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ABSTRACT

A comparative study was carried out of nuclear data calculated by the LEOPARD and WIMSD-4 codes for a typical PWR cell. Few-group macroscopic cross-sections, spectral indices, burnup and power distribution were analysed.

1. INTRODUCTION

In a nuclear reactor project, core studies account for a large part of the total cost since one of the objectives is to extract the highest amount of energy with the use of the smallest possible quantity of fuel. Table 1 gives the fuel cycle costs relating to 1985 taken from Ref. [1]. The Angra-1 reactor (PWR) used [2] approximately 50 tonnes of uranium for its initial fuel load. On the basis of the data in Table 1, and applying the conversion factors for enriched uranium and natural uranium [3], we find that the costs amount to about $59 million. If all costs relating to reprocessing ($\approx$ 60% of the initial value) are computed, we shall have values of the order of $94 million. Therefore, economic considerations justify the search for new core calculation alternatives with a view to optimization of resources. For this purpose, all the factors involved in the calculation process should be as correct as possible. It is necessary to have complete mastery of the technology involved and also to utilize practical results obtained with computer codes of other more developed centres in order to ensure the use of the best calculation sequence and the best available nuclear data. In the case of Brazil, for reasons which we shall not go into here, confidence in the data used in the calculations comes from the fact that codes used in other countries were utilized. Although such codes have approximations in their theory, they give good results if they are used with due care. A typical example is the LEOPARD code [4] which is used to obtain few-group cross-sections or the HAMMER code [5] which, in its original version, does not calculate burnup but contains few approximations in its theory.

Since we have no cell calculation code developed by our own efforts in the country, we do not have a standard for calculation to which we can refer in evaluating a new code. We encountered this problem [8] when we tested the WIMSD-4 code for generation of few-group cross-sections. This code, widely accepted in Europe, contains very few approximations in terms of transport theory and has a flexibility for calculation which is not found in the codes mentioned above. Thus, the purpose of the present work is to make a comparative study of few-group cross-sections for a typical fuel cell in thermal reactors. All these comparisons were carried out in relation to LEOPARD.

We first describe the cell under consideration and the cross-sections obtained. In the case of this cell, some burnup steps were carried out and this gave the quantity of ^{235}U and ^{238}U lost and the quantity of ^{239}Pu produced. A "boron curve" was obtained, in qualitative terms only, for this cell by comparing the quantity of boron needed to maintain its criticality over a specific time interval. We obtained, also in qualitative terms, the power distribution for a fuel element consisting of an arrangement of 16 x 16 positions without the presence of control rods.

2. A TYPICAL CELL

In order to study a typical PWR cell, we chose a cell of the Angra-1 reactor with 2.1 wt% enrichment, which is described in Refs [4, 5]. It essentially consists of a central region containing UO_2 with an outer radius of 0.4095 cm, a cladding region, including the gap, with an outer radius of 0.4750 cm and a moderator region containing water, which included the structural materials. Figure 1 gives the diagram of the cell. The concentrations of materials present can be obtained from Appendices A and B and from the input data for LEOPARD and WIMSD-4.

3. COMPARISON OF RESULTS

Using the data on this cell, we constructed the input archives for LEOPARD and WIMSD-4 in accordance with Appendices A and B. Thanks to its flexibility WIMSD-4 allows the user to select the theory to be applied to solve the transport equation (integral or differential), together with the number of energy groups to be used in the calculations. The sensitivity of the results to the different options is studied in Refs [6, 7]. In this specific case, we used an integral solution by the collision probability method and eight energy groups, which were collapsed into two, by conventional methodology [10] so that we could compare the results, as shown in Table 2.

In this table, we note that the few-group cross-sections generated by the two codes exhibit some differences and have the integral parameters given in Table 3.

This table shows that the greatest discrepancies in the results occur in the spectral indices which include ^{238}U. This indicates that in WIMSD-4 the cross-section data for ^{238}U, especially capture, need to be revised, as is corroborated by the conclusions in Ref. [9].

As to burnup, we considered the loss of ^{235}U and ^{238}U and the production of ^{239}Pu in six burnup steps, as shown in Table 4. In these calculations, the same boron concentration was maintained in the two codes.

It will be seen that the per cent differences in the ^{235}U concentrations given by the two codes increase at each step of the burnup process, although they are less than 1%.

In LEOPARD the depletion of ^{235}U is faster, underestimating the lifetime of the fuel in the reactor. This assumption was further verified and the results are given in Fig. 2. As to ^{238}U, it is to be noted that its concentration is the same for both codes but the production of ^{239}Pu is

slightly higher in WIMSD-4. Although this behaviour may appear contrary to the earlier observations, it should be remembered that the decay chains are different in the two codes.

In order to test the lifetime of the fuel elements, we devised a strategy to obtain a "boron curve". It was obviously not a conventional procedure but served our purpose of comparison, at least in qualitative terms. The strategy consisted in seeking, by trial and error, the boron concentration to be inserted or withdrawn from the cell so that K_X was always the same at each burnup step. Assuredly, a moment will come when there will be no more boron in the cell to be withdrawn in order to compensate for the burnup of fuel and to maintain the initial K_X. This will then be the "lifetime" of this fuel. The procedure was applied to the two codes and the results are shown in Fig. 2.

In this curve we give the results obtained by LEOPARD using two data libraries, one of which was the original library [4] based on ENDF/B-II and the other [11] based on ENDF/B-IV. We do so because of the results and conclusions contained in report [12] which showed that LEOPARD used with a data library based on ENDF/B-IV yielded good results in the calculation of power distribution but that the results related to the boron curve did not satisfy the needs. The use of a data library based on ENDF/B-II gave a better boron curve but a worse power distribution. Thus, in Fig. 2 we see that the results given by WIMSD-4 are closer to those obtained by LEOPARD with the original library (ENDF/B-II). Earlier results [2] using LEOPARD with the original library also showed that the boron curve was underestimated in relation to the results supplied by the manufacturer. Thus, Fig. 2 leads us

to believe that WIMSD-4 should reproduce the manufacturer's results with sufficient accuracy.

In Appendix C we give the per cent errors in power distribution obtained by WIMSD-4 and LEOPARD (with ENDF/B-IV) for a fuel element comprising 16 x 16 positions, of which 21 do not contain fuel rods but only moderator. The 2DB code [13] was used for these calculations and account was taken of the reflecting boundary condition on the four sides of the element. These errors were calculated in relation to the values given in [7], which contain a spatial correction to take into account the position of the fuel element in the reactor, but this correction was not applied to our calculations. Since the element under study was situated very close to the centre of the reactor, it was assumed to have very little influence on the results. Therefore, with these considerations, the results displayed very few discrepancies, the greatest ones being around the positions containing only moderator. In this table, the first figure in each position is the value of power obtained from the reference, while the second represents the per cent error, calculated by LEOPARD, in relation to the reference value, and the third that calculated by WIMSD-4.

4. CONCLUSIONS

From the results of these comparisons we can conclude that, although WIMSD-4 shows differences in few-group cross-sections, in comparison with LEOPARD, it gives good results in terms of overall behaviour such as the "boron curve" or power distribution. Thus, even though better results were demonstrated only qualitatively, the use of WIMSD-4 can save resources and, consequently, there is need for full studies in terms of core calculation. In carrying out these new studies it is of vital importance that institutions

which will actually use these results should participate since we could then not only benefit from persons with great experience in these types of calculation but also verify the calculations experimentally and perhaps define a new highly flexible standard like WIMSD-4.

5. REFERENCES

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Table 1. Representative data on fuel cycle cost for 1985 ($)

Unit cost of ore	107.8	$/kg U_3O_8
Unit cost of conversion	12.6	$/kg UF_6
Unit cost of enrichment	103.0	$/kg/SWU
Unit cost of fabrication	152.0	$/kg fresh U
Unit cost of transport	22.8	$/kg fresh U
Unit cost of storage	3.3	$/kg burnt U
Unit cost of reprocessing	230.0	$/kg burnt U
Unit cost of waste	81.0	$/kg burnt U
Unit cost of plutonium	37.3	$/kg fissile Pu

Table 2. Cell-homogenized macroscopic cross-sections

Groups	Group 1				Group 2		
Const.	D	Σ_a	$\nu\Sigma_f$	$\Sigma^s_{1,2}$	D	Σ'_a	$\nu\Sigma_f$
LEOPARD	1,3199E+00	1,0167E-02	6,0063E-03	1,4974E-02	4,0091E-01	8,2844E-02	1,1187E-01
WIMSD-4	1,6942E+00	9,8049E-03	6,0034E-03	1,2679E-02	5,1012E-01	7,9991E-02	1,0740E-01

Table 3. Integral parameters calculated for the cell

Int. parameter	k_∞	ρ^{28}	δ^{25}	δ^{28}	C^*
LEOPARD	1,04270	3,2480	0,1813	0,0877	0,8522
WIMSD-4	1,05055	3,1796	0,1815	0,0951	0,8507

ρ^{28} = Ratio between epithermal and thermal captures in ^{238}U;
δ^{25} = Ratio between epithermal and thermal fissions in ^{235}U;
δ^{28} = Ratio between fissions in ^{238}U and those in ^{235}U;
C^* = Ratio between captures in ^{238}U and fissions in ^{235}U.

Table 4. Concentrations of ^{235}U, ^{238}U and ^{239}Pu in different burnup steps

	Step 1 - 0,0 MWD/T			Step 2 - 100,0 MWD/T		
	U-235	U-238	Pu-239	U-235	U-238	Pu-239
LEOPARD	4,8345E-04	2,2254E-02		4,8066E-04	2,2252E-02	1,9119E-06
WIMSD-4	4,8345E-04	2,2254E-02		4,8070E-04	2,2252E-02	1,9212E-06
	Step 3 - 200,0 MWD/T			Step 4 - 2.200,0 MWD/T		
	U-235	U-238	Pu-239	U-235	U-238	Pu-239
LEOPARD	4,7790E-04	2,2250E-02	3,7861E-06	4,2615E-04	2,2207E-02	3,4834E-05
WIMSD-4	4,7798E-04	2,2250E-02	3,7709E-06	4,2766E-04	2,2207E-02	3,5014E-05
	Step 5 - 4.200,0 MWD/T			Step 6 - 6.200,0 MWD/T		
	U-235	U-238	Pu-239	U-235	U-238	Pu-239
LEOPARD	3,8233E-04	2,2165E-02	5,7499E-05	3,4406E-04	2,2122E-02	7,4753E-05
WIMSD-4	3,8482E-04	2,2165E-02	5,7651E-05	3,4725E-04	2,2122E-02	7,4783E-05

Atoms/barn.cm units.

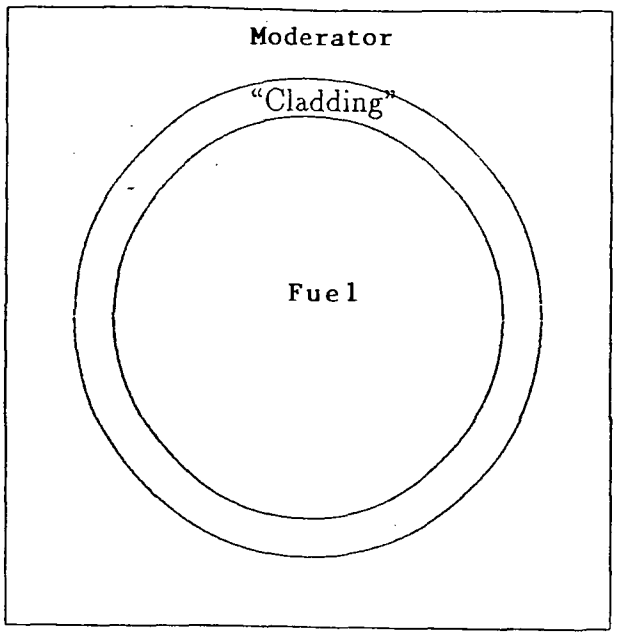

Fig. 1. Diagram of a typical fuel cell.

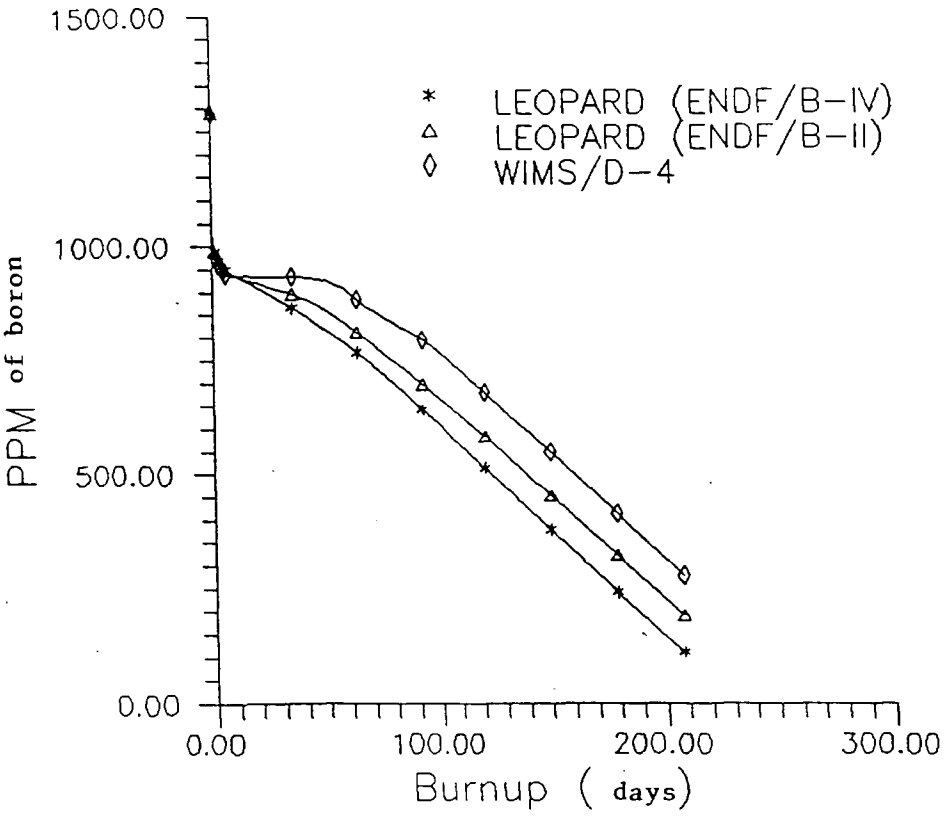

Fig. 2. Boron curve for the fuel cell.

APPENDIX A

Input data for LEOPARD

```
*****************************************************************
****                                                         ****
****                      leopard                            ****
****                                                         ****
****                                                         ****
*****************************************************************
ANGRA I - 2.1 W/O FUEL PIN - BOL TO XE-EQUILIBRIUM
  1  3  0  0  0  1  1  0  0  0  0  0  0  1  0  0  0  0
          99          1.0
          19      1.0E-10
          21      1.0E-10
          22      1.0E-10
          23      1.0E-10
          24      1.0E-10
           3                  -0.41783
         100                              0.992420
           6                              0.001903
           7                              0.003855
          11                              0.001822
         777          0.0
          18       -0.021
          29         1290
         777          0.0
      612.77      778.888     352.805        307.8   0.0004588
    0.409575      0.47498      1.2319
      2250.0                     0.95
         1.0      108.698        0.0                       0.84
           1      0.24000     1290.0
           2      34.1880     1290.0
           3     34.42800      990.0
           4       34.428      970.0
           5       34.548      955.0
           6      690.948      950.0
           7      690.948      865.0
           8      690.378      765.0
           9      691.518      640.0
          10      690.948      510.0
          11      690.948      375.0
          12      690.948      240.0
          13      690.948      110.0
         777          0.0        0.0
```

APPENDIX B

Input data for WIMSD-4

```
*****************************************************************
****                                                         ****
****                        wimsd/4                          ****
****                                                         ****
****                                                         ****
*****************************************************************
35000
CELL 6
SEQUENCE 2
NGROUP 8 2
NMESH 9
NREGION 3
NMAT 3 1
NREACT 2
PREOUT
INITIATE
* ANGRA I - 2.1 W/O FUEL PIN - BOL TO XE-EQUILIBRIUM
MATERIAL 1 -1 1052.04 1 235.4 4.8345E-04 2238.4 2.2254E-02$
         16 4.5475E-02 3239.1 1.1E-10
MATERIAL 2 -1 625.96 2 91 3.8990E-02
MATERIAL 3 -1 580.95 3 2001 4.7146E-02 16 2.3573E-02  $
       1010 1.0028E-05 56 1.6137E-04 58 3.5196E-04 52 1.4977E-04
ANNULUS 1 0.4123 1
ANNULUS 2 0.4759 2
ANNULUS 3 0.6986 3
REGULAR 1
FEWGROUPS 5 14 27 33 40 45 55 69
MESH 3 2 4
POWERC 1 34.73 0.01 1
SUPPRESS 0 0 1 1 1 1 0 1 1 1 1 0 0 1 1
BEGINC
SIGPUNCH
BUCKLING 1.0E-10 4.588E-04
LEAKAGE 5
THERMAL 2
DIFFUSION 2 7 1
BEEONE 1
DNB 1 0.0 0.0 4.5475E-02 0.0
DNB 2 0.0 0.0 0.0 0.0
DNB 3 4.7146-02 0.0 2.3573-02 0.0
PARTITION 45 69
PRINTC 1 1 0 1
REACTIONS 235.4 1052.04 2238.4 1052.04
BEGINC
```

```
POWERC 1 34.73 1.4345 2
BEGINC
BEGINC
MATERIAL 3 -1 580.95 3 1010 7.6182E-06
POWERC 1 34.73 1.4395 2
BEGINC
BEGINC
MATERIAL 3 -1 580.95 3 1010 7.0351E-06
POWERC 1 34.73 28.7895 2
BEGINC
BEGINC
MATERIAL 3 -1 580.95 3 1010 6.0634E-06
POWERC 1 34.73 28.7895 2
BEGINC
BEGINC
MATERIAL 3 -1 580.95 3 1010 4.7808E-06
POWERC 1 34.73 28.7895 2
BEGINC
POWERC 0. 0.
BEGINC
BEGINC
```

APPENDIX C

Per cent errors in power distribution

1,11	1,10	1,10	1,11	1,12	1,13	1,12	1,12	1,12	1,13	1,14	1,13	1,12	1,11	1,11	1,10
-8,2	-4,6	-2,1	-1,2	-0,5	-0,5	0,8	-0,4	-1,0	-2,5	-3,6	-3,4	-3,8	-4,5	-6,9	-5,9
-2,5	0,9	2,7	2,6	2,3	1,6	3,4	2,6	2,1	0,3	-1,3	-0,4	0,0	0,2	-1,5	-0,1
1,10	1,10	1,11	1,12	1,14	1,17	1,14	1,14	1,14	1,15	1,18	1,15	1,13	1,11	1,10	1,09
-4,6	-2,7	-1,2	1,6	1,3	0,3	2,6	0,2	-1,4	-1,6	-3,1	-1,7	-1,0	-1,2	-2,6	-2,2
0,8	2,2	2,5	3,6	2,0	-1,1	3,0	1,5	0,4	-0,6	-4,1	-0,8	1,1	2,4	2,2	3,3
1,10	1,11	1,13	1,18	1,20	0,00	1,19	1,18	1,18	1,19	0,00	1,20	1,19	1,14	1,10	1,09
-2,2	-1,3	1,0	0,0	0,2	0,0	3,5	3,0	-2,8	-0,8	0,0	-0,6	-2,4	-1,2	1,2	0,4
2,6	2,4	2,4	-2,1	-3,0	0,0	0,0	0,3	-3,4	-2,9	0,0	-3,6	-4,4	0,1	4,9	5,1
1,11	1,12	1,18	0,00	1,21	1,22	1,19	0,00	1,23	1,19	1,22	1,22	0,00	1,18	1,12	1,09
-1,6	1,2	-0,4	0,0	2,6	2,1	7,2	0,0	-6,8	-1,2	-0,7	-0,3	0,0	0,1	1,6	3,6
2,3	3,4	-2,3	0,0	-1,8	-2,6	2,8	0,0	-9,5	-2,8	-4,5	-4,4	0,0	-2,0	3,7	7,4
1,12	1,14	1,20	1,21	1,20	1,21	1,18	1,18	1,18	1,18	1,22	1,20	1,22	1,20	1,14	1,10
-1,2	0,4	-0,8	1,5	1,2	2,9	4,4	5,3	0,0	1,1	-0,3	1,7	0,7	0,4	1,4	4,2
1,9	1,4	-3,7	-2,5	-1,8	-1,3	1,8	2,2	-1,2	-0,4	-4,3	-1,4	-3,7	-3,0	2,0	7,1
1,13	1,17	0,00	1,22	1,21	0,00	1,19	1,16	1,16	1,19	0,00	1,22	1,22	0,00	1,17	1,11
-1,5	-1,1	0,0	-1,2	1,0	0,0	2,8	4,0	4,2	3,4	0,0	1,4	2,5	0,0	0,4	4,3
0,9	-2,0	0,0	-4,9	-2,7	0,0	-0,2	3,0	3,1	0,2	0,0	-3,0	-2,4	0,0	-1,0	6,4
1,12	1,14	1,19	1,19	1,18	1,19	1,16	1,16	1,16	1,16	1,20	1,18	1,20	1,20	1,14	1,11
-0,4	0,4	-1,2	-1,9	-0,2	0,9	2,5	2,7	8,5	6,9	2,5	5,2	5,3	1,4	2,6	3,2
2,5	1,5	-3,2	-3,3	-1,3	-1,6	1,9	2,1	5,8	4,9	-1,1	2,4	0,8	-2,1	3,1	5,8
1,12	1,14	1,18	1,23	1,18	1,16	1,16	1,19	0,00	1,16	1,17	1,19	0,00	1,18	1,13	1,10
-1,2	-1,6	-3,2	-7,6	-1,6	0,6	-0,4	-1,1	0,0	8,7	3,4	3,6	0,0	3,0	2,5	4,3
2,0	0,3	-3,7	-10,0	-2,3	0,7	-0,1	-2,9	0,0	6,0	1,8	0,4	0,0	0,3	3,8	7,4
1,12	1,14	1,18	0,00	1,18	1,16	1,16	1,19	1,19	1,16	1,17	1,19	1,24	1,18	1,13	1,10
-0,6	0,0	2,6	0,0	4,0	1,6	-1,7	-6,8	-1,1	2,4	0,4	-2,7	-9,0	-2,8	0,9	3,6
2,5	1,4	0,0	0,0	1,3	1,3	-0,9	-6,6	-2,9	1,9	-0,2	-3,7	-11,6	-3,4	2,7	6,9
1,13	1,15	1,19	1,19	1,18	1,19	1,16	1,16	1,16	1,16	1,17	1,19	1,20	1,20	1,14	1,11
-1,7	0,1	3,2	6,7	3,6	1,4	0,6	-2,0	-0,2	2,5	6,0	-1,8	-3,7	-3,1	0,6	2,0
0,9	0,6	-0,2	2,4	1,2	-1,2	0,6	-1,1	0,1	1,9	3,3	-3,1	-5,2	-5,2	1,6	5,0
1,14	1,18	0,00	1,22	1,22	0,00	1,20	1,17	1,17	1,17	0,00	1,22	1,23	0,00	1,17	1,12
-2,9	-2,0	0,0	1,8	0,3	0,0	-2,0	-2,0	-0,2	6,7	0,0	-0,9	-3,1	0,0	-1,0	0,9
-0,7	-3,3	0,0	-2,8	-3,8	0,0	-4,2	-1,9	-0,6	3,8	0,0	-4,7	-6,9	0,0	-2,0	3,3
1,13	1,15	1,20	1,22	1,20	1,22	1,18	1,19	1,19	1,19	1,22	1,21	1,23	1,21	1,14	1,11
-2,9	-1,1	0,1	0,2	1,0	-1,4	-0,5	-3,9	1,9	1,7	0,6	-0,9	-2,7	-2,9	0,5	1,2
0,0	-0,3	-3,1	-4,0	-1,9	-5,0	-1,6	-4,6	-0,8	-0,8	-3,6	-3,9	-6,7	-5,8	1,5	4,2
1,12	1,13	1,19	0,00	1,22	1,22	1,20	1,24	0,00	1,20	1,23	1,23	0,00	1,14	1,13	1,10
-3,6	-0,8	-2,3	0,0	-0,8	-1,3	-4,1	-9,7	0,0	4,6	-0,2	-1,8	0,0	8,8	-1,1	0,8
0,2	1,3	-4,3	0,0	-4,7	-5,0	-5,5	-12,1	0,0	0,3	-4,8	-6,0	0,0	6,8	1,1	4,7
1,11	1,11	1,14	1,18	1,20	0,00	1,20	1,18	1,18	1,20	0,00	1,21	1,19	1,14	1,11	1,09
-4,4	-1,2	-1,4	-0,4	-0,9	0,0	-3,4	-3,2	2,6	1,0	0,0	-2,0	-2,2	-1,3	-1,3	0,2
0,3	2,5	0,1	-2,3	-3,8	0,0	-5,4	-3,7	0,0	-2,3	0,0	-5,2	-4,2	0,1	2,4	5,0
1,11	1,10	1,10	1,12	1,14	1,17	1,14	1,13	1,13	1,14	1,17	1,14	1,13	1,11	1,09	1,09
-6,9	-2,7	1,0	1,1	0,4	-1,1	0,4	0,7	2,3	2,4	0,3	1,2	-0,8	-1,2	-0,3	-2,3
-1,5	2,2	4,8	3,4	1,4	-2,1	1,5	2,6	3,7	2,9	-1,1	2,0	1,3	2,5	4,6	3,2
1,10	1,09	1,09	1,09	1,10	1,11	1,11	1,10	1,10	1,11	1,12	1,11	1,10	1,09	1,09	1,09
-5,9	-2,3	0,1	3,1	3,5	3,2	1,9	3,5	4,1	3,0	1,8	1,7	1,1	0,3	-2,2	-3,6
-0,1	3,2	5,0	7,1	6,6	5,6	4,9	6,8	7,2	5,7	3,9	4,7	4,9	5,1	3,3	2,3

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