The purpose of this study is to analyze the temperature effect on the infinite multiplication factor of light water moderated UO₂ lattices KRITZ: 2-1 and KRITZ: 2-13, and UO₂-PuO₂ lattice KRITZ: 2-19 of the Sweden KRITZ reactor. To quantify the contribution of each component of the infinite multiplication factor to the temperature coefficient, calculations were performed for the three configurations of KRITZ benchmark at two temperatures: room temperature 20°C and an elevated temperature 245°C, using MCNPX which is a continuous energy Monte Carlo reference code for the calculations of neutron transport. Nuclear data needed for this work were processed by means of the NJOY99 system and the most recent libraries JENDL-4, JENDL-3.3, JEFF-3.1, ENDF/B-VII, and ENDF/B-VII.1. The performed studies on the temperature coefficient have shown an agreement between our calculations and those obtained from the final report published by the OECD in 2005 (NEA, 2005).

**INTRODUCTION**

During the reactor operation, numerous parameters such as temperature, pressure, power level, and cooler flow are continuously monitored and controlled to ensure safe and stable operation of the reactor. The specific effects of changes in these parameters vary greatly depending upon reactor design. One of the most significant effects during reactor operation is the temperature coefficient effect on the reactivity. The temperature coefficient which is the relative change of a physical property with respect to changes in temperature is considered as one of the most important physical quantities used to assess the inherent safety of a reactor. Temperature variation in a reactor induces changes in the microscopic reaction rates and in the moderator density and consequently, in the infinite multiplication factor. This results in the addition of either positive or negative reactivity and hence changes in reactor power. The temperature dependence of the infinite multiplication factor is considerably important in connection with the transient behavior of a reactor and this fact has associated nuclear criticality safety issues and must therefore be investigated since it has a large influence on the estimation of operational reactivity balance. In this research, the effect of temperature on the infinite multiplication factor has been analyzed in order to ascertain the polarity, magnitude and effects of fuel and moderator temperatures on its physical components for the safe operation of the “KRITZ experiments” including a series of light-water-moderated lattices with uranium rods, and mixed-oxide rods.

**Description of the reactor KRITZ**

The KRITZ reactor operated at Studsvik, Sweden, during the first half of the 1970s. Each core comprised a lattice of light water moderated pins on a square pitch, surrounded by a light water reflector. The core was controlled to criticality using a combination of water height and dissolved boron. The experiments subject to this analysis were performed at nominal temperatures of 20°C and 245°C. Three lattices were studied: experiment 2:1, comprising 1.86% enrichment UO₂ pins on a 1.485 cm pitch; experiment 2:13, comprising 1.86% enrichment UO₂ pins on a 1.635 cm pitch; and experiment 2:19, consisting of MOX rods containing 1.5% PuO₂ on a 1.8 cm pitch. Axial buckling measurements at both hot and cold conditions and a core specification are available from the final report of reference (NEA, 2005).

**Description of experimental configurations**

The vertical and horizontal cross-sections of the reactor KRITZ are shown schematically in Fig. 1 and Fig. 2, respectively (NEA, 2005).
Tables 1 and 2 give the main parameters of the three configurations and rods data respectively (NEA, 2005).

**MATERIALS AND METHODS**

**The Pin Cell Model:** In our analysis of infinite multiplication factor, the adopted KRITZ reactor pin cell model was treated as a single fuel rod immersed in light water with total reflection to simulate an infinite medium (Fig. 3). Analysis based on the pin cell gives an idea on the importance of different components contributing to the reactivity temperature coefficient RTC and is very useful in determining sources of discrepancy between different codes and different nuclear data libraries.

**MCNPX code:** MCNP is a general-purpose Monte Carlo N-Particle transport code. It can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems. The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by surfaces.

Pointwise cross section data are handled. For neutron, all reactions, given in a particular cross-section evaluation (such as ENDF/B-VII), are taken into account. The recent version MCNPX (version 2.7.0) is provided with a visual Editor which permits to handle input file creation, particles track visualization, geometry and tallies plots.

**The NJOY99 code:** The NJOY nuclear data processing system is a modular computer code, developed in the Los Alamos National laboratory of the U.S. since 1974. Used for converting evaluated nuclear data in ENDF format into libraries useful for application in both deterministic and Monte Carlo computational codes (MacFarlane and Muir, 1994).

**Theoretical consideration:**

For the maintenance of a self-sustaining chain reaction, it is necessary that each neutron produced in fission initiates another fission. The minimum requirement is that each nucleus undergoing fission must produce on the average, at least one neutron that will cause the fission of another nucleus. This condition is conveniently expressed in terms of the infinite multiplication factor. We have used, instead of four, five factors to describe the infinite multiplication factor $k_{\infty}$ in order to account for the (n,2n) reactions (Erradi et al., 2003; Alain Santamarina et al., 2004). Our five factors formula is the following:

$$k_{\infty} = \chi \cdot \varepsilon \cdot p \cdot f \cdot \eta$$  \hspace{1cm} (1)

Where, $\chi$ is the factor corresponding to the neutron amplification related to (n,2n) reaction, $\varepsilon$ is the fast fission factor, $p$ is the resonance escape probability, $f$ is the thermal utilization factor and $\eta$ is the thermal fission factor.

To better understand the important role and impact of each of the five factors on neutron multiplication, we examine each of them more quantitatively in terms of neutron flux, reaction rates and cross sections in thermal (T), intermediate (I), and fast (F) energy ranges.

**Fast fission factor**

$\varepsilon$ is the ratio of total number of fission neutrons produced to the number of thermal fission neutrons (Elmer E.Lewis, 2008). We have:

$$\varepsilon = \frac{\int f \cdot \sum_1^f \phi(E) \cdot \sigma_{n}(E) \cdot \varepsilon \cdot f \cdot \eta}{\int \phi(E) \cdot \sigma_{n}(E) \cdot \varepsilon \cdot f \cdot \eta}$$  \hspace{1cm} (2)

The subscript $f$ represents fuel.
The resonance escapes probability

\[ p = \frac{V_f \sum_a(E)\sigma_f(E)\rho(E)dE + V_m \sum_a(E)\sigma_a(E)\rho(E)dE}{V_f \sum_a(E)\sigma_f(E)\rho(E)dE + V_m \sum_a(E)\sigma_a(E)\rho(E)dE} \]  

(3)

Where \( V_f, V_m \) are the volumes of fuel and moderator respectively, \( \sum_a \) and \( \sum_f \) are the macroscopic absorptions cross section of the moderator and fuel respectively.

The thermal utilization factor

\[ f = \frac{V_f \sum_a(E)\sigma_f(E)\rho(E)dE}{V_f \sum_a(E)\sigma_f(E)\rho(E)dE + V_m \sum_a(E)\sigma_a(E)\rho(E)dE} \]  

(4)

Where the subscripts \( f, m, c \) denote fuel, moderator and cladding respectively.

Thermal fission factor

\[ \eta = \frac{f C_f}{f C_f + (1-f) C_m} \]  

(5)

The different components of \( p, f, \) and \( \eta \) are deduced from MCNP calculation.

The reactivity temperature coefficient \( \alpha_T \) which is defined as the change in reactivity with respect to temperature is expressed as (Erradi et al., 2003; Alhassan et al., 2010, 2011):

\[ \alpha_T = \frac{d \rho}{dT} = \frac{d}{dT} \left( \frac{n}{K_{eff}} \right) = \frac{1}{K_{eff}} \frac{dK_{eff}}{dT} \]  

(6)

Where, reactivity \( \rho \) defining the fractional departure of a system from criticality (Alhassan et al., 2010, 2011), and \( K_{eff} \) is the effective multiplication factor.

From the basic relationship between \( K_{eff}, K_x \) and \( P_{NL} \) the non-leakage probability, we obtain from Eq.(4) (Erradi et al., 2003; Alhassan et al., 2011):

\[ \alpha_T = \frac{1}{K_{eff}} \frac{dK_{eff}}{dT} = \frac{1}{K_x} \frac{dK_x}{dT} + \frac{1}{P_{NL}} \frac{dP_{NL}}{dT} \]  

(7)

Equation (5) can be written as:

\[ \alpha_T = \alpha_T^c + \alpha_T^L \]  

(8)

Where, the first term is the temperature coefficient of the infinite multiplication factor and the second term represents the
leakage temperature effect. By using the five factors formula, 
\[ \alpha_{K_e} = \frac{1}{K_e} \frac{dK_e}{dt} = \frac{1}{K_e} \frac{df}{dt} + \frac{1}{K_e} \frac{d\sigma_f}{dt} + \frac{1}{K_e} \frac{d\sigma_c}{dt} + \frac{1}{K_e} \frac{d\sigma_d}{dt} + \frac{1}{K_e} \frac{d\eta}{dt} \]  

(9)

The effect of temperature on each factor could be quantified by calculating

\[ \frac{1}{f^2} \frac{df}{dt} = \frac{1}{f^2} \frac{\Delta f}{\Delta t} = \frac{1}{f(20^\circC) - f(245^\circC)} (\frac{f(245^\circC)}{245^\circC} - \frac{f(20^\circC)}{20^\circC}) \]  

(10)

To analyze the temperature effect on five factors, the variation of material densities with temperature was taken into account and all the corresponding cross sections were processed at 20°C and 245°C.

RESULTS AND DISCUSSION

Validation of KRITZ Monte Carlo modeling

The validation of our MCNP models for the three experiments KRITZ: 2-1, KRITZ: 2-13 and KRITZ: 2-19 is carried through the reproduction of the infinite multiplication factor at two temperatures 20°C and 245°C without boron concentration for different nuclear data libraries and compared to the results presented in reference (NEA, 2005). The participants in this benchmark have provided 11 solutions for the infinite multiplication factor by calculation only, thus we compare our results with their average, our MCNPX calculations are shown in table 3. Calculation-Reference difference is computed in terms of C-R relative values.

We note that most of the results obtained by almost libraries overestimate the values of \( k_e \) presented in reference (NEA, 2005) for the three configurations and two temperatures, a few results underestimate the reference values in high temperature for MCNPX simulations. However the differences between MCNPX simulation results and those of reference (NEA, 2005) are less than 1% and become smaller for simulations carried at high temperature.

The best results are obtained by JEFF-3.1 for KRITZ: 2-19 at both room and elevated temperature. For KRITZ: 2-1 at room temperature JENDL-3.3 gives the best agreement; however at elevated temperature all the neutron cross section evaluations allow to reproduce correctly the values given in reference (NEA, 2005), except JENDL-3.3 and JEFF-3.1 that largely underestimate the \( K_e \) values. For KRITZ: 2-13 the best results are obtained at 20°C by JENDL-3.3, and at 245°C by the three ENDF/B7, ENDF/B7.1 and JENDL-4 evaluations.

Validation of the five factor formula of \( K_e \)

The previous calculations show that our MCNPX models of KRITZ experiments reproduce well the reference value of \( K_e \). After this validation, we propose to quantify each factor in the formula of \( K_e \). The integral results obtained from the five factors formula are compared to those obtained directly from MCNPX simulations.

MCNP allows a direct calculation of the infinite multiplication factor, thing that allows us to make a validation of the five factors formula. According to Tables 4, 5 and 6 we see that all the results of calculated infinite multiplication factor by the five factors formula are in good agreement with those obtained directly from the simulation for all geometries and all libraries at the two temperatures of interest.

The contribution of each of the five factors to the temperature coefficient of \( K_e \)

The temperature dependence of \( K_e \) has a significant influence on the estimation of operational reactivity balance. In this work, we have quantified the temperature effect on \( K_e \) using the infinite multiplication factor values calculated directly by MCNP at two temperatures, 20°C and 245°C (using \( \alpha_{K_e} = \frac{1}{K_e} \frac{dK_e}{dt} \)), and compared them to those deduced from the Monte Carlo computing of the five factors

\[ \left( \alpha_{K_e} = \frac{1}{K_e} \frac{df}{dt} + \frac{1}{K_e} \frac{d\sigma_f}{dt} + \frac{1}{K_e} \frac{d\sigma_c}{dt} + \frac{1}{K_e} \frac{d\sigma_d}{dt} + \frac{1}{K_e} \frac{d\eta}{dt} \right) \]

Results are compared to the published values of \( K_e \) available in reference (NEA, 2005).

According to the results of reference (NEA, 2005), for the temperature range 20°C to 245°C, the temperature coefficients related to the infinite multiplication factor are -13.3 pcm/°C, -6.99 pcm/°C, 5.28 pcm/°C for KRITZ: 2-1, KRITZ: 2-13 and KRITZ: 2-19 respectively. We note in general a good agreement between these values and our results \( \alpha_{K_e} \) calculated by the \( K_e \) values got directly from the MCNP simulation.

From the tables above, it can be observed that the fast fission factor increases with temperature increase and its contribution to the temperature coefficient of the infinite multiplication factor was positive for the three fuels but more significant for the UO\(_2\) fuels; this can be attributed to the water density effect; since an increase in moderator temperature reduces the number of neutron collisions per unit volume and hence leads to an increase in the fast to thermal ratio (Alhassan et al., 2010). In UO\(_2\) fuels with higher amount of U\(^{238}\) is fissioned by some of the fast neutrons and thereby making available more neutrons in the reactor core.

With increasing temperature the absorption resonances broaden thereby increasing the absorption of neutron so the resonance escape probability decrease and contributes negatively in the temperature coefficient of the infinite multiplication factor; this is due to Doppler broadening (Alhassan et al., 2011).

The positive contribution of the temperature coefficient of the thermal utilization factor which is related to the water density effect; an increase in moderator temperature reduces the capture in the moderator (Erradi et al., 2003). The contribution of \( \alpha_{\sigma_d} \) is more significant in KRITZ: 2-19 than KRITZ: 2-13 and KRITZ: 2-1 relatively to the temperature effect resonance escape probability that influence the neutrons portion that pass to the thermal region.

As we can observe the temperature coefficient of the thermal fission factor was negative and it is more significant in KRITZ: 2-19 than KRITZ: 2-1 and KRITZ: 2-13. This temperature effect is mainly due to the spectral shift effect which is more
the standard deviation is given in pcm.

Table 3. Comparison of $K_{\infty}$ values obtained directly by MCNP and reference ones*

<table>
<thead>
<tr>
<th>Nuclear data library</th>
<th>Réf $K_{\infty}$</th>
<th>ENDF/B7.1</th>
<th>ENDF/B7</th>
<th>JENDL-4</th>
<th>JENDL-3.3</th>
<th>JEFF-3.1</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>20°C</td>
<td>245°C</td>
<td>20°C</td>
<td>245°C</td>
<td>20°C</td>
</tr>
<tr>
<td></td>
<td></td>
<td>T</td>
<td>z</td>
<td>e</td>
<td>p</td>
<td>f</td>
</tr>
<tr>
<td></td>
<td></td>
<td>20°C</td>
<td>245°C</td>
<td>20°C</td>
<td>245°C</td>
<td>20°C</td>
</tr>
<tr>
<td></td>
<td></td>
<td>20°C</td>
<td>245°C</td>
<td>20°C</td>
<td>245°C</td>
<td>20°C</td>
</tr>
</tbody>
</table>

*: the standard deviation is given in pcm.

Table 4. Monte Carlo calculation of $K_{\infty}$ from five factors formula for KRITZ: 2-1

<table>
<thead>
<tr>
<th>Nuclear data library</th>
<th>Réf $K_{\infty}$</th>
<th>ENDF/B7.1</th>
<th>ENDF/B7</th>
<th>JENDL-4</th>
<th>JENDL-3.3</th>
<th>JEFF-3.1</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>20°C</td>
<td>245°C</td>
<td>20°C</td>
<td>245°C</td>
<td>20°C</td>
</tr>
<tr>
<td></td>
<td></td>
<td>T</td>
<td>z</td>
<td>e</td>
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<td></td>
<td></td>
<td>20°C</td>
<td>245°C</td>
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<td>245°C</td>
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<tr>
<td></td>
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<td>20°C</td>
<td>245°C</td>
<td>20°C</td>
<td>245°C</td>
<td>20°C</td>
</tr>
</tbody>
</table>

Table 5. Monte Carlo calculation of $K_{\infty}$ from five factors formula for KRITZ: 2-13

<table>
<thead>
<tr>
<th>Nuclear data library</th>
<th>Réf $K_{\infty}$</th>
<th>ENDF/B7.1</th>
<th>ENDF/B7</th>
<th>JENDL-4</th>
<th>JENDL-3.3</th>
<th>JEFF-3.1</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>20°C</td>
<td>245°C</td>
<td>20°C</td>
<td>245°C</td>
<td>20°C</td>
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<td>T</td>
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<td>p</td>
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<tr>
<td></td>
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<td>20°C</td>
<td>245°C</td>
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<td>245°C</td>
<td>20°C</td>
<td>245°C</td>
<td>20°C</td>
</tr>
</tbody>
</table>

*KRITZ: 2-13*
<table>
<thead>
<tr>
<th>Nuclear data library</th>
<th>ENDF/B7.1</th>
<th>ENDF/B7</th>
<th>JENDL-3.3</th>
<th>JENDL-4</th>
<th>JEFF-3.1</th>
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</thead>
<tbody>
<tr>
<td>( \alpha )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( T ) 20°C</td>
<td>1.00114</td>
<td>1.00129</td>
<td>1.00114</td>
<td>1.00095</td>
<td>1.00108</td>
</tr>
<tr>
<td>( Z )</td>
<td>±0.0032</td>
<td>±0.004</td>
<td>±0.005</td>
<td>±0.008</td>
<td>±0.009</td>
</tr>
<tr>
<td>( \beta )</td>
<td>±0.0032</td>
<td>±0.004</td>
<td>±0.005</td>
<td>±0.008</td>
<td>±0.009</td>
</tr>
<tr>
<td>( \epsilon )</td>
<td>±22</td>
<td>±22</td>
<td>±22</td>
<td>±22</td>
<td>±22</td>
</tr>
<tr>
<td>( \eta )</td>
<td>±50</td>
<td>±50</td>
<td>±50</td>
<td>±50</td>
<td>±50</td>
</tr>
</tbody>
</table>

### Table 6. Monte Carlo calculation of \( K_a \) from five factors formula for KRITZ: 2-19

<table>
<thead>
<tr>
<th>( K_a ) (MCNP EBC)*</th>
<th>1.28885</th>
<th>1.30421</th>
<th>1.28744</th>
<th>1.30472</th>
<th>1.28679</th>
<th>1.30414</th>
<th>1.28858</th>
<th>1.30823</th>
<th>1.28090</th>
<th>1.30061</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha )</td>
<td>±22</td>
<td>±22</td>
<td>±22</td>
<td>±22</td>
<td>±22</td>
<td></td>
<td>±22</td>
<td>±22</td>
<td>±22</td>
<td>±22</td>
</tr>
<tr>
<td>( \beta )</td>
<td>±50</td>
<td>±50</td>
<td>±50</td>
<td>±50</td>
<td>±50</td>
<td>±50</td>
<td>±50</td>
<td>±50</td>
<td>±50</td>
<td>±50</td>
</tr>
</tbody>
</table>

*: five factors formula

### Table 7. Contribution of each component of \( K_a \) to the temperature coefficient for KRITZ: 2-1

| \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) |
|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) |

| \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) |
|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) | \( \alpha \) |

**Ref**
dominant for KRITZ: 2-19 because the thermal fission factor is enrichment dependent. For the temperature range 20°C to 245°C, the temperature coefficients obtained by the sum of the effects is higher than those got from the $K_\infty$ values given directly from the MCNP simulation, this due to the compensation of the effects in the second relation.

In KRITZ: 2-1 and KRITZ: 2-13 all libraries give similar results, while for KRITZ: 2-19 the best results are given by JENDL-4 and JEFF-3.1.

**Conclusion**

This paper presented the results of cell calculations by Monte Carlo method implemented in MCNPX code for the three KRITZ 2 experiments. $K_\infty$ values and the temperature coefficient are investigated by using different nuclear data based on JEFF-3.1, ENDF/B-VII.1, ENDF/B-VII, and JENDL-4, at 20°C and 245°C. The calculated $K_\infty$ values with the above evaluations show a good agreement with the values in the reference which allows the validation of our MCNPX modeling and the qualification of our nuclear data. From the RTC calculations we can note that KRITZ: 2-1 and KRITZ: 2-13 are most safe than KRITZ: 2-19 because their RTC are negative. The results we obtained are excellent, which leads us to extend our study to a $k_{eff}$ calculated taking into account the leakage probability, and, making a calculation of KRITZ, TCA and Creole benchmarks assemblies. Our study will be completed by a sensitivity study of each parameter.

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MCNPX™ USER’S MANUAL”, Version 2.7.0, LA-CP-11-00438, Manuel/ Los Alamos National Laboratory, April 2011

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