upper limits for these defects (design values) which are assured by quality control measurements. The release of radionuclides from the coated particles depends primarily on the initial as-manufactured defects and on main-

2. US AND FRG FUEL DESIGN

Table 2-1: Comparison of US and FRG Reference Fuel Particle Nominal Characteristics

	US REFERENCE		FRG REFERENCE
	Fissile	Fertile	Fissile
Kernel			
Composition	UCO	ThO ₂	UO ₂
Carbon/Uranium	0.29	-	-
Oxygen/Uranium	1.63	-	2.0
Diameter [μm]	350	500	500
Enrichment [%]	19.8	-	10.6
Density [Mg/m^3]	10.7	9.8	10.9
Heavy Metal Loading [g]	$2.1 \cdot 10^{-4}$	$5.6 \cdot 10^{-4}$	$5.7 \cdot 10^{-4}$
Coating Thickness [μm]			
Buffer	100	65	95
Inner PyC	50	50	40
SiC	35	35	35
Outer PyC	40	40	40

taining coating integrity of standard (defect-free) particles. Therefore, the quality or condition of the fuel particle after manufacture and prior to the initiation of an accident is a key input to any release model.

Expected values used for characterizing US and FRG fuel particles to be inserted in calculations for risk analyses are specified in Table 2-2.

Particles that have all coatings defective or failed are called exposed kernels and can release all types of radionuclide species. However, the kernel itself is still a substantial barrier to radionuclide release even at MHTGR/HTR accident temperatures.

2. US AND FRG FUEL DESIGN

The total fraction of "free" uranium specification limits the amount of fissile material outside an intact SiC coating. It comprises both the uranium in particles with a defective SiC layer and the heavy metal contamination of the graphite which is another important source of radionuclide release during accidents.

Table 2-2 presents the US and FRG fuel specifications.

According to the GA approach, a particle is classified as either releasing or non-releasing (either has or does not have the potential to release radionuclides). A standard particle has all coating layers intact and therefore is non-releasing for essentially all radionuclides. If the SiC coating is defective or failed and the OPyC layer is intact, the particle is releasing. Such particles tend to retain more of the gaseous rather than the metallic radionuclides.

The US program distinguishes between heavy metal contamination and particles with failed SiC layer through the use of separate measurement techniques. A wet leach technique is used to measure the uranium content outside an intact or failed SiC layer after manufacturing. This uranium is not expected to be in the form of a kernel and is treated as heavy metal contamination. If the

Table 2-2: Comparison of US and FRG Fuel Specifications for
As-Manufactured Defects (Mean Values)

Defect or Failure	US	FRG
Total Fraction of "Free" Uranium (Contamination plus SiC Defects)	$\leq 6.0 \cdot 10^{-5}$	$3.0 \cdot 10^{-5}$
Heavy Metal Contamination	$\leq 1.0 \cdot 10^{-5}$	$1.5 \cdot 10^{-5}$
Exposed Kernels	-	$1.5 \cdot 10^{-5}$
Missing Buffer	$\leq 5.0 \cdot 10^{-5}$	-
Defective SiC, Intact OPyC	$\leq 5.0 \cdot 10^{-5}$	-
Missing or Defective IPyC	$\leq 4.0 \cdot 10^{-5}$	-
Missing or Defective OPyC	$\leq 1.0 \cdot 10^{-4}$	-

2. US AND FRG FUEL DESIGN

SiC layer is defective due to manufacturing, then the OPyC layer is expected to remain intact. The burn leach technique will burn off the OPyC thereby allowing the measurement of both the heavy metal contamination and the fraction of particles with failed SiC coating. The US value for the heavy metal contamination in the fuel rod matrix material is $1 \cdot 10^{-5}$. The total fraction of "free" uranium in the US fuel element is $6 \cdot 10^{-5}$ and is composed of the heavy metal contamination and defective SiC layers.

The US program also specifies defect levels for missing buffer, missing or defective IPyC, and missing or defective OPyC layers all of which are non-releasing as long as the SiC layer is intact. This detailed specification provides input to similarly detailed fuel failure models which give increased understanding and confidence that the as-manufactured fuel will perform as expected.

In contrast, **KFA/ISF** does not explicitly distinguish between releasing and non-releasing coated particles. The kernel and the single layers are characterized by temperature dependent "effective" fission product transport data to be inserted into KFA/ISF reference diffusion model. An originally intact particle which experiences a failed coating is treated like an exposed kernel in this model. Particles with an intact coating are practically non-releasing for fission gases and iodine even under elevated temperature conditions.

The FRG program uses a burn leach measurement technique which determines all uranium sources which are not covered by an intact silicon carbide coating. It comprises both particles with a defective or failed SiC layer and uranium contamination of the fuel element matrix graphite and the OPyC layer. The expected fraction of "free" uranium is specified at $3 \cdot 10^{-5}$. The partition of this value into two even contributions from contamination and from defective particles as specified in Table 2-2, was made by KFA/ISF in 1986 to be used in radionuclide release calculation. This even division should be conservative since the measured uranium contamination in matrix graphite of modern FRG fuel was recently found to be around or even less than $1 \cdot 10^{-6}$ resulting from natural uranium, i.e. with respect to fissile uranium, the contamination fraction which is relevant for fission product release, is even lower.

2. US AND FRG FUEL DESIGN

3. QUALITATIVE COMPARISON OF US AND FRG FUEL PARTICLE FAILURE AND RADIONUCLIDE RELEASE MODELS

All calculation models for fuel particle failure and fission product release and the corresponding code names presented here are summarized in Table 3-1 at the end of this section.

3.1 Fuel Particle Failure Models

The dominant source of radionuclide release from a small-sized HTGR core during a core heatup accident are as-manufactured heavy metal contamination and as-manufactured defective fuel particles that have failed coatings due to normal operating conditions.

3.1.1 GA Modeling Approach

According to US models used at GA, fuel particles can fail by the following mechanisms during accident conditions:

1. Pressure vessel failure in standard (intact) particles
2. Pressure vessel failure in particles with defective or missing single coatings
3. Failure of the SiC layer by fission product corrosion of the silicon carbide (OPyC layer remains intact)
4. Failure of the SiC layer by thermal decomposition of the silicon carbide (OPyC layer remains intact)

US models for accident conditions assume that the fraction of particles with missing buffer layer fail completely during normal operation producing exposed kernels.

The SORS code (Ref. 1) is used by GA to predict fuel particle failure due to elevated temperatures during accident conditions.

The GA **pressure vessel model** is considered to be one possible independent mechanism for a complete failure of the particle coating. It has the structure of a Weibull equation being dependent on the accident temperature only. The model equation signifies the final value to be reached as soon as the maximum fuel temperature is reached. The model includes the assumption for a constant fraction of fission gas released from the particle kernels during the core heatup accident sequence of the US-MHTGR.

For standard particles as well as for the other possible defective particles, the pressure vessel failure is insignificant for (temperature) conditions that small-sized modular HTGR experience.

Another mechanism for a particle failure used by GA is modeled in the **Integrated Failure and Release Model for Standard Particles** developed by Goodin and Nabielek in 1985 (Ref. 2). It is based on a more empirical approach to interpret the failure and release behavior of TRISO particles. The cesium 137 release measured in laboratory simulations of HTGR transients is assumed to be the direct indicator of a failed SiC layer. The subsequent delay of krypton release observed in the heating experiments is attributed to the time required for fission gases to diffuse through the remaining intact OPyC. In this model, interactions of fission products with the SiC layer leading to silicon carbide corrosion are the dominant failure mechanism for temperatures below 2000 °C. A corrosion rate expressed by a thinning of the SiC layer was derived by Montgomery in independent experiments (Ref. 3). For temperatures above 2000 °C, thermal decomposition of the silicon carbide becomes the dominant failure mode. A thinning rate of the SiC layer due to thermal decomposition has been measured

3. QUALITATIVE COMPARISON OF US AND FRG FUEL PARTICLE FAILURE AND RADIONUCLIDE RELEASE MODELS

by Benz in independent laboratory work at temperatures between 2000 °C and 2200 °C (Ref. 4).

The empirical approach is statistical in nature since it assumes that both the SiC layer thickness and the rates of silicon carbide corrosion and thermal decomposition are variables with statistical distributions. The intersection of the distributions determines the fraction of the SiC coatings that have failed. The convolution integral forming the solution to these compound distributions has been shown to be approximated well by a Weibull distribution for either corrosion (c) or thermal decomposition (d). The corrosion or decomposition frequency factor is then modeled using an Arrhenius relationship.

$$\phi(t,T) = 1 - e^{-\ln 2 \times \zeta^m} \quad (3-1)$$

where ζ : a so-called "action" integral

$$\zeta = \int k(T) dt$$

and k : SiC degradation rate [s^{-1}]

$$k = k_o * e^{-Q/(R*T)}$$

T : Temperature

t : Time

m : Weibull Parameter

a) SiC Corrosion

$$\log k_{o,c} = -A + 3 \cdot \log T_i + \log f_{SiC} \quad (3-2)$$

3. QUALITATIVE COMPARISON OF US AND FRG FUEL PARTICLE FAILURE AND RADIONUCLIDE RELEASE MODELS

where $k_{o,c}$: frequency factor for corrosion rate [s^{-1}]
 Q_c : activation energy (after Montgomery)
 $Q_c = 252$ [kJ/mole]
 A: constant, $A = 36.53$ for oxidic fuel
 $A = 36.70$ for carbidic fuel
 The "oxidic" value of A is used in the calculations for the US UCO fuel.
 T_i : irradiation temperature [K]
 f_{SiC} : Fission density [m^{-3}]
 m_c : Weibull parameter, $m_c = 3.3$ for single experiments
 $m_c = 1.6$ for core predictions

b) SiC thermal decomposition

$$\log k_{o,d} = -1.58 + 2.67 \cdot \log T_i + 0.61 \cdot \log \Gamma \quad (3-3)$$

where $k_{o,d}$: frequency factor for decomposition rate [s^{-1}]
 Q_d : activation energy (after Benz)
 $Q_d = 545$ [kJ/mole]
 T_i : irradiation temperature [K]
 Γ : Fast fluence [$10^{25}/m^2$, $E > 0.1$ MeV]
 m_d : Weibull parameter, $m_d = 2.2$ for single experiments
 $m_d = 1.5$ for core predictions

The two Weibull parameters m_c and m_d which have been derived from experiments, are valid for an individual particle batch. For predictions referring to a complete HTGR core where many batches of fuel are combined, Weibull parameters are recommended which conservatively include an additional interbatch variation leading to a decreased slope of the failure curve.

Additional experimental data have become available since 1985 and coefficients from the 1985 approach have been updated in the **1988 revision of the Integrated Failure And Release Model for Standard Particles** (Ref. 5). In this pro-

3. QUALITATIVE COMPARISON OF US AND FRG FUEL PARTICLE FAILURE AND RADIONUCLIDE RELEASE MODELS

posed model revision, the SiC thermal decomposition process is assumed to be the controlling failure mechanism even at lower temperatures. Observations of SiC failure in heating tests have been interpreted in this way eliminating the need to model corrosion-induced SiC failure.

The proposed SiC degradation rate is modeled using an Arrhenius relationship just as in the 1985 model. A lower limit of the frequency factor is incorporated in the model due to a better agreement with the observations from low exposure AVR fuel under heating conditions.

The activation energy incorporated in the model equation is the same derived for SiC thermal decomposition (see equation (3-3)). In cases where the lower limit is exceeded, the frequency factor exhibits a weak dependence on the fast neutron fluence and a strong dependence on the irradiation temperature. These dependencies are the result of the fitting procedure carried out, they do not contain any physical meaning.

In addition, statistical limitations of the data base result in the conservative GA assumption of a lower limit of $6 \cdot 10^{-6}$ for total fuel failure under accident conditions for any position in the core.

3.1.2 KFA/ISF Modeling Approach

According to the accepted models used by KFA/ISF (Ref. 6) for the determination of TRISO particle failure under accident conditions, the mechanisms by which a particle can fail are principally the same as those assumed by GA, except there is no explicit distinction between particles with single defective or missing coatings:

1. Pressure vessel failure in standard (intact) particles
2. Failure of the SiC layer by fission product corrosion of the silicon carbide (OPyC layer remains intact)

3. QUALITATIVE COMPARISON OF US AND FRG FUEL PARTICLE FAILURE AND RADIONUCLIDE RELEASE MODELS

3. Failure of the SiC layer by thermal decomposition of the silicon carbide (OPyC layer remains intact)

The above mentioned failure mechanisms are used in two different independent calculation models which differ in the way particle failure is interpreted.

The KFA/ISF reference particle failure model determines the fraction of failed TRISO particles under accident conditions by using a **pressure vessel model** combined with a silicon carbide degradation process. In this model coded in PANAMA-I (Ref. 4), the result of a particle failure is an exposed kernel indicated by the measured krypton gas release. A TRISO particle is supposed to fail as soon as the internal gas pressure imposing a tension on the coating exceeds its strength. The SiC layer is considered to represent the pressure vessel, the OPyC layer is neglected conservatively. Additionally, the model includes the weakening of the strength of the SiC layer by irradiation exposure and a silicon carbide corrosion by radionuclide attack. The PANAMA-I code has been extended to be also applicable to coated particles with UCO kernels.

a) Pressure Vessel Failure and SiC Corrosion

The probability for a pressure vessel failure of a TRISO particle is given by:

$$\phi(t, T) = 1 - e^{-\ln 2 \cdot (\sigma_t / \sigma_o)^m} \quad (3-4)$$

where σ_t : tension [Pa] induced in the SiC layer
by internal gas pressure

$$\sigma_t = \frac{r \cdot p}{2 \cdot d_o} \cdot \left(1 + \frac{\dot{v} \cdot t}{d_o} \right) \quad (3-5)$$

3. QUALITATIVE COMPARISON OF US AND FRG FUEL PARTICLE FAILURE AND RADIONUCLIDE RELEASE MODELS

with r : medium radius of the SiC layer [m]
 d_o : original thickness of the SiC layer [m]
 p : inner pressure of fission gases [Pa]
 v : thinning velocity [m/s]
 $v = 5.87 \cdot 10^{-7} \cdot e^{-179500/(R \cdot T)}$
 t : time [s]

and σ_o : strength of the SiC layer [Pa]
 $\sigma_o = \sigma_o(\Gamma)$
 m : the Weibull parameter for strength distribution
 $m = m(\Gamma)$

SiC strength σ_o and the corresponding Weibull parameter m are characteristics of the silicon carbide of the particle batch and have been measured independently for many particle batches by crack tests on SiC rings. The induced tension σ_t contains the corrosive attack on the SiC layer. The inner gas pressure p is derived from the ideal gas law being dependent on various contributions such as the fission yield for stable gases, burnup, gas release from the particle kernels (Booth model (Ref. 7)), and oxygen production (independent measurements for UO_2 and $(Th,U)O_2$ at Seibersdorf/Austria, negligible for UCO) resulting in CO formation.

Thermal decomposition of the silicon carbide dominant at higher temperatures is modeled as a second failure mechanism in PANAMA-I. The particle failure is empirically described by a Weibull distribution:

$$\phi(t, T) = 1 - e^{-\alpha \cdot t^\beta} \quad (3 - 6)$$

3. QUALITATIVE COMPARISON OF US AND FRG FUEL PARTICLE FAILURE AND RADIONUCLIDE RELEASE MODELS

where ζ : "action" integral

$$\zeta = \int k(T) dt$$

and k : SiC degradation rate [s^{-1}] (after Benz)

α , β : empirical constants

$$\alpha = 0.693, \quad \beta = 0.88 \quad \text{for unbonded particles}$$

$$\alpha = 0.0001, \quad \beta = 4. \quad \text{for particles in a fuel sphere}$$

The low β value for unbonded particles in the Weibull equation 3-6 corresponds to a relatively high level of predicted particle failure at typical small HTGR accident temperatures whereas the failure fraction for particles in a fuel ball (high β value) is practically negligible at these conditions.

The fraction of particles failed by thermal decomposition is handled in the same way as the pressure vessel failed particle fraction i.e. the failure results in a bare kernel without any coating.

The PANAMA-I code predicts conservative results in the lower temperature range as postcalculations of heating experiments have shown especially with respect to the assumed irradiation influence. Conservativisms are attributed to an annealing effect of irradiation-induced damage at elevated temperatures which is not taken into account, and a possibly lower strength of the SiC layer measured in SiC ring crack tests rather than in a complete coated particle within a sphere or rod.

The joint US/FRG **Integrated Failure and Release Model for Standard Particles** from 1985 (Ref. 2) was chosen by KFA/ISF as a second independent method for particle failure and cesium/krypton release calculations to identify differences between the reference way (Ref. 6) and the new more empirical approach. The result of a particle failure here is a failed SiC layer while the OPyC layer still remains intact. This interpretation is indicated by the measurement of cesium release and delayed gas release. The German version coded in PANAMA-II uses the same model equations with respect to the particle failure under accident conditions as GA does in the SORS code. Therefore, identical

3. QUALITATIVE COMPARISON OF US AND FRG FUEL PARTICLE FAILURE AND RADIONUCLIDE RELEASE MODELS

results ought to be expected with both codes when using the same boundary conditions.

The **revision** of this model from 1988 (Ref. 5) with the new Goodin recommendations is available at KFA/ISF in a preliminary coded version called PANAMA-III. Its calculational results of particle failure fractions should also be in agreement with corresponding GA results.

In contrast to this revised version of the statistical model, the other particle failure models (original version of the statistical model, pressure vessel failure model) do not specify a lower limit for a total TRISO particle failure fraction under accident conditions.

3.2 Radionuclide Release Models

The SORS code (Ref. 1) is used by GA to predict radionuclide release from fuel and graphite due to elevated temperatures during accident conditions. In addition to release from heavy metal contamination, the US safety analyses methods consider releases from four types of fuel particles:

1. Standard particles which have intact coatings at the start of an accident and which are non-releasing for all gaseous and metallic radionuclides except for silver.
2. Defective particles which have missing or defective OPyC or IPyC coatings and an intact SiC layer and which are non-releasing except for silver.
3. Defective particles which have a missing or defective SiC layer and an intact OPyC coating and which are releasing though they tend to retain gaseous radionuclides

3. QUALITATIVE COMPARISON OF US AND FRG FUEL PARTICLE FAILURE AND RADIONUCLIDE RELEASE MODELS

4. Exposed kernels which have all coatings failed and which can release any radionuclide species

The items 1 and 2 are based on the philosophy of the **Integrated Failure and Release Model for Standard Particles** (Ref. 2) assuming a radionuclide release when the SiC layer is defective or has failed. Cesium release is the direct indicator for a SiC coating defect since no retention in the pyrocarbon layers is taken into account. However, gaseous species are found to be significantly retained in an intact OPyC layer.

Besides this, the GA model includes kernel retention for failed particles at temperatures below 1600 °C. This retention effect in the kernels reduces both the metallic and gaseous radionuclide release from the fuel. Data from heating experiments show that the effect of kernel retention is negligible at temperatures above 1600 °C. For accident conditions in the MHTGR, GA models would predict a significant amount of kernel retention especially in the cooler regions of the core.

According to the methodology of KFA/ISF documented in Ref. 6, the **diffusion model** FRESCO (Ref. 8) has been selected as reference code to describe the release behavior of radionuclides from the fuel particle and the spherical fuel element under normal operating and accident conditions.

The FRESCO model contains the treatment of the heavy metal contamination as well as the following two types of fuel particles:

1. Standard particles which have intact coatings at the start of an accident and which are practically non-releasing for all gaseous, but possibly releasing for metallic radionuclides at elevated temperatures
2. Exposed kernels which have all coatings failed and which can release any radionuclide species by diffusion

Intact particles that are assumed to fail during the accident turn into exposed kernels while the inventory of the coating at that time is immediately set

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free into the matrix graphite. This is a conservative assumption since the experience has shown that the release of fission products from exposed kernels is higher than from constrained failed (10 μm laser drilled pinhole through the coating) particles - similar to particles with a breached coating.

The diffusion model is the classical approach for calculating the temperature dependent transport of fission products in concentration gradients by finding a numerical solution of the Fickian equation.

$$\frac{\partial c}{\partial t} = D_{\text{eff}}(T) \cdot \left[\frac{\partial^2 c}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial c}{\partial r} \right] - \lambda \cdot c + \dot{Q} \quad (3-7)$$

where c: concentration of fission products [m^{-3}]
 t: time coordinate [s]
 r: location coordinate [m]
 D_{eff} : "effective" diffusion coefficient [m^2/s]
 T: temperature [K]
 λ : decay constant [s^{-1}]
 Q: source rate of fission products [$\text{m}^{-3}\text{s}^{-1}$]

The fission product release rate from the particle is then dependent on the concentration gradient at the surface ($r = r_p$):

$$\dot{F}_p = -4 \cdot \pi \cdot r_p^2 \cdot D_{\text{eff}} \cdot \frac{\partial c}{\partial r} \Big|_{r=r_p} \quad (3-8)$$

The diffusion coefficient D_{eff} is usually given as an Arrhenius type relation dependent on temperature only. "Effective" means that a single diffusion coefficient is supposed to be sufficient to describe all possible transport mechanisms within a homogenized medium. Diffusion data for various fission product species

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in different reactor materials were collected over many years, often being revised and compared to experiments. The transport data are correlated such that the model realistically, at least conservatively predicts the observed data.

The fraction of failed particles (= exposed kernels) due to accident temperatures is given either by the results of a PANAMA-I calculation (see previous chapter 3.1) or by input (for instance by a failure fraction which is correlated to observed krypton release).

The **Integrated Failure and Release Model for Standard Particles** (Ref. 2) is used by KFA/ISF as a second parallel method for calculating fission product release to be compared with the reference model FRESCO in combination with PANAMA-I. With respect to cesium and krypton release, this model is used in the original version as it was proposed by the authors in 1985, i.e. cesium release is identical to the predicted fraction of failed particles. In contrast to GA, no kernel retention of fission products at accident temperatures < 1600 °C is assumed.

Another difference to GA modeling is the way of determining the release of fission gases and iodine through an intact OPyC layer. Nabelek proposed for the 1985 version the following equation describing an approximate solution for the diffusive release through a spherical shell, i.e. the OPyC layer (Ref. 9):

$$R = 1 - (1 + 0.5 \cdot \gamma) \cdot e^{-3 \cdot \gamma \cdot \delta / d} \quad (3-9)$$

where $\gamma = d / r_i$

$\delta = \int D \, dt$

and d : OPyC layer thickness [μm]

r_i : inner radius of OPyC layer [μm]

D : diffusion coefficient for krypton in OPyC [m^2/s]

A two-component diffusion coefficient for krypton in pyrocarbon has been derived from various US and FRG heating experiments (Refs. 6 + 2).

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According to the philosophy of this model, the fraction of fission gas release from particles with a defective OPyC coating is identical to that of the cesium release. It has not yet been extended to predict strontium and silver release. Iodine release, however, is supposed to be comparable to fission gas release at accident conditions.

3.2.1 Heavy Metal Contamination

The US model for radionuclide release from heavy metal contamination is included in SORS (Ref. 1). The model assumes a diffusive release mechanism from a contamination particle which is less retentive than an exposed kernel. The SORS code then combines the release from heavy metal contamination with transport through the graphite to predict the release into the coolant channel. Metallic radionuclides such as cesium are assumed to be instantaneously released from the heavy metal contamination into the surrounding graphite matrix. For fission gases such as iodine and krypton, the contamination has some retention capability based on GA experimental data for temperatures up to 1600 °C.

The diffusion model FRESCO (Ref. 8) is used in KFA/ISF calculations to predict the release of radionuclides from heavy metal contamination. The given fraction of heavy metal contamination is assumed to be homogeneously distributed in the matrix graphite of the spherical fuel element in the initial state. The diffusive release from the fuel element is then calculated according to the transport data recommended in Ref. 6. For metallic radionuclides, "effective" diffusion coefficients have been derived by Hoinkis in experiments with irradiated A3 matrix graphite (Ref. 10). For iodine transport in matrix graphite, a distinction is made between graphite grains (which initially contain the heavy metal contamination) and grain boundaries. Diffusion data for iodine (and fission gases) in the grains have been experimentally found by Müller at low temperatures (Ref. 11). The iodine transport out of the grains onto the grain boundaries is supposed to be very quick at temperatures > 1250 °C, no retention capability

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is assumed. Experiments with iodine and fission gases similar to those performed by GA, but for matrix graphite, are planned in the near future.

The FRESCO model predicts release from the spherical fuel element resulting from heavy metal contamination. The approach used in SORS predicts the release from the contamination followed by transport of those radionuclides through the graphite. Because of the significant differences in the definition and approach used in modeling release from contamination, a quantitative comparison was judged to be inappropriate under this task since the focus of this task is the fuel particle and not the fuel element where retention and diffusion in graphite is important. This comparison could be performed under PWS S-7.

3.2.2 Standard Particles

According to GA modeling, standard (=intact) particles are of non-releasing type for all relevant metallic and gaseous fission products except for silver.

KFA/ISF modeling, however, assumes in its reference method a diffusive transport also through an intact coating described by temperature dependent transport data.

3.2.3 Exposed Kernels

The only resistance to radionuclide release from an exposed kernel is the fuel kernel itself. All other coatings are breached and assumed to offer no resistance to fission product transport.

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The US model for radionuclide release from exposed kernels contained in SORS (Ref. 1) distinguishes between metallic and gaseous nuclide species. Fickian diffusion is used to model fission metal release through the fuel kernel. The diffusion coefficients for the various nuclide groups are described using Arrhenius relationships dependent only on temperature. In some cases, the relationship consists of two branches: one branch with a lower activation energy at lower temperature, and a second branch with a higher activation energy at high temperature. Fission gas release from exposed kernels is modeled by the US using a diffusion-trapping model based on experimental data on constrained failed particles (Ref. 12).

The KFA/ISF reference method to calculate radionuclide release from exposed kernels under accident conditions is part of the diffusion model FRESCO (Ref. 8) since failed particles are handled like exposed kernels in this model. There is no distinction in the modeling approach between metallic fission products and fission gases (iodine). "Effective" transport data have been derived for both groups from heating experiments with UO_2 particle kernels which had a buffer layer only (Ref. 13). The recommended diffusion coefficients for cesium and iodine consist of a two-branch Arrhenius equation each (Ref. 6).

Both the GA and KFA/ISF models for release from exposed kernels are based on diffusion processes and are comparable in the benchmark problem. However, the data bases and diffusion models were developed independently.

3.2.4 Particles with Failed SiC Layer and Intact OPyC Layer

The Integrated Failure and Release Model for Standard Particles and its revision, respectively, (Refs. 2 + 5) define the cesium release to be equal to the fraction of particles with a failed SiC layer, but the OPyC layer of which still remains intact. Such particles are thus of releasing type for metallic fission pro-

3. QUALITATIVE COMPARISON OF US AND FRG FUEL PARTICLE FAILURE AND RADIONUCLIDE RELEASE MODELS

ducts (for which a retention in pyrocarbon is neglected) but tend to retain gaseous fission products (and iodine) within an intact OPyC layer.

Comparing the diffusion coefficients for the different coating layers shows that the SiC interlayer is the most retentive barrier of the particle. In case of a defective SiC layer, metallic fission product release from a particle is well (conservatively) approximated by the release from an exposed kernel. Transport of gaseous nuclides through an intact OPyC layer is described by the above mentioned two-component diffusion coefficient; it is practically negligible at MHTGR accident temperature conditions.

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Table 3.1: Summary of Presented Calculation Models			
Model	Code	User	Remark
Integrated Failure and Release Model for Standard Particles (also called: Statistical Model) Original Version from 1985	SORS	GA	Reference Method for Particle Failure and Radionuclide Release
	PANAMA-II	KFA/ISF	
Integrated Failure and Release Model for Standard Particles (also called: Statistical Model) Revised Version from 1988	SORS	GA	
	PANAMA-III	KFA/ISF	
Pressure Vessel Failure Model	SORS	GA	
	PANAMA-I	KFA/ISF	Reference Method for Particle Failure
Diffusion Model	SORS	GA	Reference Method for Diffusive Transport in Particle Kernel and Coatings
	FRESCO	KFA/ISF	Reference Method for Radionuclide Release

4. BENCHMARK PROBLEM

4.1 Definition of Benchmark Problem

A benchmark problem is a set of conditions for the fuel particle during a given accident transient for which the US and FRG fuel failure and release models can be applied and the results compared. The US MHTGR fuel particle design, quality and condition at the start of the transient were selected for use in the benchmark problem. The benchmark problem in this study is based upon a depressurized conduction cooldown accident (loss of coolant and loss of forced circulation accident in connection with a core heatup) in the MHTGR. The maximum fuel temperature is limited to around 1600 °C through passive heat removal by conduction and radiation to a reactor cavity cooling system surrounding the reactor vessel. Particle failure and radionuclide release is calculated with the US and FRG models for temperature histories representative of both the peak fuel location and the average fuel conditions.

4.2 Temperature Histories

The temperature histories used in the benchmark problem for comparing US and FRG models are based on the predicted peak and average temperatures during a depressurized conduction cooldown in the MHTGR. They are shown in Fig. 4-1 for the first 1000 h of the transient.

The location for the "maximum temperature" history is where the absolute peak temperature occurs during the transient. The maximum temperature history reaches its maximum of 1621 °C after 81 h and then gradually decreases to 1372 °C at 250 h and down to 782 °C after 1000 h. For the "average temperature" conditions, a particular location in the core was selected which has a temperature history similar to the average core temperature. The average temperature history peaks at 1224 °C after 90 h and then gradually decreases to

4. BENCHMARK PROBLEM

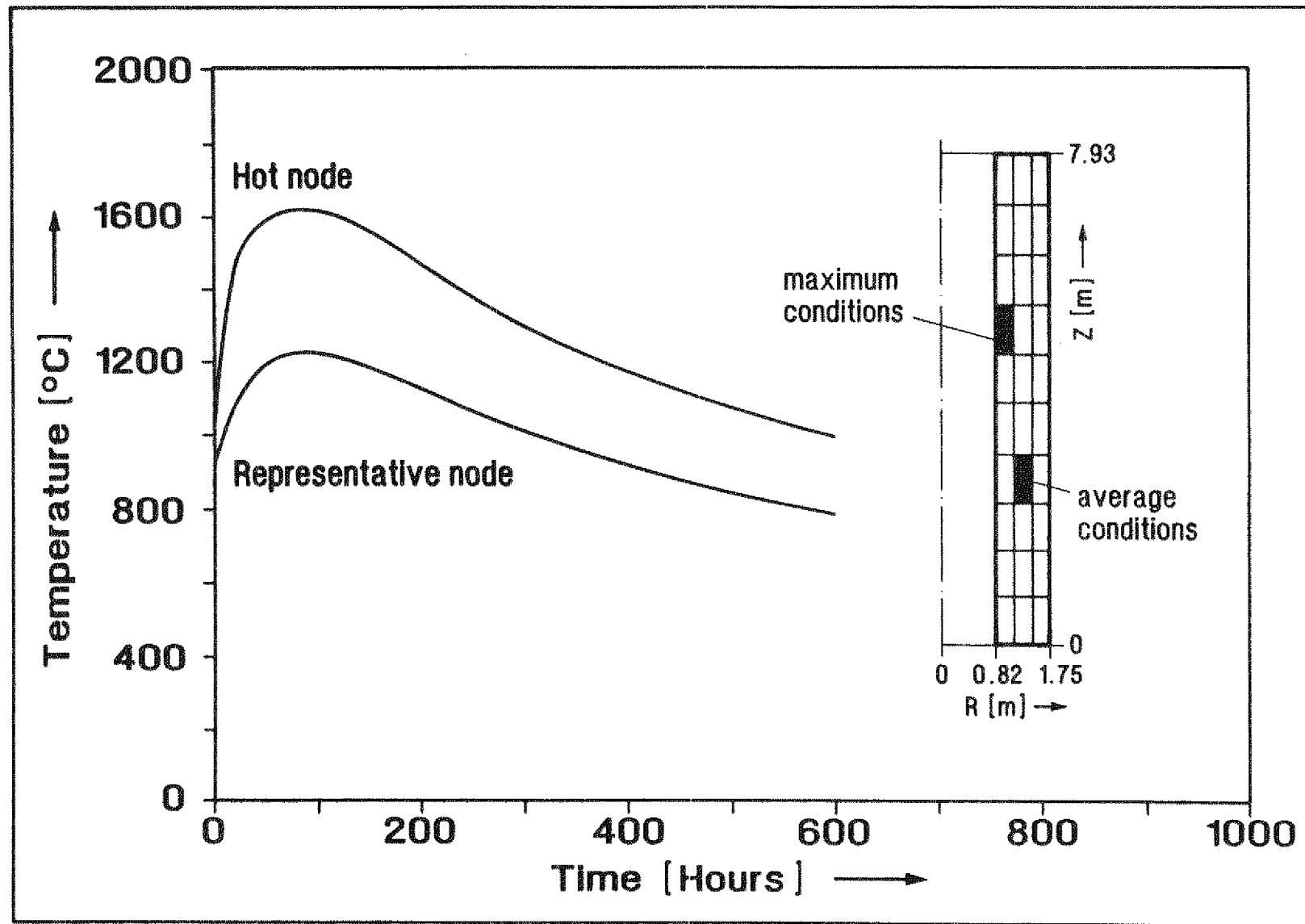


Fig. 4-1: Maximum and Average Temperature Histories for the Benchmark Problem

1053 °C at 250 h and down to 636 °C after 1000 h. The time-averaged temperature values in the first 250 hours are 1508 °C for the maximum temperature history and 1148 °C for the average temperature history.

A time of 250 hours has been selected for the comparisons in this study since beyond that time any additional fuel failure and radionuclide release is insignificant.

4.3 Initial Fuel Particle Conditions

The integrity of the US and FRG fuel at the start of an accident to be used in calculations for risk analyses is presented in Table 4-1. By far the majority of the particles are predicted to remain intact and contain all radionuclides.

US models for accident conditions assume that the fraction of particles with missing buffer layer fails completely during normal operation producing exposed kernels. For the other possible defective particles and for the standard particles, pressure vessel failure is insignificant for the operating conditions that the MHTGR or the HTR-Module experience.

The US value for exposed kernels at the start of an accident is $5 \cdot 10^{-5}$. The US also assumes an additional $6.1 \cdot 10^{-5}$ of the particles have a failed SiC layer, the most effective barrier against metallic release.

In FRG calculations performed at KFA/ISF, a particle fraction of $1.5 \cdot 10^{-5}$ with a defective coating due to manufacture (= half of the "free" uranium) is conservatively treated as exposed kernels. An additional particle fraction of $1 \cdot 10^{-4}$ (= expected value, = half of the target specification) is assumed in Ref. 6 to fail during normal operation by the end of life. The total failed fraction in KFA/ISF calculations for HTR fuel at the beginning of an accident is $6.5 \cdot 10^{-5}$ (= defect fraction in fresh fuel + half of the end-of-life value) being homogeneously distributed over the whole active core.

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Table 4-1: Comparison of US and FRG Fuel Integrity at the Start of an Accident Sequence

Defect or Failure	US	FRG
Heavy Metal Contamination	$1.0 \cdot 10^{-5}$	$1.5 \cdot 10^{-5}$
Exposed Kernels	$5.0 \cdot 10^{-5}$	$6.5 \cdot 10^{-5}$
Missing Buffer	0.	-
Defective SiC, Intact OPyC	$6.1 \cdot 10^{-5}$	-
Defective iPyC, Intact SiC	$3.0 \cdot 10^{-5}$	-
Defective OPyC, Intact SiC	$3.0 \cdot 10^{-2}$	-

These KFA/ISF assumptions for initial fuel particle conditions are a conservative choice made in 1986 (Ref. 6). New experience within the test program of modern German HTR fuel, however, has demonstrated the "free" uranium fraction in fresh fuel to be practically composed of defective particles only and a zero failure level for LEU fuel during irradiation leading to a design value of $2 \cdot 10^{-5}$ for the HTR-Module (Ref. 14).

Table 4-2: Assumed Initial Fuel Conditions for the Benchmark Problem

Parameter		
Irradiation Temperature	692 °C	Average Temperature History
	612 °C	Maximum Temperature History
Irradiation Time	1100 d	
Fast Neutron Fluence	$3.6 \cdot 10^{25} \text{ m}^{-2}$	
Burnup	15.3 % FIMA	
Fission Density	$5.8 \cdot 10^{26} \text{ m}^{-3}$	
SiC Layer Strength	480 MPa	After Irradiation
Weibull Parameter	5	After Irradiation

4. BENCHMARK PROBLEM

The focus of the benchmark problem is the fissile fuel particle which is selected to be based on the US reference fuel particle design using US fuel integrity at the start of the transient. The nominal specification of the fuel particle was presented in Table 2-1. The parameters that specify the initial fuel conditions and influence fuel particle failure and radionuclide release are presented in Table 4-2. The irradiation temperature differs between the maximum and average temperature history because different locations were selected to represent these histories.

With respect to the two different locations the model calculations refer to, they represent a volume of 1.61 m^3 at the hot node (= 2.7 % of the active core) and 2.16 m^3 at the average node (= 3.6 % of the active core). For the equilibrium cycle and assuming a uniform loading of the core, the number of particles at these specific locations is estimated to be $2.3 \cdot 10^8$ fissile and $1.3 \cdot 10^8$ fertile particles at the hot node and $1.7 \cdot 10^8$ fissile and $1.4 \cdot 10^8$ fertile particles, respectively, at the location with average conditions.

4. BENCHMARK PROBLEM

5. BENCHMARK COMPARISON OF FUEL PARTICLE FAILURE MODELS

The results of both GA and KFA/ISF fuel particle failure models are compared in this section. The comparison comprises

1. GA and KFA/ISF version of the 1985 Integrated Failure and Release Model for Standard Particles
2. GA and KFA/ISF version of the 1988 revision of the Integrated Failure and Release Model for Standard Particles
3. GA and KFA/ISF version of a pressure vessel failure
4. Comparison of all particle failure models

The benchmark comparison considers both the maximum and average fuel temperature histories.

5.1 1985 Integrated Failure and Release Model for Standard Particles

Both the KFA/ISF PANAMA-II (Ref. 6) and GA SORS (Ref. 1) methods for predicting the fraction of TRISO particles with SiC coating failures under accident conditions are based upon the 1985 Integrated Failure and Release Model for Standard Particles (Ref. 2), as discussed in Section 3.1. Therefore, results from the PANAMA-II and SORS codes should be similar with the exception of possible differences in coding techniques for the numerical solution.

Results for both "corrosion" and "thermal decomposition" failure mechanisms from the 1985 model are shown in Figures 5-1 and 5-2 for the maximum and average temperature histories, respectively. The SiC failure fractions after 250 hours of a conduction cooldown transient in the MHTGR are shown in Table 5-1 below.

5. BENCHMARK COMPARISON OF FUEL PARTICLE FAILURE MODELS

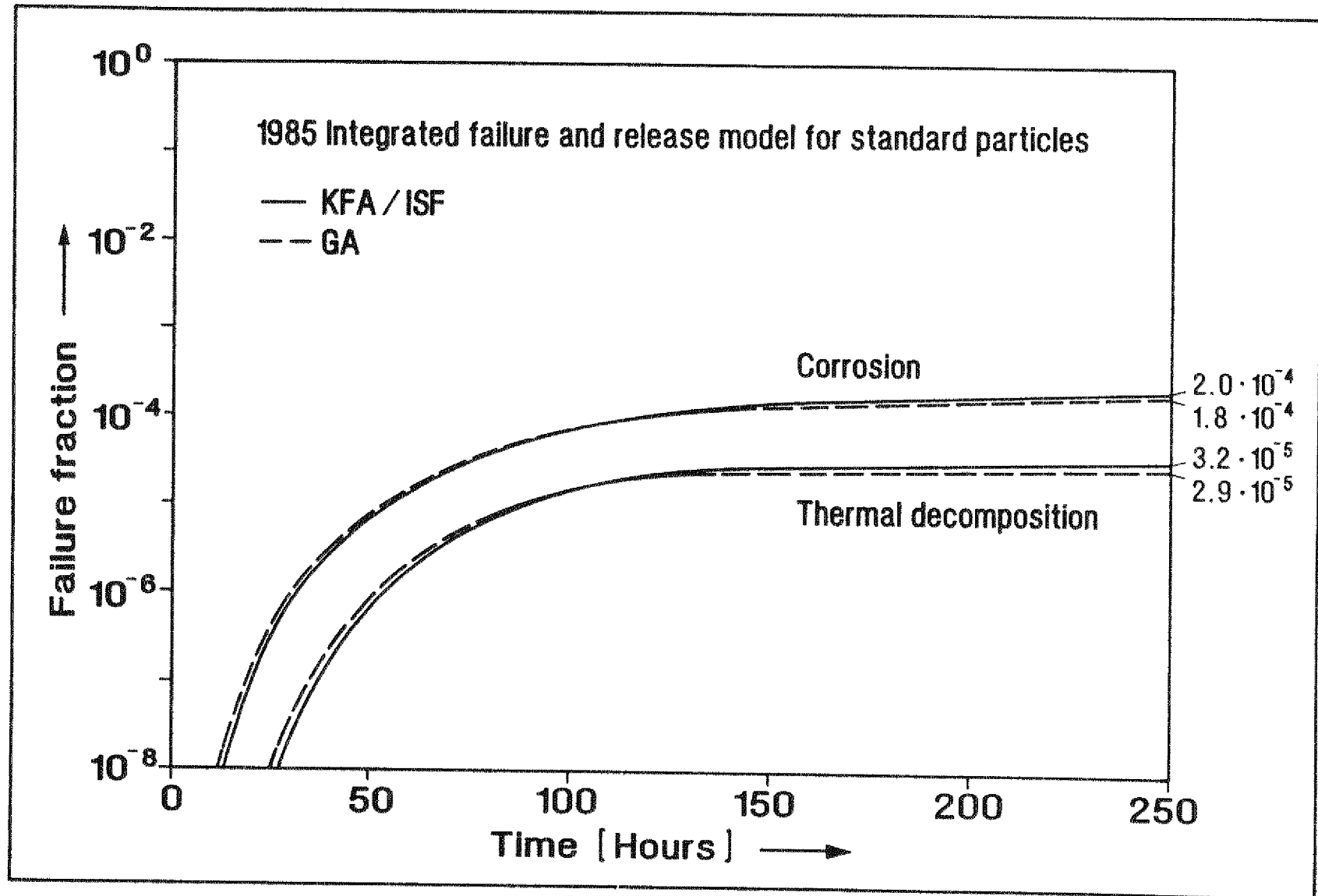


Fig. 5-1: Fuel Particle Failure for the Maximum Temperature History
Using the 1985 Integrated Failure and Release Model for
Standard Particles

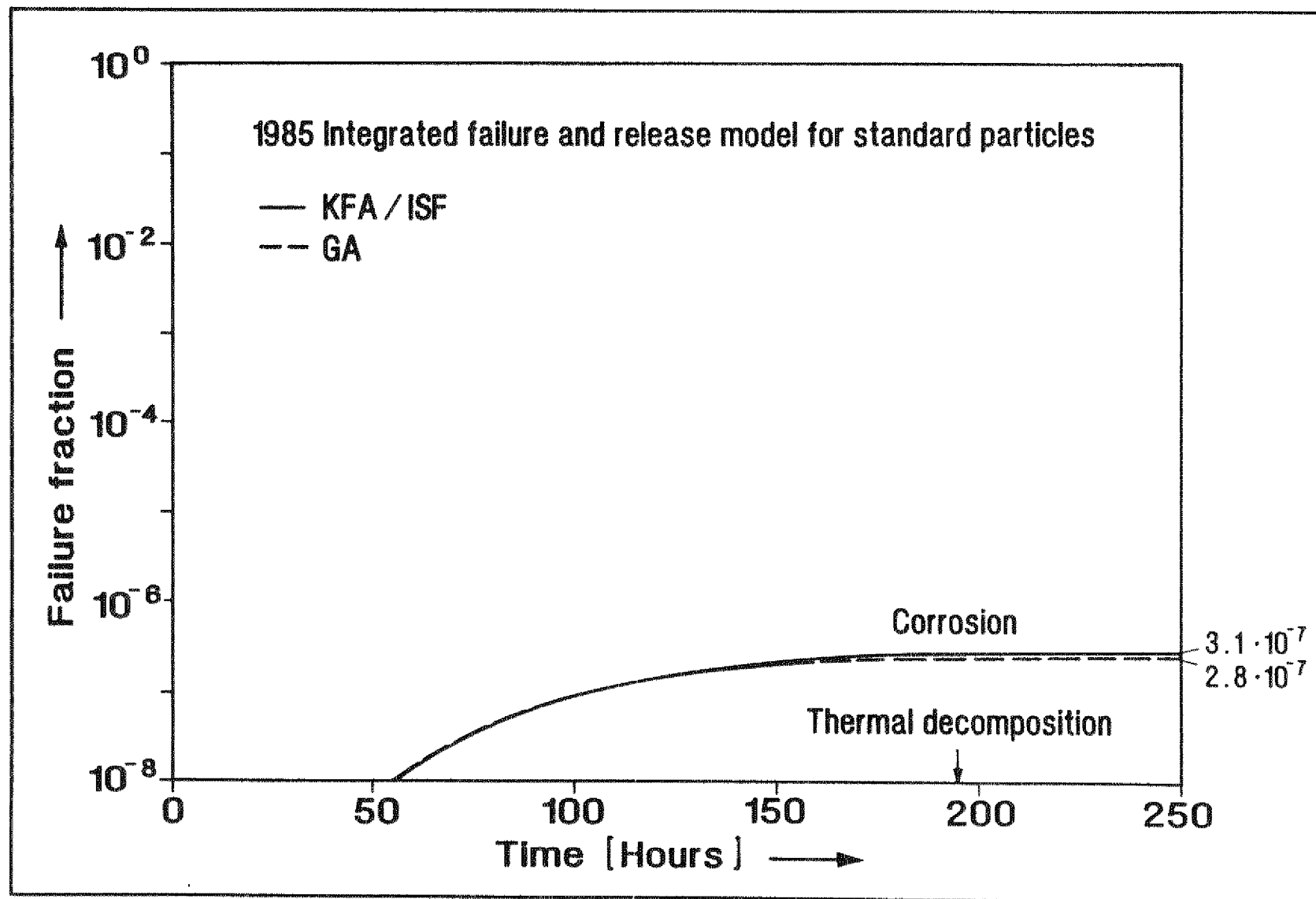


Fig. 5-2: Fuel Particle Failure for the Average Temperature History
Using the 1985 Integrated Failure and Release Model for
Standard Particles

Table 5-1: Comparison of GA and KFA/ISF Results on Failure Fractions with the 1985 Integrated Failure and Release Model for Standard Particles

Code	SiC Failure Fraction	
	Corrosion	Thermal Decomposition
<i>Maximum Temperature</i>		
SORS (GA)	1.8×10^{-4}	2.9×10^{-5}
PANAMA-II (KFA/ISF)	2.0×10^{-4}	3.2×10^{-5}
<i>Average Temperature</i>		
SORS (GA)	2.8×10^{-7}	$< 10^{-8}$
PANAMA-II (KFA/ISF)	3.1×10^{-7}	$< 10^{-8}$

The reason for the small differences between the two curves for each failure mechanism can be explained by the size of the time steps and the temperature value used within a time step. The PANAMA-II code interpolates the temperature value at the middle of the time step, while SORS utilizes the temperature at the end of the time step. The resulting fuel failure in SORS is slightly higher during the temperature rise until the maximum temperature has been reached and slightly lower thereafter.

The low fraction of particles with failed SiC layer due to thermal decomposition for the average temperature history is below scale because of the high activation energy of this degradation process and because of the low accident temperatures.

Agreement between the GA and KFA/ISF results provides verification that the independently developed codes are evaluating the 1985 model accurately.

5. BENCHMARK COMPARISON OF FUEL PARTICLE FAILURE MODELS

5.2 1988 Revision of the Integrated Failure and Release Model for Standard Particles

The calculated results for the MHTGR conduction cooldown accident with the 1988 revision of the Integrated Failure and Release Model for Standard Particles (Ref. 5) are shown in Fig. 5-3. These curves were generated using preliminary updates of PANAMA-II ($\rightarrow$ PANAMA-III) and SORS which include the 1988 revision of the model. The curves only show SiC failure fractions predicted for the maximum temperature history because the failure fractions for the average temperature history were found to be negligible. The failure fractions determined for the maximum temperature history after 250 hours are shown in Table 5-2 below.

Table 5-2: Comparison of GA and KFA/ISF Results on Failure Fractions with the 1988 Revision of the Integrated Failure and Release Model for Standard Particles

Code	SiC Failure Fraction
<i>Maximum Temperature</i>	
SORS (GA)	$2.7 \cdot 10^{-5}$
PANAMA-III (KFA/ISF)	$3.1 \cdot 10^{-5}$
<i>Average Temperature</i>	
SORS (GA)	$< 10^{-8}$
PANAMA-III (KFA/ISF)	$< 10^{-8}$

As discussed in Section 3.2, thermal decomposition is the only degradation process considered in the revised model. Due to its high activation energy, fuel failure fractions are negligible at low temperatures, as shown in results for the average temperature history (which were estimated to be less than 10^{-11}). The $6 \cdot 10^{-6}$ lower recommended fuel failure limit is not exceeded before around 80

5. BENCHMARK COMPARISON OF FUEL PARTICLE FAILURE MODELS

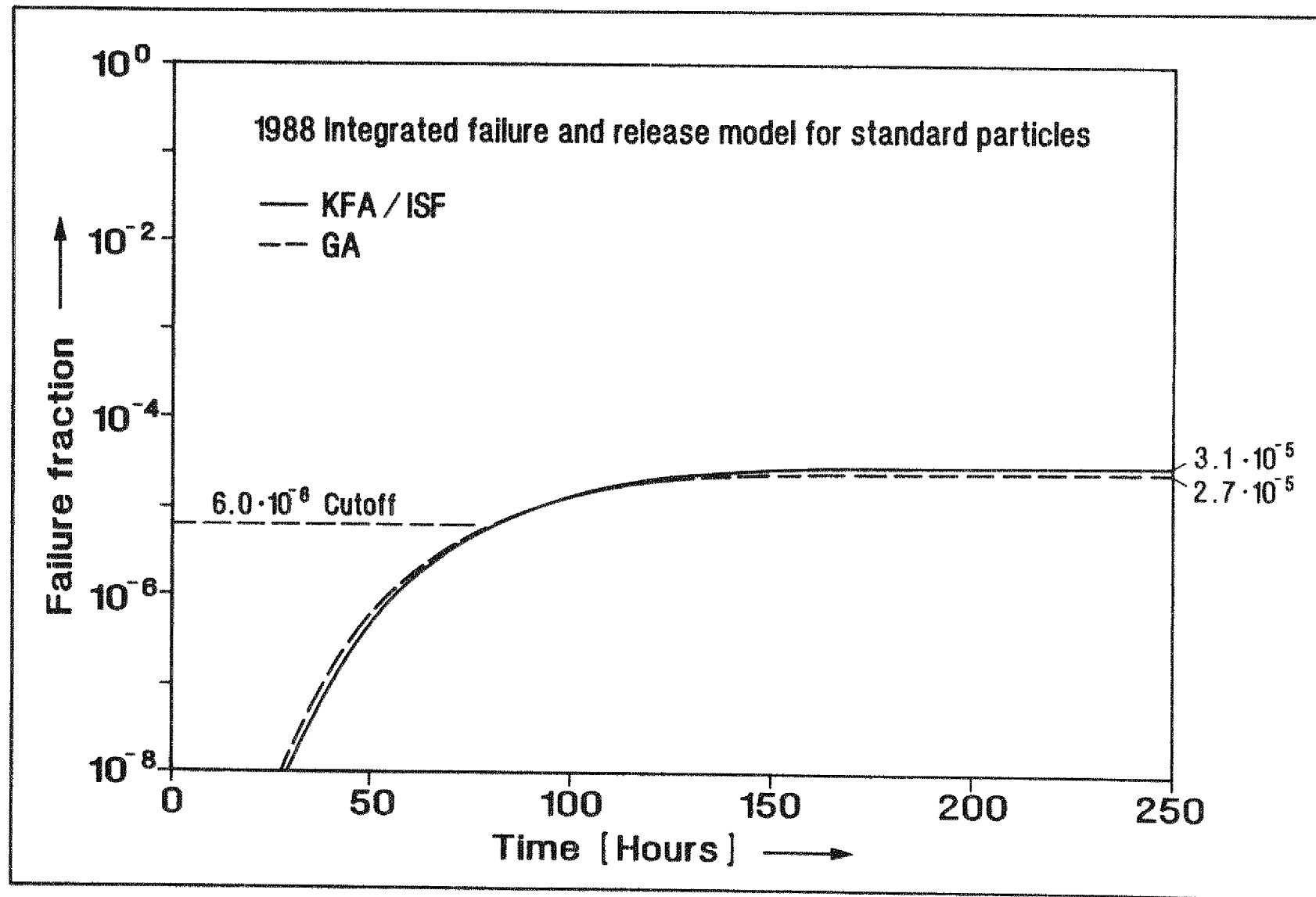


Fig. 5-3: Fuel Particle Failure for the Maximum Temperature History
Using the 1988 Revision of the Integrated Failure and Release
Model for Standard Particles

hours after start of the accident under maximum temperature conditions. However, it will not be reached at all by most parts of the active MHTGR core during a core heatup accident.

Agreement between the GA and KFA/ISF results provides verification that the independently developed codes are evaluating the 1988 model accurately.

5.3 Pressure Vessel Model

The GA and KFA/ISF method for the determination of the pressure vessel failure of TRISO particles under accident conditions comprise different failure mechanisms. The GA pressure vessel model as one failure mechanism consists of a simplified failure function which is dependent on temperature only. Corrosion and thermal decomposition induced particle failure described in the Standard Particle Failure and Release Model (Refs. 2 + 5) is added to pressure vessel failures to predict a total failure fraction. In contrast, the KFA/ISF reference method incorporates all these failure mechanisms in the pressure vessel model PANAMA-I (Ref. 4). Nevertheless, the single contributions can be separated to perform a reasonable comparison with the GA pressure vessel model. The results of the calculations are shown in Fig. 5-4 for the maximum temperature history and in Fig. 5-5 for the average temperature history.

With the assumptions for an intact US reference fissile fuel particle with an average burnup of 15.3 % FIMA (Table 4-2), the **GA pressure vessel model** leads to particle failure fractions listed in Table 5-3. The accumulated failure fraction reaches its maximum as soon as the fuel has reached its peak temperature of 1621 °C after 81 h for the hot node (Fig. 5-4) and 1224 °C after 90 h, respectively, for the average node (Fig. 5-5). No subsequent particle failure will be expected.

The **KFA/ISF pressure vessel model PANAMA-I** (Ref. 4) after insertion of the US reference fissile particle features such as geometry, a zero oxygen pro-

5. BENCHMARK COMPARISON OF FUEL PARTICLE FAILURE MODELS

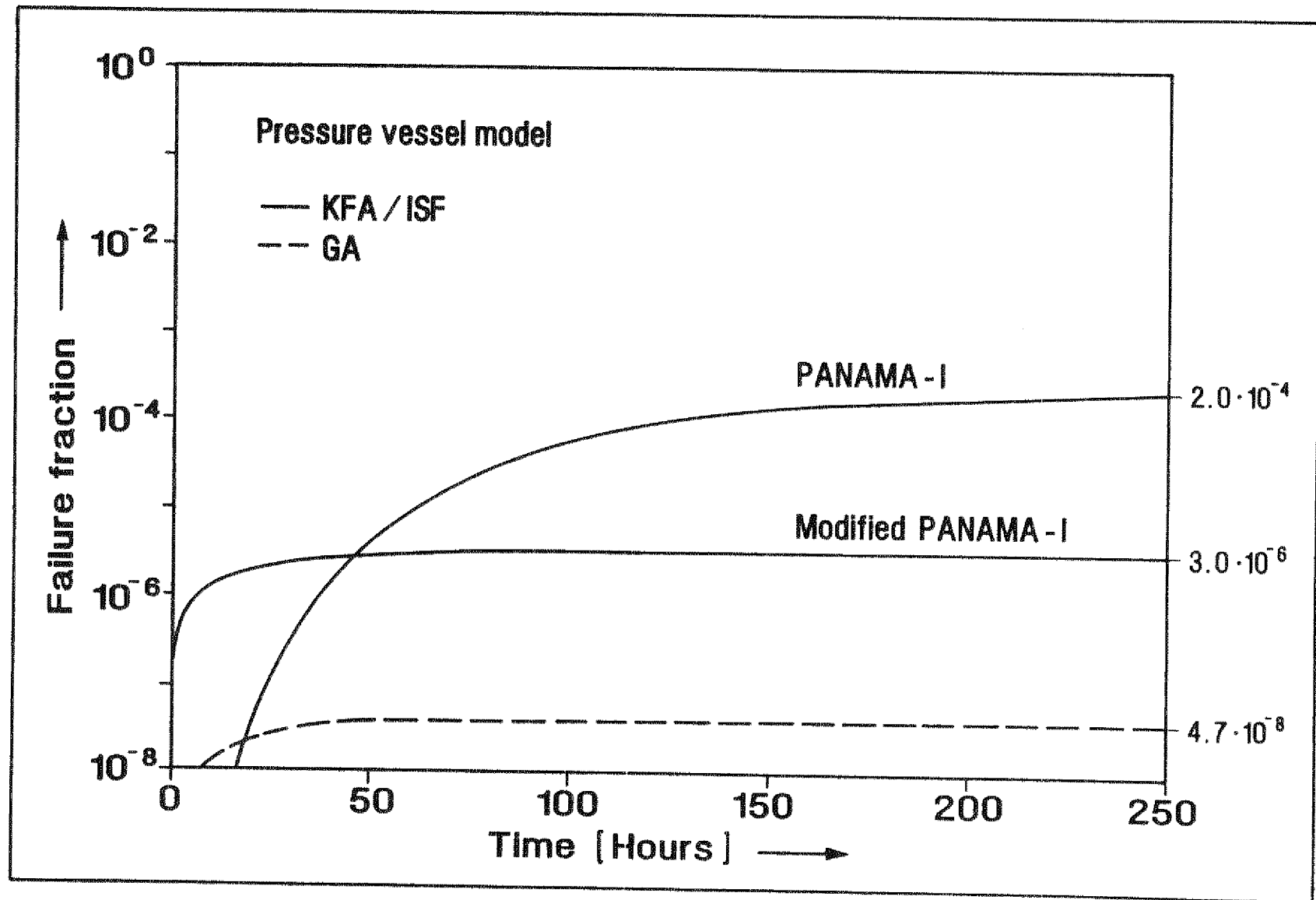


Fig. 5-4: Fuel Particle Failure for the Maximum Temperature History
 Using the Pressure Vessel Model

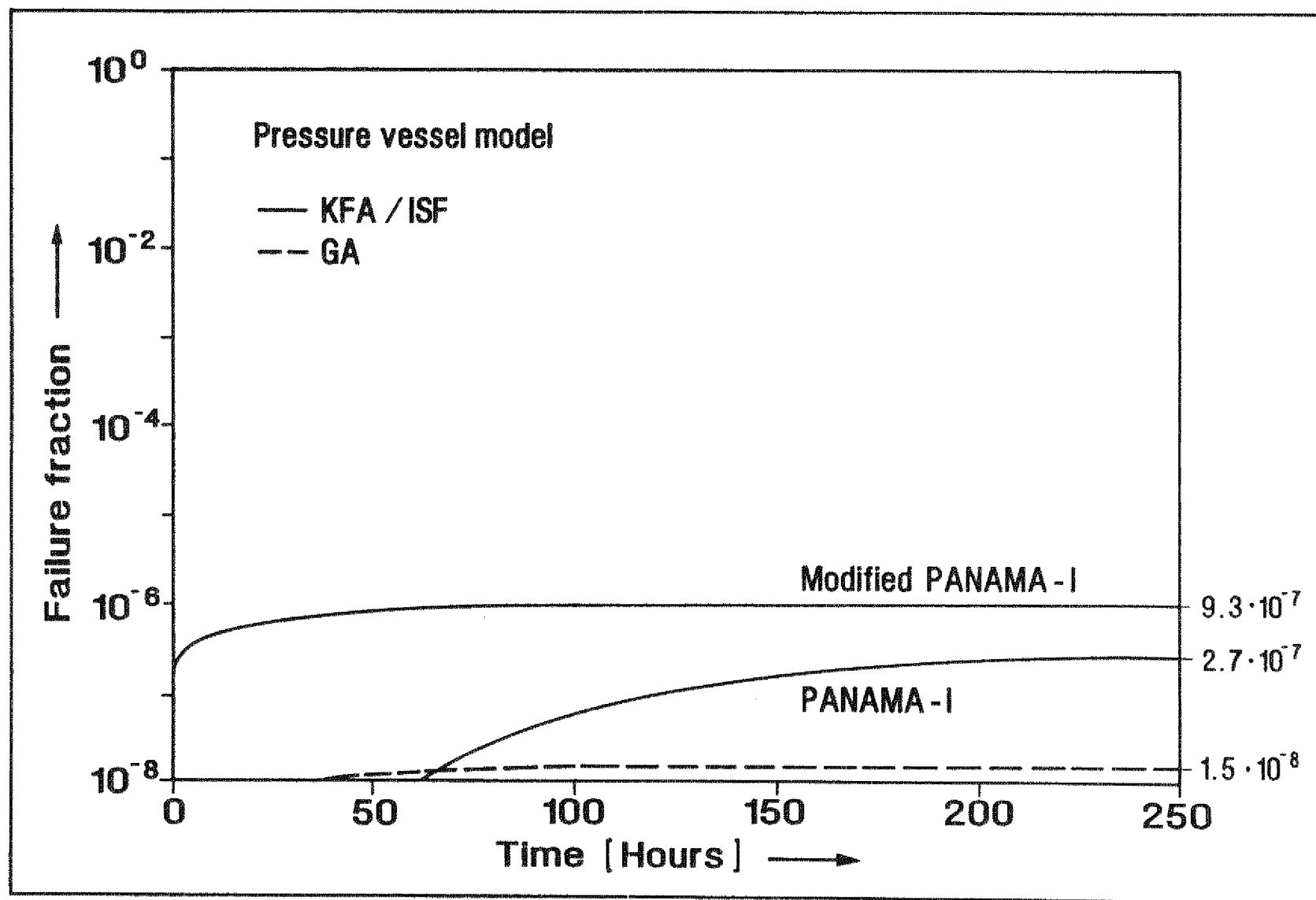


Fig. 5-5: Fuel Particle Failure for the Average Temperature History
Using the Pressure Vessel Model

duction in UCO, and the initial fuel conditions given in Table 4-2, leads to the following fractions of failed particles after 250 h (upper KFA/ISF curve in Fig. 5-4, lower KFA/ISF curve in Fig. 5-5):

Table 5-3: KFA/ISF Results on Failure Fractions with its Reference Pressure Vessel Failure Model

Code	SiC Failure Fraction
<i>Maximum Temperature</i>	
SORS (GA)	$4.7 \cdot 10^{-8}$
PANAMA-I (KFA/ISF)	$2.0 \cdot 10^{-4}$
<i>Average Temperature</i>	
SORS (GA)	$1.5 \cdot 10^{-8}$
PANAMA-I (KFA/ISF)	$2.7 \cdot 10^{-7}$

These results may be partly due to at least two different modeling assumptions used in the KFA/ISF and GA pressure vessel calculations. These assumptions are:

- Fission Gas Release from the Kernel

While the US pressure vessel model assumes a constant fraction of kernel fission gas release during the whole accident sequence, the KFA/ISF calculation determines the temperature and time dependent gas release from the kernels according to the Booth type model.

- SiC Corrosion

The KFA/ISF pressure vessel equation has an additional time dependent expression that describes the corrosion attack of fission products on the SiC layer using Montgomery experimental data (Ref. 3). (This failure mechanism is regarded separately in GA modeling.)

5. BENCHMARK COMPARISON OF FUEL PARTICLE FAILURE MODELS

Adjusting PANAMA-I for the US assumption of a constant fission gas release from the particle kernels and removing the corrosion term, removes these two differences ("modified PANAMA-I"). A comparison was then made which shows that the peak failure fraction due to this "pure" pressure vessel failure reached after 81 h (average node: 90 h) is then calculated to be (GA curves and lower KFA/ISF curve in Fig. 5-4, upper KFA/ISF curve in Fig. 5-5):

Table 5-4: Comparison of GA and KFA/ISF Results on Failure Fractions with the "Pure" Pressure Vessel Failure Model

Code	SiC Failure Fraction
<i>Maximum Temperature</i>	
SORS (GA)	4.7×10^{-8}
Modified PANAMA-I (KFA/ISF)	3.0×10^{-6}
<i>Average Temperature</i>	
SORS (GA)	1.5×10^{-8}
Modified PANAMA-I (KFA/ISF)	9.3×10^{-7}

Under both temperature conditions, the discrepancy is almost two orders of magnitude, but the absolute failure values are still negligible compared to other coating failure phenomena (see Section 5.2).

In summary, some of the differences between the KFA/ISF and GA pressure vessel models have been identified but others still exist. This area would require further effort to resolve. However, the importance of pressure vessel failure is put into perspective by comparing Figs. 5-4 and 5-6. These results show that the "pure" pressure vessel failure of particles plays a subordinate role in the given MHTGR accident scenario.

The thermal decomposition failure mechanism in PANAMA-I as discussed is an empirical approach (see equation 3-8) describing the high temperature fail-

5. BENCHMARK COMPARISON OF FUEL PARTICLE FAILURE MODELS

ure behavior either for unbonded particles or for particles embedded in a fuel sphere. Postcalculations for unbonded particles have shown a good agreement with GA and KFA experimental work for US fuel based on data well above 1600 °C. However, its extrapolation into the MHTGR/HTR accident temperature range down to 1600 °C and lower is not justified and is, therefore, not regarded in the comparison.

5.4 Comparison of All Particle Failure Models

Fig. 5-6 compares values predicted both with the pressure vessel failure model as the classical approach (KFA/ISF reference) and with the 1985 and 1988 versions of the Integrated Failure and Release Model for Standard Particles as a new and qualitatively different approach (GA reference).

The comparison between the two versions of the Integrated Failure and Release Model reveals that the particle failure fractions are predicted to be lower with the 1988 model. These results seem to be in contrast with results from the 1600 °C heating experiments in which failure fractions predicted with the new model were higher than those predicted with the old model and in good agreement with the measurements. The 1988 model is expected to predict lower failure fractions under MHTGR accident temperature transients because the time interval with sufficiently high temperatures - as compared to being sustained for hours during the heating tests - to cause higher degradation rates compared to the 1985 model is too short in a core heatup scenario to become dominant.

The comparison between the deterministic method of the KFA/ISF pressure vessel model and the 1985 Integrated Failure and Release Model shows that for the given core heatup scenario, the pressure vessel model results in about the same failure fraction after 250 hours. This result can be explained by the fact that despite the different modeling approaches of PANAMA-I and SORS, both codes contain an expression for silicon carbide corrosion based on Montgomery (Ref. 3) which is the dominant SiC degradation process under the given temper-

5. BENCHMARK COMPARISON OF FUEL PARTICLE FAILURE MODELS

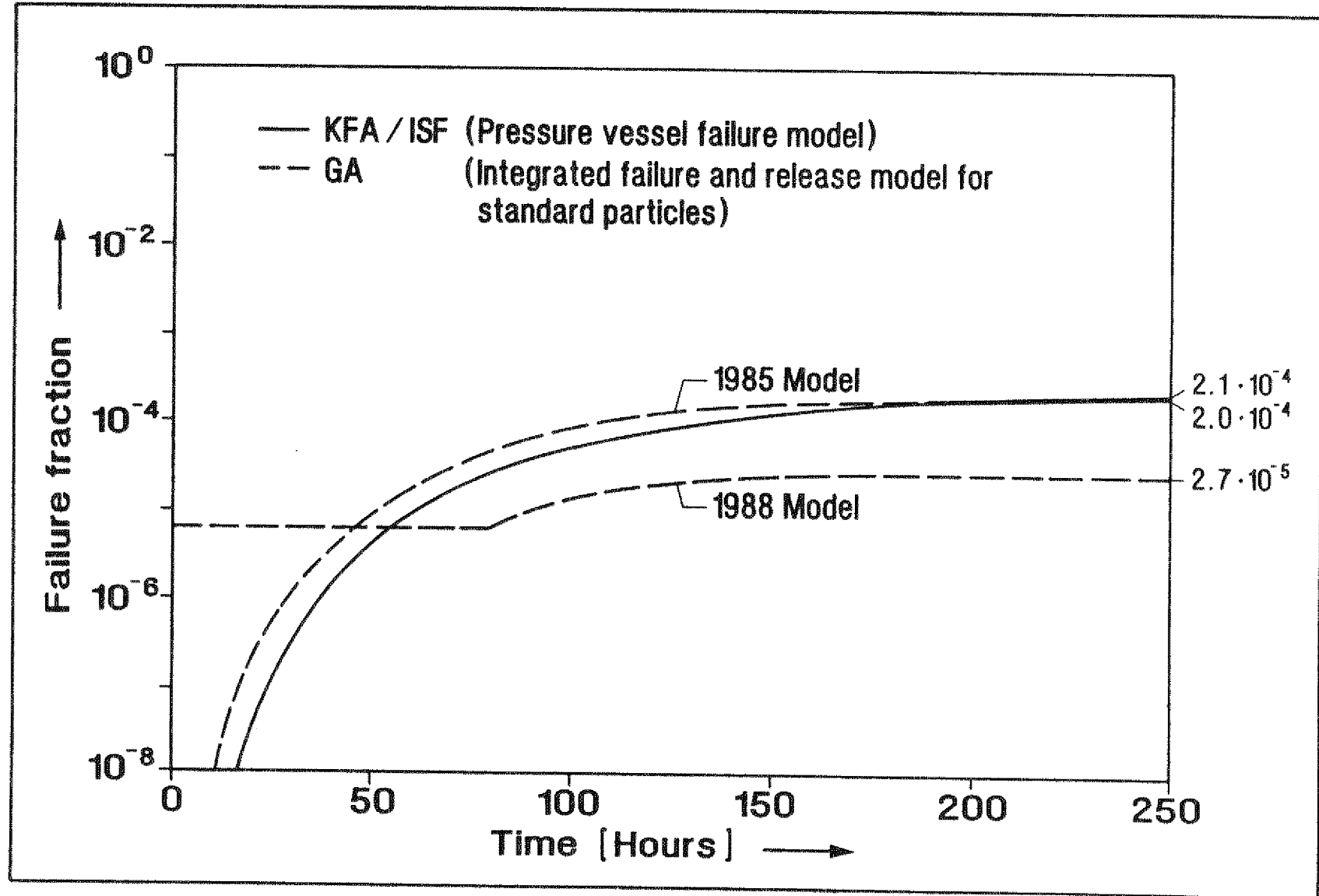


Fig. 5-6: Comparison of Fuel Particle Failure for the Maximum Temperature History Using the 1985 and 1988 Integrated Failure and Release Model for Standard Particles (GA Reference) and the Pressure Vessel Model (KFA/ISF Reference)

ature condition while the other phenomena ("pure" pressure vessel failure in PANAMA-I, thermal decomposition in SORS) are of minor importance.

However, the 1988 revision of the statistical model predicts a value lower by a factor of 7 - 8 than the reference KFA/ISF model. A reason for this difference is that the derivation of the 1988 model is based upon modern German HTR fuel while on the other hand, characteristic SiC data used in PANAMA-I for MHTGR fissile fuel have been chosen conservatively (see Table 4-2).

5. BENCHMARK COMPARISON OF FUEL PARTICLE FAILURE MODELS

6. BENCHMARK COMPARISON OF RADIONUCLIDE RELEASE MODELS

The results of both GA and KFA/ISF fission product release models are compared in this section. The comparison comprises

1. GA and KFA/ISF version of the 1985 Integrated Failure and Release Model for Standard Particles
2. GA and KFA/ISF version of the 1988 revision of the Integrated Failure and Release Model for Standard Particles
3. GA and KFA/ISF exposed fuel kernel release model
4. KFA/ISF standard particle diffusive release model
5. Comparison of all fission product release models

Fission product release from pressure vessel failed particles is not regarded in this section since the fraction of failed particles due to the "pure" pressure vessel was already found to be negligibly low. Failure fractions due to the extended PANAMA-I code (see Section 3.1.2) of KFA/ISF which are inserted in the FRESCO diffusion code to determine fission product release are handled in the same way as exposed particle kernels.

Each model is analyzed for two nuclides: iodine which illustrates gaseous radionuclide release and cesium which illustrates metallic radionuclide release. The benchmark comparison has both the maximum and average temperature histories.

6.1 1985 Integrated Failure and Release Model for Standard Particles

Both the KFA/ISF PANAMA-II (Ref. 6) and GA SORS (Ref. 1) methods for predicting the release fractions for cesium and krypton/iodine from HTGR fuel particles under accident conditions are based upon the 1985 Standard Particle Failure and Release Model (Ref. 2), as discussed in Section 3.2.

Release fractions due to both "corrosion" and "thermal decomposition" failure mechanisms from the 1985 model are shown in Figures 6-1 and 6-2 for cesium and iodine, respectively, under maximum temperature conditions. The release fractions after 250 hours of the conduction cooldown transient in the MHTGR are shown in Table 6-1 for cesium and in Table 6-2 for iodine.

6.1.1 Cesium Release

The GA version of the 1985 Integrated Failure and Release Model (Ref. 2) in the SORS code includes a particle kernel retention capability for cesium following SiC failure. The experiments that formed the basis of the 1985 statistical model were at high enough temperatures that the cesium was quickly released when the SiC failed. At the temperatures of interest during MHTGR thermal transients, data indicate significant cesium retention in the kernel such that the 1985 model was modified to incorporate this retention mechanism. Under the given maximum temperature conditions, the cesium retention by the particle kernels results in a release fraction being approximately a factor of 2 lower than the failure fraction.

The KFA/ISF code PANAMA-II is based on the 1985 model as proposed without considering a cesium holdup in the kernel. In the 1985 model, the fraction of particles with a failed SiC layer was defined to be equivalent to the fraction of cesium release from the fuel element (i.e. matrix graphite and OPyC layers were not assumed to retain cesium at elevated temperatures). Therefore, the KFA/ISF cesium release curves shown in Fig. 6-1 for the maximum temperature history, are identical to the failure fraction curves described in Section 5.

6. BENCHMARK COMPARISON OF RADIONUCLIDE RELEASE MODELS

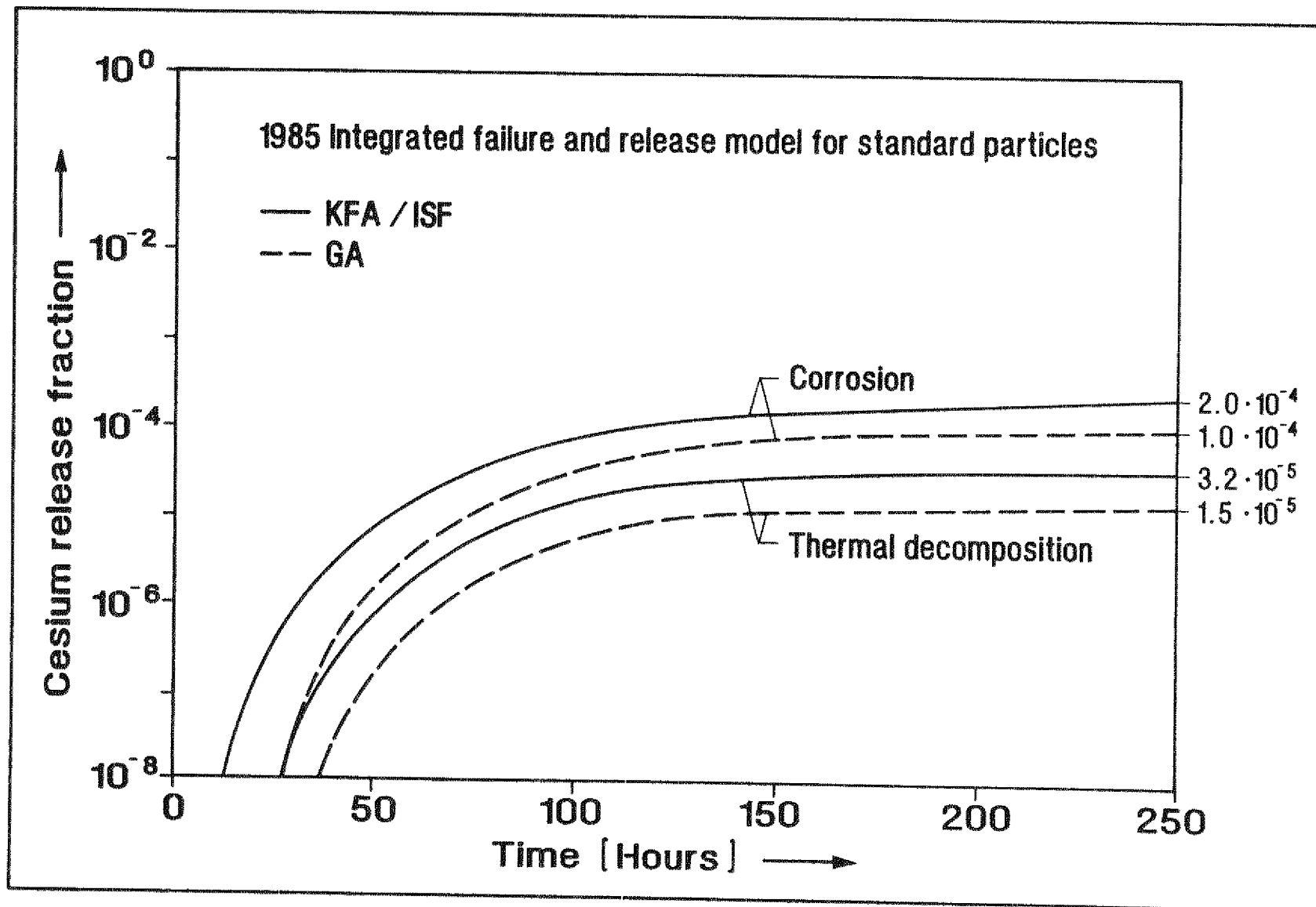


Fig. 6-1: Cesium Release from Fuel Particles Failed According to the 1985 Integrated Failure and Release Model for Standard Particles for the Maximum Temperature History

Table 6-1: Comparison of GA and KFA/ISF Results on Cesium Release with the 1985 Integrated Failure and Release Model for Standard Particles

Code	Cesium Release Fraction	
	Corrosion	Thermal Decomposition
<i>Maximum Temperature</i>		
SORS (GA)	$1.0 \cdot 10^{-4}$	$1.5 \cdot 10^{-5}$
PANAMA-II (KFA/ISF)	$2.0 \cdot 10^{-4}$	$3.2 \cdot 10^{-5}$
<i>Average Temperature</i>		
SORS (GA)	$< 10^{-8}$	$< 10^{-8}$
PANAMA-II (KFA/ISF)	$3.1 \cdot 10^{-7}$	$< 10^{-8}$

6.1.2 Iodine Release

The results for iodine release (see Table 6-2) from the GA model, which considers retention by the kernel and OPyC layer, indicated that for the maximum conduction cooldown temperature occurring, a small fraction of the iodine released by SiC corrosion and thermal decomposition mechanisms is escaping through the intact OPyC layer.

The KFA/ISF calculation based on the recommended diffusion coefficient for krypton in pyrocarbon (Ref. 6) predicts complete retention of iodine in the OPyC layer under the given time and maximum temperature conditions.

No iodine release is predicted for the average temperature history by either KFA/ISF or GA calculations.

6. BENCHMARK COMPARISON OF RADIONUCLIDE RELEASE MODELS

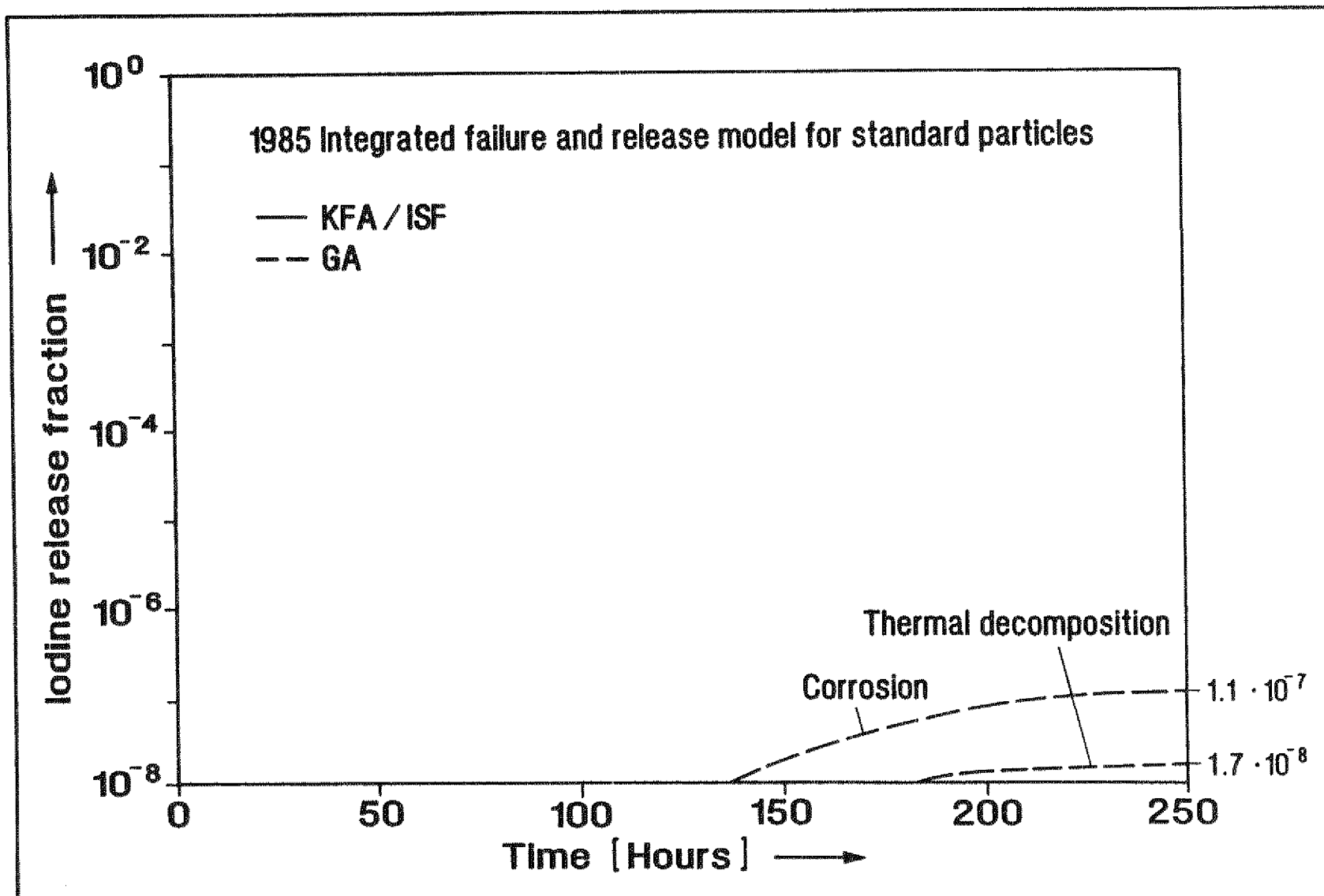


Fig. 6-2: Iodine Release from Fuel Particles Failed According to the 1985 Integrated Failure and Release Model for Standard Particles for the Maximum Temperature History

Table 6-2: Comparison of GA and KFA/ISF Results on Iodine Release with the 1985 Integrated Failure and Release Model for Standard Particles

Code	Iodine Release Fraction	
	Corrosion	Thermal Decomposition
<i>Maximum Temperature</i>		
SORS (GA)	$1.1 \cdot 10^{-7}$	$1.7 \cdot 10^{-8}$
PANAMA-II (KFA/ISF)	0.	0.

6.2 1988 Revision of the Integrated Failure and Release Model for Standard Particles

Although the failure fractions from the 1985 and 1988 versions of the Integrated Failure and Release Model differ (Refs. 2 + 5), the same models are used to predict fission product release from failed particles. Therefore, the conclusions regarding release that apply to the 1985 model also apply to the 1988 model.

6.3 Exposed Fuel Kernel Release Model

For the purpose of comparing the release calculations, the fraction of initially exposed fuel particle kernels was set at $5 \cdot 10^{-5}$. The calculated cesium release curves from the initially exposed kernels are shown in Figures 6-3 and 6-4, those for iodine are shown in Figures 6-5 and 6-6. The fractional release values after 250 hours in relation to the assumed fraction of particle kernels are summarized in Table 6-3.

6. BENCHMARK COMPARISON OF RADIONUCLIDE RELEASE MODELS

6.3.1 Cesium Release

The **KFA/ISF** modeling of the release behavior from defective or failed particles assumes that the transport is governed by diffusion from the exposed particle kernel into the graphite (Ref. 6). The results only exhibit fission product release from the particle kernels during the accident transient. The calculation for the maximum temperature history indicates that the exposed kernels have almost lost their total cesium inventory within 100 hours. The cesium release from the exposed kernels for the average temperature history increases more slowly. After 250 hours, the fraction of cesium outside the kernel is $2.1 \cdot 10^{-5}$, which corresponds to approximately 60 % of the initial cesium inventory within the exposed fuel kernel.

The corresponding **GA** cesium release curve for the maximum temperature history rises more rapidly during the initial stages of the transient, but then slows down and remains below the **KFA/ISF** curve. After 250 hours, the cesium release fraction is $2.5 \cdot 10^{-5}$ which is 50 % of the initial cesium inventory of the exposed kernels and is a factor of 2 lower than the 100 % release predicted with the **KFA/ISF** diffusion model. The predicted release fraction from exposed particle kernels after 250 hours for the average temperature history is $1.4 \cdot 10^{-5}$, which is a factor of 1.5 lower than values predicted with the **KFA/ISF** models.

6. BENCHMARK COMPARISON OF RADIONUCLIDE RELEASE MODELS

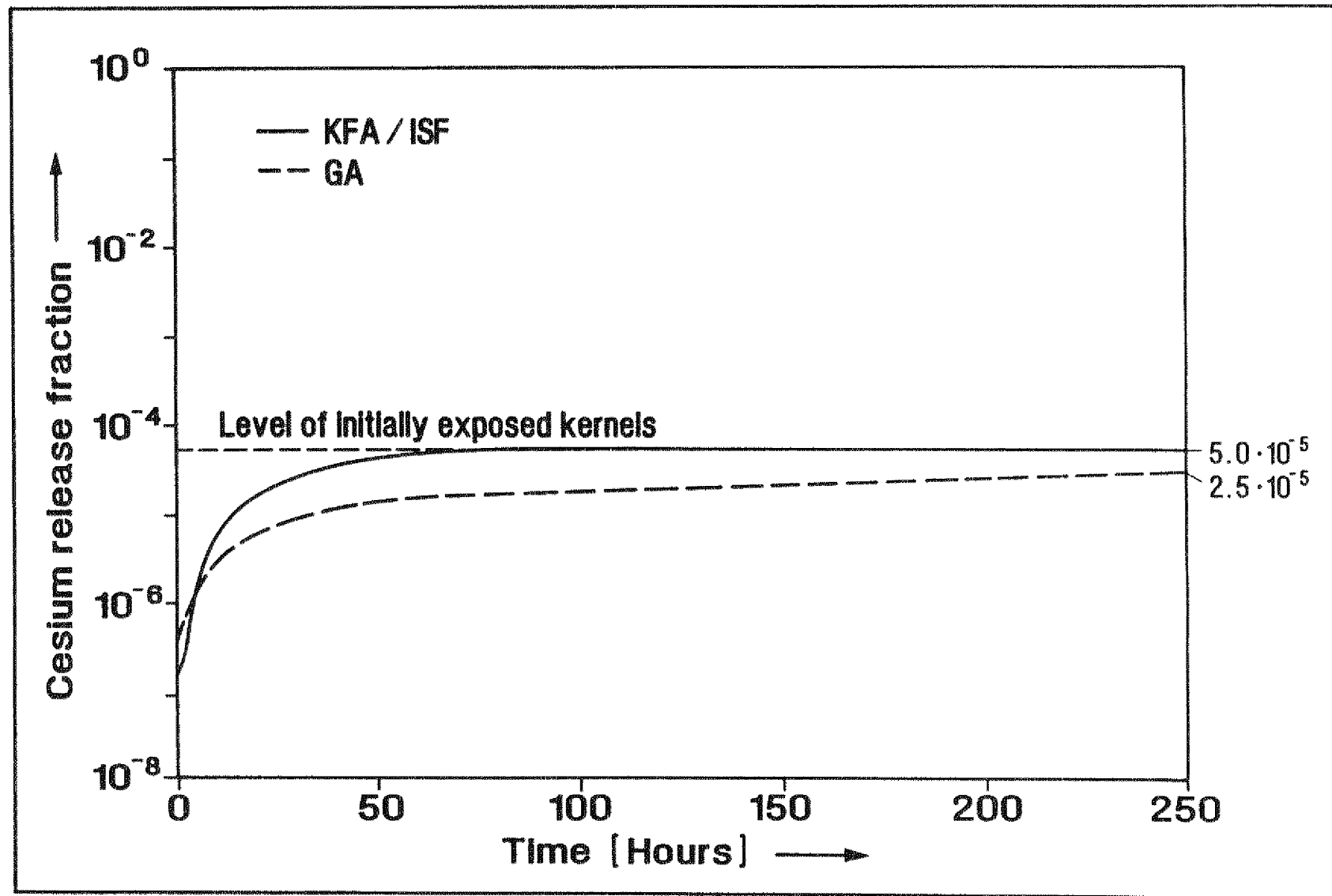


Fig. 6-3: Cesium Release from Exposed Particle Kernels
for the Maximum Temperature History

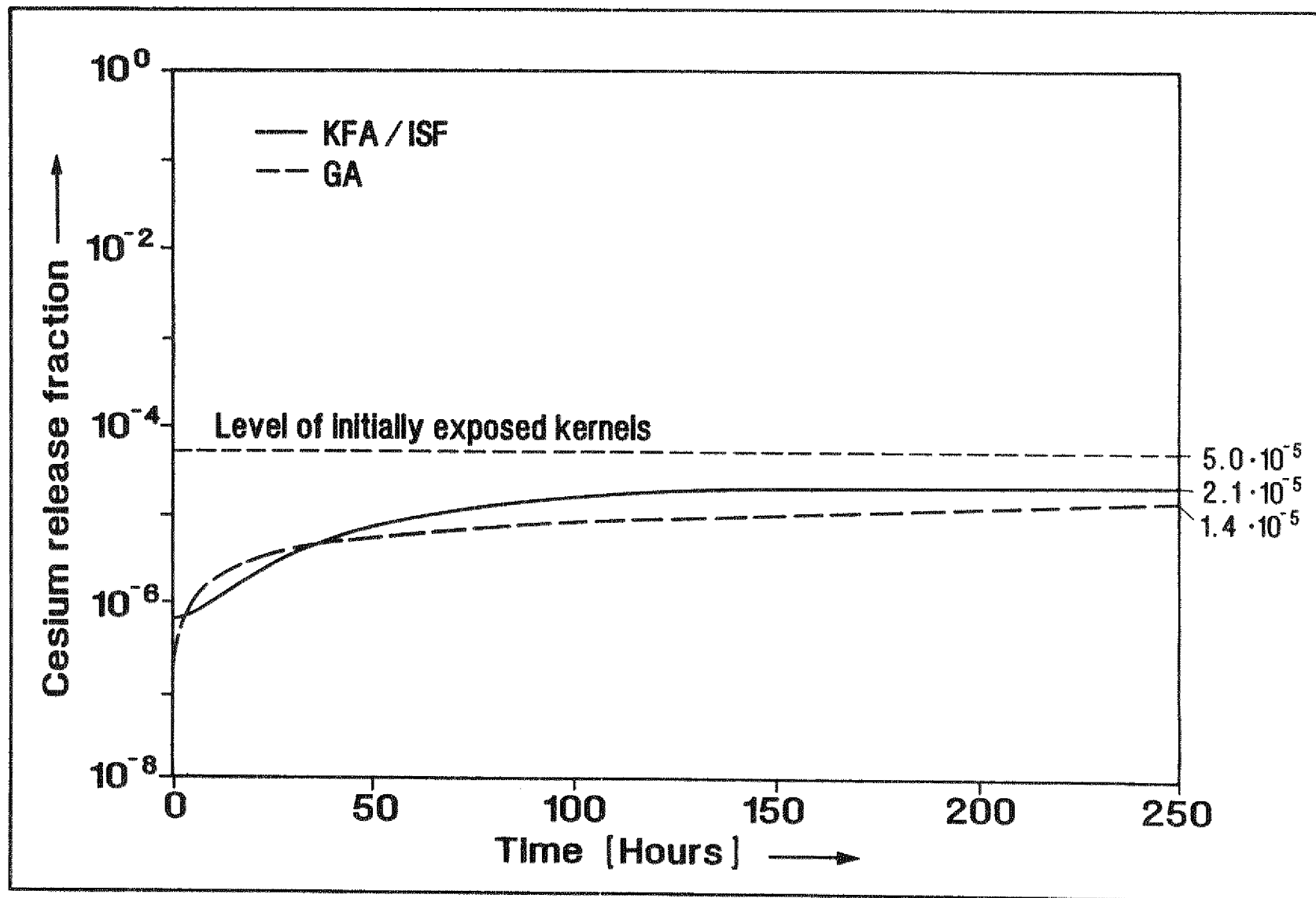


Fig. 6-4: Cesium Release from Exposed Particle Kernels
for the Average Temperature History

Table 6-3: Comparison of GA and KFA/ISF Results on Release Fractions from Exposed Particle Kernels (in Relation to the Assumed Defect Fraction of $5 \cdot 10^{-5}$) after 250 h

Code	Release Fraction [%]	
	Cesium	Iodine
<i>Maximum Temperature</i>		
SORS (GA)	50	56
FRESCO-II (KFA/ISF)	100	90
<i>Average Temperature</i>		
SORS (GA)	28	2
FRESCO-II (KFA/ISF)	42	11

6.3.2 Iodine Release

A similar conclusion as for cesium can be drawn about iodine release from the initially exposed particle kernels based upon the results shown in Figures 6-5 and 6-6. According to the **KFA/ISF** diffusion model, iodine transport should be slower than cesium in the kernel material since the diffusion coefficient is smaller. Results for the maximum temperature history in Fig. 6-5 show that the release fraction reaches $4.5 \cdot 10^{-5}$ after about 150 hours and remains constant through the remainder of the 250 hours. For the average temperature history (Fig. 6-6), the iodine release occurs gradually. The release fraction is $5.4 \cdot 10^{-6}$ after 250 hours, which is equivalent to a fuel retention fraction of 90 %.

In the **GA** calculation for the maximum temperature history, a steep rise in the release is seen within the first 10 hours, followed by a gradual rise. After 250 hours, a release fraction of $2.8 \cdot 10^{-5}$ is expected, which corresponds to an iodine retention fraction of approximately 40 %. The GA calculation for the average temperature history indicates that most of the iodine is retained within the kernel.

6. BENCHMARK COMPARISON OF RADIONUCLIDE RELEASE MODELS

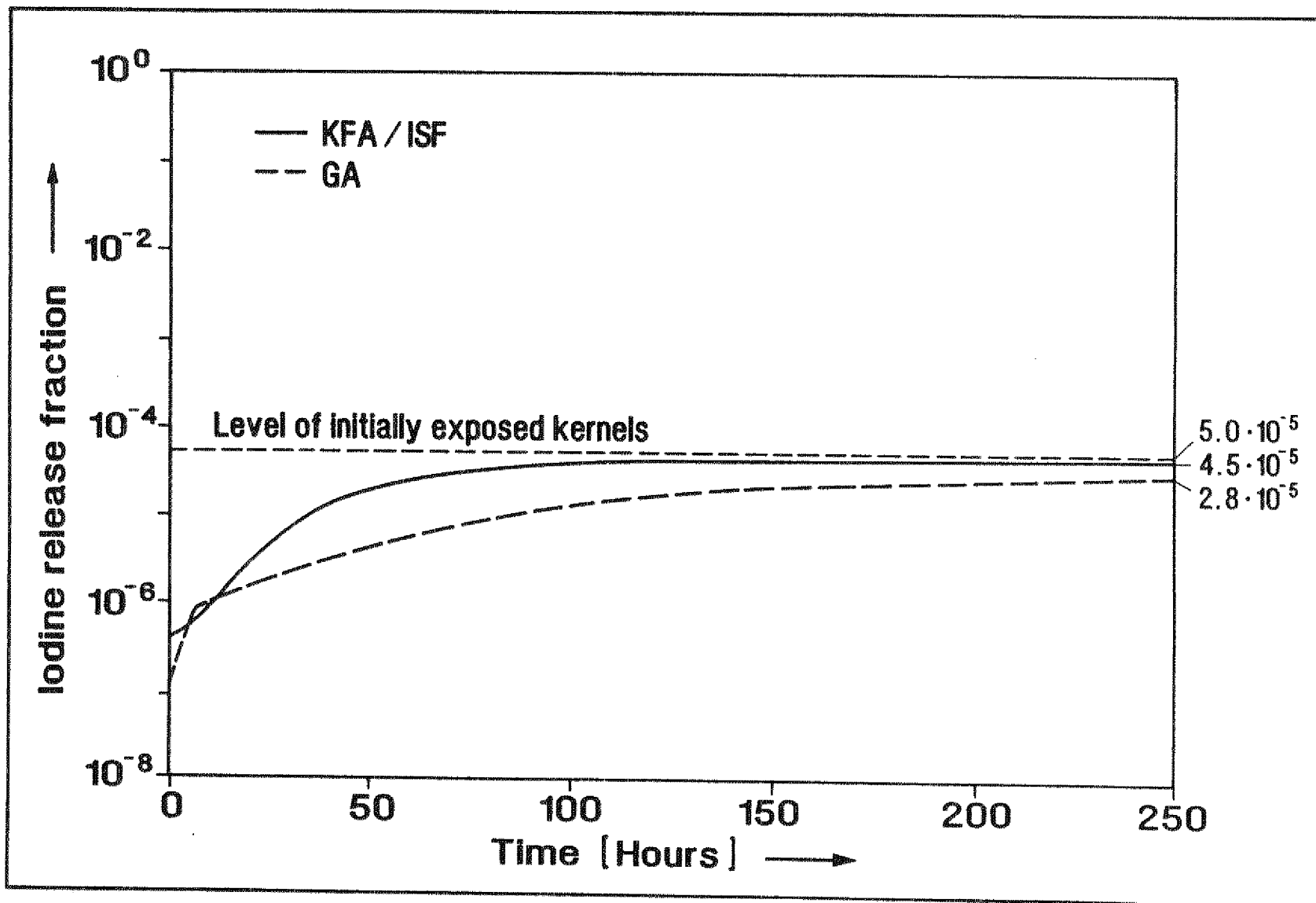


Fig. 6-5: Iodine Release from Exposed Particle Kernels
for the Maximum Temperature History

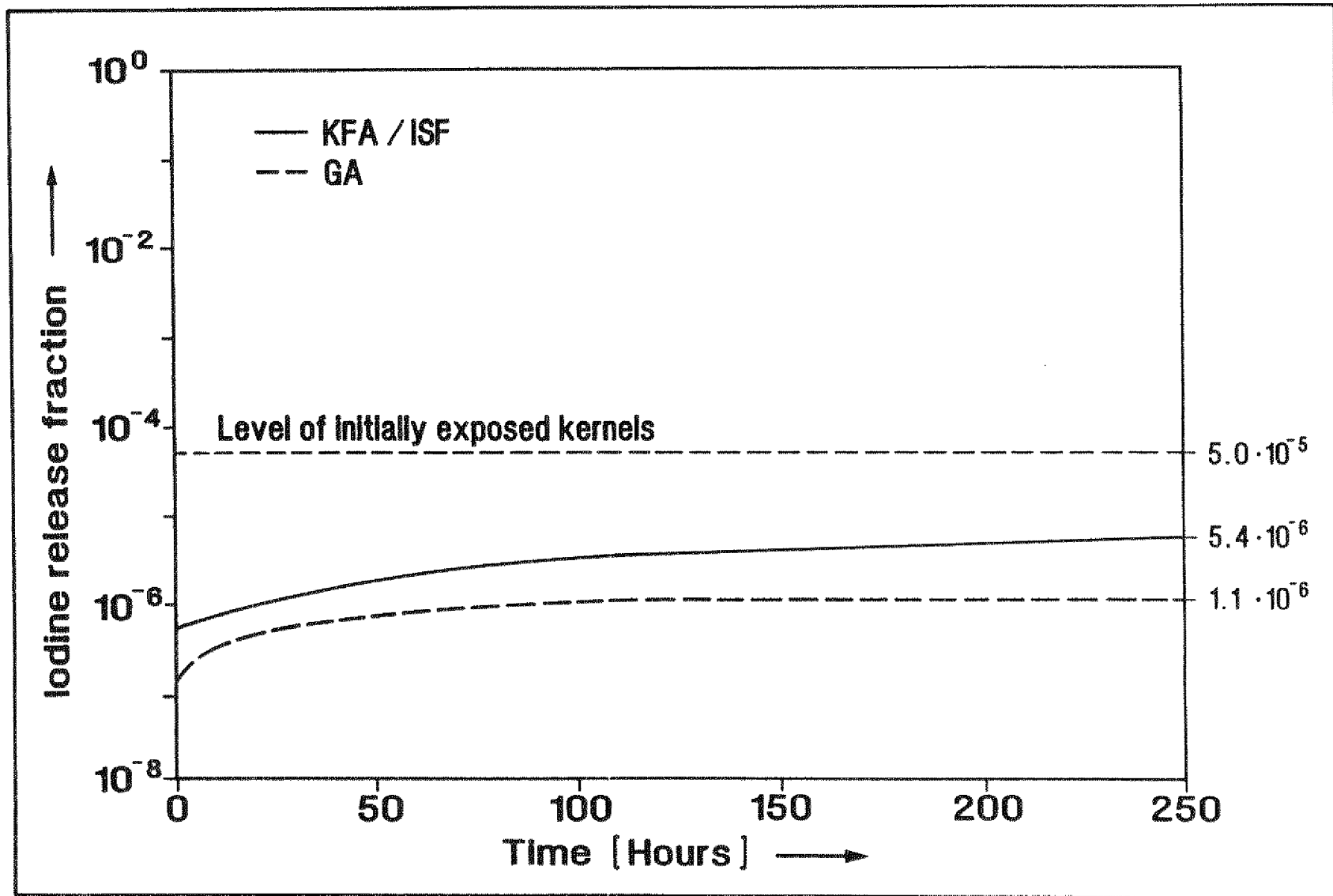


Fig. 6-6: Iodine Release from Exposed Particle Kernels
for the Average Temperature History

After 250 hours, the release fraction is predicted to be $1.1 \cdot 10^{-6}$, which corresponds to only a 2 % release of the exposed kernel inventory.

GA release estimates are up to 50 % lower due to either a different modeling approach and/or to different temperature interpolation schemes. The KFA/ISF model is based on bare kernel release data while the GA model is based on data for constrained failed particles. Experience has shown that the fission product release from exposed kernels is higher compared to that from constrained failed particles. Further study is required in order to resolve this difference.

6.4 Standard Particle Diffusive Release Model

According to GA modeling philosophy, standard particles are of non-releasing character and therefore not expected to release any fission products, except for silver at high temperatures.

Regarding standard particles in KFA/ISF modeling, the FRESCO code (Ref. 8) is used to determine the diffusive release of fission products. Transport data in the SiC layer which is the most retentive layer of the coating, has been subject to many studies. It has been already shown that the diffusion coefficient of cesium in silicon carbide recommended by Myers for accident conditions (Ref. 6) leads to overestimating the experimental results for modern German HTR fuel and definitely requires its revision. A better approach which was found to well describe the actual experimental data is a diffusion coefficient for silicon carbide with a different structure also derived by Myers (Ref. 6).

The calculation of the cesium release from standard particles shown in Fig. 6-7 for maximum temperature conditions is based on the more realistic diffusion data in the SiC layer. The release fraction after 250 hours is $5.0 \cdot 10^{-4}$ being 2 orders of magnitude lower compared to a calculation based on the earlier reference diffusion coefficient. For average temperature conditions, the cesium release from standard particles remains below 10^{-8} in both cases.

6. BENCHMARK COMPARISON OF RADIONUCLIDE RELEASE MODELS

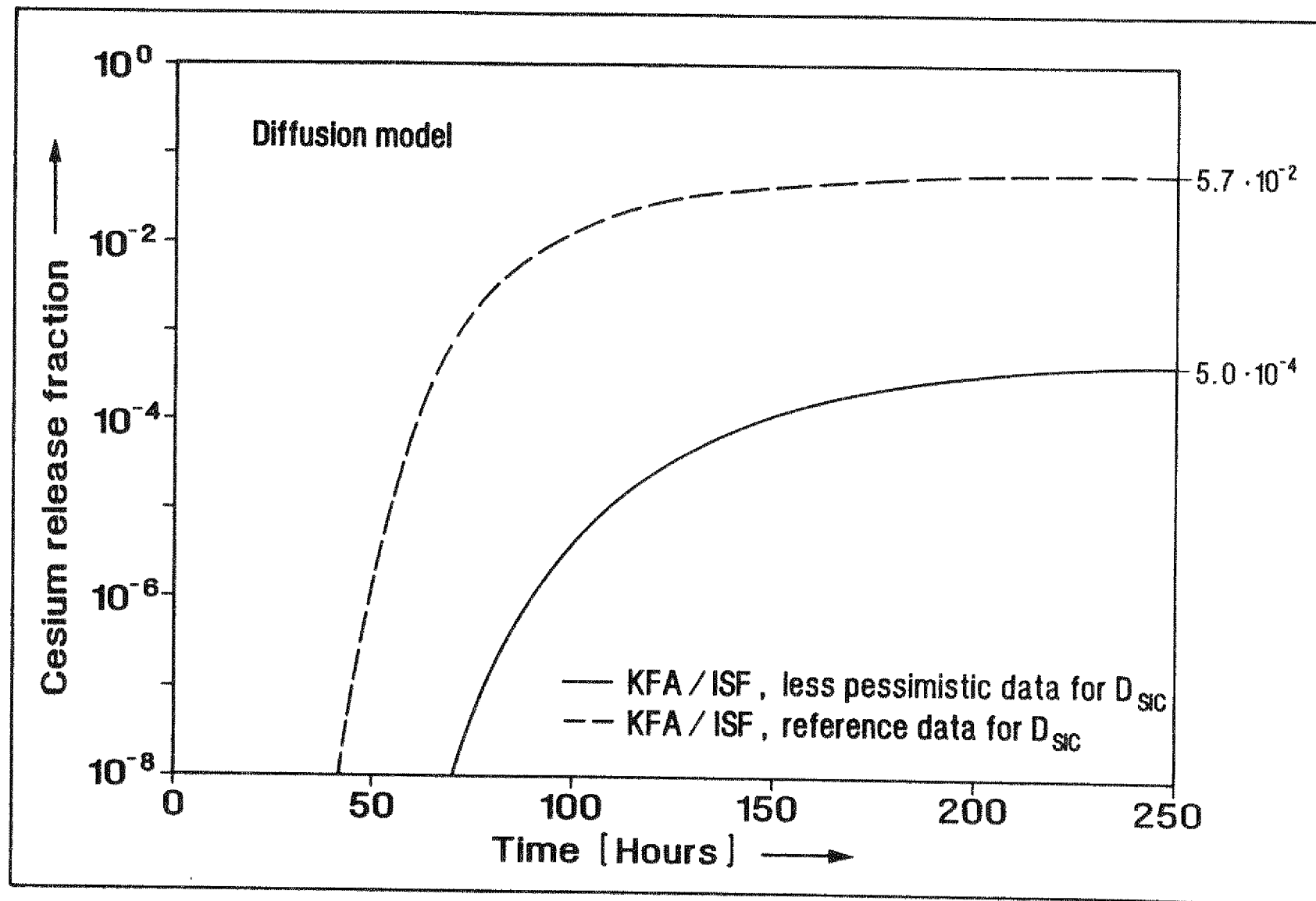


Fig. 6-7: Cesium Release from Standard Fuel Particles According to the Diffusion Model for the Maximum Temperature History

No iodine is expected to escape from particles with an intact coating layer in both GA and KFA/ISF modeling.

6.5 Comparison of All Fission Product Release Models

Regarding the comparison of each side's prediction of fission product release under the given maximum temperature condition using reference methods (Fig. 6-8), one still has to keep in mind that the philosophy the modeling is based upon is different among the codes. With respect to cesium release, the GA results with the 1985 statistical model referring to originally standard (= intact) particles the SiC layer of which has failed, are compared with KFA/ISF results with the diffusion model referring to intact particles which remain intact. The qualitative difference between the two cesium curves shown in Fig. 6-8 - later and steeper rise of the KFA/ISF curve compared to GA's - is due to the different assumptions for the modeled thermally activated processes and the corresponding activation energies (KFA/ISF: diffusion in SiC, GA: SiC corrosion). The cesium release fraction after 250 h is calculated by KFA/ISF to be $5.0 \cdot 10^{-4}$ which is higher than the GA result of $1.2 \cdot 10^{-4}$ gained with the 1985 statistical model. A reason for it could be given by the fact that the diffusion model takes account of a diffusive transport in the matrix graphite. On the other hand, the 1985 statistical model has been derived by correlating the SiC failure directly with the measured cesium release from the fuel element (neglecting a cesium holdup in the graphite), thus resulting in a smaller effective permeability of the SiC layer, i.e. a smaller cesium release from the coated particles. The KFA/ISF version of the 1985 statistical model also predicts a higher cesium release value (not shown in the Fig.), since it does not take into account a retention in particle kernels at temperatures lower than 1600 °C.

With respect to iodine release, no adequate comparison of the results can be made. The KFA/ISF pressure vessel model assumes an exposed kernel remaining after a particle failure where fission gas or iodine release is determined

6. BENCHMARK COMPARISON OF RADIONUCLIDE RELEASE MODELS

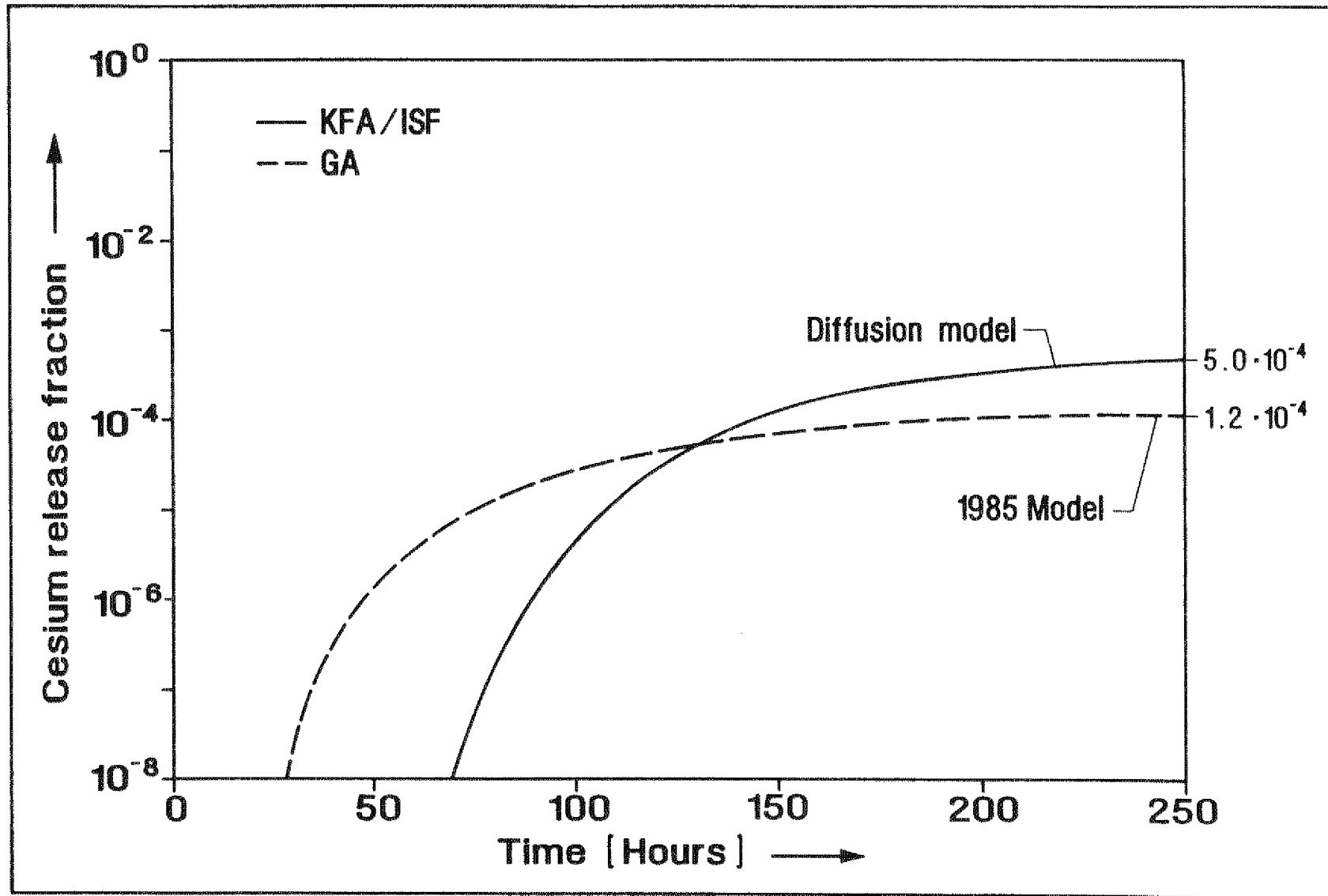


Fig. 6-8: Comparison of Cesium Release for the Maximum Temperature History
Using the GA and KFA/ISF Reference Models

according to the Booth model. In contrast, the 1985 statistical model used by GA assumes a particle with a failed SiC layer and a still intact OPyC layer which is a highly efficient barrier for fission gases and iodine. The comparison of iodine release fractions from exposed kernels has already been described in Section 6.3.2.

6. BENCHMARK COMPARISON OF RADIONUCLIDE RELEASE MODELS

7. SUMMARY AND CONCLUSIONS

The objective of this study, as described in Section 1, is to compare US and FRG HTGR fuel failure and release models. The models utilized by GA and KFA/ISF are described within this document, and differences in modeling assumptions are identified. For those models with comparable assumptions, differences are quantified by comparing results obtained from each country's models for a benchmark calculation in which a conduction cooldown is simulated for the US reference MHTGR design. Important conclusions in comparing model assumptions and release results are summarized in Sections 7.1 and 7.2, fields for further work are listed in Section 7.3.

7.1 Qualitative Comparison of US and FRG Models

The qualitative comparison of US and FRG fuel failure and release models identified several similarities and differences in modeling assumptions and inputs involving fuel quality, standard and defective particles, and heavy metal contamination, as summarized below:

1. Fuel Quality

A key input to any release model is the quality or condition of the fuel particle after manufacture and prior to the initiation of an accident.

The US program specifies defect levels for each coating layer of the TRISO coated fuel particle. The detailed specification of the US program provides input to similarly detailed fuel failure models which give increased understanding and confidence that the as-manufactured fuel will perform as expected. The US fuel specifications for heavy metal contamination and failed SiC fractions are based on separate measurement techniques.

7. SUMMARY AND CONCLUSIONS

In contrast, the **FRG** program does not explicitly differentiate between particles with defect levels for each single coating layer. The German modeling approach relies on the subdivision of the measured uranium outside an intact SiC layer into two contributions: a) heavy metal contamination in the OPyC layer and fuel element graphite and b) particles with a defective SiC layer (conservatively handled like exposed kernels in the model).

2. Standard Particles

For the modeling of SiC failure in standard particles, **GA** uses the 1985 US/FRG Integrated Failure and Release Model for Standard Particles and is considering the use of the 1988 revised version of this joint US/FRG statistical model. Experimental evidence used in the development of the 1985 US/FRG model shows that the failure of standard particles at temperatures below 1800 °C indicated by the release of cesium can be explained by corrosion and thermal decomposition resulting in particles with a defective SiC layer and a still intact OPyC layer. In the 1988 version, fuel failure is modeled by assuming thermal decomposition of the SiC coating only but defining a lower limit for failure fraction.

The statistical models also predict fission product release from standard particles by predicting their failure. The US has included kernel retention at temperatures < 1600 °C in their release estimates for gaseous and metallic fission products although this was not part of either the original 1985 or the revised 1988 model. The models were developed using experimental data at temperatures ≥ 1600 °C in which kernel retention was assumed to be negligible. However, at the lower temperatures typical of small HTGR's, kernel retention should not be ignored.

The **KFA/ISF** method to describe particle failure is based on the physical model of a pressure vessel which also includes the SiC degradation processes of corrosion and thermal decomposition. The use of the 1985 and 1988 versions of the US/FRG statistical model is being evaluated. The pressure vessel failure mechanism creates bare particle kernels indicated by the observed krypton gas release. In several heating exper-

7. SUMMARY AND CONCLUSIONS

iments at temperatures ≥ 1700 °C, single events of a spontaneous release of krypton have been observed which can be interpreted as a pressure vessel failure of a particle coating. Such events are not covered by the US/FRG statistical model and have to be regarded separately.

The German method for describing fission product release consists of a diffusion model. Characteristic transport data have been derived for relevant fission products in the kernel and the coating layers from various heating experiments. For predictive purposes, realistic data are chosen; however, in cases with a poor data base conservative data are used.

3. Defective Particles

In the GA calculations, pressure vessel failure is important only for predicting coating failure of defective particles such as the particles with missing buffer layer. Otherwise, pressure vessel failure is a negligible failure mechanism of the SiC layer in comparison to the mechanisms specified in the US/FRG model. Both GA and KFA/ISF have release models for exposed kernels based on a diffusion transport process.

4. Heavy Metal Contamination

The GA model for release from heavy metal contamination assumes a diffusive release mechanism from a contamination particle which is less retentive than an exposed kernel as supported by US experimental evidence. The GA model combines the release from heavy metal contamination with transport through the graphite to predict the release into the coolant channel.

The KFA/ISF model assumes the fission products which originate from the contamination fraction to be uniformly distributed throughout the spherical fuel element. Its transport behavior through the matrix graphite together with those fission products which have escaped the fuel particles (and which is uniformly distributed, too) is described by diffusion data derived from experiments.

7. SUMMARY AND CONCLUSIONS

Because of the significant differences in the definition and approach used in modeling release from contamination, a quantitative comparison was judged to be inappropriate and was not included in this study.

7.2 Quantitative Comparison of US and FRG Models

The quantitative comparison of US and FRG models is based on the analysis of a benchmark problem. The benchmark problem used average and maximum temperature histories from a depressurized conduction cooldown for the MHTGR using US fuel quality and fuel design. The results of the comparison are noted below:

1. Standard Particle Failure

Similar results were obtained for the particle failure predicted by GA and KFA/ISF reference models for MHTGR core heatup temperatures. The fractions after 250 hours were almost the same despite the different modeling approaches of PANAMA-I and SORS because of the SiC corrosion mechanism after Montgomery (Ref. 3) which is incorporated in both models and which is dominant in the given temperature range.

Failure fraction results from thermal corrosion and decomposition of the SiC layer were nearly identical. Although each country's models are based upon the 1985 version of the US/FRG Integrated Failure and Release Model for Standard Particles, the agreement in the results provides verification since the codes were independently developed. Failure fractions obtained from the 1988 version of the US/FRG Integrated Failure and Release Model for Standard Particles, were also nearly identical. Its results were much lower than values obtained with the 1985 version. The 1988 version incorporates more recent experimental data which was expected to lower the failure rates in the temperature range of interest.

7. SUMMARY AND CONCLUSIONS

2. Standard Particle Release

The fractions of cesium release from the particles predicted with each country's reference model for the maximum temperature history differ at least by a factor of 4 (comparison between the 1985 statistical model and the diffusion model). The explanation for it could be given by the fact that the 1985 model predicting the lower release fraction was derived under the assumption of no retention in the matrix graphite, i.e. release from particles being equivalent to release from fuel element, while the diffusion model takes account of a retention in graphite resulting in a higher release from the coated particles into the graphite described by a higher diffusion coefficient in silicon carbide. There is still a need to correctly interpret the few existing experimental data on cesium release from the fuel particles into the graphite to come to an adequate modeling of the release process.

Release estimates from standard particles that have failed according to the 1985 and 1988 joint US/FRG models exhibited similar functional behavior. However, US cesium release fractions were around 50 % lower due to the modeling of kernel retention at temperatures < 1600 °C in the US models. The FRG models do not include kernel retention according to the original definition. The 1985 and 1988 models assume that kernel retention is negligible because the experimental data upon which these models are based, are at higher temperatures (≥ 1600 °C) than those experienced during MHTGR loss of cooling accidents.

3. Exposed Kernel Release

Each country's results for exposed kernel release exhibited similar functional behavior. However, GA release estimates were up to 50 % lower due to either a different modeling approach (iodine release) or to a different diffusion data base (cesium release). This difference would need further study in order to be resolved.

In conclusion, differences exist in the fuel performance modeling of the US and FRG as represented by GA and KFA/ISF. The difference in the fuel specification is given by a different degree of detailing into the particle components

7. SUMMARY AND CONCLUSIONS

and in itself produces different modeling procedures but it is not fundamental. Fundamental differences, however, exist in both countries' modeling approaches when describing the same phenomena of particle failure and fission product release behavior observed in experiments. Nevertheless, a large part of both sides' results is in good agreement; identified differences can be resolved by putting effort into further studies. In general, all presented codes have shown their ability to describe fission product release behavior under accident conditions at least in a conservative way thus being appropriate for use in safety analyses.

The differences identified in this document provide valuable information in the understanding of US and FRG release models for future development of consistent models. The comparison of the calculational results provides valuable support to the verification and validation of those models in the independently developed computer codes of GA and KFA/ISF.

7.3 Future Work

The comparison of calculational results received with both GA and KFA/ISF methodology to describe fission product release behavior from TRISO particles have led to different aspects which should be subject to future work:

- Radionuclide release from heavy metal contamination was found to be outside the scope of this work. Experimental data on iodine and fission gas release from fuel rod matrix material has already been obtained by GA. Similar experiments regarding matrix graphite are under way at KFA (Ref. 15). These data should be compared under a different task of the 'Safety' subprogram as well as the ongoing theoretical work about fission product transport in graphite (Ref. 16).
- Differences in calculated fission product release from exposed particle kernels should be clarified by reviewing the experimental basis of the used

7. SUMMARY AND CONCLUSIONS

transport data and if necessary carrying out additional heating experiments.

- Results from post-heating examinations like measurements of fission product inventories in graphite and single coated particles (IMGA) which should provide a better understanding of fission product release behavior, should be considered in future joint modeling efforts.

7. SUMMARY AND CONCLUSIONS

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