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APPROXIMATE CALCULATION OF THE INTERGRANULAR GAS FRACTION AND THE INTRAGRANULAR GAS DRIVEN SWELLING FOR SAS4A

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ZEISIG: Approximate Calculation of the Intergranular Gas Fraction and the Intragranular Gas Driven Swelling for SAS4A

Abstract:

A simple model has been devised for estimating, under steady-state irradiation conditions and for operational transients, the fraction of intergranular gas residing in fast reactor fuel and the intragranular gas driven swelling. The total gas retention in the fuel, the grain size and the irradiation conditions (mainly time dependent temperatures) must be known. Use has been made of parts of the fission gas model contained in the code LAKU and of results calculated with this code. The routine (named ZEISIG) is intended for insertion into the fast reactor accident model SAS4A as an extension of its fission gas model for steady-state reactor operation.

ZEISIG: Näherungsweise Berechnung des intergranularen Gasanteils und des intragranularen gasgetriebenen Schwellens für SAS4A

Zusammenfassung:

Ein einfaches Modell ist entwickelt worden zu dem Zweck, den intergranularen Gasanteil und das intragranulare Schwellen im Brennstoff Schneller Reaktoren bei stationärer Bestrahlung und bei Betriebstransienten zu bestimmen. Die gesamte Gasrückhaltung im Brennstoff, die Korngröße und die Bestrahlungsbedingungen (im wesentlichen die zeitabhängigen Temperaturen) müssen bekannt sein. Zum Teil werden Modellvorstellungen aus dem Code LAKU benutzt, zum Teil Rechenergebnisse dieses Codes. Das Modell (namens ZEISIG) ist für einen Einbau in den Reaktor-Unfallcode SAS4A bestimmt zur Erweiterung seines Spaltgasmodells für stationären Reaktorbetrieb.

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1. INTRODUCTION

The gaseous fission products formed during the irradiation of reactor fuel have an important influence on the behaviour of the fuel during steady-state irradiation and, even more so, during reactor transients. Any code that attempts to model the behaviour of reactor fuel under off-normal conditions must therefore include a model for fission gas behaviour. Quite sophisticated fission gas models have been developed and verified on experiments with fuel samples or whole pins. The code developed for this purpose in Karlsruhe is called LAKU /1-4/ and has already been extensively documented. However, this kind of code is not suited for insertion into whole-core accident codes, since it needs far too much computer time. Simpler models have to be devised for this kind of application.

The whole-core accident code SAS4A /5/ contains such a very simple model for the fission gas effects. The influence of the gases during off-normal reactor transients is modelled taking into account the separate effects of the gas contained inside the fuel grains - this intragranular gas becomes active only after a time delay - and the gas residing on the surface of the grains and in pores between the grains, the intergranular gas, that acts practically instantaneously. The space dependent amount of intragranular and intergranular gas contained in the fuel at the start of the transient must, of course, be known for this model to be applied. The fission gas model for the steady-state preirradiation contained in SAS4A calculates only the space dependent total amount of gas retained in the fuel, but does not provide the intergranular gas fraction. This quantity has to be specified in the input by the user, and it is not space dependent, but is one single value to be used throughout the whole core. This kind of modelling is somewhat too simple, since intergranular gas fractions during steady-state irradiations depend on the irradiation temperature and the burnup and end, e. g., to lower values in the colder regions of the core.

There is a second deficiency of the steady-state fission gas model contained in SAS4A: The intragranular gas driven swelling is assumed to be negligible compared to the intergranular gas driven swelling and is thus not taken into account. This approximation is acceptable for high irradiation temperatures, which cause most of the fission gas to leave the grains. It gives faulty results at low irradiation temperatures, when most of the fission gas remains inside the grains, causing a quite substantial swelling.

SAS4A should thus be equipped with a more refined fission gas model for the steady-state irradiations, that is able to calculate the space dependent intergranular gas fraction and the intragranular gas driven swelling. It must be a fast-running code, since modelling an entire core involves normally calculations for 20-30 representative pins. Operational transients are often part of a preirradiation and thus have to be included in the model. The fission gas model for off-normal transients, however, is not changed by such a refinement, which serves only to supply more realistic starting values to that part of the code. The only feature to be added to the fission gas model for off-normal transients is the ability to handle space dependent intergranular gas fractions.

A fast method has thus been devised to calculate approximately the intergranular gas fraction and the intragranular gas driven swelling under steady-state irradiation conditions and for operational transients. It relies for certain parameters (irradiation temperatures, fission gas production rate, amount of gas released etc.) on the calling programme. The method is based partly on the fission gas model LAKU and partly on calculational results from this code. The main features of the fast method are:

1. Calculation of the gas release from the interior of the fuel grains with a simplified model using very large time steps, average values for the gas concentrations in the grains, and postulating, as far as possible, equilibrium conditions.

2. The intragranular bubble densities are described with parametric functions derived from LAKU-results. They depend on temperature and grain radius, and weakly on the radial temperature gradient. A relaxation function based on physical considerations is used for modelling the changing bubble densities after step changes of the irradiation temperature.

3. An upper limit on the intergranular gas fraction derived from LAKU-results and depending on the irradiation temperature is enforced for higher burnups.

4. The equilibrium intragranular gas concentration is used for long irradiations at constant or nearly constant temperatures.

The physical model will be outlined in the next chapter. This is followed by a presentation of some calculational results, which are compared with the results of the LAKU-model. A chapter on the computer realization of the model terminates the presentation. The programme has been called ZEISIG: **Z**one-wise **E**sti-mate on **I**ntragranular **S**welling and **I**ntergranular **G**as.

2. THE PHYSICAL MODEL

As has been mentioned already, the reactor core is modelled in SAS4A by defining a number of representative pins (each with its cladding and its share of coolant and structure material, which are of no interest for the fission gas model). Each pin is subdivided into several axial nodes, and the radial distributions inside the pin are represented by a number of radial nodes for each axial node. The fission gas model ZEISIG depends only on local parameters and has thus to be called up once per (steady-state irradiation) time step for each radial node in each axial node in each representative pin.

ZEISIG relies on the calling programme for all parameters SAS4A calculates or requires as input data for the steady-state preirradiation. The most important are the time step length, fuel temperature and radial temperature gradient, grain size, fuel porosity and fission gas production rate. The gas released from the fuel is also to be provided by the calling programme, since it is calculated by the fission gas model of the steady-state preirradiation part in SAS4A, and it is not intended to change this part of the model. For a complete list of the data to be provided by the calling programme see chapter 4. ZEISIG returns to the calling programme two data per radial node: The intragranular gas driven swelling and the intergranular gas fraction.

The modelling used in ZEISIG is based on the much more elaborate model LAKU, as has been mentioned already. As far as the modelling in ZEISIG is the same as in LAKU, only the main features will be outlined below, but without going into great detail and especially without discussing those details of fission gas behaviour, that are still not very well understood and for which a number of alternate models exist. The reader who wishes more information is referred to the publications on LAKU /1-4/. The main purpose of this chapter is to give a detailed account of those parts of the model that differ from LAKU, i. e. the simplifications of some parts of the LAKU-model and the numerical approximations to LAKU-results.

2.1. Choice of time steps

There is, of course, a time step length imposed on ZEISIG by the calling programme; this step will be called the external step in the following. ZEISIG does not pose any restrictions on the length of the external step, thus performing its calculations for any step sizes and irradiation conditions defined by the calling

programme. This may have to be changed, if difficulties arise when the code is actually coupled to a programme.

The external time step may be sufficiently long for basic changes to take place in the fuel. The process of interest for a fission gas model is grain growth, since the grain size is one of the fundamental parameters for gas release. Therefore the external time step may be subdivided into several internal ones, if the grain size changes considerably. This is done automatically by the code. Different internal time step sizes are employed for the different radial zones in one cross section of the fuel. The grain growth is the only criterion for defining the internal step size. When it is zero, only one time step is employed, i. e. the internal time step equals the external one. Otherwise the step size is such that the fourth power of the grain radius does not change by more than 5% per step (fourth power, because this corresponds to the law of grain growth contained in the LAKU-model). The time steps are chosen in such a way that the 5% change is always just maintained; they grow thus slowly due to the detailed form of the grain growth law. The 5% limit has been varied initially and has proven necessary for arriving at adequate numerical results.

One remark must be made regarding the notation to be used in the following: Subscript 0 refers always to the beginning, t to the end of an internal time step; subscript i denotes the end of an external time step, i-1 the end of the foregoing external time step.

2.2. Explicit calculation of the time dependent intragranular gas concentration

There are two ways of arriving at the intergranular gas fraction I, if the total amount of gas remaining in the fuel is known: Either the amount of intergranular gas is calculated directly by estimating the gas content of the intergranular bubbles and the fuel porosity not linked to the exterior of the pellet (the "closed" porosity); or the amount of intragranular gas is calculated and subtracted from the total gas retained. The second possibility is chosen in ZEISIG.

At the beginning of an irradiation, gas formation starts in the fuel matrix, and the physical processes determining gas release and gas redistribution in the fuel have not had enough time for any equilibrium conditions to be established. There are two equilibrium conditions that will be attained, if the irradiation is continued sufficiently long at constant conditions:

1. An equilibrium between the resolved gas being precipitated into intragranular bubbles and the gas in these bubbles being reintroduced into the fuel

matrix by an interaction with energetic fission products. The time for reaching this equilibrium is quite short compared to the duration of a steady-state irradiation. Therefore ZEISIG uses the assumption that the equilibrium has already been attained at any time during the irradiation. When this assumption leads to errors, as may happen for operational transients with large temperature changes in time spans of hours, corrections are foreseen (see sections 2.5 and 2.7). Thus the usefulness of ZEISIG is limited to steady-state irradiations and operational transients, whereas reactor transients with a duration of a few seconds or less can definitely not be treated with the method.

2. The second equilibrium condition is only being reached after a prolonged irradiation at constant conditions: An equilibrium between the gas being formed in the grains and the gas being released to the surface of the grains. The gas concentration in the grain has then reached an equilibrium value. This value is employed, if the irradiation conditions remain constant or nearly constant for a long time, but otherwise the gas release from the grain has to be calculated explicitly.

The explicit calculation of the intragranular gas concentration, employing only the first equilibrium condition, is presented first. The calculation of the equilibrium gas concentration following from the second equilibrium condition is detailed in section 2.6.

The basic balance equation relates the time dependent volumetric gas production rate, β, to the intragranular gas in solid solution, c, the gas in intragranular bubbles, b, and the gas that has left the interior of the grain, g (g comprises the intergranular gas and the gas that has totally escaped from the fuel):

$$\int_0^t \beta(t')\,dt' = c(t) + b(t) + g(t) = G(t) \qquad (1)$$

t	time
G	total amount of gas created during the irradiation

The rate of gas release from the grain is thus

$$\dot{g}(t) = \beta - \dot{c}(t) - \dot{b}(t) \qquad (2)$$

From the equations developed in /1/ for $\dot{c}$ and $\dot{b}$ and the equilibrium between gas precipitation and resolution follows:

$$\dot{g}(t) = \beta(1 - Z) + ZA_1b + ZA_2c \qquad (3)$$

A_1, A_2 and Z depend on the irradiation conditions, mainly on the fuel temperature and the grain size. A_1 is the inverse time constant for the release of intragranular bubbles to the grain surface:

$$A_1 = \frac{1}{\tau_1} + \frac{1}{\tau_2} + \frac{1}{\tau_3}$$

τ_1	time constant for grain boundary sweeping
τ_2	time constant for pore migration
τ_3	time constant for steady-state intragranular bubble migration

The physical processes described by $\tau_1 - \tau_3$ are sweeping processes that occur at intermediate and high temperatures. The amount of gas released by them depends on the irradiation temperature and the grain size for all three. Grain boundary sweeping is a consequence of grain growth. The sweeping effect of pore migration depends on (apart from the temperature and the grain size, as already mentioned) the amount of fuel porosity and on the temperature gradient, which is also an important parameter for steady-state intragranular bubble migration. All sweeping processes are treated in LAKU, and their time constants can be found in ref. /1/.

A_2 is the inverse time constant for the release of the intragranular gas in solid solution. The release is mainly due to the migration of the atomic gas to the grain surface, but at higher irradiation temperatures a small amount is released by grain boundary sweeping and pore sweeping.

$$A_2 = \frac{1}{\tau_1} + \frac{1}{\tau_2} + F_a$$

$1/F_a$	time constant for the migration of resolved gas to the grain surface
F_a	$= 15D_g/a^2$ for spherical grains
D_g	diffusion coefficient of resolved gas
a	grain radius

Z is a correction for the deviation of the actual space dependent gas distribution in the grain from the equilibrium shape /6/.

The equilibrium between precipitation and resolution can be written as

$$b = \alpha c \tag{4}$$

$$\alpha = \frac{4\pi D_g n r}{\eta + A_1} \tag{5}$$

n, r number density and radius of intragranular bubbles

η inverse resolution time constant

From eq.'s (2) - (4) follows:

$$\dot{c} + \dot{b} = Z\beta - (c + b)Z\frac{A_1\alpha + A_2}{1 + \alpha} \tag{6}$$

If one now introduces the assumption that all time dependent coefficients in eq. (6) can be replaced by suitable average values for a time interval Δt, the solution is

$$c_t + b_t = \frac{\beta(1 + \alpha)}{A_1\alpha + A_2} + \left(c_0 + b_0 - \frac{\beta(1 + \alpha)}{A_1\alpha + A_2}\right)\exp\left(-\frac{(A_1\alpha + A_2)Z}{1 + \alpha}\Delta t\right) \tag{7}$$

c_0, b_0 initial values of c and b

c_t, b_t values of c and b at the end of the interval

When the sum c+b has been calculated, the separate values of c and b can be deduced from eq. (4).

Eq. (7) is the basic equation used for calculating the gas distribution, even when the second equilibrium condition is employed afterwards for correcting the results. Since averaged values for the coefficients are employed, the programme has to proceed in the following way:

1. The external time interval must be subdivided in such a way, that the numerical error introduced by averaging remains acceptable. This leads to the internal time steps mentioned in section 2.1.

2. An iteration must be executed in each internal time step in order to arrive at sufficiently good values for the coefficients depending on the final results b_t and c_t (α does via r; see section 2.4).

2.3. Calculation of intragranular gas driven swelling and intergranular gas fraction

When the calculation of the intragranular gas content has reached the end of the external time step, the intragranular gas driven swelling S and the intergranular gas fraction I remain to be determined from c_i and b_i, the intragranular gas in solid solution and in bubbles at the end of the external time step.The intragranular gas driven swelling is the sum of the intragranular bubble volume and the amount of swelling associated with the gas in solid solution (2Ω per gas atom):

$$S = \frac{4\pi}{3} n_i r_i^3 + c_i 2\Omega L$$

n_i, r_i	n and r at end of external time step
Ω	molecular volume
L	Avogadro's number (the gas concentrations are assumed to be given in mol/cm^3)

The quantity of gas retained in the fuel at the end of the external time step, Q, is determined by SAS4A. The quantity of intergranular gas, g_I, follows as

$$g_I = Q - c_i - b_i$$

and the intergranular gas fraction is

$$I = \frac{g_I}{Q}$$

S and I are passed to the calling programme.

2.4. Intragranular bubble number density and radius

The intragranular bubble size and density have been assumed to be known in section 2.2. They are calculated in LAKU from the irradiation conditions and the amount of gas present in the grain. This calculation requires, however, much smaller internal time steps than those envisaged for ZEISIG, especially for changing irradiation temperatures. Therefore a simplified approach has been chosen for ZEISIG, by deducing a parametric representation from results of calculations with LAKU.

The number density of the intragranular bubbles depends mainly on the irradiation temperature, but also to some extent on the preconditioning (especially when the irradiation temperature changes), the grain size and the radial temperature gradient. It is calculated in two steps. First an asymptotic number density n_{as} typical for the actual irradiation temperature is defined. It depends, apart from the actual irradiation temperature T (in °K), on the grain radius a (in cm) and the radial temperature gradient ∇T (in °K/cm):

$$n_{as} = \frac{10^{f_1(T)} f_2(T) f_3(a, a_g(T))}{f_4(T, \nabla T)} \quad [cm^{-3}] \tag{8}$$

with the additional condition

$$n_{as} \leq 10^{17} \quad [cm^{-3}]$$

Among the different functions in eq. (8), f_1 contains the main temperature dependence:

$$T \geq 1524°K: \; f_1(T) = \min\left(17, 31016.28 - \frac{4.91T}{1428}\right)$$
$$T \leq 1524°K: \; f_1(T) = \min\left(17, 392.32 - \frac{.34T}{242}\right)$$

f_2 corrects for details in the temperature dependence:

$$T \geq 2023°K: \; f_2(T) = \max(.3, 1. - .00125(T - 2023))$$
$$1723°K < T < 2023°K: \; f_2(T) = 1 + \max\left(0, .5\frac{2023 - T}{300}\right)$$
$$1430°K \leq T \leq 1723°K: \; f_2(T) = 1 + \max\left(0, .5\frac{T - 1473}{250}\right)$$
$$1360°K < T < 1430°K: \; f_2(T) = 1.1 - .1\frac{|T - 1395|}{35}$$
$$1300°K \leq T \leq 1360°K: \; f_2(T) = 1$$
$$T < 1300°K: \; f_2(T) = .5 + \max(.1, (T - 900).00125)$$

f_3 takes into account the effect of the grain size and depends on, in addition to the grain radius, the upper limit to the grain size, a_g. This limit increases with increasing irradiation temperatures; it has been measured on UO_2 irradiated at constant conditions. Though a does not exceed a_g when the irradiation temperature remains constant, it may well do so under irradiation conditions changing with time. This happens, when there is first a time interval at high temperatures

leading to fast grain growth, followed by an interval at temperatures that are so low, that the limiting value falls below the actual value reached in the foregoing interval. - For the numerical value of a_g, see ref. /1/.

$$f_3(a, a_g(T)) = \min(a, a_g(T))$$

except when $T > 1750°K$ and $a_g(T) < a$; then:

$$f_3(a, a_g(T)) = \min(a, a_g(T)) + \left[a_g(T) \cdot \left(2 - \frac{a_g(T)}{a} \right) - \min(a, a_g(T)) \right] \cdot \min(1, \max(0, .01T - 17.5))$$

f_4 corrects for the effect of the temperature gradient (bubble losses due to bubble migration in the temperature gradient at higher irradiation temperatures):

$$f_4(T, \nabla T) = .0005\left(1 + .7\nabla T \frac{\max(0, T - 1500)}{4.5 \times 10^6} \right)$$

This completes the set of functions needed for calculating the asymptotic bubble number density. As a second step, the number density n_t at the end of an internal time interval is calculated from the number density at its beginning, n_0, and n_{as} with a relaxation function:

$$n_t = n_0 e^{-\zeta \Delta t} + n_{as}\left(1 - e^{-\zeta \Delta t}\right) \qquad (9)$$

with

$$\zeta = .01\eta \quad \text{for } n_0 > n_{as}$$
$$\zeta = \tau_n \beta \quad \text{for } n_0 < n_{as}$$

τ_n (not to be confounded with τ_1-τ_3) is given by

$$\tau_n = 10^{\max(.725 + .002T,\ 1.475 + .0015T)} \quad \text{for } T \geq 1300°K$$
$$\tau_n = 10^{(-.475 + .003T)} \quad \text{otherwise}$$

The bubble number density is thus updated at the end of each internal time step with eq. (9).

The bubble radius is normally calculated from the reduced Van-der-Waals equation, as in LAKU:

$$\frac{b}{n} RT = \left(\frac{4\pi}{3} r^3 - \frac{b}{n} w \right) \left(\frac{2\gamma}{r} + p \right) \qquad (10)$$

R	universal gas constant
w	Van-der-Waals constant
γ	surface tension of fuel
p	pin internal pressure

A first estimate of the bubble radius at the end of the internal time step has always to be made at the beginning of this step, in order to define an average value of α for the step. Normally $r_t = r_0$ is used as a first approximation. After calculating b_t with eq.s (4) and (7), a new value of r_t is deduced from eq. (10). If the new value deviates too much from the estimate, the calculation is repeated with the new value, and this iteration is performed up to 5 times, if necessary.

A slightly different approach is taken for the first internal time step after changing the irradiation temperature. The bubble radius may change very much in this case due to the intragranular gas being redistributed into or out of the bubbles, and thus r_0 may not be a good first approximation for r_t. The following empirical relation is used under these conditions (with r in cm):

$$r = \max(5 \times 10^{-8}, \min(4.332 \times 10^{-7} - 1.4 \times 10^{-10} T, -1.09 \times 10^{-7} + 2.45 \times 10^{-10} T)) \cdot \left(\frac{\min(a, a_g(T))}{.0005} \right)^{.8}$$

This value is used only as a first estimate after changing the irradiation temperature, and is replaced by the radius resulting from eq. (10) after the first iteration in the first internal time step has been performed.

2.5. Special approximations and corrections

It has been mentioned in section 2.2 already, that average values have to be employed for the coefficients of eq. (6). Among these, Z, A_1 and A_2 are only weakly time dependent and thus only a small error is introduced by averaging. α, however, depends on both the bubble radius and number density which change more quickly. It has been found, that it is normally sufficient to use the average value of the product nr at the beginning and the and of an internal time step. A

special problem arises for the first internal time step, however, when the irradiation temperature changes.

Since the initial value of nr is always the one at the end of the foregoing step, it relates in this case to the old irradiation temperature. At the beginning of a step with a new temperature occur very fast intragranular gas redistributions between the resolved gas and the gas in bubbles, that cause the bubble parameters to adapt quickly to the conditions posed by the new temperatures. The time needed for these changes is so small that there is no large contribution to the average value of nr during the redistribution; the gas release from the grain remains small, too. Thus the effective quantity of intragranular gas at the beginning of the first internal time step, $b_0 + c_0$, is nearly the same as the value at the end of the last external time step, $b_{i-1} + c_{i-1}$, but the value of nr to be used for defining the average may differ quite significantly from the known value $n_{i-1}r_{i-1}$. Calculating explicitly the initial redistributions costs quite a lot of computer time in LAKU. Thus a suitable estimate for the long-term changes of nr in the first internal time step must be found without explicitly employing the values after redistribution.

This is done by noting that, according to eq. (10) and neglecting the pin internal pressure (which for intragranular bubbles is always small compared to the bubble surface tension) and the Van-der-Waals constant (this introduces an error for small bubbles, but is otherwise acceptable), nr^2 is proportional to b. In addition, c and b grow or decrease in roughly the same manner; therefore b may be replaced by the total intragranular gas content $c + b$, thus evading the evaluation of the initial gas redistribution. With these two facts in mind the following approximation has been chosen for averaging:

$$nr \sim c + b$$

$$\overline{nr} \simeq n_t r_t .5\left(1 + \frac{b_{i-1} + c_{i-1}}{b_t + c_t}\right) \qquad (11)$$

with subscript t denoting the values at the end of the first internal time step. This approximation has been inserted in ZEISIG, compared to results of the LAKU-model and found to be sufficient.

Another problem may arise at medium irradiation temperatures after long irradiations with changing temperatures. The intergranular gas fraction tends then to a small value which the code sometimes is not able to reproduce, due to an accumulation of errors. Therefore the results of the LAKU-model have been analyzed, and a maximum intergranular gas fraction f_{max} is defined, which may not be ex-

ceeded by the results of ZEISIG. This limit is enforced under the following conditions:

$$a \geq 15\ \mu m\ ,\quad 1400°K \leq T \leq 2000°K\ ,\quad \omega < 4 \tag{12}$$

ω relates to the equilibrium conditions to be presented in the next section. A large value of ω means that equilibrium conditions have been reached, and a correction of the intergranular gas fraction is not necessary in this case, since the equilibrium gas concentrations are always sufficiently well approximated.

If the conditions given by eq.s (12) are fulfilled, the maximum intergranular gas fraction is deduced from the following considerations: The quantity of gas g_o in "open" fuel porosity (porosity connected to the exterior of the fuel) is, according to the ideal gas equation:

$$g_o = \frac{pP}{RT}$$

P fraction of fuel porosity

The quantity of intergranular gas, g_I, remains near but somewhat above this value, under the conditions given by eq.s (12). The approximate value deduced from LAKU-results is given by:

$$g_I = g_o(1 + \max(0, .01(2100 - T)(1 - 1000G)))$$

where G (and also βt below) are in mol/cm^3. The upper limit for the intergranular gas fraction is then given by

$$I_{max}(\infty) = \frac{g_I}{G}$$

This value is not realized immediately, if the intergranular gas fraction I_{i-1} at the start of an external time interval is above this limit (e. g. due to a foregoing irradiation at a different temperature). The actual upper limit at any time t during the external time interval i is therefore calculated from a relaxation relation:

$$I_{max}(t) = I_{i-1} + (I_{max}(\infty) - I_{i-1})\left(1 - e^{-3 \times 10^4 \beta t}\right)$$

Apart from this condition, and at all times and under all irradiation conditions, I is always kept within its physically meaningful limits, i. e. $0 \leq I \leq 1$.

2.6. Equilibrium values

As has been mentioned above, the solutions deduced from eq.s (4) and (7) tend to accumulate errors, due to the approximations used and the averaging over large time steps. The errors become the larger the longer an irradiation continues at constant or nearly constant conditions. This can be corrected, however, since these are exactly the conditions for reaching equilibrium gas concentrations, which can be calculated with good precision. The technique used in ZEISIG is thus the following: At the beginning of an irradiation or after a large change of the irradiation temperature, the calculation is performed using only eq.s (4) and (7); when the irradiation has proceeded sufficiently long at the same temperature, the equilibrium gas concentration is calculated in addition and used for correcting the results of eq.s (4) and (7); the weight of this correction is then increased as long as the irradiation continues at approximately the same temperature, until the equilibrium gas concentration practically replaces the solution of eq.s (4) and (7). When the irradiation temperature changes, the process starts anew, but may lead more early to the equilibrium state, depending on the difference between the old and the new irradiation temperature.

One can deduce from the equation for the equilibrium gas concentration to be presented below, that the concentration depends strongly on the irradiation temperature and also on the grain size. It therefore changes as long as the grains continue growing. The time until equilibrium conditions are reached depends in the same way on the same parameters. One can thus expect the approach to equilibrium to be quantitatively different for different irradiation temperatures.

In the following, the equation for the equilibrium gas concentration is presented first. Then the parameter ω is introduced, which is used for deciding on whether the correction is to be applied. If it is, ω is also used for calculating the weight the equilibrium gas concentration is to be assigned. After a somewhat lengthy presentation of all equations used for calculating ω, the section ends with the derivation of the final solution from the result of the explicit calculation and the equilibrium gas concentration.

The equation for the equilibrium gas concentration can be deduced from eq.s (3) and (4) by noting, that the amount of gas leaving the grain equals the gas cre-

ated in the equilibrium case. Thus with $\dot{g} = \beta$, the following equation results from eq.s (3) and (4):

$$f(b_{eq}) = \alpha\beta - b_{eq}(A_1\alpha + A_2) = 0 \qquad (13)$$

This is an implicit equation for b_{eq}, since α, A_1 and A_2 depend on the bubble radius $r(b_{eq})$. It is solved easily by an iteration with the Newton-Raphson-method. The equilibrium gas concentration of the resolved intragranular gas, c_{eq}, is then calculated from eq. (4).

The decision on whether the equilibrium gas concentration is to be used for correcting is much more involved. The numerical results are quite sensitive to the correction, and thus the criteria were only partly derived from physical considerations. Testing on realistic cases lead to the addition of rectifications for a number of special situations.

The time for reaching the equilibrium conditions depends on F_a, the time constant for the release of resolved intragranular gas. Therefore the quantity ω measures the irradiation time in units F_a. It depends, as F_a does, on the diffusion coefficient of the resolved intragranular gas (and and thus on the irradiation temperature) and on the grain size.

If the grain size and irradiation temperature would not vary during an irradiation, defining ω would be quite straightforward. Assuming the value of ω at the start of the external time interval, ω_0, is known (it may differ from the value at the end of the foregoing external time interval, ω_{i-1}, see below), ω_i at the end of the external time step would be given by

$$\omega_i = \omega_0 + \Delta t_e F_a \qquad (14)$$

ω_0 value of ω at start of first internal time step in an external time step
Δt_e length of the external time step

The variable parameters must be taken into account, however. When F_a changes from a value $F_{a,0}$ to a value $F_{a,i}$, ω is renormalized to a value ω':

$$\omega' = \omega \cdot \frac{F_{a,i}}{F_{a,0}} \qquad (15)$$

Combining eq.'s (14) and (15) results in

$$\omega_i = \frac{F_{a,i}}{F_{a,0}} (\omega_0 + \Delta t_e F_{a,0}) \tag{16}$$

Eq. (16) is used to calculate the increase of ω during one whole external time step; intermediate values are not needed, because the correction with the equilibrium gas concentration is only applied at the end of an external time step.

A second renormalization must be performed on ω at the beginning of each external time step. If the irradiation temperature in the foregoing external time interval has been the same as in the one to be calculated, the value of ω is kept constant, i. e. $\omega_0 = \omega_{i-1}$. If the irradiation temperature is changed, ω_0 has to be different from ω_{i-1}, too.

The formalism for deciding on an appropriate value of ω_0 will be first explained for low irradiation temperatures. This is the only case when the old value of ω needs not to be taken into account for estimating the new one. At low temperatures the bulk of the intragranular fission gas is in solid solution in the fuel matrix, i. e. the gas in intragranular bubbles can be neglected. The equilibrium gas concentration can then be directly written down /1/:

$$c_{eq} = \frac{\beta}{F_a} \tag{17}$$

The effective gas concentration c_0 at the beginning of an external time step at low temperatures is the sum $c_{i-1} + b_{i-1}$ at the end of the foregoing step, since any bubble gas can be assumed to be quickly transferred back into the fuel matrix due to resolution. ω_0 is inferred from the difference between c_{eq} and $c_{i-1} + b_{i-1}$, using

$$\frac{c_{i-1} + b_{i-1}}{c_{eq}} = 1 - e^{-\omega_0} \tag{18}$$

Combining eq.s (17) and (18) yields:

$$\omega_0 = -\ln\left(1 - \frac{(c_{i-1} + b_{i-1})F_a}{\beta}\right) \tag{19}$$

This formalism for calculating ω_0 is used for irradiation temperatures up to 1700°K; beyond this temperature the intragranular bubble gas component becomes important and the equations following below are employed. It may also happen at low but rising irradiation temperatures, that $c_{i-1} + b_{i-1} > c_{eq}$; then the programme switches also to the following formalism.

When gas precipitation and resolution start playing a significant role, the equilibrium gas concentration cannot be so easily calculated, but c + b remains proportional to the gas production rate β and inversely proportional to F_a; F_a consists of a term depending on the grain radius, which remains constant upon changing the irradiation temperature, multiplied by the gas diffusion coefficient. One can thus try to approximate the change of the equilibrium gas concentration by (with subscripts i-1 and i denoting the values in the foregoing and the actual external time interval):

$$\begin{aligned} c_{eq}(T_i) + b_{eq}(T_i) &= (c_{eq}(T_{i-1}) + b_{eq}(T_{i-1}))\,\frac{D_g(T_{i-1})\beta_i}{D_g(T_i)\beta_{i-1}} \\ &= (c_{eq}(T_{i-1}) + b_{eq}(T_{i-1}))V' \end{aligned} \tag{20}$$

In addition, an equation linking the actual and the equilibrium gas concentration with the value of ω at the end of the foregoing time step, ω_{i-1}, and at the beginning of the actual time step, ω_0, is postulated, analogous to eq. (18):

$$\begin{aligned} \frac{c_{i-1} + b_{i-1}}{c_{eq}(T_{i-1}) + b_{eq}(T_{i-1})} &= 1 - e^{-\omega_{i-1}} \\ \frac{c_{i-1} + b_{i-1}}{c_{eq}(T_i) + b_{eq}(T_i)} &= 1 - e^{-\omega_0} \end{aligned} \tag{21}$$

Combining eq.'s (20) and (21) and solving for ω_0 yields:

$$\omega_0 = -\ln(1 - V) \tag{22}$$

with

$$V = (1 - e^{-\omega_{i-1}})V'$$

V may become bigger than 1. This happens easily, when the irradiation temperature increases, since the equilibrium gas concentration decreases in this case and may fall below the value of c + b attained in the foregoing time interval. The

equilibrium is then approached from bigger values and not from smaller ones, as is the rule. It has been found suitable to replace V by 1/V in this case. - If V (or its inverse value for V>1) exceeds the limit .9999546 = $1\text{-}e^{-10}$, ω_0 is assigned the value 10 for numerical reasons; at values of ω exceeding 10 the equilibrium gas concentration practically replaces the numerical results, and the further growth of ω needs not to be treated in detail, anyway.

So far the physical considerations for calculating ω have been presented. They were tested in ZEISIG, and though they give quite sensible results in many cases, it turns out that a number of correction are necessary for special situations. The first two are applied only if T>1700°K or V>1:

$$\text{If } \omega_{i-1} > 3 \text{ and } \omega_0 < \omega_{i-1}\text{: } \omega_0 = \omega_0 + 1.5\sqrt[4]{\omega_{i-1} - 3}$$

$$\text{If } T_{i-1} < T_i \text{ and } V > 1 \text{ and } V' < 3\text{: } \omega_0 = \omega_{i-1}\left(\frac{3}{2} + \frac{|V' - 2|}{2}\right)$$

The following corrections are always applied:

$$\text{If } T_{i-1} < T_i \text{ and } \omega_0 > \omega_{i-1}\text{: } \omega_0 = \min(\omega_0, \omega_{i-1} \times \min(3, V'))$$

$$\text{If } \omega_0 < \omega_{min}\text{: } \omega_0 = \omega_{min}$$

$$\text{If } \omega_0 + \Delta tF_{a,0} \geq 2 \text{ and } \omega_i < 2 \text{ and } G(t) > 50\ \mu mol/cm^3\text{: } \omega_i = \omega_0 + \Delta tF_{a,0}$$

The minimum value of ω used above is given by:

$$\omega_{min} = 2.3$$

$$\text{If } V > 1 \text{ and } \omega_0 < \omega_{i-1} \text{ and } a > agT\text{: } \omega_{min} = 2.3 \cdot \frac{a_g(T)}{a}$$

$$\text{If } T \leq 1600°K \text{ or } G(t) < 20\ \mu mol/cm^3\text{: } \omega_{min} = 0$$

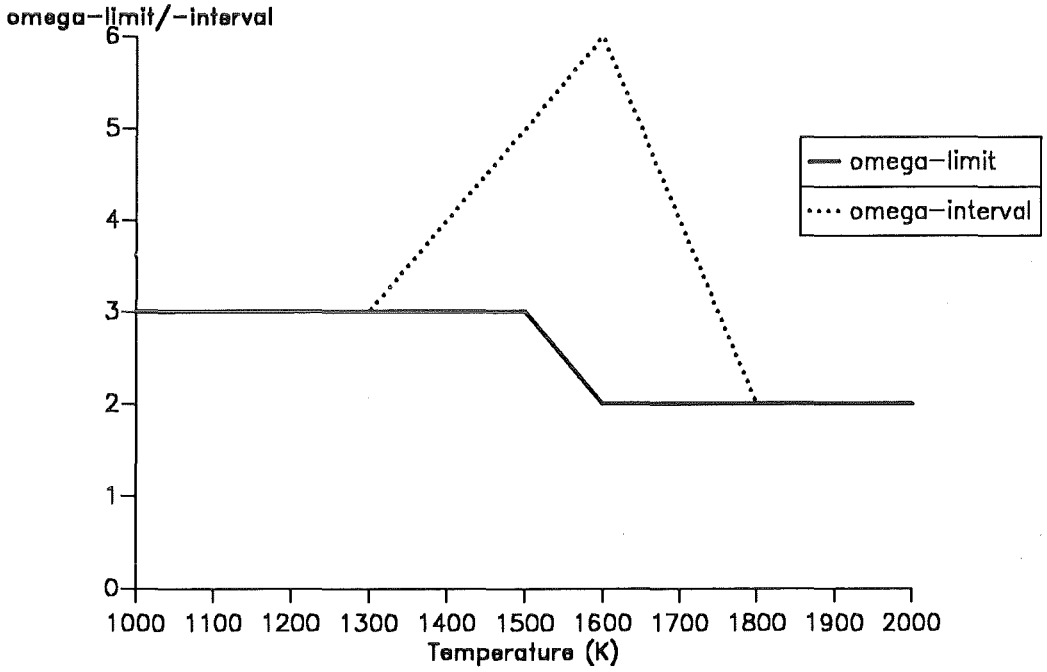
linear increase of ω_{min} from 0 to 2.3 resp. $2.3 \cdot \frac{a_g(T)}{a}$
in the intervals $1600°K < T < 1700°K$
and $20\ \mu mol/cm^3 < G(t) < 70\ \mu mol/cm^3$

This completes the equations applied for the calculation of ω. With the value of ω at the end of the external time step established, the decision on whether the solution of eq.s (4) and (7) is to be corrected can be taken. No correction is to be applied for small values of ω; therefore a value ω_{lim} is defined, which has to be exceeded by ω, before any correction is made. ω_{lim} can be expected to lie between 2 and 3, since 2-3 times its time constant should be sufficient for a process to approach its equilibrium (for an exponential approach to equilibrium, 2-3 times

the time constant corresponds to a deviation between 13 and 5%). Testing established, in fact, a value of 3 for lower and 2 for higher temperatures; the exact temperature dependence of ω_{lim} used in ZEISIG can be deduced from the figure below.

When ω exceeds ω_{lim}, the equilibrium gas concentration is used for correcting; this is done by suitably weighting and adding the two solutions. The weight of the equilibrium gas concentration should grow with growing ω. A temperature dependent interval ω_{int} is used for this purpose, which determines, together with ω and ω_{lim}, the weight of the equilibrium solution. The numerical value of ω_{int} has been arrived at in the same way as that of ω_{lim} and is also shown in the figure below. It is to be noted, that ω_{int} equals ω_{lim} for very high and very low temperatures, but that a much larger value has to be used in the intermediate region. This is probably due to the establishment of equilibrium conditions being retarded by grain growth effects.

Temperature dependent parameters for using equilibrium solution



The weight of the equilibrium solution in the correction is defined by

$$W = 1 - \exp\left(- \frac{\omega - \omega_{lim}}{2\omega_{int}} \right)$$

Note that W=0 for $\omega = \omega_{lim}$, and that W approaches 1 for increasing ω. The corrected solution is given by

$$(c_i + b_i) = (1 - W)(c_t + b_t) + W(c_{eq} + b_{eq})$$

c_i, b_i values of c and b at the end of the external time step
c_t, b_t values of c and b at the end of the last internal time step

After correcting the sum c+b, eq. (4) is again used for deriving the individual values of b_i and c_i.

2.7. Corrections for steps in irradiation temperatures

Steady-state irradiations include not only time intervals at constant conditions but also operational transients. These cause short-time changes to the gas distribution, which are modelled by LAKU but not by ZEISIG, due to its reliance on long time steps and equilibrium conditions. An approximate treatment of these effects is warranted whenever they influence the long-time behaviour of the gases.

One of the effects has been mentioned already in section 2.5: The redistribution of the resolved intragranular gas and the gas in intragranular bubbles and the resulting change of the bubble parameters n and r. Three other short-time effects due to temperature changes have to be included in the model in order to arrive at acceptable results.

The first effect occurs for increasing irradiation temperatures. In this case the pressure in the intragranular gas bubbles is also increased, and this excess pressure is only relaxed gradually due to bubble growth. According to the LAKU-model the bubbles have an enhanced mobility as long as their excess pressure persists. This may lead to an enhanced release of intragranular bubbles for sufficiently fast temperature ramps to higher temperatures. The quantity of intragranular gas released in this way is normally not very large, but the bubbles arriving on the grain faces may interlink and cause venting of part or even all of the intergranular gas, thus decreasing the intergranular gas fraction. The whole process takes, typically, only seconds or minutes and can thus be modelled as an instantaneous gas release for the purposes of the ZEISIG-model.

The model for calculating the number of intragranular bubbles released and their gas content has been transferred practically unaltered from LAKU to ZEISIG (its

details can be found in /2/). The ensueing release of intergranular gas is then calculated by using a simple approximation of LAKU-results. A temperature dependent limit to the intragranular gas released, $\Delta(b + c)_{lim}$ is defined:

$$\begin{aligned}\Delta(b + c)_{lim} &= 1.5\ \mu mol/cm^3 && \text{for } T \leq 1550°K\\ &= 1.5 + .01(T - 1550)\ \mu mol/cm^3 && \text{for } 1550°K < T < 1700°K\\ &= 3.0\ \mu mol/cm^3 && \text{for } T \geq 1700°K\end{aligned}$$

The intergranular gas release fraction R_I as a function of the actually occurring intragranular gas release, $\Delta(b + c)$, is:

$$\begin{aligned}R_I &= 0 && \text{for } \Delta(b + c) \leq \Delta(b + c)_{lim}\\ &= 2 - \frac{\Delta(b + c)}{\Delta(b + c)_{lim}} && \text{for } \Delta(b + c)_{lim} < \Delta(b + c) < 2\Delta(b + c)_{lim}\\ &= 1 && \text{for } \Delta(b + c) \geq 2\Delta(b + c)_{lim}\end{aligned}$$

The second and third effects both occur for decreasing temperatures; they concern the number density of the intragranular bubbles and the gas release during the initial readjustment of the equilibrium between precipitation and resolution. The intragranular bubble number density tends - asymptotically - to higher values as temperatures decrease (except for very low temperatures). There is, however, an initial decrease of the bubble number density for decreasing temperatures, which is due to a sharp decrease of the term for bubble formation. The way it is modelled in LAKU, this term depends on the diffusion coefficient for resolved gas - which decreases strongly with temperature - and on the square of the concentration of the resolved gas. The resolved gas concentration may experience some quick initial growth due to bubble gas resolution, but its further growth to values offsetting the decrease of the diffusion coefficient occurs only gradually with the time constant of fission gas formation. There is therefore an initial short time interval after a reduction of the irradiation temperature during which the bubble number density may decrease.

The equation for the short term formation and destruction of intragranular bubbles is deduced from the model employed in LAKU /1/:

$$\dot{n} = -\eta n + (n_s - n)4\Omega L^2 D_g \sqrt[3]{12\Omega\pi^2}\,(c_0 + \Delta c_0)^2 \qquad (23)$$

n_s number of potential bubble sites

Δc_0 is time dependent and is the short-term increase of the resolved gas due to resolution of bubble gas. Resolved gas is quickly precipitated back into the bubbles at temperatures above 1750°K, and thus Δc_0 can be approximated by 0 in this case. The resolved gas component starts growing gradually at temperatures below 1750°K, and the precipitation back into the bubble becomes small below 1400°K. Furthermore Δc_0 decreases, when the difference of the old and the new irradiation temperature decreases. The time constant for resolution is $1/\eta$. With all this in mind, and neglecting the increase of the resolved gas due to fission gas production, which is much slower than the precipitation-resolution processes, Δc_0 is approximated by:

$$\Delta c_0 = b_0 F(T_i, T_{i-1} - T_i)\left(1 - e^{-\eta t}\right)$$
$$F(T_i, T_{i-1} - T_i) = \min\left(1, \frac{T_{i-1} - T_i}{200}\right) \min\left(1, \max\left(0, 5 - \frac{T_i}{350}\right)\right) \qquad (24)$$

There is no need for solving eq.s (23) and (24) explicitly. The time constant for Δc_0 to reach its asymptotic value is $1/\eta$; with a typical value of 10^{-4} s for η, this is normally much smaller than the external time interval. The time constant for the changes in n is $1/\eta$ or less, as is evident from eq. (23). It is thus sufficient to replace Δc_0 in eq. (23) by its final value b_0F and to calculate the asymptotic value of n, n_∞, from eq. (23) with $\dot{n} = 0$. The result is:

$$n_\infty = n_s \frac{A(c_0 + b_0 F(T_i, T_{i-1} - T_i))^2}{\eta + A(c_0 + b_0 F(T_i, T_{i-1} - T_i))^2}$$

with

$$A = 4\Omega L^2 D_g \sqrt[3]{12\Omega\pi^2}$$

The correction to be applied to the bubble number density at the beginning of the external time interval is

$$\Delta n = \min(0, n_\infty - n_{i-1})(1 - 1/V')$$

n_{i-1} bubble number density at end of foregoing external time step

The factor (1-1/V') has been added to ensure, that the correction reduces to zero for identical irradiation conditions. This may not happen automatically, because n_{i-1} is the result of the approximations described in section 2.4, which may not be

totally consistent with eq.s (23) and (24); also, these two equations are themselves approximations. (1-1/V') is practically 1 for strongly differing irradiation conditions.

The correction Δn is applied to the bubble number density before calculating the first internal time step, if this step exceeds $2/\eta$. If it does not, the correction is distributed linearly over several internal time steps, until the total time exceeds $2/\eta$. If the external time step is less than $2/\eta$, the correction is reduced accordingly.

The third effect concerns the gas release during the time needed for establishing the equilibrium between precipitation and resolution. This effect is not covered by the treatment developed in section 2.2, which works with the assumption that the equilibrium has already been established. The additional gas release occurring initially after a decrease of the irradiation temperature is

$$\dot{g} = -\dot{b}(1 - Z)$$

This is approximated in ZEISIG by

$$\Delta g = (b_0 - b_t)(1 - Z)$$

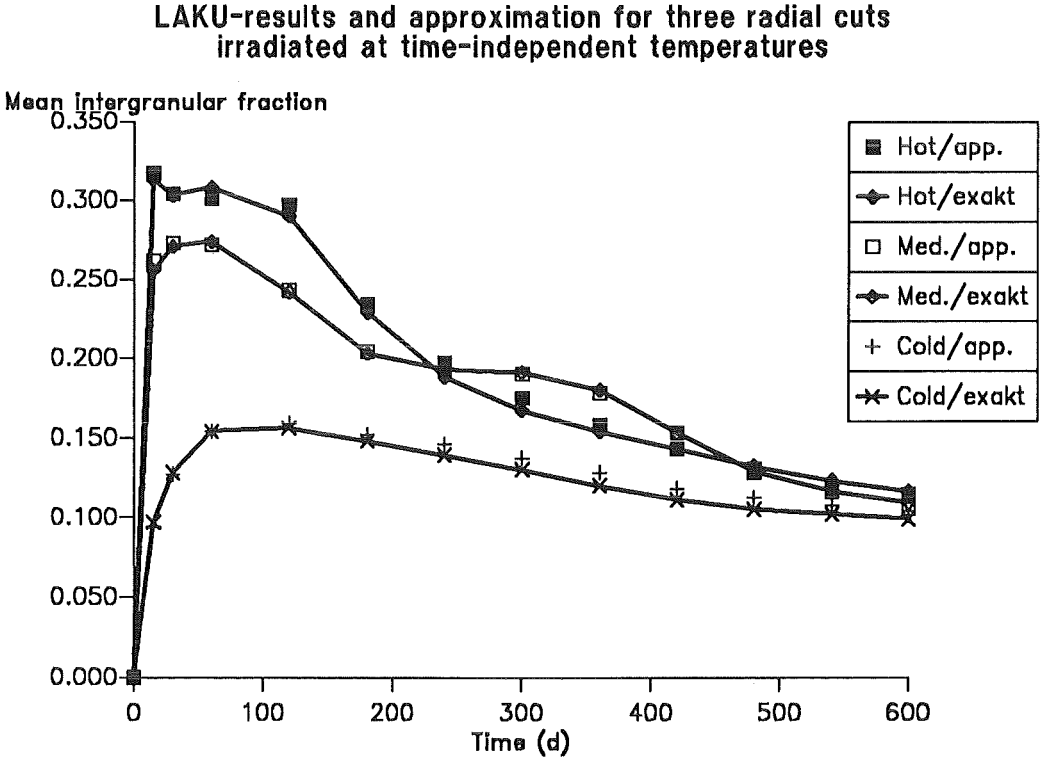
The sum $c_t + b_t$ is diminished by this quantity after calculating the gas behaviour in a time step, whenever the temperatures have changed from the foregoing step.

3. COMPARISON OF RESULTS FROM ZEISIG AND LAKU

A comparison of the results of the code with the results of the Karlsruhe model LAKU will be presented for five test cases. All cases are calculations for one axial cut through a pin, with the irradiation temperatures depending on the radial position in the pin. The first case is the base calculation at constant temperatures, whereas all other cases are modelled on real reactor irradiations.

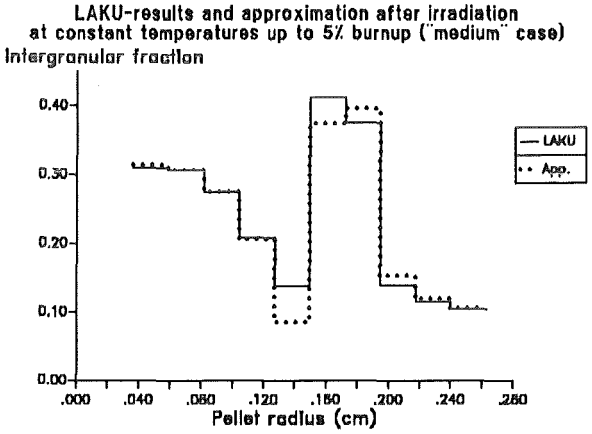
3.1. Irradiation at constant temperatures

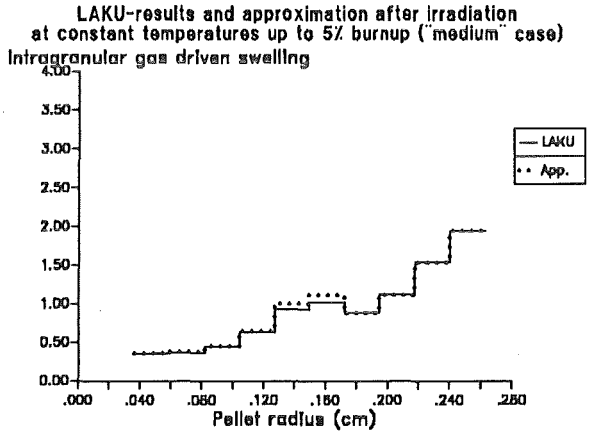
The first case is an irradiation with temperatures and gas production rates remaining constant in time, up to a 10at% burnup. The pin internal pressure increases slowly. Three variants are calculated, which are referred to as "cold" (fuel temperature 1579°K at pin center, 922°K at the surface), "medium" (2000°K / / 1001°K) and "hot" (2360°K / 1087°K). 10 radial nodes are employed. The external time step sizes vary from 7.5 days at the beginning of the irradiation to 15 days after 1at% burnup. - The following figure shows the time dependent radially averaged intergranular gas fraction as calculated by the LAKU-model (marked "exact") compared to the results of the ZEISIG-routine (marked "app.").

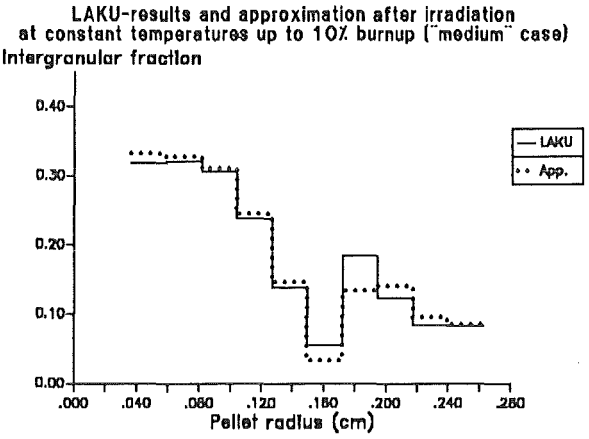


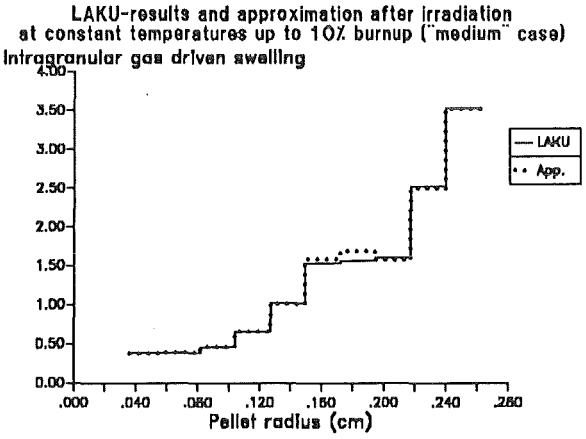
The intergranular gas fraction, as calculated by LAKU, exhibits always the same behaviour: There is an initial rise corresponding to the accumulation of gas on grain faces and in pores; then gas starts to be released due to the interlinkage of pores and grain face bubbles, and the intergranular gas fraction drops to an equilibrium value. It is obvious from the figure, that ZEISIG is very well able to reproduce these results.

The next four figures show the radial distribution of the intergranular gas fraction and the intragranular gas driven swelling for the "medium" case, at 5 and 10at% burnup, again as calculated by LAKU and ZEISIG. The agreement is satisfactory.





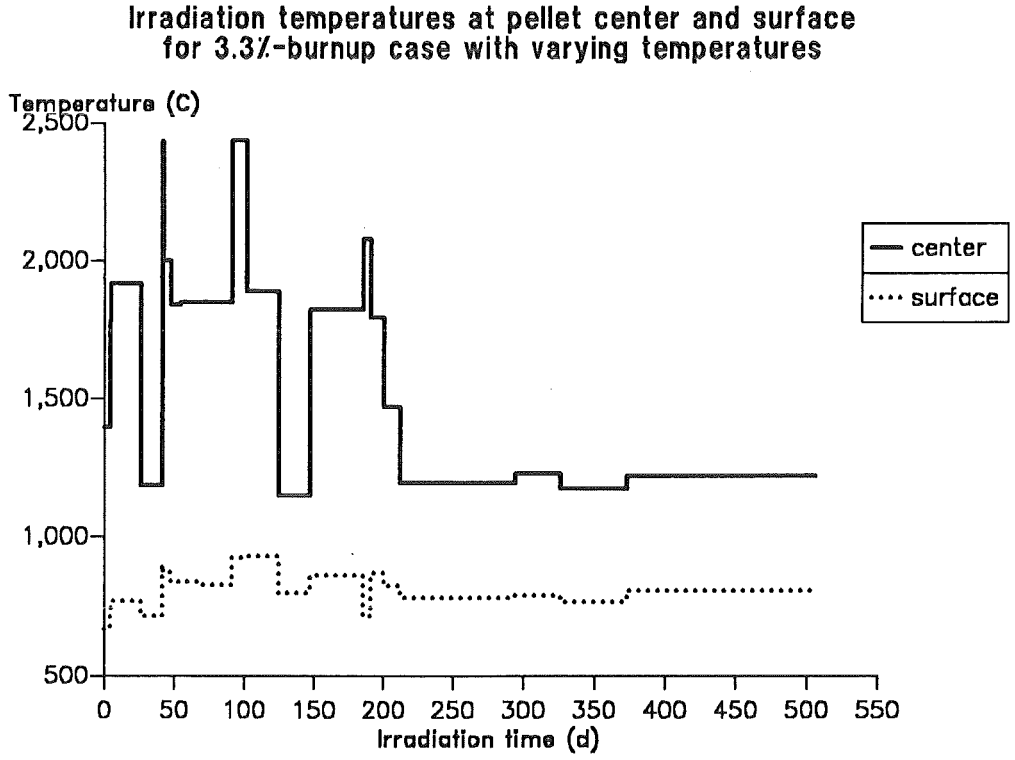


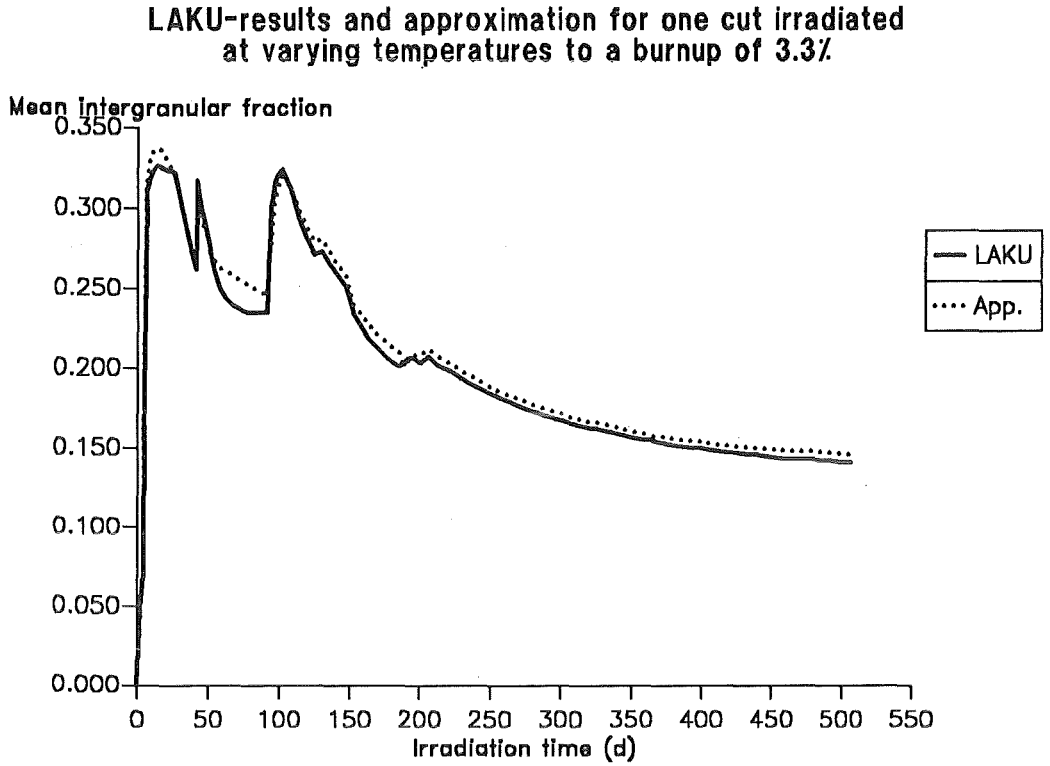


3.2. Varying temperatures: Low burnup, low final temperatures

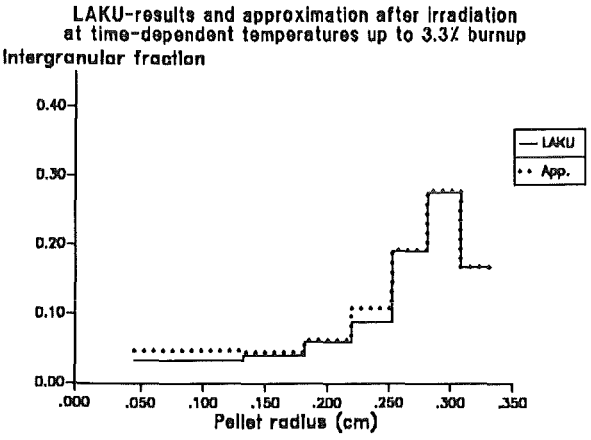
The second case has 20 time intervals with varying temperatures and gas production rates, up to a 3.3at% burnup (the CABRI-1 Rig2 irradiation /7/ near the hottest axial node is employed as a model for this case). Medium to low temperatures characterize the irradiation with only a few short intervals at higher temperatures at the beginning. 7 radial nodes are employed. The external time step size is kept below 14 days, with smaller step sizes at the beginning of the irradiation.

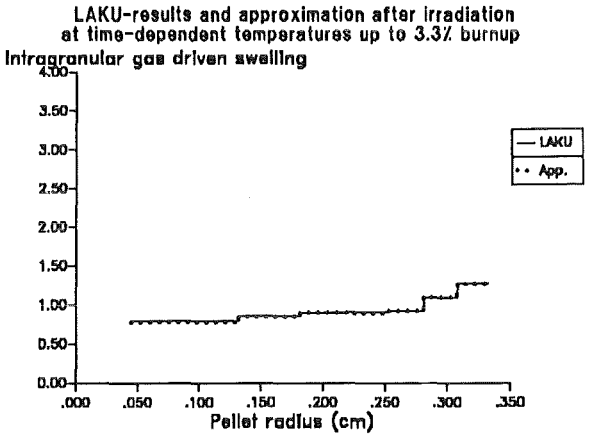
The next two figures show the time dependent temperatures at the inner and the outer surface of the fuel, and the corresponding time dependent radially averaged intergranular gas fraction as calculated by LAKU and ZEISIG. The intergranular gas fraction exhibits the same basic time dependent behaviour as in the case of constant temperatures, with a few spikes reflecting the time intervals at high temperatures.





The radial distribution of the intergranular gas fraction and the intragranular gas driven swelling at the end of the irradiation are shown in the next two figures.



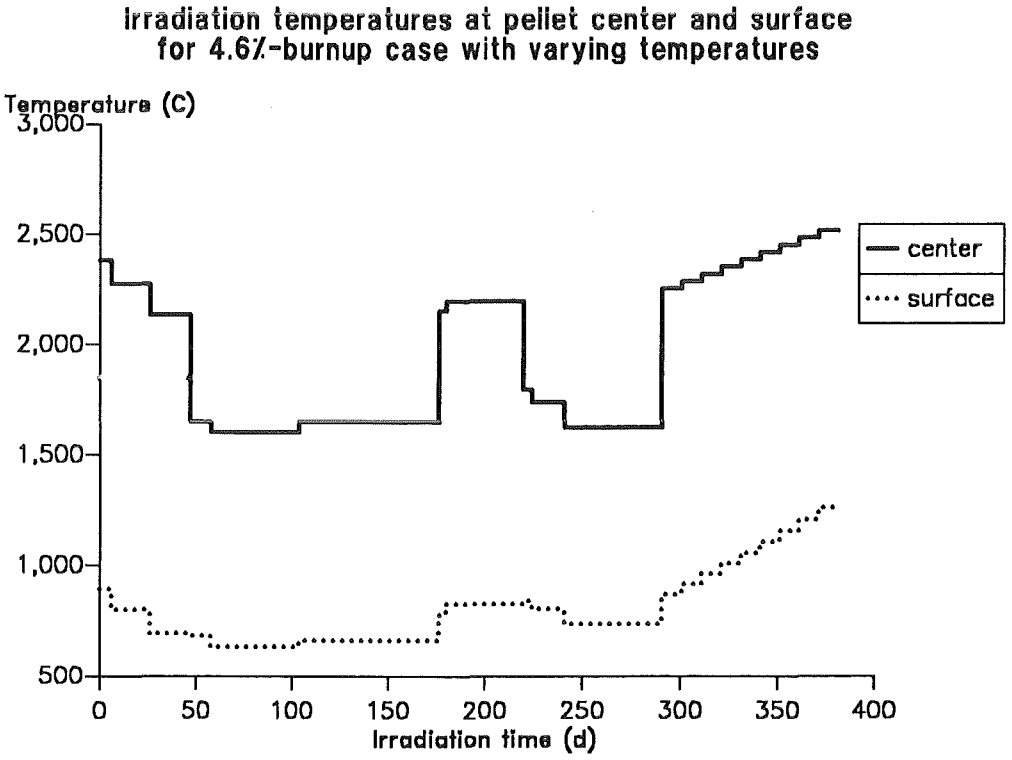


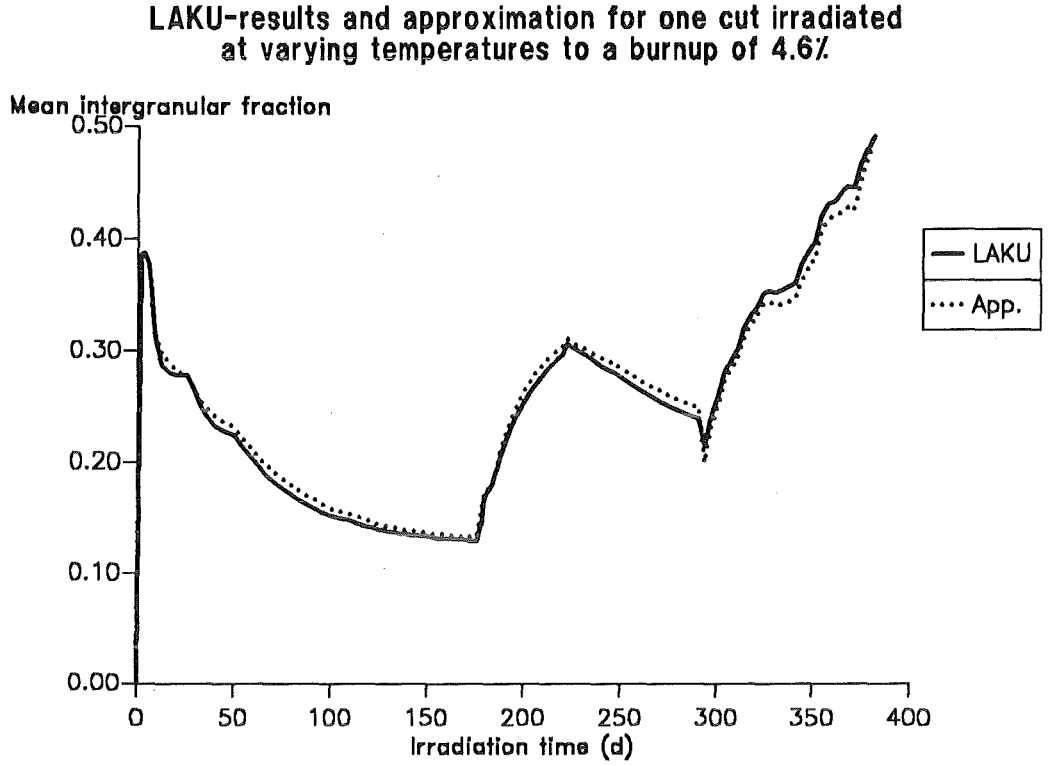
The agreement of the ZEISIG-results with those of LAKU is very good.

3.3. Varying temperatures: Medium burnup, temperature ramp at end of irradiation

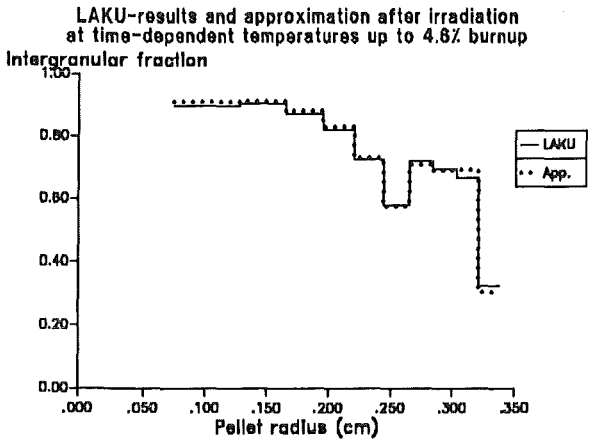
The third case has again 20 time intervals with varying temperatures and gas production rates, up to a 4.6at% burnup (the CABRI-1 Rig3 irradiation /7/ near the hottest node is the model for this case). The temperatures vary between high and medium for this irradiation, with a sustained temperature rise at the end. 10 radial nodes are employed. The external time step sizes are below 7 days during the whole irradiation, and remain below 3.5 days during the final ramp.

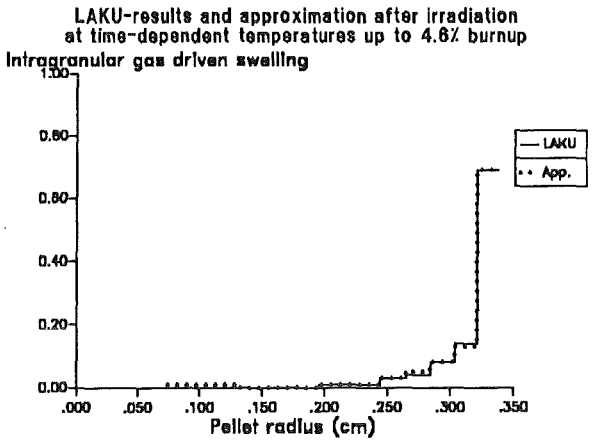
The time dependent temperatures and averaged intergranular gas fraction are shown in the next two figures. There is a gradual increase of the intergranular gas fraction at the end of the irradiation due to the rising temperatures, which ZEISIG is well able to reproduce.





The radial distribution of the intergranular gas fraction and the intragranular gas driven swelling at the end of the irradiation are shown in the next two figures. Much gas has been released during the final temperature rise, and thus the intragranular gas driven swelling is very low everywhere except in the outermost node. What little gas remains resides mainly on the grain surfaces, and therefore the intergranular gas fraction is very high in all radial nodes except the outermost one.



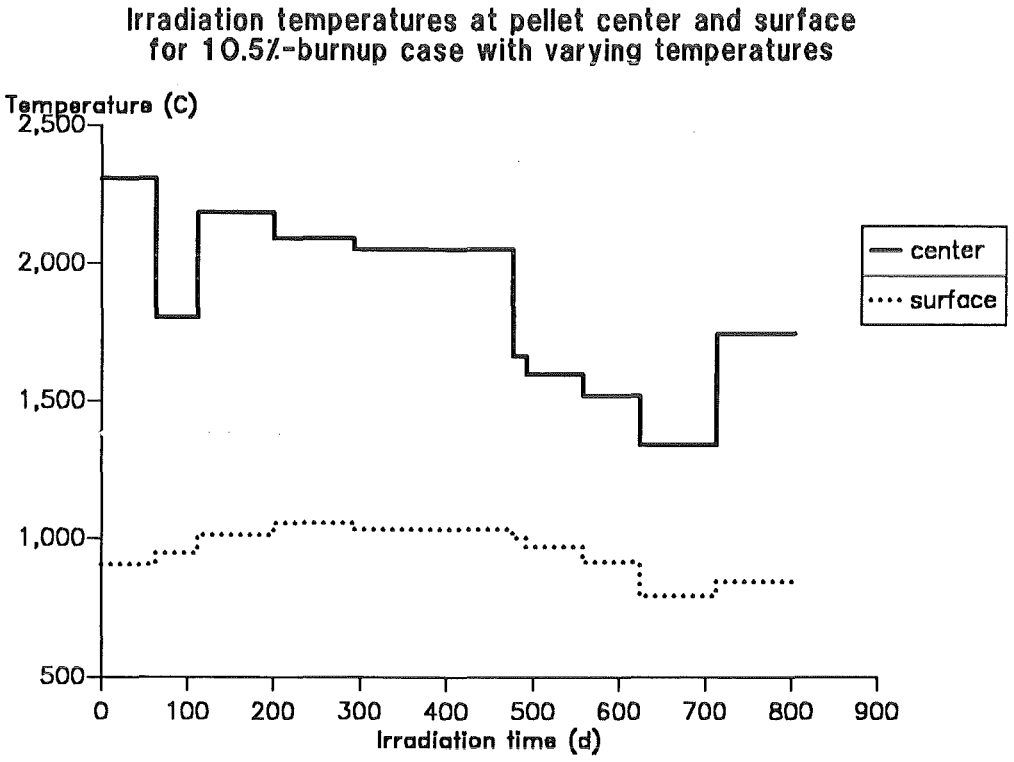


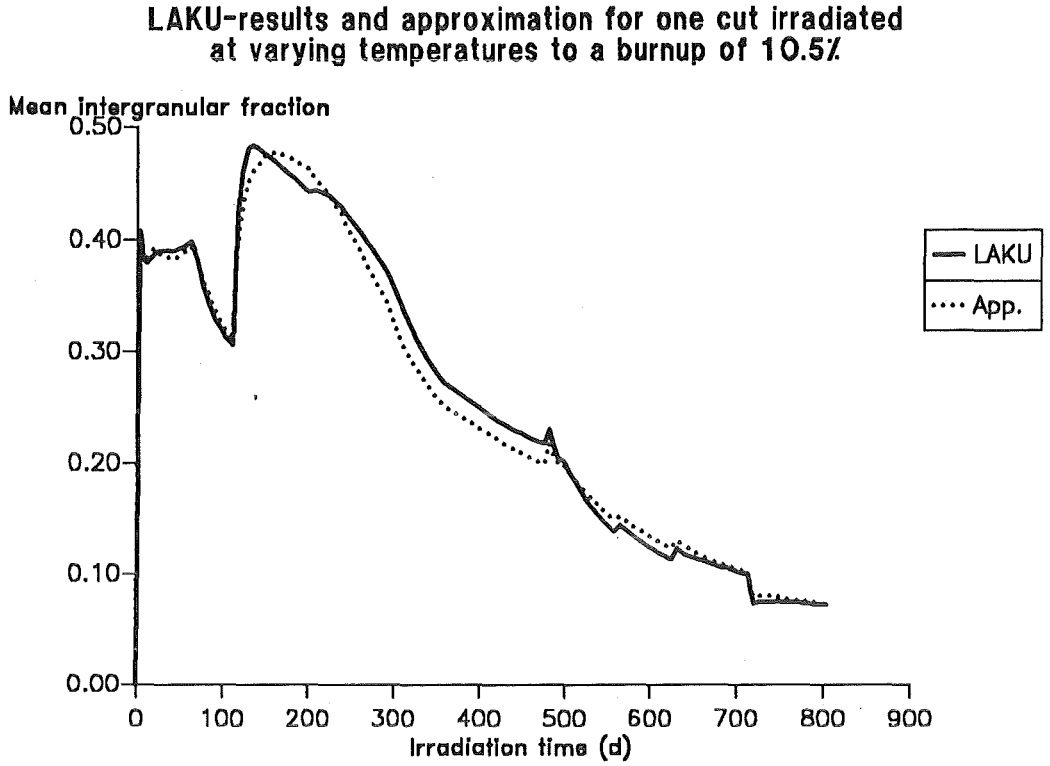
The results of ZEISIG agree again very well with those of LAKU.

3.4. Varying temperatures: High burnup, medium temperatures

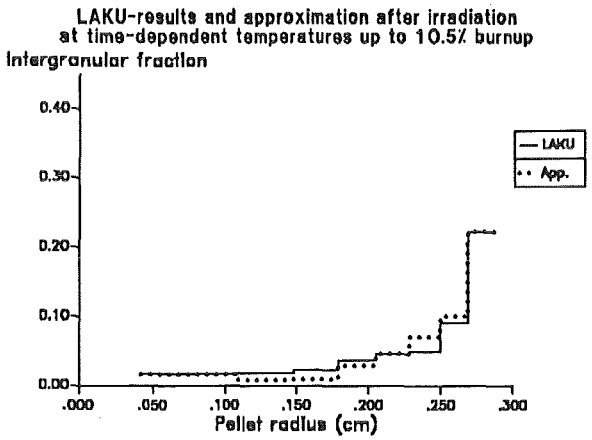
The fourth case is an irradiation with 10 time intervals with varying temperatures and gas production rates, up to a 10.5at% burnup (the CABRI-2 Viggen-4 irradiation /7/ near the hottest node is the model for this case). The temperatures vary between high and medium, with medium temperatures at the end of the irradiation. 8 radial nodes are employed. The external time step sizes remain below 10 days for the whole calculation.

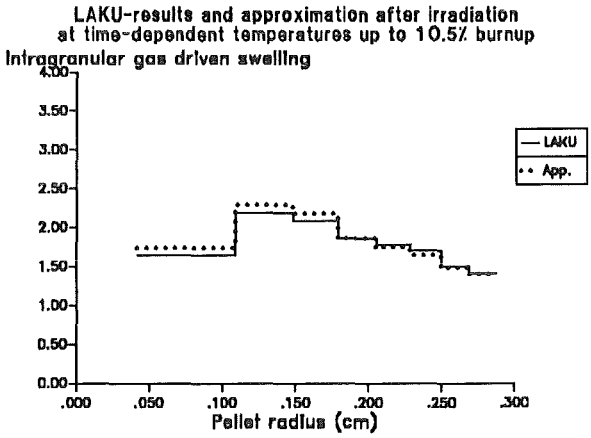
The time dependent temperatures and the averaged intergranular gas fraction are again shown first:





This case exhibits the basic behaviour discussed in section 3.1 and thus presents no problem for ZEISIG. Below follow the radial distributions at the end of the irradiation:





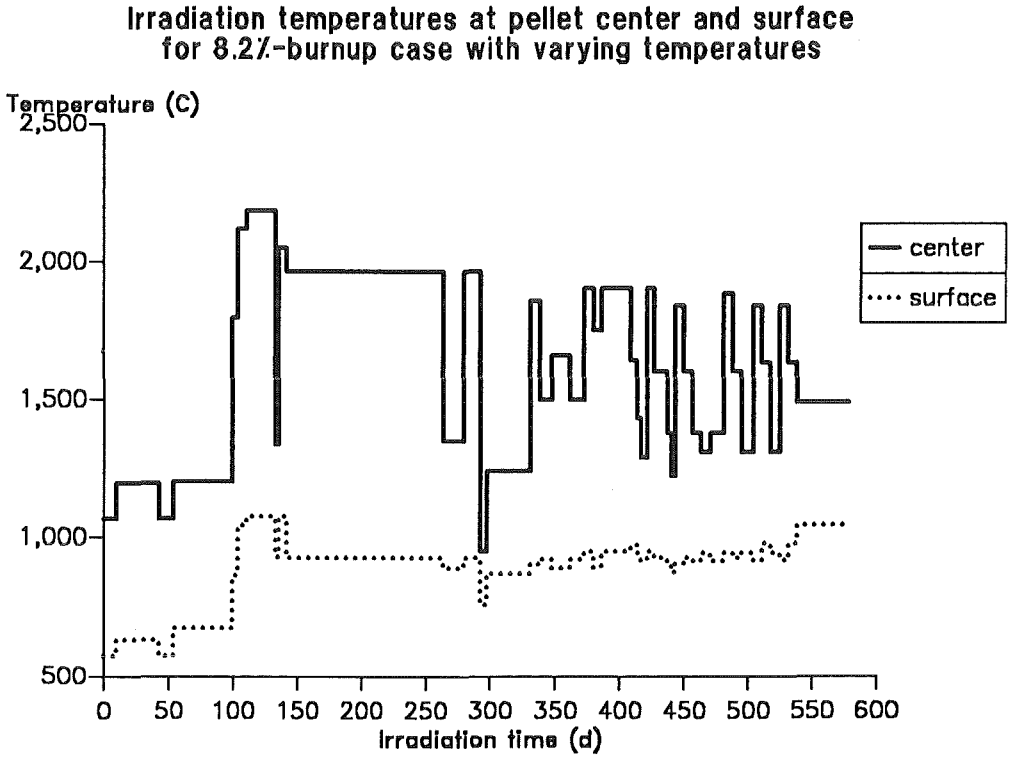
The agreement is very good. It should be mentioned here however, that there is as yet no model for the development of the outer rim region at high burnups in LAKU and also not in ZEISIG, which follows the LAKU-model closely. The inter-

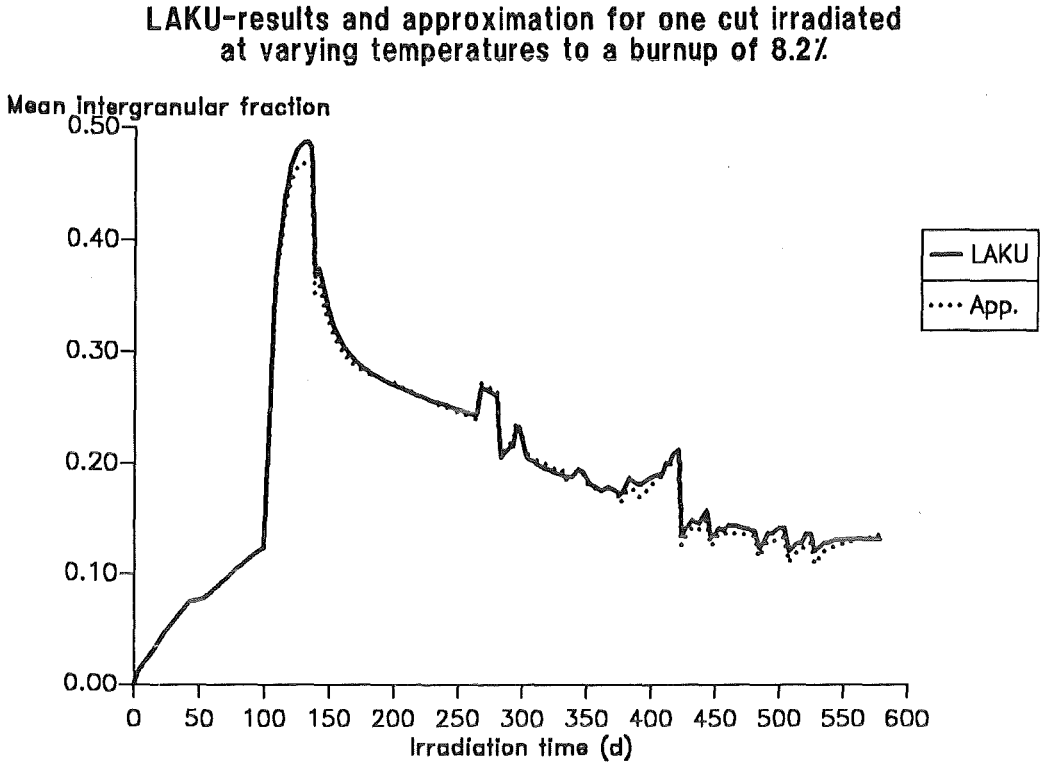
granular gas fraction as calculated by ZEISIG for this case is therefore probably too low in the outermost nodes. The same is probably true for the next case.

3.5. Varying temperatures: High burnup, medium temperatures, many temperature changes

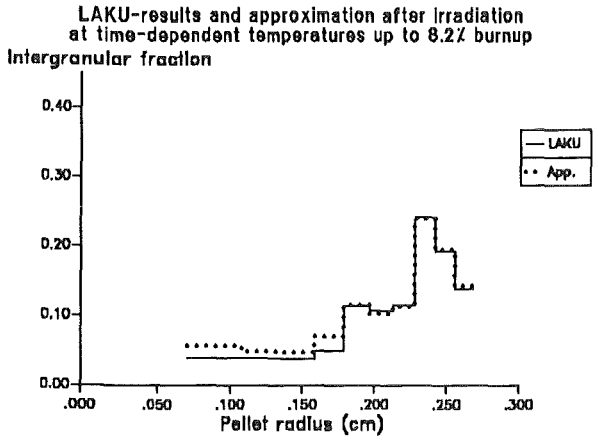
The last example is an irradiation with 42 time intervals with varying temperatures and gas production rates, up to an 8.2at% burnup (an irradiation in the German KNK-reactor /8/ is the model for this case). The temperatures are mostly moderate. This is the most complicated irradiation history comprising many temperature changes and short time intervals. 10 radial nodes are employed, and the external time step sizes remain below 6 days.

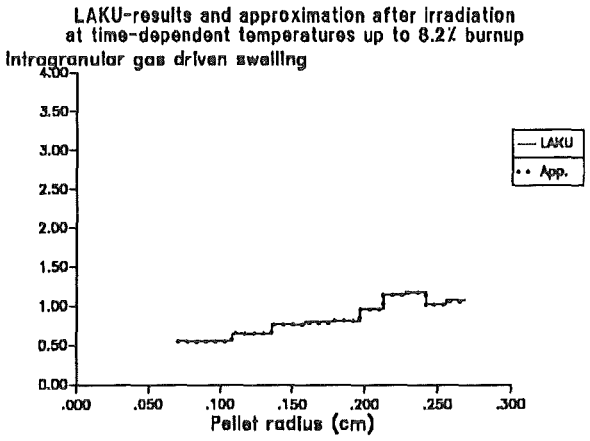
The next two figures show the time dependent temperatures and the radially averaged intergranular gas fraction.





The agreement is excellent. The radial distribution of the intergranular gas fraction is also well predicted, as can be seen in the first of the next two figures, and the agreement for the intragranular gas driven swelling is excellent, as in the foregoing cases.





When all results are taken together, it can be stated that the model is very well able to reproduce the results of the LAKU-model.

4. PROGRAMMING CONSIDERATIONS

The model depends on the results of the calling programme (e. g. SAS4A) for the following parameters: Total gas produced, total gas retained in the fuel, grain size, fuel porosity, pin internal pressure at beginning and end of time step, mean fuel temperature and radial temperature gradient during the time step, mean fuel temperature in the foregoing time step, creation rate of gas, time step length.

It returns to the calling programme: Intragranular gas driven swelling, fraction of intergranular gas.

Storage to be reserved per spatial point to be calculated: At present 19 floating point variables, if iterations in time are required, 12 otherwise.

CPU-time for: 1 channel with 20 axial nodes, 10 radial nodes in the fuel, 500 d irradiation in 10 h-time steps: ~100 s on an IBM-3090.
Gain in computer time, compared to LAKU: A factor of 40-80, depending on the case.

Length of programme: ~600 FORTRAN-statements.

Present status: The routine has been prepared for insertion into SAS4A, but a routine organizing the transfer of data from and to SAS4A remains to be written.

5.CONCLUSIONS

The fast-running code ZEISIG has been developed on the basis of the more elaborate fission gas behaviour model LAKU, with the aim of improving the fission gas modelling in the preirradiation part of the SAS4A reactor accident model. The results of the LAKU-model can be very well reproduced by the new model. The coupling to the SAS4A-code remains to be performed.

Acknowledgements:

The author whishes to gratefully acknowledge the helpful and valuable discussions with E. A. Fischer and R. Fröhlich.

Table of symbols:

A_1	inverse time constants for the release of intragranular bubbles
A_2	inverse time constants for the release of intragranular resolved gas
a	grain radius
a_g	upper limit on the grain size
b	gas in intragranular bubbles
b_{eq}	equilibrium value of b after long times at constant conditions
b_i	b at end of external time step
b_{i-1}	b at end of foregoing external time step
b_t	b at end of an internal time step
b_0	b at beginning of an internal time step
c	intragranular gas in solid solution
c_{eq}	equilibrium value of c after long times at constant conditions
c_i	c at end of external time step
c_{i-1}	c at end of foregoing external time step
c_t	c at end of an internal time step
c_0	c at beginning of an internal time step
Δc_0	short-term increase of c_0 after decrease of irradiation temperature
D_g	diffusion coefficient of resolved gas
F_a	inverse time constant for the migration of resolved gas to the grain surface (excluding sweeping effects)
$F_{a,i}$	value of F_a at end of external time step
$F_{a,0}$	value of F_a at beginning of external time step
f_1-f_4	functions for calculating the asymptotic bubble number density
G	total amount of gas created during the irradiation
g	gas released from the interior of the grain
g_i	quantity of intergranular gas
g_o	gas in open porosity according to ideal gas equation
I	intergranular gas fraction
I_{i-1}	intergranular gas fraction at end of foregoing external time step
I_{max}	maximum intergranular gas fraction
L	Avogadro's number
n	number density of intragranular bubbles
n_{as}	asymptotic bubble number density of intragranular bubbles
n_{i-1}	n at end of foregoing external time step
n_s	number of potential bubble sites
n_t	n at end of internal time step
n_0	n at beginning of internal time step
P	fraction of fuel porosity

p	pin internal pressure
R	universal gas constant
r	radius of intragranular bubbles
r_{i-1}	r at end of foregoing external time step
r_t	r at end of internal time step
T	irradiation temperature
T_i	irradiation temperature in external time interval i
T_{i-1}	irradiation temperature in forgoing external time interval
∇T:	temperature gradient
t	time
Δt	length of internal time interval
Δt_e	length of external time interval
V'	factor measuring the difference in irradiation conditions, see eq. (18)
w	Van-der-Waals constant
Z	correction for the time constant $1/F_a$
α	factor relating the time constants for precipitation and resolution
β	gas production rate
γ	surface tension of fuel
ζ	relaxation parameter for bubble number density
η	inverse resolution time constant
τ_n	relaxation parameter for bubble number density
τ_1	time constant for grain boundary sweeping
τ_2	time constant for pore migration
τ_3	time constant for steady-state intragranular bubble migration
Ω	molecular volume
ω	factor measuring the approach to equilibrium
ω_i	ω at end of external time step
ω_{i-1}	ω at end of foregoing external time step
ω_{int}, ω_{lim}	parameters for calculating weighting function from ω
ω_{min}	minimum value of ω
ω_0	ω at beginning of external time step

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/8/ K. Schleisiek, KfK: private communication