



**HTR-N & N1**  
**High-Temperature Reactor Physics and Fuel Cycle Studies**  
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Document Title

**IRI results for the plutonium cell burnup benchmark**

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| Rev. | Date       | Description                                              |
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| 0    | 27/05/2003 | First version by J.L. Kloosterman, Delft Univ. of Techn. |
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## 1. INTRODUCTION

In the framework of a plutonium cell burnup benchmark [1] defined within the HTR-N/N1 project [2], calculations have been done with the SCALE [3] computer code system and the JEF2.2 nuclear data library [4]. From the SCALE code system, we used the BONAMI-S code for the resonance treatment in the unresolved energy region, the NITAWL-II code for the resonance treatment in the resolved energy region, and the XSDRNPM-S code for the cell-weighting calculations. The Dancoff factor used in the resonance shielding was calculated by an analytical procedure [5] and took into account the double heterogeneity of the fuel. The actual burnup calculations were done using the ORIGEN-S fuel depletion code and a nuclear data library based on JEF-2.2 and EAF3 [6]. All codes were coupled to each other via PERL scripts and via own-made FORTRAN programs.

The whole sequence of cell-weighting calculations and burnup calculations for the fuel were repeated several times to calculate the  $k_{\infty}$  and the composition of the fuel as a function of burnup. Furthermore, at each burnup time step, the temperature reactivity coefficient was calculated.

Results are reported on plutonium composition types B and C (first and second generation plutonium) and with a plutonium mass of 1.0 g per Fuel Element (FE) for type B and 1.5 g per FE for type C. For a further specification of the these composition and cases, see Ref [1].

## 2. RESULTS PLUTONIUM COMPOSITION B (1.0 GRAM / FE)

The  $k_{\infty}$  of the fuel and the uniform temperature coefficient (UTC) were calculated after 0, 10, 100, 200, 300, 400, 500, 600, 700, 800 MWd/kgHM. Because the double heterogeneity was not taken into account in the cell-weighting procedure (except for the calculation of the Dancoff factor), a uniform temperature of 1073 K has been assumed. The UTC has been determined by calculating the  $k_{\infty}$  at a temperature of 1173 K for all nuclides. Results are given in Table 1. The isotopic composition and the microscopic absorption and fission cross sections of the nuclides available in our nuclear data library are given in Table 2, 3, and 4, respectively.

Table 1: Results for the  $k_{\infty}$  and the FTC for plutonium composition B.

| Burnup time step<br>(MWd/kgPu) | $k_{\infty}$ | UTC (pcm/K) |
|--------------------------------|--------------|-------------|
| 0                              | 1.3714       | -9.65       |
| 10                             | 1.3364       | -7.77       |
| 100                            | 1.3028       | -7.48       |
| 200                            | 1.2756       | -7.50       |
| 300                            | 1.2483       | -7.67       |
| 400                            | 1.2181       | -7.68       |
| 500                            | 1.1758       | -7.64       |
| 600                            | 1.0990       | -7.06       |
| 700                            | 0.8657       | -2.69       |
| 800                            | 0.2545       | -12.0*      |

\*Because of the low value of  $k_{\infty}$  this value is highly suspicious.

Table 2: Atomic density for some nuclides ( $\text{barn}^{-1} \text{cm}^{-1}$ ) as a function of burnup (MWd/kgPu).

| Nuclide | 0         | 100       | 400       | 600       | 800       |
|---------|-----------|-----------|-----------|-----------|-----------|
| Pu-238  | 6.011e-04 | 5.765e-04 | 5.003e-04 | 4.211e-04 | 2.490e-05 |
| Pu-239  | 1.245e-02 | 9.514e-03 | 2.644e-03 | 3.637e-04 | 3.342e-06 |
| Pu-240  | 5.445e-03 | 5.363e-03 | 4.090e-03 | 2.209e-03 | 1.341e-05 |
| Pu-241  | 3.009e-03 | 3.437e-03 | 3.465e-03 | 1.897e-03 | 5.460e-06 |
| Pu-242  | 1.547e-03 | 1.609e-03 | 2.108e-03 | 2.738e-03 | 2.026e-03 |
| Am-241  | 1.000e-20 | 3.788e-05 | 1.005e-04 | 5.880e-05 | 4.312e-09 |
| Am-242m | 1.000e-20 | 3.096e-07 | 1.524e-06 | 8.608e-07 | 8.005e-11 |
| Am-243  | 1.000e-20 | 1.133e-04 | 4.446e-04 | 7.041e-04 | 9.093e-04 |
| Cm-242  | 1.000e-20 | 2.895e-06 | 3.805e-05 | 7.100e-05 | 4.666e-05 |
| Cm-243  | 1.000e-20 | 9.490e-09 | 5.170e-07 | 1.581e-06 | 1.654e-06 |
| Sr-90   | 0.000e+00 | 4.487e-05 | 1.717e-04 | 2.477e-04 | 3.090e-04 |
| Zr-93   | 1.000e-20 | 8.594e-05 | 3.308e-04 | 4.771e-04 | 5.866e-04 |
| Nb-94   | 0.000e+00 | 1.767e-10 | 5.956e-10 | 7.454e-10 | 7.200e-10 |
| Tc-99   | 1.000e-20 | 1.378e-04 | 5.390e-04 | 7.687e-04 | 7.445e-04 |
| Pd-107  | 1.000e-20 | 8.562e-05 | 3.579e-04 | 5.567e-04 | 7.016e-04 |
| Sn-126  | 0.000e+00 | 7.744e-06 | 3.164e-05 | 4.833e-05 | 6.315e-05 |
| I-129   | 1.000e-20 | 3.235e-05 | 1.339e-04 | 1.974e-04 | 1.984e-04 |
| Cs-135  | 1.000e-20 | 8.715e-05 | 2.884e-04 | 3.627e-04 | 5.402e-04 |
| Cs-137  | 0.000e+00 | 1.568e-04 | 6.162e-04 | 9.117e-04 | 1.168e-03 |
| Sm-147  | 1.000e-20 | 1.217e-06 | 1.888e-05 | 3.503e-05 | 2.367e-05 |
| Sm-151  | 1.000e-20 | 1.322e-05 | 1.737e-05 | 9.505e-06 | 3.289e-06 |
| Eu-154  | 1.000e-20 | 6.007e-07 | 1.126e-05 | 2.868e-05 | 4.081e-05 |

Table 3: Microscopic absorption cross section for some nuclides (barn) as a function of burnup (MWd/kgPu).

| Nuclide | 0         | 100       | 400       | 600       | 800       |
|---------|-----------|-----------|-----------|-----------|-----------|
| Pu-238  | 2.564e+01 | 2.745e+01 | 4.377e+01 | 7.657e+01 | 1.636e+02 |
| Pu-239  | 1.784e+02 | 2.012e+02 | 3.655e+02 | 6.753e+02 | 1.304e+03 |
| Pu-240  | 1.480e+02 | 1.495e+02 | 1.728e+02 | 2.176e+02 | 2.365e+02 |
| Pu-241  | 1.442e+02 | 1.583e+02 | 2.703e+02 | 4.890e+02 | 9.903e+02 |
| Pu-242  | 5.167e+01 | 5.078e+01 | 4.394e+01 | 3.319e+01 | 1.479e+01 |
| Am-241  | 1.559e+02 | 1.678e+02 | 2.522e+02 | 4.088e+02 | 6.948e+02 |
| Am-242m | 6.441e+02 | 7.098e+02 | 1.266e+03 | 2.368e+03 | 5.061e+03 |
| Am-243  | 9.498e+01 | 9.355e+01 | 8.652e+01 | 7.503e+01 | 4.885e+01 |
| Cm-242  | 7.267e+00 | 7.307e+00 | 7.578e+00 | 8.044e+00 | 9.496e+00 |
| Cm-243  | 1.284e+02 | 1.302e+02 | 1.458e+02 | 1.759e+02 | 2.498e+02 |
| Zr-93   | 1.784e+00 | 1.758e+00 | 1.634e+00 | 1.406e+00 | 9.520e-01 |
| Tc-99   | 1.559e+01 | 1.544e+01 | 1.463e+01 | 1.316e+01 | 1.015e+01 |
| Pd-107  | 5.462e+00 | 5.319e+00 | 4.770e+00 | 3.717e+00 | 1.435e+00 |
| I-129   | 3.054e+00 | 3.212e+00 | 4.564e+00 | 7.237e+00 | 1.388e+01 |
| Cs-135  | 3.509e+00 | 3.243e+00 | 3.270e+00 | 3.442e+00 | 4.030e+00 |
| Sm-147  | 4.211e+01 | 3.866e+01 | 3.537e+01 | 3.256e+01 | 2.826e+01 |
| Sm-151  | 4.593e+02 | 4.899e+02 | 8.147e+02 | 1.473e+03 | 3.269e+03 |
| Eu-154  | 1.408e+02 | 1.427e+02 | 1.631e+02 | 2.038e+02 | 3.108e+02 |

Table 4: Microscopic fission cross section for some nuclides (barn) as a function of burnup (MWd/kgPu).

| Nuclide | 0         | 100       | 400       | 600       | 800       |
|---------|-----------|-----------|-----------|-----------|-----------|
| Pu-238  | 2.146e+00 | 2.185e+00 | 2.554e+00 | 3.305e+00 | 5.411e+00 |
| Pu-239  | 1.110e+02 | 1.250e+02 | 2.270e+02 | 4.197e+02 | 8.151e+02 |
| Pu-240  | 3.881e-01 | 3.823e-01 | 3.423e-01 | 2.689e-01 | 9.676e-02 |
| Pu-241  | 1.074e+02 | 1.176e+02 | 1.997e+02 | 3.603e+02 | 7.315e+02 |
| Pu-242  | 2.512e-01 | 2.465e-01 | 2.135e-01 | 1.558e-01 | 3.817e-02 |
| Am-241  | 1.308e+00 | 1.392e+00 | 1.976e+00 | 3.057e+00 | 4.962e+00 |
| Am-242m | 5.280e+02 | 5.814e+02 | 1.033e+03 | 1.928e+03 | 4.109e+03 |
| Am-243  | 2.479e-01 | 2.433e-01 | 2.139e-01 | 1.628e-01 | 5.530e-02 |
| Cm-242  | 8.181e-01 | 8.411e-01 | 1.042e+00 | 1.447e+00 | 2.444e+00 |
| Cm-243  | 1.100e+02 | 1.114e+02 | 1.242e+02 | 1.488e+02 | 2.083e+02 |

### 3. RESULTS PLUTONIUM COMPOSITION C (1.5 GRAM / FE)

The  $k_{\infty}$  of the fuel and the temperature coefficients (UTC and FTC) were calculated at intervals of 25 days up till the total irradiation time of 1200 full power days (corresponding to a burnup of 800 MWd/kgPu). Results are given in Table 5 and in Figure 1. The FTC is determined from  $k_{\infty}$  values at a 50 K higher temperature by only raising the temperature of the fuel nuclides (actinides and fission products), while the UTC is determined by raising the temperature of the fuel and moderator together. It is seen that the FTC itself already provides a negative temperature coefficient during the whole range of burnup. The isotopic composition and the microscopic absorption and fission cross sections of the nuclides available in our nuclear data library are given in Table 6, 7, and 8, respectively.

Table 5: Results for the  $k_{\infty}$  and the UTC and FTC for plutonium composition C.

| Burnup time step<br>(MWd/kgPu) | $k_{\infty}$ | UTC (pcm/K) | FTC (pcm/K) |
|--------------------------------|--------------|-------------|-------------|
| 0                              | 1.1056       | -12.37      | -3.09       |
| 50                             | 1.0744       | -10.48      | -3.05       |
| 100                            | 1.0721       | -10.47      | -3.08       |
| 150                            | 1.0697       | -10.56      | -3.10       |
| 200                            | 1.0670       | -10.65      | -3.13       |
| 250                            | 1.0635       | -10.70      | -3.16       |
| 300                            | 1.0589       | -10.79      | -3.17       |
| 350                            | 1.0521       | -10.47      | -3.18       |
| 400                            | 1.0416       | -10.04      | -3.09       |
| 450                            | 1.0232       | -9.36       | -2.93       |
| 500                            | 0.9882       | -7.94       | -2.66       |
| 550                            | 0.9112       | -5.22       | -2.21       |
| 600                            | 0.7158       | 0.55*       | -1.61*      |
| 650                            | 0.3658       | 6.05*       | -1.12*      |
| 700                            | 0.2409       | -17.99*     | -0.95*      |
| 750                            | 0.2877       | -21.51*     | -0.76*      |
| 800                            | 0.3196       | -20.59*     | -0.55*      |

\*Because of the low value of  $k_{\infty}$  this value is highly suspicious.

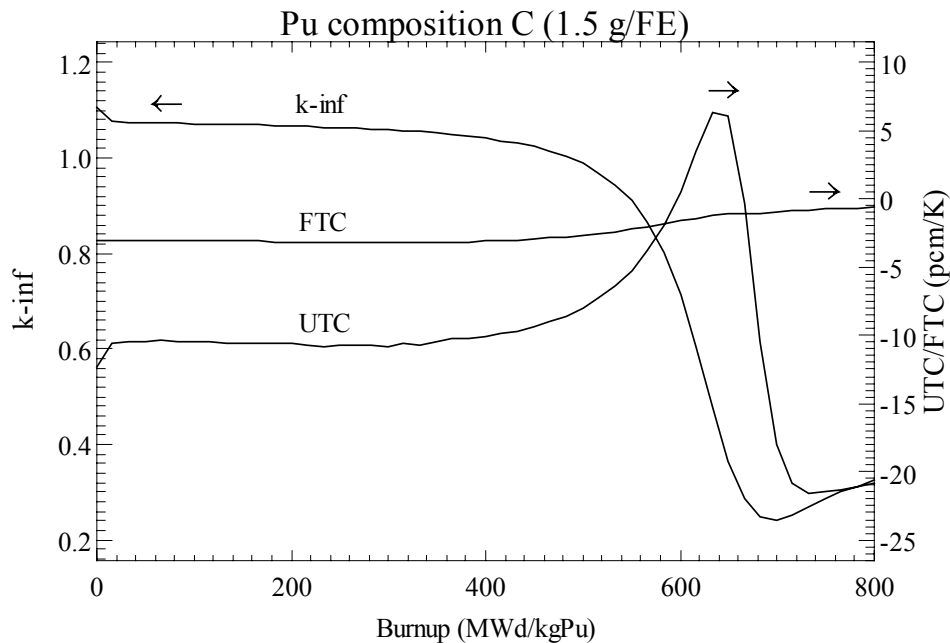


Figure 1: The  $k_{\infty}$  and the UTC and FTC as a function of burnup.

Table 6: Atomic density for some nuclides ( $\text{barn}^{-1} \text{cm}^{-1}$ ) as a function of burnup (MWd/kgPu).

| Nuclide | 0         | 100       | 400       | 600       | 800       |
|---------|-----------|-----------|-----------|-----------|-----------|
| Pu-238  | 1.137e-03 | 1.068e-03 | 8.607e-04 | 5.102e-04 | 7.287e-07 |
| Pu-239  | 6.219e-03 | 4.105e-03 | 5.824e-04 | 6.970e-05 | 9.088e-08 |
| Pu-240  | 7.897e-03 | 6.707e-03 | 2.835e-03 | 5.012e-04 | 2.822e-06 |
| Pu-241  | 3.508e-03 | 4.110e-03 | 2.950e-03 | 3.937e-04 | 6.761e-07 |
| Pu-242  | 4.247e-03 | 4.184e-03 | 4.522e-03 | 4.695e-03 | 1.291e-03 |
| Am-241  | 1.000e-20 | 6.392e-05 | 1.151e-04 | 1.270e-05 | 2.779e-10 |
| Am-242m | 1.000e-20 | 6.849e-07 | 1.783e-06 | 1.693e-07 | 6.848e-12 |
| Am-243  | 1.000e-20 | 3.601e-04 | 1.114e-03 | 1.457e-03 | 5.395e-04 |
| Cm-242  | 1.000e-20 | 7.160e-06 | 6.659e-05 | 7.893e-05 | 1.092e-05 |
| Cm-243  | 1.000e-20 | 3.826e-08 | 1.395e-06 | 2.716e-06 | 3.323e-07 |
| Se-97   | 0.000e+00 | 0.000e+00 | 0.000e+00 | 0.000e+00 | 0.000e+00 |
| Rb-87   | 0.000e+00 | 1.997e-05 | 7.556e-05 | 1.100e-04 | 1.384e-04 |
| Sr-90   | 0.000e+00 | 4.213e-05 | 1.578e-04 | 2.278e-04 | 2.740e-04 |
| Zr-93   | 1.000e-20 | 8.044e-05 | 3.026e-04 | 4.372e-04 | 5.161e-04 |
| Mo-93   | 0.000e+00 | 0.000e+00 | 0.000e+00 | 0.000e+00 | 0.000e+00 |
| Nb-94   | 0.000e+00 | 1.347e-10 | 3.849e-10 | 4.650e-10 | 4.110e-10 |
| Tc-99   | 1.000e-20 | 1.350e-04 | 5.087e-04 | 7.015e-04 | 4.043e-04 |
| Pd-107  | 1.000e-20 | 9.288e-05 | 3.931e-04 | 5.948e-04 | 6.428e-04 |
| Sn-126  | 0.000e+00 | 7.964e-06 | 3.286e-05 | 4.972e-05 | 5.962e-05 |
| I-129   | 1.000e-20 | 3.105e-05 | 1.259e-04 | 1.797e-04 | 8.027e-05 |
| Cs-135  | 1.000e-20 | 8.860e-05 | 2.850e-04 | 3.476e-04 | 7.877e-04 |
| Cs-137  | 0.000e+00 | 1.536e-04 | 5.998e-04 | 8.838e-04 | 1.088e-03 |
| Sm-147  | 1.000e-20 | 1.942e-06 | 2.469e-05 | 3.931e-05 | 4.238e-06 |
| Sm-151  | 1.000e-20 | 1.176e-05 | 1.173e-05 | 4.495e-06 | 6.377e-07 |
| Eu-154  | 1.000e-20 | 1.001e-06 | 1.709e-05 | 3.787e-05 | 8.959e-06 |

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Table 7: Microscopic absorption cross section for some nuclides (barn) as a function of burnup (MWd/kgPu).

| Nuclide | 0         | 100       | 400       | 600       | 800       |
|---------|-----------|-----------|-----------|-----------|-----------|
| Pu-238  | 2.335e+01 | 2.534e+01 | 4.530e+01 | 1.073e+02 | 1.654e+02 |
| Pu-239  | 1.627e+02 | 1.869e+02 | 3.766e+02 | 9.155e+02 | 1.326e+03 |
| Pu-240  | 1.077e+02 | 1.167e+02 | 1.789e+02 | 2.689e+02 | 2.358e+02 |
| Pu-241  | 1.316e+02 | 1.466e+02 | 2.793e+02 | 6.744e+02 | 1.004e+03 |
| Pu-242  | 3.885e+01 | 3.849e+01 | 3.379e+01 | 2.208e+01 | 1.453e+01 |
| Am-241  | 1.407e+02 | 1.536e+02 | 2.522e+02 | 5.200e+02 | 7.080e+02 |
| Am-242m | 5.588e+02 | 6.306e+02 | 1.303e+03 | 3.341e+03 | 5.125e+03 |
| Am-243  | 9.047e+01 | 8.779e+01 | 7.995e+01 | 6.263e+01 | 4.829e+01 |
| Cm-242  | 7.346e+00 | 7.389e+00 | 7.702e+00 | 8.563e+00 | 9.515e+00 |
| Cm-243  | 1.226e+02 | 1.244e+02 | 1.442e+02 | 2.014e+02 | 2.516e+02 |
| Zr-93   | 1.846e+00 | 1.819e+00 | 1.663e+00 | 1.245e+00 | 9.376e-01 |
| Tc-99   | 1.586e+01 | 1.567e+01 | 1.471e+01 | 1.204e+01 | 1.004e+01 |
| Pd-107  | 5.685e+00 | 5.526e+00 | 4.843e+00 | 2.896e+00 | 1.368e+00 |
| I-129   | 2.852e+00 | 3.026e+00 | 4.667e+00 | 9.629e+00 | 1.404e+01 |
| Cs-135  | 3.578e+00 | 3.285e+00 | 3.318e+00 | 3.652e+00 | 4.035e+00 |
| Sm-147  | 4.294e+01 | 3.882e+01 | 3.531e+01 | 3.080e+01 | 2.823e+01 |
| Sm-151  | 4.058e+02 | 4.414e+02 | 8.476e+02 | 2.107e+03 | 3.305e+03 |
| Eu-154  | 1.304e+02 | 1.333e+02 | 1.629e+02 | 2.421e+02 | 3.128e+02 |

Table 8: Microscopic fission cross section for some nuclides (barn) as a function of burnup (MWd/kgPu).

| Nuclide | 0         | 100       | 400       | 600       | 800       |
|---------|-----------|-----------|-----------|-----------|-----------|
| Pu-238  | 2.106e+00 | 2.150e+00 | 2.601e+00 | 4.040e+00 | 5.448e+00 |
| Pu-239  | 1.009e+02 | 1.158e+02 | 2.339e+02 | 5.702e+02 | 8.290e+02 |
| Pu-240  | 3.781e-01 | 3.737e-01 | 3.353e-01 | 2.102e-01 | 8.982e-02 |
| Pu-241  | 9.805e+01 | 1.090e+02 | 2.064e+02 | 4.972e+02 | 7.415e+02 |
| Pu-242  | 2.385e-01 | 2.336e-01 | 1.979e-01 | 1.055e-01 | 3.354e-02 |
| Am-241  | 1.202e+00 | 1.291e+00 | 1.970e+00 | 3.803e+00 | 5.054e+00 |
| Am-242m | 4.584e+02 | 5.167e+02 | 1.063e+03 | 2.716e+03 | 4.161e+03 |
| Am-243  | 2.398e-01 | 2.340e-01 | 2.008e-01 | 1.174e-01 | 5.092e-02 |
| Cm-242  | 7.693e-01 | 7.944e-01 | 1.042e+00 | 1.800e+00 | 2.467e+00 |
| Cm-243  | 1.049e+02 | 1.064e+02 | 1.226e+02 | 1.694e+02 | 2.098e+02 |



|              |                           |                                                              |                  |
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