

## Alicia Mullins

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**From:** David Pickett  
**Sent:** Tuesday, April 09, 2002 11:18 AM  
**To:** cgrossman@cnwra.swri.edu  
**Subject:** RE: RE: Gold Sim  
**Attachments:** kd kc calc.xls

**Follow Up Flag:** Follow up  
**Flag Status:** Flagged

Chris,

I re-did the calculation. See the new "Pickett" worksheet in the attached file. I get a log-normal mean of  $1e04$ , and std dev of 10. So they're using the Pu distribution discussed on p 386, as opposed to the Am value they said they were going to use (mean  $1e05$ , Table 6-90, p 387). So we've got a flag to raise here. I suspect that, since writing the report, they decided to go with separate numbers for Am(+ Th?) and Pu (+ Pa?).

Let me know if you agree with my interpretation after you've had a look at the TSPA Model document sections I discussed below.

David

-----Original Message-----

**From:** cgrossman@cnwra.swri.edu [mailto:cgrossman@cnwra.swri.edu]  
**Sent:** Tuesday, April 09, 2002 8:50 AM  
**To:** dpickett@cnwra.swri.edu  
**Subject:** Re: RE: Gold Sim

David-

That should be it then. I plugged the data set into Excel and plotted a histogram of the log (Data/0.03). The log of the distribution looks normal. The mean comes out close to DOE's value. Not sure about the SD though. The file is attached. I'll send a short write up of what I have done shortly. That way you can send Dave a compiled write up of what we have accomplished for his summary.

Chris

----- Original Message -----

**From:** David Pickett <dpickett@cnwra.swri.edu>  
**Date:** Monday, April 8, 2002 4:38 pm  
**Subject:** RE: Gold Sim

> It looks like the TSPA-SR Model document may have sufficient  
> information.  
> Look at pages 386-387. It says Kc is calculated by multiplying Kd for  
> colloids by the colloid concentration. The latter number is taken to  
> be 0.03 mg/L (p 386). The colloid Kd is sampled. It says on p 386 that  
> the americium value is used, although they mention a Pu value. The Kd  
> distribution used (Table 6-90, p 387) is log-normal with  $1e05$  ml/g  
> geometric mean and 10 std deviation. It looks like what happens is,  
> offline of GoldSim, the distribution is sampled 100 times and each  
> value is multiplied by  
> 0.03 mg/L  
> (presumably with units handled correctly), producing the lookup table.

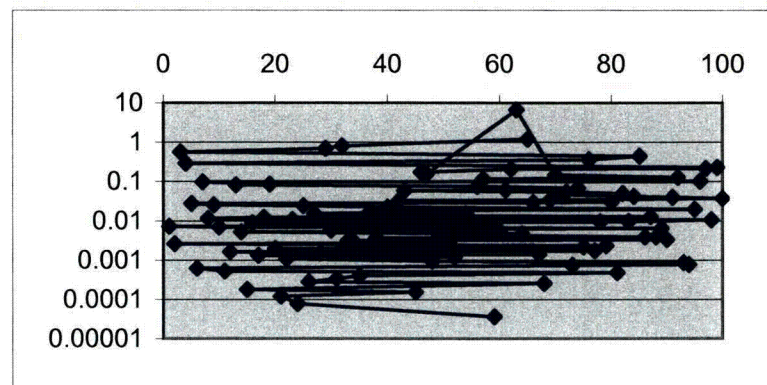
> I guess this is done separately for Pu+Pa and Am+Th (see Table 6- 91).  
> But if the text is to be believed, the same Kd distribution is used in  
> each case.  
>  
> It looks like a way to check this would be to take the data from the  
> table, divide each value by 0.03 mg/L (treat units so that results  
> will be in ml/g), and plot the results. Is it consistent with the  
> given distribution for Kd?  
>  
> We can look at this together, if you like.  
>  
> David  
>  
> -----Original Message-----  
> From: cgrossman@cnwra.swri.edu [mailto:cgrossman@cnwra.swri.edu]  
> Sent: Monday, April 08, 2002 2:42 PM  
> To: dpickett@cnwra.swri.edu  
> Subject: Gold Sim  
>  
>  
> David-  
>  
> I am having trouble locating the 1-D Table input 'KC\_PU\_GW\_COLLOID' in  
> the AMRs I have searched several and find no mention of it..  
> Could you  
> look up in the GoldSim file to see what the parameter is a function of  
> and what it affects? Also, is there any description associated with  
> this parameter?  
>  
> Its location is  
> TSPA\_Model\Saturated\_Zone\_Transport\SZ\_Input\_Parameters  
>

| SZ_Index | KC_PU_... | KC/0.03     | -Ln(KC/0.03) |
|----------|-----------|-------------|--------------|
| 65       | 0.035386  | 1.179533333 | 0.165119     |
| 32       | 0.023992  | 0.799733333 | 0.223477     |
| 29       | 0.020579  | 0.685966667 | 0.376926     |
| 3        | 0.016832  | 0.561066667 | 0.577916     |
| 85       | 0.013092  | 0.4364      | 0.829196     |
| 76       | 0.010652  | 0.355066667 | 1.03545      |
| 4        | 0.008751  | 0.2917      | 1.232029     |
| 99       | 0.006745  | 0.224846667 | 1.492337     |
| 97       | 0.00636   | 0.21199     | 1.551216     |
| 62       | 0.006178  | 0.205936667 | 1.580187     |
| 46       | 0.005112  | 0.170393333 | 1.769646     |
| 47       | 0.004623  | 0.154083333 | 1.870262     |
| 63       | 0.19713   | 6.571       | 1.882666     |
| 70       | 0.004424  | 0.14746     | 1.914198     |
| 92       | 0.003811  | 0.127033333 | 2.063306     |
| 57       | 0.003475  | 0.11582     | 2.155718     |
| 96       | 0.003039  | 0.101286667 | 2.2898       |
| 7        | 0.002927  | 0.097563333 | 2.327254     |
| 19       | 0.00256   | 0.085336667 | 2.461151     |
| 13       | 0.002444  | 0.081463333 | 2.507602     |
| 56       | 0.002243  | 0.07478     | 2.593205     |
| 74       | 0.002032  | 0.06772     | 2.692374     |
| 61       | 0.001811  | 0.060373333 | 2.807208     |
| 43       | 0.001752  | 0.05839     | 2.840611     |
| 72       | 0.001634  | 0.05445     | 2.910472     |
| 82       | 0.001485  | 0.049513333 | 3.005513     |
| 71       | 0.001398  | 0.046583333 | 3.066512     |
| 84       | 0.001253  | 0.04177     | 3.175577     |
| 91       | 0.001187  | 0.039573333 | 3.2296       |
| 100      | 0.001106  | 0.03686     | 3.300628     |
| 69       | 0.001021  | 0.034023333 | 3.380709     |
| 42       | 0.000966  | 0.032194333 | 3.435965     |
| 80       | 0.000907  | 0.030249    | 3.498292     |
| 66       | 0.000869  | 0.028962333 | 3.541759     |
| 5        | 0.000825  | 0.027499333 | 3.593594     |
| 9        | 0.000762  | 0.025383667 | 3.673649     |

Mean = 4.612897  
Std Dev = 2.243778

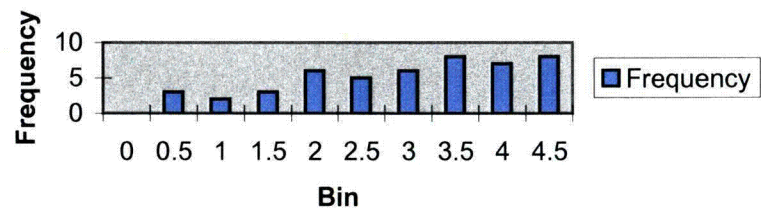
| 0    | Bin | Frequency |
|------|-----|-----------|
| 0.5  | 0   | 0         |
| 1    | 0.5 | 3         |
| 1.5  | 1   | 2         |
| 2    | 1.5 | 3         |
| 2.5  | 2   | 6         |
| 3    | 2.5 | 5         |
| 3.5  | 3   | 6         |
| 4    | 3.5 | 8         |
| 4.5  | 4   | 7         |
| 5    | 4.5 | 8         |
| 5.5  | 5   | 9         |
| 6    | 5.5 | 8         |
| 6.5  | 6   | 8         |
| 7    | 6.5 | 6         |
| 7.5  | 7   | 6         |
| 8    | 7.5 | 4         |
| 8.5  | 8   | 4         |
| 9    | 8.5 | 2         |
| 9.5  | 9   | 2         |
| 10   | 9.5 | 2         |
|      | 10  | 0         |
| More |     | 1         |

|    |          |             |          |
|----|----------|-------------|----------|
| 25 | 0.000717 | 0.023912667 | 3.733347 |
| 40 | 0.000665 | 0.02218     | 3.808564 |
| 95 | 0.000586 | 0.019530333 | 3.935786 |
| 41 | 0.000554 | 0.018466    | 3.991824 |
| 37 | 0.000534 | 0.017807667 | 4.028126 |
| 39 | 0.000489 | 0.016304    | 4.116345 |
| 27 | 0.000456 | 0.015204667 | 4.186153 |
| 54 | 0.000447 | 0.014914    | 4.205455 |
| 44 | 0.000409 | 0.013641333 | 4.294651 |
| 87 | 0.00038  | 0.012673667 | 4.368229 |
| 18 | 0.000365 | 0.012158    | 4.409768 |
| 8  | 0.000348 | 0.011605667 | 4.456262 |
| 23 | 0.000321 | 0.010698333 | 4.537667 |
| 98 | 0.000314 | 0.010479667 | 4.558318 |
| 83 | 0.000289 | 0.009623667 | 4.64353  |
| 78 | 0.00028  | 0.009321333 | 4.67545  |
| 16 | 0.000264 | 0.008816333 | 4.731149 |
| 53 | 0.00024  | 0.008013667 | 4.826607 |
| 58 | 0.000234 | 0.007808    | 4.852606 |
| 1  | 0.000217 | 0.007226333 | 4.930024 |
| 10 | 0.000209 | 0.006952667 | 4.96863  |
| 89 | 0.000193 | 0.006436333 | 5.045796 |
| 55 | 0.000187 | 0.006224667 | 5.079235 |
| 30 | 0.000171 | 0.005711667 | 5.165244 |
| 60 | 0.000167 | 0.005571667 | 5.190061 |
| 14 | 0.000156 | 0.005188333 | 5.261343 |
| 49 | 0.000143 | 0.004766333 | 5.346178 |
| 64 | 0.000139 | 0.004621667 | 5.377    |
| 50 | 0.000131 | 0.004376    | 5.43162  |
| 86 | 0.000117 | 0.003894667 | 5.548147 |
| 88 | 0.000116 | 0.003869333 | 5.554673 |
| 38 | 0.000109 | 0.003625667 | 5.619717 |
| 90 | 9.87E-05 | 0.00329     | 5.716868 |
| 33 | 9.50E-05 | 0.003166667 | 5.755076 |
| 34 | 8.90E-05 | 0.002966667 | 5.820316 |
| 51 | 8.20E-05 | 0.002733333 | 5.902233 |
| 2  | 7.74E-05 | 0.00258     | 5.959966 |

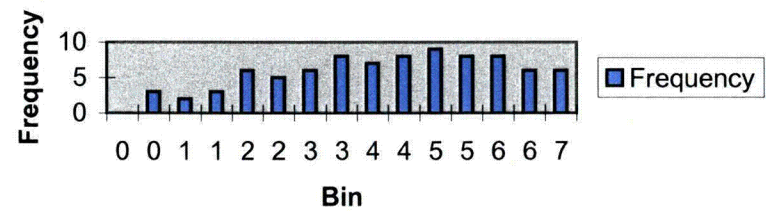


|    |          |             |          |
|----|----------|-------------|----------|
| 79 | 7.00E-05 | 0.002333333 | 6.060457 |
| 75 | 6.45E-05 | 0.00215     | 6.142287 |
| 20 | 5.90E-05 | 0.001966667 | 6.231415 |
| 36 | 5.83E-05 | 0.001943333 | 6.243351 |
| 77 | 5.12E-05 | 0.001706667 | 6.373213 |
| 12 | 4.83E-05 | 0.00161     | 6.431521 |
| 28 | 4.39E-05 | 0.001463333 | 6.527038 |
| 67 | 4.16E-05 | 0.001386667 | 6.580852 |
| 17 | 3.94E-05 | 0.001313333 | 6.635187 |
| 52 | 3.61E-05 | 0.001203333 | 6.72266  |
| 22 | 3.20E-05 | 0.001066667 | 6.843217 |
| 48 | 2.81E-05 | 0.000936667 | 6.973183 |
| 93 | 2.54E-05 | 0.000846667 | 7.074203 |
| 94 | 2.28E-05 | 0.00076     | 7.182192 |
| 73 | 2.21E-05 | 0.000736667 | 7.213375 |
| 6  | 1.85E-05 | 0.000616667 | 7.391182 |
| 11 | 1.57E-05 | 0.000523333 | 7.555292 |
| 81 | 1.42E-05 | 0.000473333 | 7.655711 |
| 35 | 1.21E-05 | 0.000403333 | 7.815747 |
| 31 | 1.02E-05 | 0.00034     | 7.986565 |
| 26 | 8.42E-06 | 0.000280667 | 8.178343 |
| 68 | 7.72E-06 | 0.000257333 | 8.265138 |
| 15 | 5.34E-06 | 0.000178    | 8.633727 |
| 45 | 4.58E-06 | 0.000152667 | 8.787254 |
| 21 | 3.64E-06 | 0.000121333 | 9.016969 |
| 24 | 2.35E-06 | 7.83333E-05 | 9.454537 |
| 59 | 1.08E-06 | 0.000036    | 10.23199 |

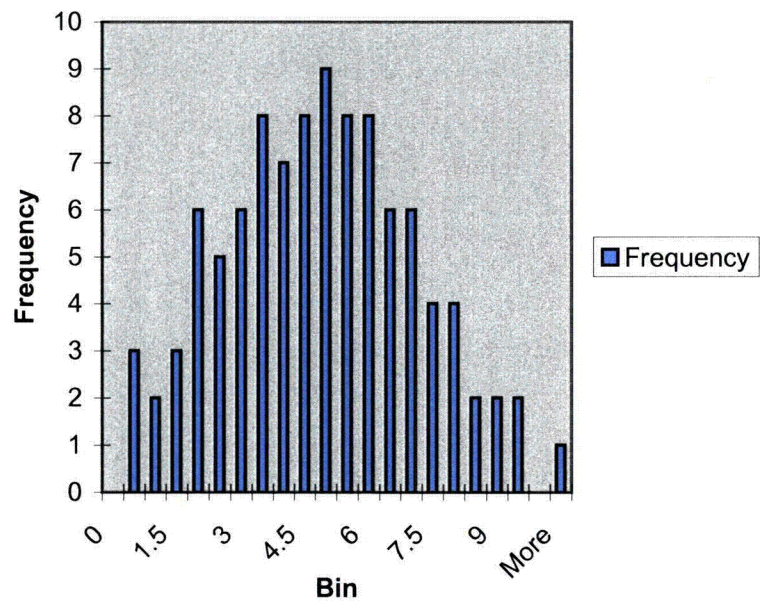
**Histogram**



**Histogram**



**Histogram**



| SZ_Index | KC_PU_...  | calc Kd, L/g | calc Kd, ml/g | log         |         |             | Bin  | Frequency |
|----------|------------|--------------|---------------|-------------|---------|-------------|------|-----------|
| 65       | 0.035386   | 1179.533333  | 1179533.333   | 6.071710218 | average | 4.01443113  | 0    | 0         |
| 32       | 0.023992   | 799.7333333  | 799733.3333   | 5.902945198 | std dev | 1.010564135 | 0.25 | 0         |
| 29       | 0.020579   | 685.9666667  | 685966.6667   | 5.836303012 |         |             | 0.5  | 0         |
| 3        | 0.016832   | 561.0666667  | 561066.6667   | 5.749014468 |         |             | 0.75 | 0         |
| 85       | 0.013092   | 436.4        | 436400        | 5.639884742 |         |             | 1    | 0         |
| 76       | 0.010652   | 355.0666667  | 355066.6667   | 5.550309903 |         |             | 1.25 | 0         |
| 4        | 0.008751   | 291.7        | 291700        | 5.464936429 |         |             | 1.5  | 0         |
| 99       | 0.0067454  | 224.8466667  | 224846.6667   | 5.351886454 |         |             | 1.75 | 1         |
| 97       | 0.0063597  | 211.99       | 211990        | 5.326315375 |         |             | 2    | 1         |
| 62       | 0.0061781  | 205.9366667  | 205936.6667   | 5.313733679 |         |             | 2.25 | 2         |
| 46       | 0.0051118  | 170.3933333  | 170393.3333   | 5.231452599 |         |             | 2.5  | 3         |
| 47       | 0.0046225  | 154.0833333  | 154083.3333   | 5.187755665 |         |             | 2.75 | 4         |
| 63       | 0.19713    | 6571         | 6571000       | 6.817631467 |         |             | 3    | 5         |
| 70       | 0.0044238  | 147.46       | 147460        | 5.16867423  |         |             | 3.25 | 7         |
| 92       | 0.003811   | 127.0333333  | 127033.3333   | 5.103917694 |         |             | 3.5  | 7         |
| 57       | 0.0034746  | 115.82       | 115820        | 5.063783561 |         |             | 3.75 | 10        |
| 96       | 0.0030386  | 101.2866667  | 101286.6667   | 5.005552279 |         |             | 4    | 10        |
| 7        | 0.0029269  | 97.56333333  | 97563.33333   | 4.98928663  |         |             | 4.25 | 9         |
| 19       | 0.0025601  | 85.33666667  | 85336.66667   | 4.931135675 |         |             | 4.5  | 9         |
| 13       | 0.0024439  | 81.46333333  | 81463.33333   | 4.910962177 |         |             | 4.75 | 8         |
| 56       | 0.0022434  | 74.78        | 74780         | 4.873785461 |         |             | 5    | 7         |
| 74       | 0.0020316  | 67.72        | 67720         | 4.830716949 |         |             | 5.25 | 6         |
| 61       | 0.0018112  | 60.37333333  | 60373.33333   | 4.780845155 |         |             | 5.5  | 4         |
| 43       | 0.0017517  | 58.39        | 58390         | 4.766338475 |         |             | 5.75 | 3         |
| 72       | 0.0016335  | 54.45        | 54450         | 4.735997884 |         |             | 6    | 2         |
| 82       | 0.0014854  | 49.51333333  | 49513.33333   | 4.694722165 |         |             | 6.25 | 1         |
| 71       | 0.0013975  | 46.58333333  | 46583.33333   | 4.668230562 |         |             | 6.5  | 0         |
| 84       | 0.0012531  | 41.77        | 41770         | 4.620864475 |         |             | 6.75 | 0         |
| 91       | 0.0011872  | 39.57333333  | 39573.33333   | 4.597402633 |         |             | 7    | 1         |
| 100      | 0.0011058  | 36.86        | 36860         | 4.566555331 |         |             | 7.25 | 0         |
| 69       | 0.0010207  | 34.02333333  | 34023.33333   | 4.53177686  |         |             | 7.5  | 0         |
| 42       | 0.00096583 | 32.19433333  | 32194.33333   | 4.507779436 |         |             | 7.75 | 0         |
| 80       | 0.00090747 | 30.249       | 30249         | 4.480711022 |         |             | 8    | 0         |
| 66       | 0.00086887 | 28.96233333  | 28962.33333   | 4.461833548 |         |             | 8.25 | 0         |
| 5        | 0.00082498 | 27.49933333  | 27499.33333   | 4.439322165 |         |             | 8.5  | 0         |
| 9        | 0.00076151 | 25.38366667  | 25383.66667   | 4.404554356 |         |             | 8.75 | 0         |

|    |            |             |             |             |
|----|------------|-------------|-------------|-------------|
| 25 | 0.00071738 | 23.91266667 | 23912.66667 | 4.37862801  |
| 40 | 0.0006654  | 22.18       | 22180       | 4.345961542 |
| 95 | 0.00058591 | 19.53033333 | 19530.33333 | 4.290709656 |
| 41 | 0.00055398 | 18.466      | 18466       | 4.266372831 |
| 37 | 0.00053423 | 17.80766667 | 17807.66667 | 4.250607018 |
| 39 | 0.00048912 | 16.304      | 16304       | 4.212294167 |
| 27 | 0.00045614 | 15.20466667 | 15204.66667 | 4.181976904 |
| 54 | 0.00044742 | 14.914      | 14914       | 4.173594139 |
| 44 | 0.00040924 | 13.64133333 | 13641.33333 | 4.134856821 |
| 87 | 0.00038021 | 12.67366667 | 12673.66667 | 4.10290228  |
| 18 | 0.00036474 | 12.158      | 12158       | 4.084862139 |
| 8  | 0.00034817 | 11.60566667 | 11605.66667 | 4.064670093 |
| 23 | 0.00032095 | 10.69833333 | 10698.33333 | 4.029316125 |
| 98 | 0.00031439 | 10.47966667 | 10479.66667 | 4.020347469 |
| 83 | 0.00028871 | 9.623666667 | 9623.666667 | 3.983340572 |
| 78 | 0.00027964 | 9.321333333 | 9321.333333 | 3.969478039 |
| 16 | 0.00026449 | 8.816333333 | 8816.333333 | 3.945288002 |
| 53 | 0.00024041 | 8.013666667 | 8013.666667 | 3.903831274 |
| 58 | 0.00023424 | 7.808       | 7808        | 3.892539805 |
| 1  | 0.00021679 | 7.226333333 | 7226.333333 | 3.858917991 |
| 10 | 0.00020858 | 6.952666667 | 6952.666667 | 3.842151408 |
| 89 | 0.00019309 | 6.436333333 | 6436.333333 | 3.808638528 |
| 55 | 0.00018674 | 6.224666667 | 6224.666667 | 3.7941161   |
| 30 | 0.00017135 | 5.711666667 | 5711.666667 | 3.756762854 |
| 60 | 0.00016715 | 5.571666667 | 5571.666667 | 3.745985126 |
| 14 | 0.00015565 | 5.188333333 | 5188.333333 | 3.71502787  |
| 49 | 0.00014299 | 4.766333333 | 4766.333333 | 3.678184411 |
| 64 | 0.00013865 | 4.621666667 | 4621.666667 | 3.664798619 |
| 50 | 0.00013128 | 4.376       | 4376        | 3.641077313 |
| 86 | 0.00011684 | 3.894666667 | 3894.666667 | 3.590470294 |
| 88 | 0.00011608 | 3.869333333 | 3869.333333 | 3.587636145 |
| 38 | 0.00010877 | 3.625666667 | 3625.666667 | 3.559387874 |
| 90 | 9.87E-05   | 3.29        | 3290        | 3.517195898 |
| 33 | 9.50E-05   | 3.166666667 | 3166.666667 | 3.500602351 |
| 34 | 8.90E-05   | 2.966666667 | 2966.666667 | 3.472268752 |
| 51 | 8.20E-05   | 2.733333333 | 2733.333333 | 3.436692598 |
| 2  | 7.74E-05   | 2.58        | 2580        | 3.411619706 |

|      |      |   |
|------|------|---|
| 9    | 9    | 0 |
| 9.25 | 9.25 | 0 |
| 9.5  | 9.5  | 0 |
| 9.75 | 9.75 | 0 |
| 10   | 10   | 0 |
| More |      | 0 |



|    |          |             |             |             |
|----|----------|-------------|-------------|-------------|
| 79 | 7.00E-05 | 2.333333333 | 2333.333333 | 3.367976785 |
| 75 | 6.45E-05 | 2.15        | 2150        | 3.33243846  |
| 20 | 5.90E-05 | 1.966666667 | 1966.666667 | 3.293730757 |
| 36 | 5.83E-05 | 1.943333333 | 1943.333333 | 3.2885473   |
| 77 | 5.12E-05 | 1.706666667 | 1706.666667 | 3.232148706 |
| 12 | 4.83E-05 | 1.61        | 1610        | 3.206825876 |
| 28 | 4.39E-05 | 1.463333333 | 1463.333333 | 3.165343266 |
| 67 | 4.16E-05 | 1.386666667 | 1386.666667 | 3.141972076 |
| 17 | 3.94E-05 | 1.313333333 | 1313.333333 | 3.118374967 |
| 52 | 3.61E-05 | 1.203333333 | 1203.333333 | 3.080385947 |
| 22 | 3.20E-05 | 1.066666667 | 1066.666667 | 3.028028724 |
| 48 | 2.81E-05 | 0.936666667 | 936.6666667 | 2.971585065 |
| 93 | 2.54E-05 | 0.846666667 | 846.6666667 | 2.927712462 |
| 94 | 2.28E-05 | 0.76        | 760         | 2.880813592 |
| 73 | 2.21E-05 | 0.736666667 | 736.6666667 | 2.867271019 |
| 6  | 1.85E-05 | 0.616666667 | 616.6666667 | 2.790050474 |
| 11 | 1.57E-05 | 0.523333333 | 523.3333333 | 2.718778398 |
| 81 | 1.42E-05 | 0.473333333 | 473.3333333 | 2.67516709  |
| 35 | 1.21E-05 | 0.403333333 | 403.3333333 | 2.605664116 |
| 31 | 1.02E-05 | 0.34        | 340         | 2.531478917 |
| 26 | 8.42E-06 | 0.280666667 | 280.6666667 | 2.448190837 |
| 68 | 7.72E-06 | 0.257333333 | 257.3333333 | 2.410496046 |
| 15 | 5.34E-06 | 0.178       | 178         | 2.250420002 |
| 45 | 4.58E-06 | 0.152666667 | 152.6666667 | 2.183744223 |
| 21 | 3.64E-06 | 0.121333333 | 121.3333333 | 2.083980129 |
| 24 | 2.35E-06 | 0.078333333 | 78.33333333 | 1.893946608 |
| 59 | 1.08E-06 | 0.036       | 36          | 1.556302501 |

