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**AN ANALYSIS OF SORS: A COMPUTER PROGRAM
FOR ANALYZING FISSION PRODUCT RELEASE FROM
HTGR CORES DURING TRANSIENT TEMPERATURE EXCURSIONS**

J.M. Dickey

HTGR SAFETY DIVISION

Date Published - April 1978

**DEPARTMENT OF NUCLEAR ENERGY BROOKHAVEN NATIONAL LABORATORY
UPTON, NEW YORK 11973**

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ABSTRACT

The code SORS was written by General Atomic to calculate the release of fission products from the fuel into the primary coolant during a hypothetical uncontrolled transient temperature excursion. The code assumes that the graphite core remains structurally intact. The release from the fuel particles is calculated using a coarse time step for several sections of the core. For the non-volatile elements, the code calculates a diffusion rate and an evaporation rate in each section of the core. The expression used for the evaporation rate is found to be incompatible with the rest of the assumptions used in the calculation.

I. Introduction

An analysis of a maximum hypothetical fission product release is required for the evaluation of a reactor site.¹ This release is estimated assuming an uncontrolled core heat-up resulting from a non-mechanistic loss of cooling. The fuel particle coatings and the graphite moderator will delay the escape of the fission products from the core of a high temperature gas cooled reactor, HTGR, to the interior of the pre-stressed concrete reactor vessel, PCRV. The fission products may then leak out of the PCRV into the containment. The code SORS² was written by Schwartz et. al. to treat the first stage in the release of the fission products during a transient temperature excursion, namely from the core of the reactor to the primary coolant circuit.

The core of an HTGR consists of several graphite blocks which contain the fuel. The core is cooled by helium gas which circulates through coolant channels bored in the graphite. The core and the primary coolant system is encased in a PCRV. Under normal operating conditions the helium is at a pressure of about 725 psia and is circulated by 3 turbine driven axial flow compressors at a rate of 11×10^6 lb/hr. There are, in addition, three auxiliary cooling loops in case of failure of the main cooling system. In the hypothetical accident to be considered it is assumed that all the circulators have failed so there is no forced circulation of the He. Such a failure would result in an immediate reactor trip. The subsequent decay of the fission products would generate a considerable amount of heat. In the absence of forced circulation this heat cannot be removed sufficiently quickly by conduction and radiation, therefore the

temperature of the core is not maintained within the range of normal operating conditions, but will gradually rise to the sublimation temperature of graphite. Schwartztrauber and Silady³ have estimated that after about 10 hours, the maximum temperature anywhere in the core will be about 4800°F, and after about 50 hours, about one third of the core will be at 6500°F.

Before the accident occurs, almost all the fission products present will be contained within the fuel particles. Some fission products may be plated out on surfaces of the primary coolant circuit. These amounts are expected to be small, in a reactor which has a normal operating history, so the effect of lift off will not be discussed here. As the temperature of the core increases we can describe qualitatively what may be expected to occur. There will be no immediate release of the fission products, as the particle coatings are almost impervious until the temperature has risen several hundred degrees above operating temperatures. However, in the course of time, during the assumed accident, as the temperature reaches higher values, the fission products can diffuse through the coatings and the coatings themselves are eventually degraded. The expected performance of the coatings as a function of temperature and past fluence must be based on experimental data and is necessary input for the calculation. The fuel particles are packed in a graphite binder and stacked in holes drilled in graphite blocks. One may conservatively assume that the most volatile elements, the rare gases and the halogens, are released directly into the primary coolant circuit after escaping from the fuel particles. So for these elements it is only necessary to calculate the release from the fuel particles; this is done in the version of the code, SORSD. The release of the non-volatile elements on the other hand is retarded by the

graphite moderator. These elements must diffuse across the graphite web to the coolant channel surface and evaporate directly from this surface. Initially this process will merely result in a redistribution of the fission products as the mobile elements will evaporate from the hotter regions of the core and redeposit in the cooler regions. As the cooler parts of the core heat up and the reflector also heats up, eventually some of the atoms can escape from the core into the upper plenum. The version SORSG of the basic code SORS calculates these stages of the release of the non-volatile fission products. In the analysis used in SORS of a loss of coolant accident, it is assumed that the integrity of the graphite core is maintained, that carbon is lost from the core only through sublimation and that the amount lost is negligible.

The code SORS is described in detail in a licensing topical report, GA-LTR-10.² The output of the code has been quoted in several Safety Analysis Reports, e.g. Fort St Vrain FSAR,⁴ Fulton PSAR⁵ and GASSAR,⁶ and also in the Accident Initiation and Propagation Analysis (AIPA) report.⁷ The results from SORS also have been used as a source term for the dispersal from the containment in other studies.⁸ One version of SORS was received from General Atomic on March 10, 1975. This version calculated only the release from the fuel and incorporated the fuel model described in GA-LTR-10.² Two other versions of the code, SORSD and SORSG, were received from General Atomic on February 10, 1976. The later version used a different fuel model, which is similar to that described in the AIPA report.⁷ This report is based on an analysis of these versions of the codes and the published documentation.²

The objective of this work is to examine the adequacy of the code SORS as a means of calculating the consequences of the postulated accident scenario. The analysis considers such questions as whether the mathematical model is adequate or whether the computational technique is appropriate; the report discusses the relative importance of different factors, insofar as they bear on the choice of the mathematical approximations used in the code. It was not the purpose of this study to exercise the code. Chapter 2 describes the core of an HTGR. Chapter 3 describes the data and models of the physical processes used in the code. Chapter 4 describes the mathematical structure of the code. Chapters 5-7 describe the stages in the migration of a fission product. Chapter 8 summarizes the observations.

II. Core design and the mathematical model used in SORS

The fuel is contained in spherical fuel particles which have a ceramic coating (Fig. 2.1). The fissile fuel is uranium enriched with ^{235}U in the form of UC_2 . The particles of UC_2 are 200 μm in diameter and have a triso coating consisting of a low density pyrocarbon buffer layer followed by a high density pyrocarbon layer, a SiC layer and an outer high density pyrocarbon layer. The fertile fuel particles contain kernels of ThO_2 whose diameter is 500 μm . These particles have a biso coating consisting of an inner buffer layer of low density pyrocarbon and an outer layer of high density pyrocarbon. At normal operating temperatures the fuel particle coatings are almost impermeable to the fission products. The rate at which fission products can leak out of the particles increases as the temperature is raised. At a sufficiently high temperature, the coatings fail and the fission products can escape readily. The fuel particle behavior is

discussed further in Chapter 5.

The fuel particles are mixed with carbonized pitch and graphite flour and the mixture is formed into cylindrical fuel rods. The fuel rods have a diameter of .618 in and are 31.22 in long. The fuel elements are hexagonal blocks of graphite through which are drilled an array of holes (Fig. 2.2). Some of these holes contain a fuel rod or burnable poison and the remaining holes are the coolant channels along which the helium flows. Each standard fuel element contains 132 fuel rods and 72 coolant channels. The fuel rods are sealed in the fuel holes by a graphite plug. Eight fuel elements are stacked in a vertical column and similar blocks of graphite are placed at the top and bottom to act as reflectors. The coolant channels of adjacent elements are aligned by dowel pins. The columns are arranged in refueling regions each of which contains 7 columns except at the outer edge of the core. The active core, in a proposed design for a 3000 MWt reactor, contains 402 fuel columns and is surrounded by a permanent side reflector consisting of graphite (Fig. 2.3). The core is supported on graphite blocks and held in place by a lateral restraint structure. One quarter of the fuel is replaced each year. The fluence experienced by a given fuel particle depends on its location in the core as well as the age of the fuel and operating history of the reactor. Consequently the inventory of fission products will vary from one particle to another. The core is modelled mathematically in a simple cylindrical geometry (Fig. 2.4). The core is divided into up to 14 concentric radial regions and 10 axial segments, one corresponding to each fuel element, and two for the top reflector. The properties of each radial region are calculated by averaging

over the fuel elements in the corresponding annular portion of the reactor core. Thus spatial variations within the core are partially taken into account. For example, for each segment the fraction of the fuel which is 1, 2, 3 or 4 years old is calculated from the arrangement of the refueling regions and this information is used as data by the code.

The objective of SORS is to calculate the time taken for the fission products to migrate from the fuel particles to the upper plenum. The migration of the atoms is modelled as a succession of barriers; this is shown figuratively in Fig. 2.3. The first stage of the calculation concerns the release from a fuel particle. This is discussed in detail in Chapter 5. It is assumed that the fission product atoms can move freely through the loose graphite binder surrounding the fuel particles. The volatile fission products are hardly retarded by the graphite matrix, but escape directly from the fuel particles into the primary coolant. Two further stages in the calculation are required for the non-volatile fission products, the diffusion through the graphite matrix and evaporation at the coolant channel surface; these stages are discussed in Chapters 6 and 7.

III. Physical data and models required for the calculation

In this chapter we discuss the data that must be supplied for the calculation. Some of this data is fixed for a particular plant, e.g. geometrical data concerning the dimensions of the core of a 3000 MWt plant. Other data are based on the results of experimental tests or are taken from the output of another code. Insofar as there is some uncertainty in the latter data it is necessary to determine the sensitivity of the release rates predicted by SORS to variations in the data. Some physical properties

are not known directly and so general considerations must be used to generate the required data. Following is a list of the data used by SORS together with the references on the sources.

- 1) Geometrical data concerning the reactor.
 - a) Physical data determined by the plant under consideration, e.g. diameter of coolant channels, size of graphite blocks.
 - b) Data determined by the mathematical model of the core, e.g. number and size of the regions into which the core is divided.
- 2) Mathematical data for the computation.

For example, initial time step, number of significant figures, maximum error in the integration.
- 3) Historical data, which depend on the prior operating history of the reactor.
 - a) Inventory of fission products in the core at the start of the incident. The inventory will depend on the time elapsed since the last refueling and also on the power level during the past 4 years. The amounts of short lived fission products will attain an equilibrium value, but the amounts of longer lived fission products will increase approximately linearly with time. The amount of fission products will be at a maximum just prior to refueling. The inventory used as input in SORS has been calculated using the code RAD.⁹ This code takes account of the different fission yields of ^{235}U and ^{233}U . RAD also partially calculates the effects of the parents and grandparents of an isotope, but it does not calculate the results of neutron capture.

- b) Distribution of fission products in the core.

RAD estimates the total inventory of fission products throughout the core. The fission products are not uniformly dispersed but the concentration will vary from one part of the core to another. This variation is expressed by supplying a power factor for each axial node and a power factor for each radial node. The fraction of the inventory in a given portion of the core is then given by $P_A P_R V$, where P_A and P_R are the relevant axial and radial power factors and V is the volume of the portion of the core. The product $P_A P_R$ varies from .54 to 1.28 in the sample data. The power distributions in the different refueling regions are calculated using core physics codes¹⁰ and the power factor for each radial region is calculated by averaging over the included refueling regions.

- c) The relative amounts of biso and triso fuel particles for each radial region.

- 4) Decay schemes and data for the decay chains.

The code allows for decay chains with a maximum of 6 members and for a simple branching pattern (Fig. 3.1).

- 5) Temperature history of the core.

The temperature history of each region of the core is calculated by the parallel code CORCON.³ The two aspects of the problem, the migration of the fission products and temperature evolution of the core, have been decoupled in SORS. The consistency of this assumption could be checked by using the results of SORS in

a second iteration of CORCON; a discussion of such an iteration is outside the scope of this review, which is restricted to a consideration of SORS. The temperature of the core rises slowly. Fig. 3.2 shows the average and maximum temperature of the core versus time; after 10 hours the average temperature is about 3000°F and after 20 hours 4200°F. The temperature evolution varies in different parts of the core. Fig. 3.3 shows the temperature sequence for the segments in the central region of the core.

6) Coolant flow rate and pressure.

Following a pipe rupture the helium escapes into the containment. The change in pressure is calculated in the code CONTEMPG.¹¹ If the containment remains intact the pressures in the PCRV and the containment reach equilibrium with a value of 39.8 psia after about 100 seconds. The pressure then falls to 29.0 psia at 20 minutes and 27.8 psia at 24 hours. In this accident it is assumed that there is no forced circulation so that the flow of helium is due to natural convection caused by the hot core. Because of the large resistance to flow, the flow rate will be very slow and has been estimated by H. W. Che and G. J. Malek, using the code RECA,¹² to range from .034 lb/hr at about .1 hr to $5. \times 10^{-5}$ lb/hr at about 50 hours. The corresponding Reynolds numbers are 6.9 and 0.0041 so the flow is laminar and far below the transition to turbulent flow, which occurs at Reynolds numbers of about 2000.

7) Fuel release characteristics.

As the temperature rises the capacity of the fuel particles to

retain the fission products decreases. The probability of fission products escaping from the fuel particles at different temperatures is needed for the code. Experimental data is available based on both in pile and out of pile tests. The experimental results have a wide spread and several models have been suggested based on the results.^{2,13} The data and these models have been reviewed extensively in two topical reports.^{14,15} So it is unnecessary to discuss the validity of the basic data; this report is concerned with the extent to which the variations in the data and the different empirical models affect the calculations in SORS, namely the release curves for different isotopes. This topic is discussed in detail in Chapter 5. The data for some elements are similar so the elements are grouped into 10 classes shown in Table 3.1, and parameters for each class are specified.

- 8) Diffusion coefficients in graphite and partition coefficient between the graphite binder and graphite blocks.

Norman¹⁶ has reviewed the available data. Experimental values for the diffusion coefficients are available only for Sb and a few other elements.¹⁶ For the remaining elements Norman suggests the data in Table 3.2, which are based on a heuristic relationship between the activation energy for diffusion and the vapourization energy. This expression involves a considerable extrapolation from known experimental results. Another variable which affects the diffusion of an impurity is the partition of the impurity between the two types of graphite in the core, the loose binder

graphite and the graphite blocks. Once again there is only slight experimental data so there could be deviations from the value of 15 suggested by Norman.¹⁶

9) Vapour pressure.

Experimental vapour pressure data are available for many elements and their carbides. The data have been collected and reviewed by Norman.¹⁶ For Cs, Rb, Ba and Sr Freundlich isotherms are used above a critical concentration C_0 , and Langmuir isotherms are used for lower concentrations:

$$\text{for } C < C_0 \quad \ln P = A + \frac{B}{T} + (A' + \frac{B'}{T}) \ln C$$

$$\text{and for } C > C_0 \quad \ln P = A + \frac{B}{T} + (A' + \frac{B'}{T}) \ln C_0 + \ln \frac{C}{C_0}$$

where P is the pressure

T is the temperature

C is the concentration

A, B, A', B' are the vapour pressure constants, Table 3.3.

For Cs a value of $C_0 = 0.078 \text{ moles/m}^2$ has been observed; the same value is adopted for the other 3 elements. For the remaining elements an Arrhenium equation is used. Since the chemical form, in which the element is present, is not known, the vapour pressures of the free element and the carbide are added together in SORS. This assumption overestimates the vapour pressure and so will overestimate the evaporation rate but will underestimate the deposition rate. If the surface coverage is less than a monolayer, the density of the vapour in equilibrium with the surface will be

less than the saturated vapour density of the same temperature. It is assumed that the saturation vapour density is scaled by the same fraction as the surface coverage. Another parameter is thus introduced, namely the concentration of impurity corresponding to the monolayer coverage. This has been estimated by Norman¹⁶ from geometrical considerations, based on the close packing of spheres with the appropriate atomic radii. So the expression used for the vapour pressure is:

$$\text{for } C \leq C_m \quad \log P = A - \frac{B}{T} + A' - \frac{B'}{T}$$

$$\text{and for } C > C_m \quad \log P = A - \frac{B}{T} + A' - \frac{B'}{T} + \log \left(\frac{C}{C_m} \right)$$

where P is the pressure

T is the temperature

C is the concentration

C_m is the concentration corresponding to a complete monolayer (table 3.5)

A, B are the vapour pressure constants for the element
(table 3.4)

A', B' are the vapour pressure constants for the carbide
(table 3.4).

IV. Mathematical equations and computational techniques used in SORS

The procedure adopted in SORS is to describe the problem in terms of several coupled first order differential equations with coefficients which are dependent on time. The independent variables represent the total amount of each isotope in one of the three parts of the core - the fuel,

the graphite or the primary coolant. The variable coefficients represent an average probability of an atom moving from one part of the core to another, where the probability has been averaged over the whole reactor. These time dependent coefficients are calculated in separate subroutines. The differential equations are integrated numerically using Hamming's predictor - corrector technique. Since Hamming's technique is a four step method, a Runge-Kutta routine is used to set up the starting values. Hamming's method is well established and has several advantages. A comparison of the predicted and corrected values permits an estimate of the error in the integration and also enables the time step to be automatically adjusted during the course of the calculation. So the integration procedure is accurate and reliable. In general, a computation requires a numerical method which is as accurate as the equations which are to be integrated.

We will use the following notation, which is different from that used in LTR-10.²

N_i = total number of atoms of isotope i in the reactor

n_i = total number of atoms of isotope i in the fuel particles

m_i = total number of atoms of isotope i in the graphite moderator

r_i = total number of atoms of isotope i in the primary coolant circuit.

It is assumed that the atoms of the volatile elements can pass directly into the coolant after escaping from the fuel, so for the volatile elements:

$$N_i(t) = n_i(t) + r_i(t) \quad 4.1$$

The non-volatile elements are delayed in the graphite, so for the non-volatile elements:

$$N_i(t) = n_i(t) + m_i(t) + r_i(t) \quad 4.2$$

The change in the number of atoms of an isotope "i" due to radioactive decay depends on the decay constant λ_i and the probability of P_{ij} of a precursor "j" decaying into "i". So the differential equation for the total number of atoms of any isotope is:

$$\frac{dN_i}{dt} = -\lambda_i N_i + \sum_j P_{ij} N_j \quad 4.3$$

where the summation is over all precursors.

In Fig. 2.1 we show schematically the disposition of an isotope between the fuel, graphite and coolant. We can define fractional release rates, F, G, which at a given time represent the probability of an atom moving from one of these three media to another. For example if the number of atoms of a given isotope in the fuel at time t is $n(t)$ then the rate at which those atoms escape from the fuel at this time is $-F(t) n(t)$. Similarly if $m(t)$ is the number of atoms of an isotope in the graphite the rate at which these atoms move from the graphite into the primary coolant circuit can be written as $-G(t)m(t)$.

In terms of these release rates the coupled differential equations for the number of atoms in different parts of the core are as follows: For the amount in the fuel particles n_i ,

$$\frac{dn_i}{dt} = (-\lambda_i n_i + \sum_j P_{ij} n_j) - F_i n_i \quad 4.4$$

where the first bracket on the right hand side represents the effects of radioactive decay, as in Eq. 4.3, and the second term is the rate at which atoms are released from all the fuel particles. The remaining equations differ for the volatile and non-volatile elements. For volatile elements, it is assumed there is no retention in the graphite so the equation for

the amount released into the primary coolant, r_i , is

$$\frac{d}{dt} r_i = (-\lambda_i r_i + \sum P_{ij} r_j) + F_i n_i \quad 4.5$$

The term in brackets is due to decay and the last term is the release rate from the fuel. For the non-volatile elements, the corresponding equation for the amount in the primary coolant, involves instead the release rate from the graphite, $G_i m_i$,

$$\frac{d}{dt} r_i = (-\lambda_i r_i + \sum P_{ij} r_j) + G_i m_i \quad 4.6$$

The amount in the graphite, m_i is calculated from the equation for conservation of mass

$$m_i = N_i - n_i - r_i \quad 4.7$$

Having set up the mathematical formulation of the problem in this form, if the functions $F(t)$ and $G(t)$ were known, the problem would be reduced to a simple numerical integration. The combination of Hamming's method and the Runge-Kutta method would be an appropriate technique. However the release rates, F and G , have been defined in a purely formal manner. The value of these release rates represents an average over the whole reactor and depends not only on time explicitly but also on the distribution of the fission products throughout the reactor.

Stage I Release from the fuel particles, subroutine FKCALC

First we shall discuss the release from the fuel particles. Let us consider one individual fuel particle " α " and denote by v_i^α the amount of the isotope " i " in this fuel particle. For this fuel particle at a specified time there is a well defined fractional release rate f_i^α which depends on the temperature of the particle and which can be calculated from the

input data. The differential equation for v_i^α is:

$$\frac{d v_i^\alpha}{dt} = (-\lambda_i + \sum_j P_{ij} v_j^\alpha) - f_i^\alpha v_i^\alpha \quad 4.8$$

The total amount of the isotope in all fuel particles is

$$n_i = \sum_\alpha v_i^\alpha \quad 4.9$$

differentiating this equation and substituting from e.g. 4.8

$$\frac{d n_i}{dt} = \sum_\alpha \frac{d v_i^\alpha}{dt} = \sum_\alpha (-\lambda_i v_i^\alpha + \sum_j P_{ij} v_j^\alpha) - \sum_\alpha f_i^\alpha v_i^\alpha \quad 4.10$$

$$\frac{d n_i}{dt} = (-\lambda_i n_i + \sum_j P_{ij} n_j) - \sum_\alpha f_i^\alpha v_i^\alpha \quad 4.11$$

This is the exact equation governing the release from fuel particles.

Comparing the two Eqs. 4.4 and 4.11, the formal release rate for the whole core is:

$$F_i n_i = \sum_\alpha f_i^\alpha v_i^\alpha \quad 4.12$$

$$\text{or } F_i = \left(\sum_\alpha f_i^\alpha v_i^\alpha \right) / \left(\sum_\alpha v_i^\alpha \right) \quad 4.13$$

To find F_i exactly it is necessary to know the contents of each fuel particle, that is to have the solutions of the differential equations, Eq. 4.11, for all the fuel particles. So far nothing has been achieved by the introduction of the formal release rate F . The procedure adopted in SORS is to decouple the calculation of F from the solution of the equation involving decay.

F is calculated approximately in subroutine FKCALC. Eq. 4.8 is replaced by a simpler equation in which decay is neglected:

$$\frac{d v_i^\alpha}{dt} = - f_i^\alpha v_i^\alpha \quad 4.14$$

Since the decay data has been eliminated, the same equation holds for all isotopes of a given element. For simplicity we shall ignore, in the mathematical discussion, the differences between biso and triso particles and the intact and failed state. Let us consider one particular segment of the core and one element. The input data includes a table of the temperature of the segment versus time. Using the fuel failure model the release rate for the chosen element is calculated at each of the temperatures in the table. Eq. 4.14 is integrated using a simple stepwise method. Take the release rate to be constant between the times in the table then if x is the value of the release rate during a time interval δt the amount in the fuel particles falls by a fraction $e^{-x\delta t}$ in this time interval. Thus the amount of the element within the fuel particles contained in the segment, and also the release rate from the fuel particles for that segment, are calculated versus time in FKCALC. This procedure is repeated for all the segments into which the core is divided and all the classes of elements. The overall release rate from the fuel particles for the whole reactor is now calculated from Eq. 4.13. The output of FKCALC is a table of average fuel particle release rates versus time for each of the 10 classes of the elements. The main program uses this table of release rates, interpolating where necessary, to find the time dependent coefficients in the original differential Eq. 4.4. This equation is then integrated using Hamming's method. This lengthy discussion is summarized in Fig. 4.1.

Since FKCALC calculates quickly an approximate release curve from the fuel elements, it is of interest to compare this curve with the results

obtained using the full code SORS. The comparison is made in Figs. 4.2, 4.3 for a volatile isotope ^{131}I and two less volatile isotopes ^{144}Ce and ^{147}Sm . It can be seen that, for each of these three isotopes, the results from FKCALC are within a few percent of the final result calculated by SORS, despite the difference in accuracy of the integration algorithms used in the two cases. Moreover the time step used in FKCALC is very large, 1.5 hours between 4.5 and 10.5 hours, compared with the time step used in Hammings routine, which time step is initially set at 10^{-4} hours. The additional computer time has affected the results very little, in these examples.

In the exact Eq. 4.8, the amount of an isotope in a fuel particles can change due to radioactive decay or because atoms migrate out of the fuel particle. If one of these terms is much larger than the other then the simpler differential equation involving only the larger term is an adequate approximation. This will be so in the following circumstances:

- a) Short lived isotope with no precursors, i.e. $\lambda \gg f$. Such isotopes are not of interest in this problem since they will have decayed to a fraction of their initial activity before it is possible for them to be released.
- b) Long lived isotope. Since most of the release occurs in the time span 5-15 hours, the activity of isotopes with a half life greater than this time will not change much during release, so the decay term can be neglected. Fig. 4.3 shows release curves for ^{131}I , which has a half life of 8.05 days and ^{133}I which has a half life of 20.8 hours. FKCALC gives a very good approximation for ^{131}I

and even for ^{133}I gives a reasonable estimate; this estimate could be improved simply by scaling by $e^{-\lambda t}$.

- c) Short lived isotope which is the daughter of a long lived precursor. In this case the activity of the daughter at any position is determined by the activity and migration rate of the parent. An example is the parent-daughter pair ^{132}Te , half life 78 hours, and ^{132}I , half life 2.28 hours. Since Te and I are both in class 10 their migration rates are the same. Although the activity of the ^{132}I atoms originally present in the core would have decreased by a factor of about 1.1^9 in 20 hours, Fig. 4.2 shows that during this time, FKCALC provides a good approximation to the total activity of ^{132}I calculated using SORS.

The release curve and the release rate will vary in different regions of the core. Fig. 4.4 shows the release curves from FKCALC for Xe for the 8 segments into which the central part of the core is divided (for the corresponding temperature sequence see Fig. 3.3), and Fig. 4.5 shows the fractional release rates for the same segments. Typically the release from the fuel particles occurs over a period of 3-4 hours between 4 and 10 hours after the accident, although in the cooler parts of the core these

* In the codes SORS, SORSD supplied by GA, and also in published data, e.g. GASSAR⁶, account is not taken of the decay of an isotope after its release from the fuel. For example, GASSAR⁶ table 2A. 5-1, the amount of ^{135}I , half life 6.7 hours is constant between 32 and 48 hours. The correction would require a trivial change in the code.

times are larger. During the period in which most of the isotope is escaping from the fuel particle the fractional release rate is between about .1 and .25 hr^{-1} . So in solving the differential equation it is only necessary to take account of decay and migration simultaneously if the decay constant λ is near the range .1 to .25 hr^{-1} , or if the precursors of an isotope are such that $\sum_j P_{ij} \lambda_j / \lambda_i$ is in this range. An example is ^{135}I , which has a half life of 6.7 hours, and is shown in Fig. 4.6. Out of the 234 nuclides treated in SORS only about 12 have values of λ in this range, so almost all nuclides fall into the 3 categories for which either decay or migration is dominant. For those isotopes which do not fall in these categories, the procedure adopted in SORS, of dropping one of the two nearly equal terms in Eq. 4.8, introduces a large approximation. This approximation is not compensated for by using an accurate numerical integration later in the calculation. For most isotopes the results of the full code and FKCALC are equally accurate.

Stage 2 Diffusion of the non-volatile elements through the graphite and their transport by the coolant, subroutine RELEAS

After they have escaped from the fuel particles, the non-volatile fission products are still confined by the graphite matrix. The scenario assumes that the graphite matrix remains intact. In order to reach the upper plenum of the primary coolant circuit, the fission products must diffuse through the graphite to the coolant channel, evaporate at the surface of the channel and be carried out of the channel by the coolant stream. The mathematical approach in SORSG to the second stage of migration is similar to the approach taken in the release from the fuel particles so we will not repeat the details. The differential equation,

Eq. 4.6, involving the total amount of nuclides present in the graphite and coolant is solved accurately. The time dependent coefficient $\bar{Q}$, which expresses the average probability of an atom escaping from the graphite into the primary coolant over the whole reactor, is calculated in subroutine RELEAS.

In subroutine RELEAS the core is divided into 140 segments. For each segment, a differential equation for the amount of the element in the coolant channel is solved. The equation is similar to Eq. 4.14 used in FKCALC; decay is neglected and the fractional release rate represents the probability of migration from the graphite to the coolant, or vice versa. A maximal rate of release controlled by diffusion is calculated on the assumption that evaporation is instantaneous. A release rate controlled by evaporation is also calculated on the assumption that diffusion is instantaneous. The lesser of these two release rates is taken as the net release rate in the code. It is assumed that the lower value indicates the rate determining process. The differential equation is solved using a crude stepwise method and a time interval of .5 hour. The remarks made in the previous section on FKCALC about the mathematical technique for decoupling the effects of decay and transport apply equally to RELEAS. There are, in addition, several other considerations:

- 1) Since some transport phenomena depend in a non-linear manner on the concentration, e.g. Freundlich isotherms, it is necessary to treat all the isotopes of an element at the same time. This is done in RELEAS.
- 2) RELEAS calculates the transport of the isotopes of the element

under consideration. The release of progenitors from the fuel is taken into account but the transport of progenitors through the graphite is not calculated. The short lived daughter of a long lived parent is everywhere in quasi equilibrium with the parent so the transport of the daughter is determined by the migration of the parent. Any isotope falling into this category is not calculated correctly by the code.

- 3) The calculation required in FKALC was simpler in that the release from the fuel particles in one section of the core did not depend directly on the release in any other section of the core. In the present case the coolant stream carries the atoms along the coolant channels and atoms which have evaporated from one section of the core may redeposit back in another part of the core. RELEAS takes this flow along the coolant channels into account.
- 4) For any isotope, the total amount, which has been released from the fuel particles in the whole core, is used as a source term for the second stage of the release. In other words the two stages of release, out of the fuel and into the coolant, have been decoupled in SORSG. Consider one particular section of the core. The amount of an isotope available to migrate through the graphite depends on the local release rate from the fuel particles, that is on the local temperature. Thus use of an average source term for the second transport stage, instead of the true source term, will be an overestimate in those regions of the core where the temperature is lower than average, and will be an underestimate in those

regions whose temperature is higher than average. Since migration rates are higher in the hotter sections, this approximation tends to underestimate the amount released at any one time, and so this assumption is not conservative. Whether the consequences of this assumption are important depends on whether the migration rates are high at the temperature at which release occurs from the fuel. If the migration rate of an isotope is low at these temperatures then transport will not become appreciable until a later time when the temperatures have risen, and so the exact time dependence of the source term is not important.

In the treatment of the first stage of release, combining the averaging performed in FKCALC with numerical integration in the main program, did not appear to change the results appreciably. In the second stage of release because the transport process is more complex it is possible that alternately calculating an average in RELEAS and then integrating the average in the main program may introduce inaccuracies.

V. Release from the fuel particles

The first stage in the release of the fission products is their escape from the fuel particles. The volatile elements, Xe, Kr, I, Br, Se and Te are assumed to escape directly into the primary coolant but for the remaining elements the amount released from the fuel is the source term for the second stage in the release. Briefly, a fuel model provides the probability of fuel failure versus temperature, and also release rate functions versus temperature for both intact and failed particles. The data may depend on the age of the particle and the fluence and temperature history. The two

versions of SORS supplied by GA incorporated two different fuel models; one similar to that used in LTR10² and the other similar to that used in AIPA.⁷ The models are discussed in detail in references 14 and 15. These two models will be referred to as Model I and Model II. In this chapter we discuss the influence of several factors on the release from the fuel particles.

1) Results for different chemical elements

The elements are divided into 10 classes such that the experimental data for the members of any one class is similar. The first two figures, 5.1, 5.2, show the release curves for the 10 classes as calculated in FKCALC for the two fuel models. This is a convenient way of compressing the results, since it was shown Chapter 4 that for most nuclides, which have moderate or long lifetimes, the release curves, which have been calculated using the whole code, are approximately the same as the results of FKCALC. The curves from FKCALC are not smooth because of the large time step, 1.5 hours, used; 50% of the release occurs over a time span of about 5 hours, and the curves approach 100% slowly, as some portions of the core remain relatively cool for a long time.

2) Effect of fuel model used

The next four figures, 5.3 - 5.6, show the difference between the two fuel models. The results are the output of the full code. Two volatile elements ⁸⁵Kr and ¹³¹I, one moderately volatile element ¹³⁷Cs and one refractory element ⁹⁵Nb are shown. For ¹³¹I, Fig. 5.3, a member of class 10, there is a significant difference in the consequences of the two models. The time, at which 50% is released,

has been postponed about 13 hours. For ^{85}Kr , Fig. 5.4, a member of class 6, there is also a significant difference, the release curve is shifted almost 5 hours. ^{137}Cs , Fig. 5.5, is a member of class 1. This is the only class for which the second fuel model predicts release from the fuel at an earlier time than the first model. The curves are displaced by about 1/2 hour. For ^{95}Nb , Fig. 5.6, which is a member of class 7, the release from the fuel occurs about 3/4 hour later using Model 2. Figs. 5.1 - 5.6 show that differences between the models postulated to fit the empirical fuel particle data for one element results in differences between the release curves for that element comparable to the differences between the curves for different elements.

3) Effect of fuel failure characteristics

The rate at which fission products can escape from fuel particles which have intact coatings is very much less than from fuel particles whose coatings have a small hole or are cracked. A small fraction of the fuel particles have impaired coatings even as manufactured. During the normal operation of the reactor it is expected that the coatings of a few more particles will deteriorate. As the reactor heats up the pressure inside the particles will increase and more coatings will fail. The fuel particle coatings fail at lower temperatures in the first fuel model than in the second fuel model so the effects of the fuel failure characteristics are different in the two cases.

For Model I the fuel fails at temperatures at which the

release rate function from a failed particle is low. So an appreciable amount of a fission product does not escape until some time after fuel failure, when the temperature of the particle has risen. Thus the details of the temperature range, within which fuel failure occurs, are not important. To take an extreme example suppose all of the particle coatings have failed prior to the accident. On this hypothesis only the release rate data for failed particles is used in the calculation. Figs. 5.7 and 5.8 show the release curves assuming 100% failed fuel, compared with the usual failure model, for ^{131}I and ^{85}Kr . The difference is only detectable at short times less than about 5 hours; for ^{131}I there is a difference of 17% at 2 hours, 3% at 3.5 hours, 1% at 5 hours; for ^{85}Kr the difference is 21% at 2 hours, 4% at 3.5 hours and 1% at 5 hours.

In fuel Model II, by contrast, the fuel particle coatings fail at a higher temperature, so the fission products thereupon can escape rapidly. Fig. 5.9 shows the fraction of triso and biso particles, which have failed, versus time. Superimposed are the release curves for three isotopes. For the classes of elements 1-9 the release curves are close to the fuel failure curve, showing that the model for fuel failure versus temperature is the controlling factor in determining the time of release. For ^{131}I and the other elements in class 10 the escape rate function is important, as in the first fuel model.

4) Effect of temperature sequence

The temperature history of the core is provided by the code

CORCON.³ For completeness, the impact of uncertainties of the temperature sequence on the SORS results was investigated. In Fig. 4.4 the release curves are shown for Xe for 8 segments of the core in the central region. The temperature histories of these 8 segments are shown in Fig. 3.3. The release curve for a given segment depends sensitively on its temperature history. There is a big difference between the release curves for different segments. So a change in the temperature histories of the individual segments could affect the average release curve for the whole core.

5) Effect of the number of segments in the mathematical model of the core

In the first version of the code which we received, the core was divided into 56 segments, and in the second version there were 112 segments. The simplest assumption would be to consider just 1 segment, in other words to assume that the whole core is at a uniform temperature and at any time this temperature is equal to the average temperature calculated by CORCON.³ Fig. 5.10 shows the release curves for the uniform core model compared with the results based on 56 segments. The very crude calculation gives a good estimate of the time taken for about 50% of a fission product to be released. From the point of view of the accident under consideration this is the essence of the calculation. The curves for the uniform core differ in the tails at long and short times. This is to be expected, for at short times some parts of the core are at a higher temperature than the average temperature and so

the release from these parts of the core will be greater than from the uniform core. At long times some parts of the core will be much cooler than the average and will still retain the fission products. So the release curve for the core with a distributed temperature will be above the release curve for a uniform core at short times, and below for long times.

VI. Diffusion through the graphite

The evaporation rate at the surface of a coolant channel is a boundary condition for the partial differential equation describing the diffusion through the graphite. This is a complex problem, so in SOKSG, diffusion and evaporation are treated independently. The code essentially makes one of two extreme assumptions. In each small section of the core either the process is controlled solely by the rate of diffusion or solely by the rate of evaporation. In the first case it is assumed that any atoms reaching the coolant channel surface evaporate instantaneously and moreover, that the concentration profile in the graphite, and the current, have the steady state values. The actual geometry of the core is complicated so in SORSG the graphite matrix is modelled as a cylinder surrounding the fuel hole, thus the concentration profile is assumed to be logarithmic. The rate of release of an element into the coolant channel is taken to be equal to the steady state diffusion current. In the second case it is assumed that evaporation is the controlling process, and that diffusion is sufficiently rapid that the concentration profile is always uniform. In other words as atoms evaporate from, or are deposited on the surface, migration to, or from, the interior occurs immediately to maintain an even concentration.

The rate of evaporation is calculated from the vapour pressure of the element in question. In SORSG, for each section of the core, two potential release rates are calculated based on each of these two assumptions, Fig. 6.1. The smaller of these two rates is assumed to indicate which is the controlling process and this rate is then used as the net release rate.

In practice diffusion through the matrix web requires a certain amount of time, and also after the failure of the fuel it will require some time to establish either of the steady state concentration distributions assumed in SORSG. For example, initially, even if evaporation is instantaneous at the coolant channel surface, the diffusion current will be less than the steady state value and so use of the steady state current could lead to an underestimate of the time for the release of a small fraction of the fission product inventory. Moreover, especially for the more refractory elements, the diffusion rate is so slow that assumption of a uniform concentration may drastically overestimate the possible evaporation rate, since the time required to establish a uniform concentration could be years. So, some calculations were made to determine rough guide lines as to the time scale required by the diffusive process alone. These times give a lower limit on the time required for release of the fission products because of the additional time delay caused by evaporation, and also the possibility of deposition back on other cooler parts of the core.

Three simple cases, for which solutions are available,¹⁸ were considered. The geometry and data, which were given in SORSG, were used. In the first two calculations it is assumed that the evaporation rate is very high so that the concentration at the surface of a coolant channel is

always zero. For a very small release, 1 - 2%, the amount of the isotope in the fuel rod can change by a small fraction, so to estimate the time required we use the solution in which the concentration in the fuel rod is constant (Franck¹⁸ p. 84). To estimate the time required for a larger quantity to be released we use the transient solution for the release from a cylinder within which the initial distribution is specified (Franck¹⁸ p. 73). In Tables 6.1 and 6.2 are shown the results calculated for the release of a few percent and of about one third. Table 6.1 shows the estimated times at two temperatures; 2270°K, at this temperature almost all fuel particles have failed so the fission products are available to diffuse through the graphite; and 3640°K, which is the sublimation temperature of graphite, and so is the highest temperature attained by the core. From this table we see that at a constant temperature of 2270°K it would require more than 1.6 hours for a few percent of Pd to diffuse from the fuel hole to the coolant channel and longer for the elements more refractory than Pd. Even at the sublimation temperature of graphite more than 30 hours would be required for the diffusion of a few percent of the Mo and elements more refractory than Mo. So the most refractory elements will be retained in the core for long periods of time provided the graphite remains intact. Table 6.2 shows the results in terms of the temperature required for diffusion to occur in the specified time of 1 hour or 1 day.

The alternative assumption regarding diffusion in SORSG is that the concentration in the graphite web is always uniform. Because diffusion is not instantaneous, some time will elapse before the fission products have spread out uniformly from the fuel holes. Since in this model the

diffusion rates are assumed to be very rapid, compared to the evaporation rates, we will use the solution for the diffusion of an initial distribution within a cylinder, which has an impermeable surface (Franck¹⁸ p. 81). The results are shown in Tables 6.1 and 6.2. From Table 6.1 at 2270°K, we see that for Sb, about 1/2 hour is required to establish an approximately even concentration; and about 2.5 hours, at this temperature, would be required for an appreciable release, assuming no constraint were imposed on the rate of evaporation. So for elements more volatile than Sb, it is reasonable to calculate a vapour pressure based on the assumption of a uniform distribution of the element throughout the graphite. On the other hand, elements after Pd require upwards of about 16 hours at 2270°K for the concentration to become uniform, so this assumption would overestimate the vapour pressure. After about 48 hours about half the core is at the graphite sublimation temperature of 3640°K. For a section of the core at this temperature an even concentration distribution could be attained quickly, in less than 1 hour, for elements more mobile than Nd, whereas for elements more refractory than U more than a day would be required. To consider the most refractory elements, Nb and Zr, more than a year would be required to reach a uniform concentration, so obviously use of this assumption is unrealistic.

The migration of fission products from the fuel to the primary coolant involves an interplay of the two processes, diffusion and evaporation. The evaporation rate will depend on the rate at which the coolant flows through the coolant channels as well as on the temperature distribution. In SORSG we can eliminate the evaporation process and calculate a release curve in

which the delay in the graphite is due only to diffusion. This curve gives a minimum estimate of the times required for release since the steady state diffusion current is used, and redeposition of the fission products is neglected. For fast flow rates for which evaporation is rapid the release curves will be close to this estimate. If the flow rate is slow, the release curve will be displaced to larger times. Fig. 6.2 compares the curves showing the release from the fuel and the release from the graphite, assuming instantaneous evaporation and no redeposition, for ^{90}Sr . It can be seen that the release curves are displaced by about 5 hours. So for ^{90}Sr , diffusion alone implies an additional delay of about 5 hours in the release from the core.

VII. Evaporation and Deposition in the coolant channels

After the fission product atoms have diffused through the graphite matrix to the coolant channel surface they may escape from the surface and be carried along the coolant channel by the flowing helium. Further along the coolant channel atoms may deposit back on the surface and then diffuse into the graphite. This cycle may be repeated several times before an atom emerges out of the coolant channel into the upper plenum. At any place the net loss by evaporation will depend on the local temperature and surface concentration of the graphite, the flow rate of the coolant and the partial pressure of the element in the coolant.

The coolant channel is modelled by dividing it into a number of segments and the temperature is taken to be uniform within each segment. The change in temperature along the length of a coolant channel in the central portion of the core is shown in Fig. 7.1 for two different times. Fig.

3.3 shows the evolution in time of the temperature of central parts of the core. It can be seen in Fig. 7.1 that sharp discontinuities in the temperature are introduced at the boundary between two segments. However the segments are chosen to coincide with the fuel elements so the thermal conduction from one element to another will be poorer than within one element. Direct diffusion from one fuel element to another is neglected.

As the coolant flows up the coolant channels, the fission products will evaporate from the graphite wall if the partial pressure in the coolant is less than the vapour pressure at the surface of the channel. Conversely the fission products will deposit back on the graphite if the partial pressure is less than the vapour pressure. As the core heats up material will initially evaporate from the hotter central segments and be redeposited on the cooler segments at the top and on the reflector. Eventually these segments heat up and the material re-evaporates. In order to calculate the evaporation rate, the assumption is made in SORSG that the distribution of the impurity is uniform throughout each segment of the core. If all the impurity present in a given segment has originated within the fuel particles contained in that segment, this is a conservative assumption, since the concentration at the coolant surface must be less than in the interior; however as discussed in Chapter 6, this assumption may not be realistic at a temperature at which the diffusion rate is low. If we consider a portion of the top reflector, initially there are essentially no fission products present. However as the core heats up fission products will evaporate from the hot central portions of the core, will be carried up the coolant channel and will redeposit back on the top reflector. To calculate the rate of

deposition onto the top reflector the same assumption concerning diffusion is made, namely that the concentration becomes uniform instantaneously. However in this instance the direction of diffusion is in the opposite direction, from the coolant channel surface toward the interior of the matrix graphite. Moreover the reflector is at a lower temperature than the rest of the core so diffusion rates are slower. The concentration at the surface will actually be higher than that calculated using a uniform concentration and there may be a buildup of impurity at the surface, especially for elements and temperatures for which the diffusion rate is low. Thus, the effect of the assumption of infinitely fast diffusion is, in this case, to overestimate the rate of deposition, and to underestimate the probability of an impurity atom being carried out of the coolant channel. So the assumption is not conservative overall.

Development of an expression for mass transfer as described in LTR10²

We quote the following paragraph from LTR-10², section 5.4 page 5-16. A coefficient H is defined in Eq. 7.2.

"The vapor pressure at the graphite surface in a coolant channel, relative to the gas-phase partial pressure in the coolant channel, is then used in calculating the local mass transfer coefficient. The release rate from the graphite into the gas phase of the coolant channel, or rate of condensation from the coolant and re-adsorption in the graphite, is then a function of the magnitude of the mass transfer coefficient and the direction of the pressure gradient from the bulk stream to the surface of the graphite:

$$R(t) = H W \frac{P_b - P_c}{P_s}, \quad (\text{LTR-10 - 5.9}) \quad 7.2$$

where $R(t)$ = evaporation or condensation rate (g/sec),

H = local mass transfer coefficient calculated as a function of turbulent, laminar, or sublaminal flow regime defined by the local Reynolds and Schmidt numbers,

W = carrier gas flow rate (g/sec),

P_s = total system pressure (atm),

P_b = temperature- and concentration-dependent element vapor pressure at the graphite surface (atm),

P_c = element partial pressure in the coolant stream at the entrance to the core segment (atm)."

$R(t)$ is the total evaporation rate in (g/sec) so the coefficient H , defined above, is a global mass transfer coefficient for the segment of the coolant channel under consideration. The term 'local' usually denotes a transfer coefficient referred to an infinitesimal segment. The use of $R(t)$ in the code is consistent with the assumption that both $R(t)$ and H in Eq. 7.2 refer to global rates for a whole segment.

We quote the expressions given in section 5.5.3 of LTR-10² for three different flow regimes:

"5.5.3 Mass Transfer Film Coefficient

The well-known Sherwood-Pigford relationship, based on the heat mass transfer analogy, is used for the calculation

of the mass transfer coefficient. The mass transfer coefficient (H) for the effusing species through the coolant boundary layer is based on both laminar and turbulent flow considerations:

$$\text{For Reynolds number } > 2100 \text{ (turbulent flow),} \\ H \approx 0.023 / (Sc^{0.67} Re^{0.2}); \quad 7.3$$

$$\text{for Reynolds number } < 2100 \text{ and } L/(d Re Sc) < 0.07, \\ H \approx 1.86 (d/L Re Sc)^{1/3} / (Re Sc); \quad 7.4$$

$$\text{for Reynolds number } < 2100 \text{ and } L/(d Re Sc) > 0.07, \\ H \approx 3.66 / (Re Sc). \quad 7.5$$

A correction factor, Eq. 5.20 of LTR-10², is applied to account for the diffusion of the impurity through the boundary layer. Since this is approximately one for low impurity concentrations we will omit it, for simplicity, in our discussion.

Combining Eq. 7.2 with each of the possible expressions for H, we get

$$1) \text{ For } Re > 2100 \\ R(t) = [0.023 / (Re^{0.2} Sc^{0.67})] (W(P_b - P_c) / P_s) \quad 7.6$$

$$2) \text{ For } Re < 2100 \text{ and } L/(d Re Sc) < .07 \\ R(t) = [1.86 (d/L Re Sc)^{1/3} / (Re Sc)] (W(P_b - P_c) / P_s) \quad 7.7$$

$$3) \text{ For } Re < 2100 \text{ and } L/(d Re Sc) > .07 \\ R(t) = [3.66 / (Re Sc)] (W(P_b - P_c) / P_s) \quad 7.8$$

Inspection of the code indicates that the expressions used to calculate R(t) are consistent with Eqs. 7.6, 7.7, and 7.8.

Let us apply these equations to two specific examples.

Example 1 Fast flow through a short segment. We assume that the flow is turbulent so Eq. 7.6 is appropriate. If we substitute for the Reynolds and Schmitt numbers, we obtain for the evaporation rate

$$R(t) = [0.023/L/cD]^{0.67} (Vcd/\mu)^{0.2} (W(P_b - P_c), P_s) \quad 7.9$$

where V is the velocity of the fluid in cm/s

c is the density of the fluid in gm/cm³

μ is the viscosity of the fluid in gm/cm sec

d is the diameter of the channel in cm

D is the diffusion coefficient of the impurity in cm²/sec and the other symbols are defined in Eq. 7.2. This equation does not include explicitly the length of the segment. So Eq. 7.9 predicts that the same number of grams would evaporate per second from a segment twice as long as the original segment. For the flow conditions under consideration, we would expect, on physical grounds, that the concentration of the impurity in the vapour will change very slowly along the length of a tube. So the mass evaporated from a given segment should be approximately proportional to the length of that segment.

Example 2 Slow flow through a long segment. We assume that the flow is laminar and that the length of the segment is such that $(L/D \text{ Re } Sc) > 0.07$, so Eq. 7.8 is appropriate. The partial pressure of the impurity at the end of the segment, P_d , is

$$P_d = P_c + (R/W) P_s, \quad 7.10$$

Substitute for R from Eq. 7.8

$$P_d = P_c + [3.66/(Re \text{ } Sc)] (P_b - P_c). \quad 7.11$$

Substitute for the Reynolds and Schmidt numbers then

$$P_d = P_c + [3.66 D/Vd] (P_b - P_c). \quad 7.12$$

As a particular example, suppose that the partial pressure at the entrance to the segment were zero, i.e. $P_c = 0$, then Eq. 7.12 becomes

$$P_d = (3.66 D/Vd) P_b \quad 7.13$$

If we consider slower and slower flows through the same segment, this equation predicts that the partial pressure at the exit from the segment increases without limit, i.e. if $V \rightarrow 0$ then $P_d \rightarrow \infty$. Physically, this cannot happen. Evaporation only occurs if the partial pressure is less than the saturated vapour pressure, and so the partial pressure at the exit to the segment must be always less than the saturated vapour pressure.

The contradictions revealed by these two examples are due to the inconsistent use of Eqs. 7.2 and 7.3-5.

Development of an expression for mass transfer using the standard approach

We will now develop the expressions for the evaporation or condensation rate following the usual approach adopted in the literature. The discussion will be based primarily on two books: 'Transport Phenomena',²⁰ by R. B. Bird, W. E. Stewart and E. N. Lightfoot and 'Mass Transfer',²¹ by T. K. Sherwood, R. L. Pigford and C. R. Wilke. The latter book is a revision of the book which was cited by Schwartz et. al.² in the description of SORS. Expressions for the rate of mass transfer are often chosen on the basis of the analogies between mass, heat and momentum transfer, if the theoretical bases and experimental data for mass transfer are not available. We quote from 'Mass Transfer' page 159: "The close similarity of the processes of mass, heat and momentum transfer in fluids is

suggested by the fact that the basic equations expressing the fluxes have the same form The similarity of the forms of the three rate equations makes it possible to apply an analysis of one of the processes to either of the other two." Table 21.2-1 of 'Transport Phenomena' gives a list of the analogous heat transfer and binary mass transfer quantities; for example the Prandtl number in heat transfer is the analogue of the Schmidt number in mass transfer.

We will define a transfer coefficient and Nusselt number following section 21.1 of 'Transport Phenomena'. Consider a gas flowing along a mass transfer surface through which an impurity may enter the stream at a local rate, N moles/(unit area)(unit time). The diffusional contribution to N should be roughly proportional to some characteristic composition difference between the gas at the surface and in the main stream. Since we are considering a gas, it is convenient to use the difference in partial pressure of the impurity rather than the molar concentration. For a surface of area A , we can define an average mass transfer coefficient, k , by the equation

$$R(t) = k (\Delta P/P_s) A \quad 7.14$$

where $R(t)$ is the molar rate of transfer across the whole surface in mole/sec,

A is the area of the surface in cm^2 ,

ΔP is a characteristic difference in the partial pressure of the impurity (in atm),

P_s is the pressure of the flowing gas (in atm),

k is an average mass transfer coefficient in moles/(sec cm^2).

P_s should be multiplied by a correction factor. Since this correction factor is approximately equal to one for low impurity concentrations, we shall, for simplicity, omit the factor here. The same factor was omitted in the previous section. The characteristic pressure difference, ΔP , may be defined in several different ways, leading to correspondingly different definitions of the mass transfer coefficient k . For example ΔP may be defined as the initial difference in partial pressures; alternatively, ΔP may be defined as an arithmetic, or logarithmic, average over the whole surface, of the difference in partial pressures. If the transfer rate is very small these three definitions of ΔP would give the same value for the mass transfer coefficient k . However at high transfer rates, there may be a considerable difference between the different choices for k . An example, for the case of heat transfer, is shown in Fig. 13.1-3 of 'Transport Phenomena'. In practice, the logarithmic average is usually adopted.

It is useful to proceed in terms of a dimensionless number, the Nusselt number, which is derived from k . The Nusselt number, Nu , for flow through a circular tube, is defined as

$$Nu = \frac{kd}{cD} \quad 7.15$$

where d is the diameter in cm,

c is the molar concentration in moles/cm³,

D is the binary diffusion coefficient in cm²/sec.

Since the Nusselt number derives from the transfer coefficient, there is a local Nusselt number, a logarithmic Nusselt number, etc. We can rewrite Eq. 7.14 in terms of the Nusselt number, and the area of a segment,

of length L cm, of a circular channel. The molar rate of transfer for the segment is

$$R(t) = cD \text{ Nu } \pi L (\Delta P/P_s) \quad 7.16$$

To facilitate comparison with the expressions used in SORS we will rewrite this expression so that it involves the flow rate of the carrier gas, W , explicitly.

$$W = cV \pi d^2/4 \quad 7.17$$

where W is the carrier gas flow rate (moles/sec),

c is the density of the carrier gas (moles/cm³),

d is the diameter of the channel (cm),

V is the average velocity of the carrier gas (cm/sec).

In terms of the Reynolds and Schmidt numbers

$$W = \pi cDd \text{ Re Sc}/4 \quad 7.18$$

Substituting in Eq. 7.16, the molar rate of transfer for a segment is

$$R(t) = (4L/d) (\text{Nu}/\text{Re Sc}) (W\Delta P/P_s) \quad 7.19$$

'Transport Phenomena' quotes expressions for the logarithmic heat transfer Nusselt number for three flow regimes on page 399 and page 404. These expressions are based on theory and experimental data. If we substitute the analogous quantities for mass transfer we obtain the following equations for the logarithmic mass transfer Nusselt number, Nu_{1n} ,

For $\text{Re} > 20,000$

$$\text{Nu}_{1n} = .026 \text{ Re}^{0.8} \text{ Sc}^{.33} \quad 7.20$$

For $\text{Re} < 2000$ and $L/(d \text{ Re Sc}) < .1$

$$\text{Nu}_{1n} = 1.86 (d/L \text{ Re Sc})^{1/3} \quad 7.21$$

For $Re < 2000$, Nu_{ln} tends to a limit for large values of $(L/d Re Sc)$

$$\lim Nu_{ln} = 3.657 \quad 7.22$$

Sherwood et. al.,^{19,21} discuss the experimental data on mass transfer, between the surface of a liquid film and a gas stream in a wetted wall column, for turbulent flow, $Re > 2000$. They quote several empirical relationships similar to Eq. 7.24 but with slight variations in the choice of the multiplicative factor and the exponents. So it is reasonable to use Eq. 7.24 for flow rates such that $Re > 2000$.

We can now combine Eq. 7.19 with the empirical expressions given in Eqs. 7.20-22.

For $Re > 2000$

$$R(t) = (4Ld) (.026 / (Re^{0.2} Sc^{.67})) (W\Delta P_{ln} / P_s) \quad 7.23$$

For $Re < 2000$ and $L/d Re Sc < .1$

$$R(t) = (rL/d) (1.86 (d/L Re Sc)^{1/3} / Re Sc) (W\Delta P_{ln} / P_s) \quad 7.24$$

We emphasize that since Eqs. 7.20, 7.21 refer to logarithmic Nusselt numbers, the pressure differences in Eqs. 7.23 and 7.24 must also be logarithmic averages. This difference is academic only for a flow rate and length of segment such that ΔP does not change much along the length of the segment. For the third possibility which corresponds to slow flow rates and a long segment, the limiting value of Nu_{ln} must be used. However this limit must be treated consistently, since the logarithmic pressure difference diverges, so we will expand on this case in more detail.

For brevity, we will introduce a dimensionless number which we will

call the "stagnation number", S_n ,

$$S_n = L/d \text{ Re } S_c \quad 7.25$$

where L is the length of the segment,

d is the diameter of the channel,

Re is the Reynolds number,

S_c is the Schmitt number.

The stagnation number can be rewritten as a ratio of the time that the coolant takes to traverse the channel to the time that an impurity atom takes to diffuse from the wall to the center of the channel. The reason for calling this dimensionless quantity the stagnation number is apparent as it measures the degree of stagnation of the flow. In a stagnant container an impurity in the fluid will be in equilibrium with the impurity deposited on the walls of the container. For flow through a channel, if the stagnation number is large there is ample time for many atoms to diffuse into the coolant stream during the time the coolant takes to flow the length of the channel. So at the exit from the channel the construction of an impurity in the coolant will be in quasi-equilibrium with the impurity on the walls of the channel. For the case under consideration the driving force for mass transfer is the difference between the partial pressure of an impurity in the coolant and the vapour pressure of the impurity at the temperature of the graphite. How close the partial pressure, at the exit of a segment, is to the vapour pressure, within the segment, depends on the value of the stagnation number. Fig. 7.2¹⁹ shows some data and theoretical predictions for flow through tubes. The pressure at the exit of a segment tends to the stagnant limit for large values

of the stagnation number and is within 5% of the limit for values of the stagnation number greater than about 0.2.

The limiting case for slow flows corresponds to a logarithmic Nusselt number equal to about 3.66 and a pressure at the exit to the segment approximately equal to the vapour pressure. The correct limiting form for the total number of moles transferred per second in a segment is equal to the difference between the number of moles leaving the segment per second at a partial pressure equal to the vapour pressure, P_b , and the number of moles entering the segment per second at a partial pressure P_c . Assuming that we can use the perfect gas laws for both coolant and impurity

$$\frac{W}{P_s} \approx \frac{R(t)}{P_b - P_c} \quad 7.26$$

or for $Re < 2000$ and $L/d Re Sc > .2$

$$R(t) \approx W (P_b - P_c)/P_s \quad 7.27$$

To summarize, the pertinent equations which should be used to calculate mass transfer are Eqs. 7.23, 7.24 and 7.27. These can now be compared with those used in SORS, Eqs. 7.6, 7.7 and 7.8.

Comparing Eqs. 7.23 and 7.24 with Eqs. 7.6 and 7.7, we notice two differences. A geometrical factor $4 L/d$ is omitted from the equations used in SORS. Also the pressure difference at the entrance to the segment is used instead of the logarithmic average pressure differences. Comparing Eqs. 7.27 and 7.8 we see that an extra factor $(3.66/Re Sc)$ has been included in the expression used in SORS.

Application to the hypothetical accident

We will now apply the previous discussion to the hypothetical

accident under consideration. The accident scenario assumes that there is no forced circulation and so the coolant flow is induced by natural convection. Using the code RECA,¹² Schwartz et. al. estimated that the average Reynolds number varies from 6.9 at 1 hour to .0041 at 50 hours. Because of the differences in temperature the Reynolds number varies from one part of the core to another and also with time. For the flow rate of 5.67×10^3 gm mole/hr, which is used in the sample data supplied by General Atomic, the ranges of Reynolds number in the core are shown in Table 7.1. In other published data⁶ a flow rate of 5.67×10^5 gm mole/hr is used. This would increase the Reynolds number by a factor of 100. For the trial data the Reynolds numbers vary from .1 to .5, so the flow is laminar. The second dimensionless number is the Schmidt number. Values of this number range from .18 to 1.8. Table 7.1 shows the range of values of the stagnation number calculated in SORSG using the trial data. Sn varies from 247 to 2500. Even if the flow rate is increased by a factor of 100 the stagnation number is still within the limiting regime. Thus, for the flow conditions expected during the accident, the rate of transfer from coolant to the graphite and vice versa should be based on the expressions for the stagnant limit, Eq. 7.27.

The expression used for $R(t)$ in SORSG, Eq. 7.8, contains an erroneous factor equal to $(3.66/Re Sc)$. The implications of this on the further calculations cannot be predicted. For example, with the trial data supplied with the code SORSG, a typical value of this factor is about 10. Thus in one portion of the core the code will overestimate the rate of evaporation by a factor of 10, yet in another portion of the core, where

mass transfer is in the opposite direction, the code will overestimate the amount deposited back on the surface by a factor of 10. So the net effect of the error on the release rate of a fission product from the core is unpredictable. To see what the effect may be, the instructions in the code SORSG in which the evaporation rate was calculated, were changed from Eq. 7.5 to Eq. 7.7. The rest of the structure of the code was unchanged. Fig. 7.3 shows the output using the trial data supplied by GA for the two calculations. The release curve is shifted by about 10 hours for ^{90}Sr .

Effect of correlations between the time of the release from the fuel and the evaporation rate

As discussed in Chapter 4, the code is structured in such a way that the total amount of a fission product which has escaped from the fuel particles, is used as the source term for diffusion and evaporation. In other words the correlation between the release from the fuel particles in a given segment and the diffusion and evaporation within the same segment, is neglected. This approximation is only good if the migration rate through the graphite is low at the temperatures at which the material is released from the fuel. To see the possible significance of this correlation the code, modified as described previously to use Eq. 7.7, was run with the amount in the graphite at the start of the accident equal to 0%, 10% and 100%. Fig. 7.4 shows the release curves for ^{90}Sr . The three curves are close to each other and so the time at which ^{90}Sr is released from the fuel does not affect appreciably its migration through the graphite for this set of data.

Comparison of the results of SORSG with the results of EVAP

Subroutine RELEAS calculates the release rate from the graphite in

each section of the core and calculates an average of the release rates for the whole core. RELEAS is called at specified time intervals. The amount of an element within the graphite of a given section is expressed as the product of the total amount of the element in the graphite of the whole reactor and a weighting factor for the particular section. The change in the weighting factor is calculated within subroutine RELEAS. However the change in the total amount of a fission product in all of the graphite of the reactor is calculated in the main part of the program, using the average release rate from the graphite and including radioactive decay. This mathematical procedure could conceivably introduce some inaccuracies into the results.

An independent code EVAP was written to produce results which could be compared with the results of SORSG under appropriate conditions. A detailed description of EVAP is given in a report.²² In EVAP the core is divided into several sections as in SORSG. EVAP calculates only the migration along the coolant channels, it does not calculate the release from the fuel particles, the rate of diffusion or decay. It is assumed that the concentration of an impurity is uniform within each of the graphite sections. EVAP treats each radial region of the core separately. For one radial region, the coupled differential equations for the amount of an impurity within each of the sections of that region are integrated numerically from the start of the accident to the final time desired. The same procedure is followed for each of the radial regions in turn. The total amount released from the whole core is the sum of the amounts released from each radial region.

For illustration we show the results for two stable isotopes. Fig. 7.5 compares the results for ^{88}Sr and ^{149}Sm calculated by SORSG, modified as described previously, and EVAP. For Sr there is a small difference in the two curves. SORSG predicts that ^{149}Sm would be released about 20 hours earlier than is predicted by EVAP. SORSG predicts that at 20 hours after the initiation of the accident about 4.3% of the ^{149}Sm would be released. We will make a rough estimate of an upper bound for the maximum release during the first 20 hours, using a crude and overly conservative model. Assume that all the ^{149}Sm is initially in the upper half of the top reflector. The highest temperature reached in the upper half of the top reflector by 21 hours is 2621°F . At this temperature the vapor pressure of Sm would be 4.5×10^{-5} atm. The temperature of the upper half of the top reflector rises slowly during the course of the accident. For the purposes of this calculation assume that the temperature is equal to 2621°F for 20 hours. Taking the same flow rate used in SORSG the computed amount of ^{149}Sm which can be swept out of the reflector in 20 hours is about 1.5%. The difference between the 4.3% computed by SORS and the upper bound of 1.5% indicates that the mathematical procedure adopted in SORSG could introduce inaccuracies, and further analysis of the algorithms in SORS is needed to identify the source of the discrepancy.

VIII. Summary of Observations

The objective of the code SORS is to calculate the release of fission products from the fuel into the primary coolant circuit. The code calculates the release from the fuel particles and uses this release as a source term for the second stage of migration. The only physical

processes considered in the second stage are diffusion and evaporation.

The problem involves a consideration of three kinetic processes simultaneously, radioactive decay, transport out of the fuel, and transport through the graphite and in the primary coolant. The two transport rates depend both on time and on the position within the reactor, since these rates involve processes which are temperature dependent. A mathematical solution of the problem must incorporate two features, a subdivision of the core into segments and a technique for the numerical integration of the differential equations. The approach adopted in SORS is to calculate average reactor wide values for the transport rates by solving, approximately, differential equations, which neglect decay, in each segment of the core. Then the differential equations for the whole reactor incorporating both decay and the average values of the transport rates, are integrated using an accurate and sophisticated numerical technique. A simultaneous treatment of decay and transport is required only if the rates of these two processes are comparable. If the changes caused by decay are negligible then the accuracy of the final solution is determined by the averaging process, that is by the subdivision of the core and the time interval and integration technique used in calculating the changes within each segment. To repeat the integration, as done in SORS, does not increase the accuracy. If the rates of decay and transport are comparable, the procedure used in SORS to decouple these processes is questionable. The average values of the transport rate are calculated by neglecting decay in each individual segment, this neglect of one of two comparable terms in a differential equation introduces a large approximation. To

reintegrate the reactor wide differential equations, which incorporate both decay and the approximate values for the average transport rates, does not compensate for any errors, which may have been introduced in the calculation of the average transport rates.

1) Release from the fuel particles

The results from SORS are as accurate as the results calculated in FKALC, wherein a time step of about 1.5 hours has been used. The interpretation of the experimental data on the properties of the fuel particles, is one of the most important inputs to the code. A very crude calculation with one core segment and a time step of 1.5 hours gives a fair approximation, in most cases, to the results calculated using the whole code. The differences between the results based on different fuel models are large. The temperature distribution and evolution is another important set of input data.

2) Transport through the graphite and in the coolant channels

1. The release from the fuel and the second stage of transport have been decoupled. The adequacy of this approximation depends on the transport rates at the temperatures at which release from the fuel occurs. For ^{90}Sr the time at which the atoms escape from the fuel particles does not appear to affect the release into the coolant.

2. For this stage the calculation of an average transport rate and the integration of the averaged reactor wide equation proceed in parallel. The reintegration cannot improve the accuracy

over that attained in subroutine RELEAS, moreover this alteration may introduce additional errors. For example, the amount of a fission product in the graphite in a given segment is written as the product of the total amount in the graphite for the whole reactor and a weighting factor. The first term in this product is affected by what has happened in other segments of the reactor, far away from the segment under consideration. A comparison with a code which treats the migration along the coolant channels in a different manner shows that, for the conditions considered, the release curves may be displaced a few hours.

- 3) The expression used to calculate the evaporation rate is in error. This error introduces inconsistencies during the course of the calculation. The net effect of the error is indeterminate since the net evaporation rate is overestimated in some parts of the core and underestimated in other parts.

Conclusions

- 1) The calculation scheme for the release of the volatile fission products is probably adequate. The mathematical accuracy is determined primarily by the time step used in subroutine FKCALC. The accuracy of the results is dominated by the uncertainties in the experimental data, in the empirical model for release from the fuel particles and in the temperature history.
- 2) Assuming that the expression for the evaporation rate and for the mass transfer coefficient are made consistent, the results predicted by SORSG using the trial data differ slightly from the

results predicted by another independent code. We attribute these differences to the mathematical procedure used in the SORSG to average over the core and to include decay. For the non-volatile fission products the accuracy of the results is dominated by uncertainties in the temperature history of the top reflector, the flow rate of the coolant and the vapour pressure data.

Any calculations based on the code, in the form which we received it and using the expressions described in LTR-10² for the evaporation rate are incorrect. The magnitude of the error depends on the conditions specified for the accident and may be large.

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Table 3.1

Fission Product Classification by
Chemical and Thermodynamic Similarities

<u>Species Number</u>	<u>Element</u>
1	Sr
2	Rb, Cs
3	Ba, Sm, Eu
4	Ce
5	Xe
6	Kr
7	Zr, Nb, Mo, Te
8	Y, Pd, Sn, La, Pr , Nd, Pm
9	Ru, Rh
10	Se, Br, Te, Sb, I

Table 3.2

Diffusion Coefficients for Elements in Graphite^(a)

<u>Element</u>	<u>A</u>	<u>B</u>
Y	0.74	14.2
Zr	1.19	22.8
Nb	1.32	25.5
Mo	1.00	19.2
Tc	1.02	19.6
Ru	0.91	17.5
Rh	0.77	14.8
Pd	0.52	10.1
Sb	0.35	6.8
La	0.75	14.4
Ce	0.84 (0.55)	16.2 (10.5)
Pr	0.63	12.0
Nd	0.56	10.7
Pm	0.44	8.5
Sm	0.39	7.6
Eu	0.33	6.4
Th	1.03 (0.98)	19.8 (18.8)
Pa	1.13	21.7
U	0.81	15.6
Pu	0.55	10.6
Sr	0.34 (0.67)	6.5 (6.8)
Ba	0.35 (0.12)	6.7 (7.0)
Cs	0.21	4.1
Rb	0.21	4.1

(a) Literature values are shown in parentheses.

$$- \log_{10} D = A + \frac{B \times 10^3}{T},$$

where D is in cm²/sec and T is in °K
(source: Ref. 16).

Table 3.3

Freundlich Isotherms of Certain Fission Products^(a)

<u>Element</u>	<u>a</u>	<u>b</u>		
Ba	6.49	-33.7	-1.304	7.55
Sr	8.67	-36.1	-0.572	4.59
Cs	7.8	-29.84	0.2351	1.873
Rb	9.33	-31.06	-2.23	6.99

$$(a) \ln P_m = a + \frac{b \times 10^3}{T} + (c + \frac{d \times 10^3}{T}) \ln C_m$$

where P_m is in atm and C_m is in μmoles/m² reactor graphite surface area (source: Ref. 16).

Table 3.4

Vapor Pressures of Elements in a Graphite System^(a)

P_n	A	B	P_n	A'	B'
Y	4.21	25.8	Ce	6.77	29.5
YC ₂	8.70	39.3	CeC ₂	9.83	36.7
Zr	7.65	41.5	Pr	4.37	21.9
ZrC ₂	9.40	49.4	PrC ₂	7.58	31.3
Nb	8.14	46.3	Nd	3.47	19.5
NbC ₂	9.88	54.6	NdC ₂	7.00	30.4
Mo	7.40	34.9	Pm	3.93	15.5
Tc	8.09	35.6	Sm	3.72	13.8
Ru	7.27	31.9	Eu	3.28	11.6
RuC	7.97	34.9	EuC ₂	6.66	26.2
Rh	6.85	26.9	Th	6.40	36.0
RhC	7.87	32.4	ThC ₂	7.86	39.4
Pd	5.59	18.2	Pa + PaC ₂	6.99	39.2
Sb as Sb	5.35	12.4	U	4.50	28.3
Sb as Sb ₂	5.13	9.0	UC ₂	7.89	38.7
Sb as Sb ₄	2.60	5.1	Pu	3.45	19.3
La	5.16	26.1	PuC ₂	5.20	30.0
LaC ₂	7.81	33.3			

(a) $\log P_n = A - B \frac{10^3}{T}$, where P_n is in atm and T is in °K

(source: Ref. 16).

Table 3.5

Monolayer Concentrations in Graphite

(graphite assumed to have $1 \text{ m}^2/\text{g}$ surface area
and a 90.7% packing fraction allowed)

<u>Element</u>	<u>Monolayer Concentration</u> <u>($\mu\text{moles/g}$ graphite)</u>
Rb	7.8
Sr	10.4
Y	15.1
Zr	18.7
Nb	22.5
Mo	24.9
Tc	25.9
Ru	26.7
Rh	26.7
Pd	25.6
Sb	19.0
Cs	6.7
Ba	9.7
La	13.7
Ce	14.6
Pr	14.5
Nd	14.5
Pm	14.6
Sm	14.6
Eu	12.1
Th	14.7
U	25.1
Pu	20.9

(Source: Ref. 16)

Table 6.1

Approximate Diffusion Times in Hours at the Stated Temperature for:

1. Release of a few percent
2. Attainment of an even concentration
3. Release of about a third

	<u>2270°K</u>			<u>3640°K</u>		
	1	2	3	1	2	3
RB	1.7E-03	1.9E-02	5.0E-02	3.6E-04	3.9E-03	1.0E-02
CS	1.7E-03	1.9E-02	5.0E-02	3.6E-04	3.9E-03	1.0E-02
EU	2.4E-02	2.5E-01	6.7E-01	2.0E-03	2.2E-02	5.9E-02
SR	2.7E-02	2.9E-01	7.6E-01	2.2E-03	2.4E-02	6.4E-02
SA	3.3E-02	3.6E-01	9.6E-01	2.6E-03	2.8E-02	7.4E-02
SB	3.7E-02	4.0E-01	1.1E+00	2.8E-03	3.0E-02	7.9E-02
SM	9.1E-02	9.9E-01	2.6E+00	5.0E-03	5.4E-02	1.4E-01
PM	2.5E-01	2.8E+00	7.3E+00	9.9E-03	1.1E-01	2.8E-01
PD	1.6E+00	1.7E+01	4.5E+01	3.3E-02	3.6E-01	9.4E-01
PU	2.8E+00	3.0E+01	7.9E+01	4.8E-02	5.2E-01	1.4E+00
ND	3.1E+00	3.4E+01	9.0E+01	5.3E-02	5.7E-01	1.5E+00
PR	1.4E+01	1.5E+02	3.9E+02	1.4E-01	1.5E+00	4.0E+00
Y	1.6E+02	1.8E+03	4.7E+03	7.3E-01	7.9E+00	2.1E+01
LA	2.1E+02	2.2E+03	5.9E+03	8.5E-01	9.2E+00	2.4E+01
RH	3.2E+02	3.5E+03	9.3E+03	1.1E+00	1.2E+01	3.3E+01
J	8.0E+02	8.7E+03	2.3E+04	2.1E+00	2.3E+01	6.0E+01
CE	1.6E+03	1.7E+04	4.5E+04	3.3E+00	3.5E+01	9.3E+01
RU	6.9E+03	7.5E+04	2.0E+05	8.7E+00	9.4E+01	2.5E+02
MO	4.8E+04	5.2E+05	1.4E+06	3.1E+01	3.4E+02	9.0E+02
TC	7.5E+04	8.1E+05	2.2E+06	4.2E+01	4.6E+02	1.2E+03
TH	9.4E+04	1.0E+06	2.7E+06	4.9E+01	5.3E+02	1.4E+03
PA	8.2E+05	8.8E+06	2.3E+07	2.1E+02	2.2E+03	5.9E+03
ZR	2.9E+06	3.1E+07	8.2E+07	4.7E+02	5.1E+03	1.4E+04
NB	6.0E+07	6.5E+08	1.7E+09	3.5E+03	3.8E+04	1.0E+05

Table 6.2

Temperature ($^{\circ}$ F) Required for Approximate Diffusion Times of One Hour and One Day Assuming:

1. Release of a few percent
2. Attainment of an even concentration
3. Release of about a third

	<u>1 hour</u>			<u>24 hours</u>		
	<u>1</u>	<u>2</u>	<u>3</u>	<u>1</u>	<u>2</u>	<u>3</u>
RB	1156.	1629.	1913.	781.	1042.	1184.
CS	1156.	1629.	1913.	781.	1042.	1184.
EO	2130.	2915.	3392.	1517.	1944.	2176.
SR	2177.	2978.	3465.	1551.	1986.	2223.
SA	2264.	3094.	3600.	1617.	2067.	2312.
SB	2304.	3147.	3660.	1648.	2104.	2353.
OW	2658.	3620.	4208.	1912.	2430.	2714.
OW	3067.	4172.	4851.	2216.	2807.	3131.
BO	3810.	5180.	6031.	2765.	3489.	3889.
PO	4053.	5515.	6426.	2942.	3712.	4137.
NO	4106.	5590.	6517.	2981.	3761.	4191.
PR	4747.	6478.	7568.	3447.	4347.	4846.
Y	5870.			4258.	5371.	5993.
LA	5975.			4333.	5467.	6101.
PH	6187.			4484.	5659.	6317.
J	6617.			4791.	6050.	6757.
OE	6945.			5023.	6348.	7093.
OC	7684.			5542.	7016.	7849.
MC				6240.	7921.	
TC				6406.		
TH				6490.		
PA				7308.		
ZR				7801.		

Table 7.1

Dimensionless Numbers in Coolant Channel During Release of Sr

	<u>Average</u>	<u>Minimum</u>	<u>Maximum</u>
Reynolds Number	0.13 - 0.27	0.1	0.49
Schmidt Number	1.58 - 1.74	0.8	1.8
Stagnation Number	600 - 1400	247	2500

FISSILE COATED FUEL PARTICLE

FERTILE COATED FUEL PARTICLE

Figure 2.1. HTGR fuel particles.²

Figure 2.2. Large HTGR fuel element design.²

Figure 2.3. HTGR core and support arrangement.²

Figure 2.4. Typical SORS model.²

Figure 2.5. Barriers to the release of fission products.

Figure 3.1. Generalized decay chain structure.

Figure 3.2. Evolution of the average and maximum temperature of the core.

Figure 3.3. Evolution of the temperature of the 10 segments in the central part of the core.

PROCEDURE USED TO CALCULATE THE RELEASE FROM THE FUEL

Step #1 FKCALC

Equations	Separate equations for the amount of an element in each segment of the core, 4.14. Release rate in each segment calculated from empirical fuel model. Decay neglected.
Solution	Crude, using a large time step, stepwise integration.
Result	Amount of each element in each segment of the core versus time. Table of fractional release rates averaged over the core.

Step #2 Main Program

Equations	Equation for the total amount of an isotope in the fuel in the whole reactor, 4.4. Release rate is the approximate value calculated in FKCALC. Each decay chain treated separately.
Solution	Accurate, small time step, Hammings method.
Result	Total amount of an isotope within the fuel particles and total amount outside the fuel particles versus time.

Figure 4.1. Summary of mathematical approach to release from the fuel.

Figure 4.2. Comparison of the release from the fuel of ^{131}I , ^{132}I , ^{133}I predicted by FKALC and SORS.

Figure 4.3. Comparison of the release from the fuel of ^{144}Ce , ^{140}Ba predicted by FKALC and SORS.

Figure 4.4. Fraction released from fuel for each segment in the central part of the core, predicted by FKCALC.

Figure 4.5. Fractional release rate from fuel for each segment in the central part of the core, predicted by FKCALC.

Figure 4.6. Release from the fuel for ^{135}I , predicted by FKCALC and SORS.

Figure 5.1. The release from the fuel predicted by FKCALC using Fuel Model I.

Figure 5.2. The release from the fuel predicted by FKCALC using Fuel Model II.

Figure 5.3. Comparison of the two fuel models for ^{85}Kr .

Figure 5.4. Comparison of the two fuel models for ^{131}I .

Figure 5.5. Comparison of the two fuel models for ^{137}Cs .

Figure 5.6. Comparison of the two fuel models for ^{95}Nb .

Figure 5.7. The effect of the model for fuel failure using Fuel Model I, ^{131}I .

Figure 5.8. The effect of the model for fuel failure using Fuel Model I, ^{85}Kr .

Figure 5.9. The effect of the model for fuel failure using Fuel Model II.

Figure 5.10. Comparison of the release from the fuel for a uniform core with the release for a core divided into 56 segments.

CONCENTRATION PROFILES IN GRAPHITE ASSUMED IN SORSG

$$\text{NET RELEASE} = \text{LESSER OF } \begin{matrix} J_{DIF} \\ J_{EVAP} \end{matrix}$$

Figure 6.1. The two alternative approximations for diffusion used in SORSG.

Figure 6.2. The amount of ^{90}Sr released from the fuel, curve 1, and the amount that has diffused through the graphite, curve 2, on the assumption that evaporation is instantaneous and no redeposition occurs.

Figure 7.1. Variation of temperature along the coolant channels in the central portion of the core. The full curve refers to 21 hours and the dashed curve to 29 hours.

T.K. SHERWOOD AND R.L. PIGFORD

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Data on mass transfer in a wetted-wall tower with streamline flow.

X AXIS IS $\frac{\pi}{4}$ (1/'STAGNATION NUMBER') $\equiv$ GRAETZ NUMBER

Y AXIS IS $\frac{P_2 - P_1}{VP - P_1}$

Figure 7.2. Experimental data and theoretical curves for mass transfer in a fluid flowing through a cylindrical channel.

Figure 7.3. Comparison of the output of SORSG and the results predicted by the code if the expression for the evaporation rate is change to Eq. (7.27).

Figure 7.4. Comparison of the release of ^{90}Sr assuming that initially 0%, 10% or 100% of the ^{90}Sr has been released from the fuel particles.

Figure 7.5. Comparison of the results using SORSG and EVAP. The full curve is predicted by EVAP and the dashed curve is predicted by SORSG.