Optimization of HTR fuel design to reduce fuel particle failures

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Abstract

In this paper, an attempt is made to formulate criteria that can be used in the redesign of HTR fuel. A simplified fuel performance model is setup to calculate the fuel particle failure probability as a function of the TRISO particle design and the particle packing fraction. These models require knowledge of the fast neutron dose, the fuel burnup level, and the fuel temperature. In this paper, a neutronic, thermal-hydraulic and burnup calculations for the PBMR 400 MW_{th} design are used to provide the fuel performance model with the required data. It was found that the failure impact increases considerably with increasing number of particles and reactor operating temperature, but decreases with a larger buffer layer.

KEYWORDS: High Temperature Reactor, pebble bed,fuel performance, PBMR

1 Introduction

The fuel design for High Temperature Reactors (HTR) currently planned and investigated is largely based on experience from several decades ago (Dragon, AVR, HTR-Modul, etc). Trends in Very High Temperature Reactor (VHTR) intended operating conditions, such as higher fuel temperatures and higher exit burnup values, call for a reconsideration of these earlier fuel designs. Of particular interest is the fuel particle failure probability, which is expected to increase under the contemplated new operating conditions. An important question that arises is whether modifications to the fuel design can be made that reduce the chance of failure. Furthermore, the use of PuO_2 as a fuel or of coated particles containing minor actinides calls for a complete new fuel design for which design criteria and methods need to be developed.

In this paper, an attempt is made to formulate criteria that can be used in the redesign HTR fuel. A simplified fuel performance model is setup to calculate the fuel particle failure probability as a function of the TRISO particle design and the particle packing fraction. As these models require knowledge of the fast neutron dose, the fuel burnup level, and the fuel temperature, the ultimate aim of this project is to eventually couple this fuel performance model to neutronics, thermo-hydraulics and burnup calculations. This can be realized by incorporating these models into the PEBBED code [1] that is under

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development at the Idaho National Laboratory (INL). In order to validate the fuel performance model, a thermal-hydraulic calculation has been performed with THERMIX (DIREKT) [2], a neutronic calculation with DALTON [3] and a burnup calculation with SCALE5 [4] for the PBMR-400 design. The future use of PEBBED foreseen in this study restricts our fuel performance model to pebble-bed fuel designs.

2 Optimization

The aim of this study is to find the combination of design parameters that result in the lowest impact from fuel particle failures, within all imposed constraints. Among the parameters that can be varied are:

- Number of TRISO particles per fuel pebble,
- Dimensions of the fuel pebble,
- Dimensions of the TRISO coated fuel particles,
- Pebble transit time through the core,
- Helium coolant inlet and outlet temperatures,
- Mean power density in the core.

The phase space will be scanned for combinations of parameter values to find the fuel design parameters that will result in the lowest impact of fuel particle failures. Eventually, the fuel performance model will be coupled to the PEBBED code to assess the behavior of the fuel during irradiation conditions representative of operations.

3 Failure mechanisms

In the fuel performance model, two different failure mechanisms are taken into account [5]: Failure due to touching between particles, which are crunched at the pressing stage of the fuel manufacturing process, and failure due to pressure buildup in the fuel particle. For the latter mechanism, two processes are modeled: 1) production and diffusion of gaseous fission products and carbon-monoxide (CO) form the fuel kernel to the porous buffer layer, and 2) the shrinkage of the PyC layers during irradiation.

3.1 Particle failure during manufacturing

To determine the number of TRISO particles that can be assumed to be touching, a critical inter-particle distance has to be defined. Particles closer to each other than the critical distance will be assumed touching during the pressing stage of the fuel manufacturing process and a fraction of these particles will start to leak during irradiation. If this critical distance is large enough, implying small TRISO particles and large dilution, the Poisson distribution can be used for the inter-particle distance distribution and the number of defective particles in a fuel pebble can be easily calculated analytically [5]. In practice, for fuel particles having a carbon overcoat, this assumption will be valid, and the predicted number of defective particles in the sphere is given by:

$$n_{def} = N\psi\left\{1-\exp\left[-N\left(\frac{d_{crit}}{R_{fuel}}\right)^3\right]\right\} \quad (1)$$

where N is the number of fuel particles in the pebble, R_{fuel} is the outer radius of the fuel zone of the pebble, d_{crit} is the critical distance, and $\psi = 1.4 \cdot 10^{-5}$ ("impact parameter") [6]. If no carbon overcoat is applied or the conditions for validity of the Poisson distribution are no longer fulfilled, a numerical approach can be used to calculate the number of touching particles. In any case, both the impact parameter and the critical distance are empirical factors to be retrieved from experiments.

3.2 Particle failure during reactor operation

For the second mechanism, failure due to pressure buildup, the diffusion of gaseous fission product from the kernel to the porous buffer layer can be calculated after, temperature, power density, fluence and burnup is known for every time step [7,8].

3.2.1 Neutron flux and power profile

A two-dimensional R-Z model of the PBMR-400 reactor in the diffusion code DALTON is made to calculate the fast and thermal neutron flux in the reactor, as well as the power profile. The fast neutron fluence at any point in time during the life of a pebble is calculated from the fast neutron flux profile and transit time of the pebble trough the core. The pebbles are assumed to pass the core 6 times in which they experience the same neutron flux profile every time they pass the core.

3.2.2 TRISO temperature calculation

The temperature in the kernel and porous buffer layer of the TRISO coated fuel particles are calculated from the axially dependent pebble surface temperature and the axially dependent power profile, augmented with the following contributions:

1. The temperature step from the pebble surface to the surface of the fueled zone within the pebble:

$$\Delta T_1 = \frac{q'''_{fuel}}{3k_{graph}} R_{fuel}^3 \left(\frac{1}{R_{fuel}} - \frac{1}{R_{pebb}}\right) \quad (2)$$

Where k_{graph} is the thermal conductivity of graphite, taken to be 20.0 $W.m^{-1}K^{-1}$, power density q'''_{fuel} is the power density in the fuel zone of the pebble, R_{fuel} and R_{pebb} are the radius of the fuel zone and the radius of the pebble respectively.

2. The temperature step from the fueled zone surface to a TRISO particle in the fueled zone:

$$\Delta T_2 = \frac{q'''_{fuel}}{6\,k_{fuel}}\left(R_{fuel}^2 - r^2\right) \qquad (3)$$

Where k_{fuel} is the thermal conductivity of fuel zone, taken to be 20.0 W.m^{-1}K^{-1}.

3. The temperature step over the gap between the porous buffer layer and the inner PyC layer in the TRISO particle (assuming that the porous buffer layer will shrink during irradiation, thereby creating a gap between the porous buffer layer and the inner PyC layer [9]):

$$\Delta T_3 = \frac{q'''_{fuel}}{3\,k_{gap}} R_{fuel}^3 \left(\frac{1}{R_{gap}} - \frac{1}{R_{iPyC}}\right) \qquad (4)$$

Where $k_{gap} = 3.2 \cdot 10^{-4}$ W.cm^{-1}K^{-1} is the thermal conductivity of the gap, corresponding to a 74-26% Xe-CO mixture at 1200 ^{0}C [9], and R_{iPyC} is the inner radius of the inner PyC layer. The R_{gap} is the outer radius of the porous buffer layer after shrinkage. For example, if the dimensions of the TRISO particle are originally 0.04 cm radius for the kernel and 0.05 cm outer radius for the porous buffer layer $\left(= R_{iPyC}\right)$, the latter value reduces to 0.0479 cm after a 25% shrinkage of the buffer volume, leaving a gap of 0.0021 cm.

Finally the temperature profile in the fuel kernel and porous buffer layer is assumed to be uniform. The temperature is the sum of the pebble surface temperature and all temperature steps:

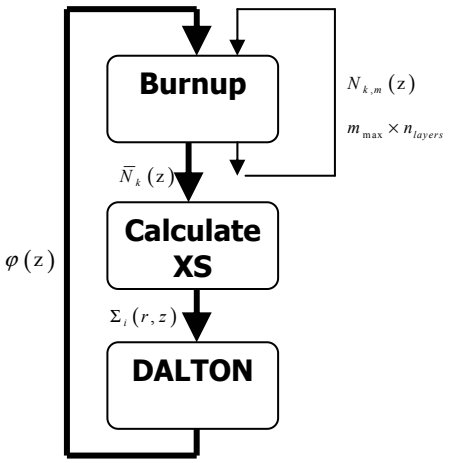
$$T_{krnl} = T_{surface} + \Delta T_1 + \Delta T_2 + \Delta T_3 \qquad (5)$$

The surface temperature is calculated with the thermal-hydraulics code THERMIX, which is supplied with a power profile from DALTON. The results of the two-dimensional R-Z model in THERMIX and DALTON are collapsed to one-dimensional axial profiles.

3.2.3 Burnup calculation

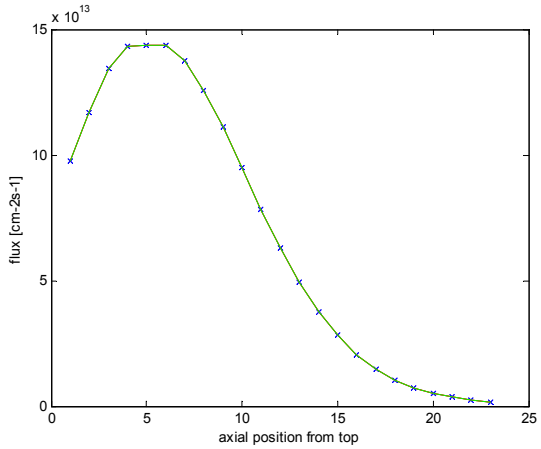
To provide information on the burnup of the pebble during its time in the reactor, a burnup calculation in SCALE5 is made. The nuclide concentrations are assumed to have reached equilibrium concentrations. The neutron flux profile remains the same over time. The burnup calculation scheme is shown in figure 1. For each axial layer z in the core and for each pass m trough the core the nuclide concentration in the pebble is calculated by using an axial flux profile that is calculated with the diffusion code DALTON. Each axial layer in the core has an equal amount of pebbles with different burnup states. The number of different burnup states is equal to the number of passes through the core. For each layer in the core the nuclide concentrations are averaged, resulting in an axial (average) nuclide concentration profile $\bar{N}_k(z)$ for each nuclide k.

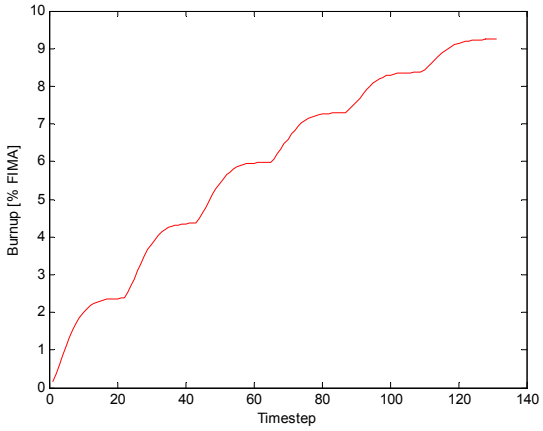
Figure 1: Burnup calculation scheme



These nuclide concentrations are then used for generating neutron cross sections for the full reactor geometry, resulting in macroscopic neutron cross sections $\Sigma(r,z)$ dependent on the radial and axial position in the reactor.
The neutronics code DALTON is used to calculated the neutron flux in R-Z geometry, which is then collapsed to a one-dimensional axial profile to supply the burnup calculation. The calculation steps are repeated several times until satisfactory results are found for k_{eff} and the final discharge burnup.
The results for axial neutron flux profiles and burnup during the life of a pebble for a simplified PBMR400 (no control rods or void regions present) geometry are shown in figure 2 and 3. The target burnup was 90 MWd/kg U and k_{eff} was 1.06.

Figures 2 and 3: Axial thermal neutron flux [$cm^{-2}s^{-1}$] and burnup [FIMA] during pebble lifetime calculated





It can be seen that the burnup of the pebble is influenced by the thermal flux profile. The

burnup increases fast when the pebble is in the region of the flux peak, while burnup speed is low at the bottom of the reactor. The increase in burnup during each pass trough the reactor decreases with each pass, because of the depletion of U^{235}, which reduces the macroscopic fission cross section.

3.2.4 Pressure buildup by diffusion of gaseous fission products

The buildup of gaseous fission products can be calculated analytically and numerically [7, 8] by solving the equation:

$$\frac{D}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C}{\partial r}\right)+S=\frac{\partial C}{\partial t} \tag{6}$$

In which, C is the fission product concentration, r is the radial position in the kernel, D is the diffusion coefficient and S the source term of fission products.
Because the analytical approach needs some unrealistic boundary conditions (a zero concentration in the porous buffer layer), the numerical approach is used in our model.
The resulting pressure on the SiC layer, caused by the fission product buildup, is calculated with the ideal gas law using the kernel temperature. Besides the pressure caused by the fission products Kr and Xe, the formation of CO is also taken into account using an empirical formula [10]:

$$O/_f = 8.32\cdot 10^{-11} t^2 \exp\left(\frac{162.7\cdot 10^3}{RT}\right) \tag{7}$$

In which $O/_f$ is the oxygen release per fission, t is the irradiation time in seconds, R the universal gas constant in J/mol.K.

3.2.5 Failure fraction distribution function

The failure fraction of the Sic layer in the kernel can be calculated using the following Weibull distribution function [3]:

$$\Phi = 1-\exp\left[-\ln(2)\left(\frac{rp}{2d}\frac{1}{\sigma_{med}}\right)^m\right] \tag{8}$$

Where p is the pressure inside the kernel, d is the thickness of the SiC layer, r is the radius of the SiC shell and σ_{med} is the median strength of the SiC.

3.3 Failure calculation methodology

Finally, to calculate the failure probability, not only the gas pressure needs to be known, but also the material properties of the graphite, which are determined by the fast neutron dose, and thus by the irradiation history of the graphite [11].
The particle is followed during its lifetime in order to calculate the maximum failure fraction that it will experience. For each position in the core and for every pass that the pebble makes trough the core, the kernel failure fraction is calculated for several regions in the fuel zone of the pebble. The failure fractions for each fuel region layer are averaged to calculate the average failure fraction in the pebble at a certain time. The failure impact

Ψ is then calculated with:

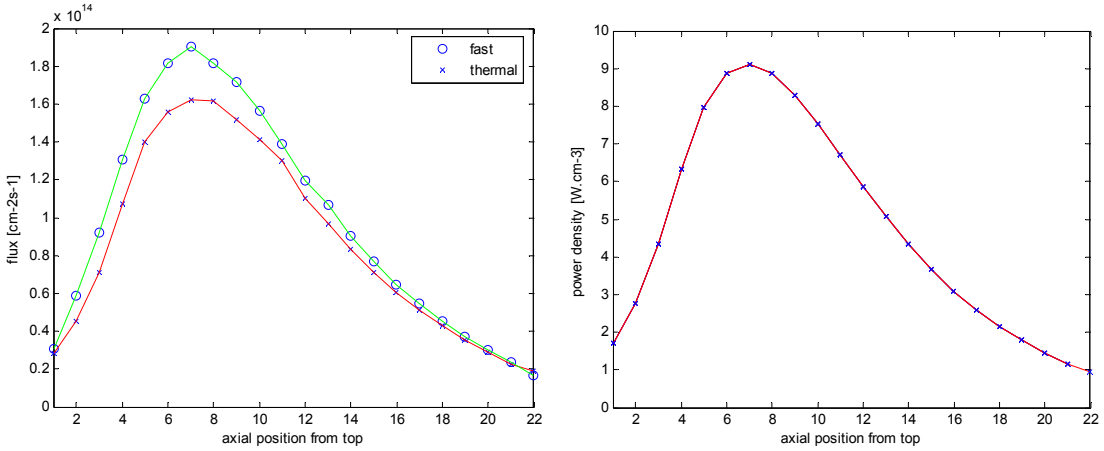
$$\Psi = \Phi V_k n_k FIMA_{\text{discharge}} \quad (9)$$

In which V_k is the kernel volume, n_k the number of TRISO particles (kernels) per pebble and $FIMA_{\text{discharge}}$ the burnup in FIMA of the discharged pebbles.

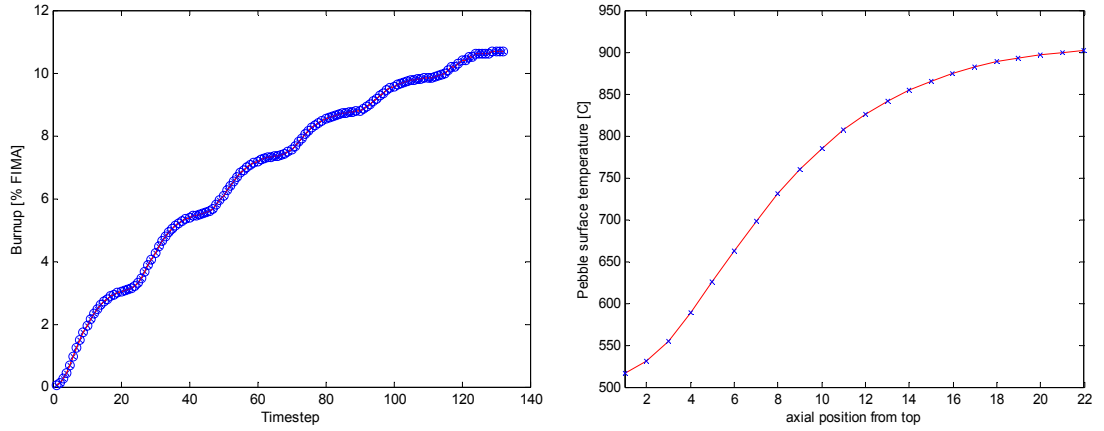
4 Calculation results of fuel particle failure

For the calculation results below, data was taken form an extensive PBMR400 model including the control rods and void regions. A fixed neutron cross section data set was used to generate the fluxes and power profile with DALTON (figures 3 and 4). The temperature profile was calculated with THERMIX and burnup profile was generated with the burnup script (figures 5 and 6).

Figures 3 and 4: Axial thermal and fast neutron flux [$cm^{-2}s^{-1}$] and axial power profile [$W.cm^{-3}$]



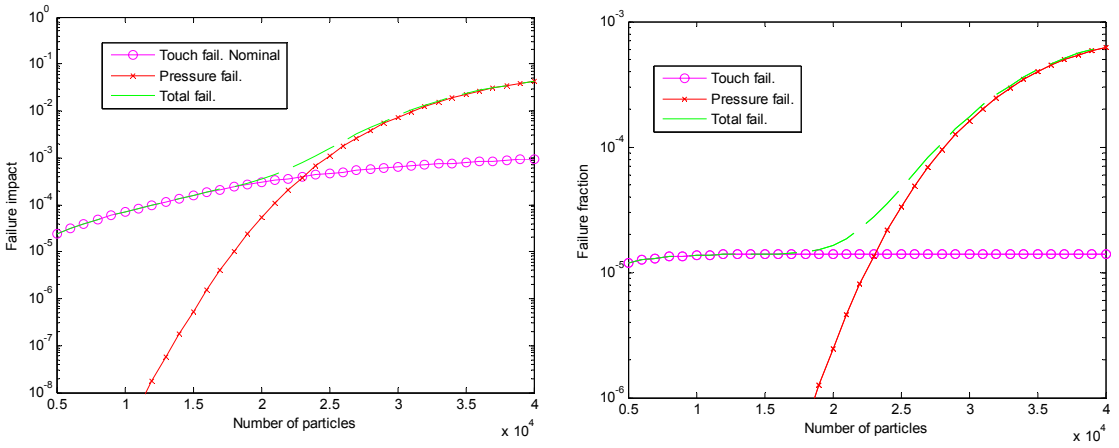
Figures 5 and 6: Burnup [% FIMA] during pebble lifetime and axial temperature [°C] profile



4.1 Particle failure for standard particle geometry using different number of particles per pebble

The standard TRISO particle geometry that is used for the PBMR and other HTR reactors is used in the calculation of the failure fraction. The number of particles per pebble is varied, which implicitly changes the required enrichment, discharge burnup and the irradiation time [5]. The required enrichment is calculated from the number of particles per pebble, requiring that the k_∞ for pebble bed material remains at a constant level. The discharge burnup is calculated from the enrichment, using a correlation from [5]. The irradiation time is calculated from the discharge burnup, while maintaining the reactor at a constant power level.
Results for several particle densities are shown figures 7 and 8. It can be seen that the total failure fraction (and failure impact) is determined by failure due to touching at low particle packing fraction, while at high packing fractions the failure by pressure increase is the dominant factor. At high particle packing fractions, the pebbles can achieve higher burnup due to the high enrichment. This will lead to more fission product build up in the buffer layer of the particle as well as increased CO production. The CO production plays an more important role in this case, because the long irradiation time increases the CO/f factor.

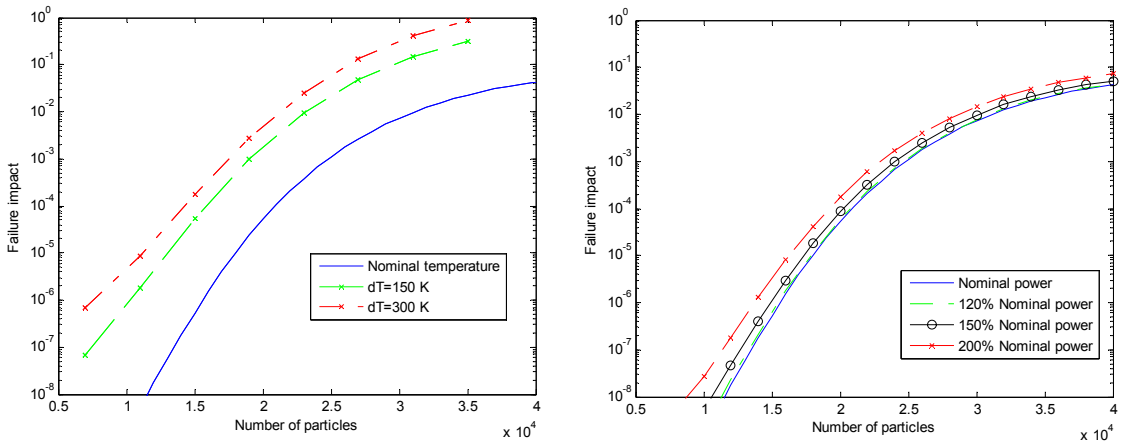
Figures 7 and 8: Failure fraction and failure impact dependent of the number of particles



4.2 Particle failure impact for increased power and temperature

Increasing the temperature in the reactor will increase the failure impact considerably (figure 9). In the calculations was assumed that the amplitude of axial temperature profile was increased with a temperature difference dT, while the power level remains the same. The temperature increase will lead to a higher internal pressure by fission products at the SiC surface.Altering the power level of the reactor, while keeping pebble surface temperatures constant, will lead to a different temperature profile in the pebble. In reality, the coolant flow has to be increased proportional to the power increase in this case. A small increase of failure impact can be recognized (figure 10).

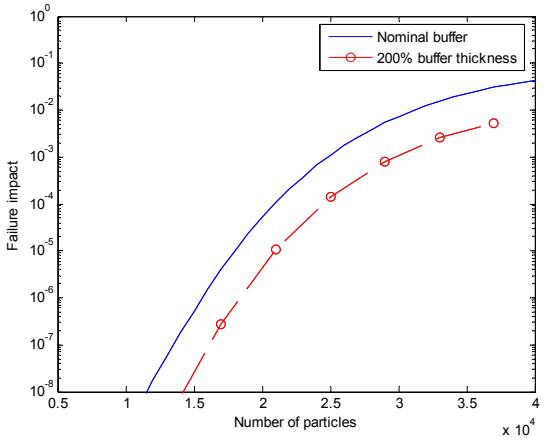
Figures 9 and 10: Failure impact for increased temperature and power cases



4.3 Particle failure impact for altered design

The thickness of the buffer layer can be increased to provide more room for the fission products. According to equation (8) the failure fraction increases with increasing SiC radius. However, the decrease in internal pressure on the SiC layer will lead to a lower failure fraction (figure 11).

Figure 11: Failure impact for nominal buffer (95 µm) and increased carbon buffer thickness (190 µm)



5 Conclusion

In this paper a TRISO fuel particle performance model is presented. Failure fractions and failure impacts are calculated successfully for different particle packing fractions, increased reactor temperature and increased reactor power for the PBMR400 design. The failure of the particles at high packing fractions is determined by the build up of pressure by fission products and CO production. The model will be expanded with swelling and creeping of the coating layers under irradiation. Furthermore, it is the goal of the authors to create and a direct coupling to the PEBBED code [1].

6 References

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