



HERA M&S Exercise Problem Description Report

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Changing the World's Energy Future

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September 2022

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ABSTRACT

The Nuclear Energy Agency (NEA) Framework for Irradiation Experiments (FIDES) program includes the High burnup Experiments for Reactivity initiated Accident (HERA) Joint Experimental Program (JEEP). The HERA project is focused on studying Light Water Reactor (LWR) fuel behavior during Reactivity Initiated Accident (RIA) conditions. The HERA experiment plan includes analytical integral experiments using test specimens tailored to investigate specific conditions of relevance as well as prototypic integral experiments focused on irradiated fuel from prototypic origin. Modeling & simulation (M&S) is a key component of any experiment program, and the HERA JEEP is coordinating a M&S exercise. The purpose of this document is to provide problem descriptions to support the HERA M&S exercise based on fuel performance modeling. The HERA M&S exercise is expected to evolve into multiple efforts in outyears. This document may be revised and expanded to incorporate those evolutions.

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1. INTRODUCTION

The Nuclear Energy Agency (NEA) Framework for Irradiation Experiments (FIDES) program includes the High burnup Experiments for Reactivity initiated Accident (HERA) Joint Experimental Program (JEEP). The HERA project is focused on studying Light Water Reactor (LWR) fuel behavior during Reactivity Initiated Accident (RIA) conditions [1]. The HERA experiment plan includes analytical integral experiments using test specimens tailored to investigate specific conditions of relevance as well as prototypic integral experiments focused on irradiated fuel from prototypic origin. Modeling & simulation (M&S) is a key component of any experiment program and, similar to the FIDES JEEP called P2M, the HERA JEEP is coordinating a M&S exercise.

The purpose of this document is to provide problem descriptions to support the HERA M&S exercise based on fuel performance modeling. Currently, the M&S scope is expected to be divided into Part I and Part II. This document currently addresses Part I only. This work has been devised to be strongly supportive of the HERA JEEP and in the context of completion of extensive RIA modeling benchmarks by the NEA Working Group for Fuel Safety over the past several years [2][3][4][5]. The HERA M&S exercise is expected to evolve into multiple efforts in outyears. This document may be revised and expanded to incorporate those evolutions.

1.1 Structure

The strategy developed for HERA naturally divides into two parts, expected to be executed serially during the remaining 2021-2024 project duration.

- Part I 2022-2023: Pre-test ‘blind’ predictions based on nominal parameters, intended to inform the experiment design and to provide unique perspective relative to past RIA modeling/experiment activities.
- Part II 2023-2024: Post-test evaluation for final data synthesis, preservation, and support to project conclusions.

Part I M&S will be the first activity to be performed with modeling case descriptions provided in this document.

1.2 Goals and Objectives

The HERA M&S for 2021-2024 is aligned with the goals of the JEEP, to study fuel behavior during RIA over its irradiation lifetime. The specific technical goal of the Part I exercise is to evaluate the effect of power pulse width on the behavior of hydrided zirconium cladding, which will indirectly provide evaluation of the overall experiment design. Depending on ultimate relative timelines, the results may impact final experiment design parameters.

In addition to technical objectives, the HERA M&S exercise is purposed to:

- Improve M&S and experiment integration;
- Facilitate community involvement in experiment design and interpretation;
- Facilitate community collaboration;
- Aid in ensuring program data meet fuel performance code needs.

2. MODELING RECOMMENDATIONS

For each code/participant, the default or user-preferred model options should be used unless otherwise specified in this document. The fuel relocation and oxidation models should be disabled. Each participant will document and/or provide a reference for modeling options used or options not available to their respective code (e.g. the cladding failure model, frictional/frictionless contact, cladding hydride models, or thermal hydraulic options).

3. PART I CASE DESCRIPTIONS

3.1 Part I Overview

The focus of the exercise simulations will be on Pellet-Cladding Mechanical Interaction (PCMI). Hydrided zirconium cladding is theorized to fail in RIA PCMI conditions under rapid loading, when cracks initiating in the brittle hydride rim propagate through the metallic substrate. Failure can be predicted if the stress intensity factor (K_I) (as a result of crack initiation in hydrides near the cladding outer diameter) is greater than some critical value (K_{IC}). The stress intensity factor is expressed in the following form:

$$K_I \propto \sigma_{11} \sqrt{\pi a} \quad (1)$$

where (a) is the crack length which can be assumed to be the depth of the hydride rim (in SRA cladding types) and σ_{11} is the normal (hoop) tensile stress field.

Thus, the vulnerability of a fuel rod to PCMI failure will depend on both the extent of the environmental degradation (depth of hydride rim) as well as the extent of the PCMI interaction. Cladding is more likely to survive transient conditions allowing time for temperature increase prior to experiencing a tensile load. The increase in temperature has two consequences. First the yield stress of zircaloy cladding decreases dramatically with increasing temperature. Therefore, at a given loading, the tensile stress field that develops in the cladding is much lower when the cladding temperature is higher, thus the stress intensity factor is also much lower for a given crack depth. The effect of longer pulses leading to higher cladding temperatures and thus lower cladding stresses is clearly seen in fuel performance models of RIA transients of different pulse widths. A simple BISON calculation on fresh fuel illustrates this phenomenon in Figure 1 below.

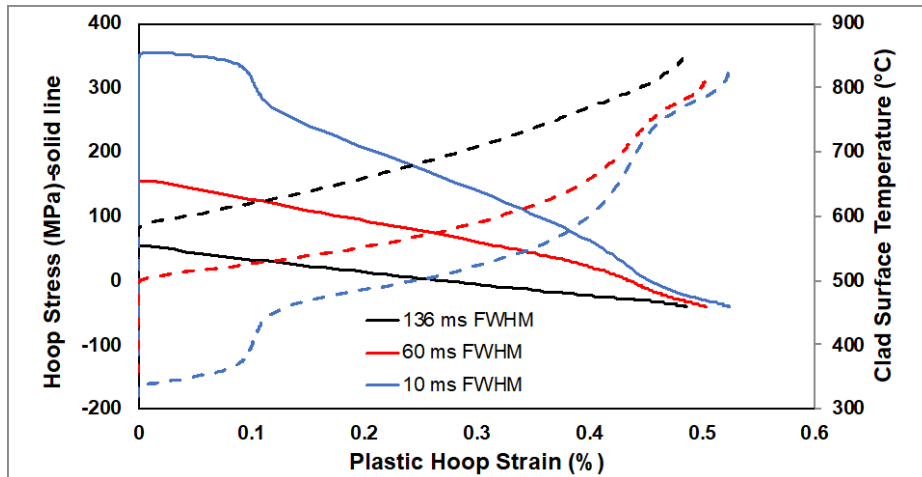


Figure 1. Cladding hoop stress during PCMI phase of RIA transients of varying pulse widths.

A second related consequence of the cladding heating rate being much faster than the loading rate (as is the case in longer transients) is that the cladding fracture toughness (critical stress intensity factor K_{IC}) begins to increase dramatically with temperature [6]. While precise determination of fracture toughness values for irradiated and hydrided zirconium alloy claddings are difficult to determine experimentally, numerous separate effects studies show at least qualitatively that the recovery of fracture toughness with increasing cladding temperature is rather dramatic [7][8].

The Part I M&S cases are based on two experiment systems from the Transient Reactor Test (TREAT) facility and the Nuclear Safety Research Reactor (NSRR) – with very similar overall boundary conditions. Each experiment uses a water-filled capsule holding a fuel specimen completely immersed in stagnant water. The main relevant distinctions between the two systems are fuel and cladding lengths and test capsule water and gas volumes. Both systems include a fresh fuel test specimen of very similar design and identical compositions. All cases are in water at room temperature and pressure conditions.

The Part I M&S case matrix is shown in Table 1. The matrix includes 14 sets of results based on 4 as-designed experiments in HERA noted by the bolded lines in the table. The primary difference between these four cases are the planned pulse width for each experiment noted in the table. Three important experiment parameters were selected as a simple sensitivity evaluation. The peak radial average enthalpy, cladding hydrogen content, and fuel outer radius (fuel-cladding gas gap width) each include two variations applied to only two pulse widths. The latter parameter variation was added later to the case matrix as Cases 13 and 14. While all cases are encouraged to be performed, the bolded lines represent priority cases to be performed by participants as a reduced study if required. This provides a minimum option for participants if resources are limited for whatever reason.

Table 1. HERA M&S Part I Case Matrix. The bolded lines represent priority cases to be performed by participants as a reduced study if required by an individual participant.

Case #	HERA Test ID	Pulse Width at FWHM (ms)	Peak Radial Average Enthalpy Increase (J/g)	Hydrogen Content/Rim t (ppm/ μ m)	Fuel Outer Radius (mm)
1	HERA-PreH-1,2	7.5	650	400/80	4.1605
2			650	200/40	4.1605
3			650	600/140	4.1605
4			550	400/80	4.1605
5			750	400/80	4.1605
13			650	400/80	4.1305
6	HERA-PreH-3,4	90	650	400/80	4.1605
7			650	200/40	4.1605
8			650	600/140	4.1605
9			550	400/80	4.1605
10			750	400/80	4.1605
14			650	400/80	4.1305
11	HERA-PreH-5,6	50	650	400/80	4.1605
12	HERA-PreH-5,6	300	650	400/80	4.1605

3.2 Specimen Description

The test specimen in all cases is based on a fresh 17x17 PWR type fuel design composed of Zry-4 cladding and UO₂ fuel. Basic specimen information is provided in the next section. The fuel system is designed to mimic certain aspects of irradiated fuel to generate Pellet-Cladding Mechanical Interaction (PCMI) behavior with cladding that is similarly mechanically degraded as some high burnup claddings. This approach is accomplished via artificially hydrogenating the cladding and specifying a small pellet-cladding gas gap.

The claddings are treated in a furnace to produce a hydride structure with similarity to prototypic hydride structures from LWRs. Figure 2 shows an example of the hydride structure produced on HERA test specimen claddings. The specific treatment employed produces a notable rim of higher

hydride concentration as seen in the figure. The nominal hydride concentration is 400 ppm with a rim thickness of approximately 80 microns. Negligible oxide is on the cladding surface.

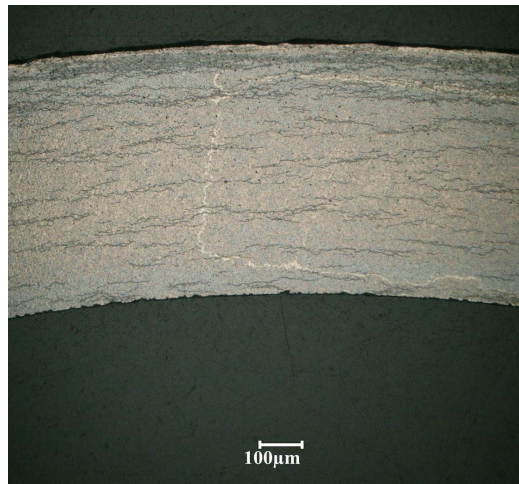


Figure 2. Metallography image showing example of hydride structure produced for HERA prehydrided tests corresponding to Part I modeling cases.

To induce Pellet-Cladding Mechanical interaction (PCMI), with similar magnitude to irradiated fuel that is effectively in contact with the cladding, the HERA experiments will use oversized fresh fuel pellets with a smaller than prototypic initial pellet-cladding gap. The specific geometry information is provided in the next section.

3.3 Primary Model Parameters

The specimen geometry is a fresh 17x17 PWR type fuel rod. Figure 3 provides a simple depiction of the specimen geometry for all cases. Table 2 provides a list of parameters needed for modeling inputs. The figure shows fuel in cladding with a fuel-cladding gap and plenum accounting for total specimen initial free volume. The test specimen is suspended in stagnant (pool) water at room temperature and pressure conditions. The total fuel mass corresponds to the dimensions provided in the table below. The fuel geometry should not include any pellet dishing or chamfers.

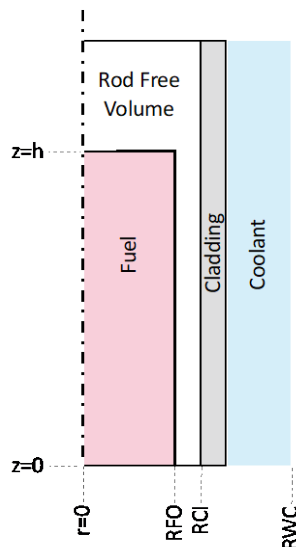


Figure 3. Schematic representation of HERA M&S geometry.

Table 2. List of specimen parameters for both TREAT and NSRR. Note the only differences are the fuel stack height and rod plenum volume.

Test Parameter	TREAT	NSRR
Fuel Composition	Fresh UO2	
Fuel Density (kg/m ³)	10475	
Cladding Type	Zry-4, stress-relief annealed (SRA)	
Hydride Composition	See Table 1	
Fuel Outer Radius (mm)	See Table 1	
Fuel Pellet Height (mm)	10.160	
# Fuel Pellets	10	12
Total Fuel Mass (g)	57.9	69.4
Cladding Inner Radius (mm)	4.1785	
Cladding Outer Radius (mm)	4.7500	
Plenum Pressure (MPa @ 20°C)	0.1	
Rod Free Volume (cc)	1.23	2.52
Bulk Water Temperature (°C)	20	
Capsule Pressure (MPa)	0.1	

All other parameters not specified (open porosity, fuel grain size, surface roughnesses, cladding properties, etc.) should be set by the performer using default values or best judgment in selection for fresh fuel in a pulse irradiation.

3.3.1 Other Capsule Parameters

For Part I modeling activities, the previous section is expected to suffice for modeling inputs. Thermal hydraulic models should be selected by individual users based on tools available that best fit the problem description. If participants are interested to model the thermal hydraulic performance of the capsule using a systems code, Figure 4 presents a schematic of a simplified representative geometry and basic hydraulic parameters with dimensions shown in Table 4.

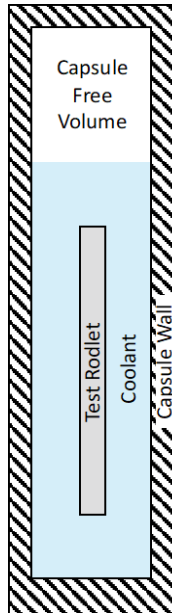


Figure 4. Schematic representation of the HERA experiment capsules.

Table 3. Basic hydraulic parameters corresponding with Figure 4. Note these parameters are not required for Part I exercise activities, though may be used as inputs to systems code calculations if desired.

Test Parameter	TREAT	NSRR
Water Outer Radius (mm)	25	120
Capsule Water Volume (cc)	280	6250
Capsule Argon Free Volume (cc)	500	2350

3.4 Specimen Input Power

For Part I activities, the specimen total power input is assumed to have to a pure Gaussian temporal profile starting from zero power. For all part I models, only the fuel specimen will generate energy (heat), all other component heating is assumed negligible for exercise purposes. The varied characteristics include the total energy and the pulse width defined as Full Width Half Maximum (FWHM). Table I provides a specification of target specimen radial average enthalpy and pulse widths for each case. Because enthalpy is also a calculated value, the specific energy inputs have been generated to provide approximately the targeted peak radial average fuel enthalpy in the case matrix. Figure 5 presents a comparison of power distributions for all pulse width variations. The power profiles are created from the Gaussian function defined below as

$$f(t) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2} \frac{(t - t_m)^2}{\sigma^2}\right) \quad \text{Equation 1}$$

where t_m is the time of peak power (chosen as 1.0 seconds). The pulse width of the power profile is adjusted as defined below

$$\sigma = \frac{FWHM}{2\sqrt{2 \ln(2)}} \quad \text{Equation 2}$$

and the magnitude is scaled as needed to target the peak radial average enthalpy.

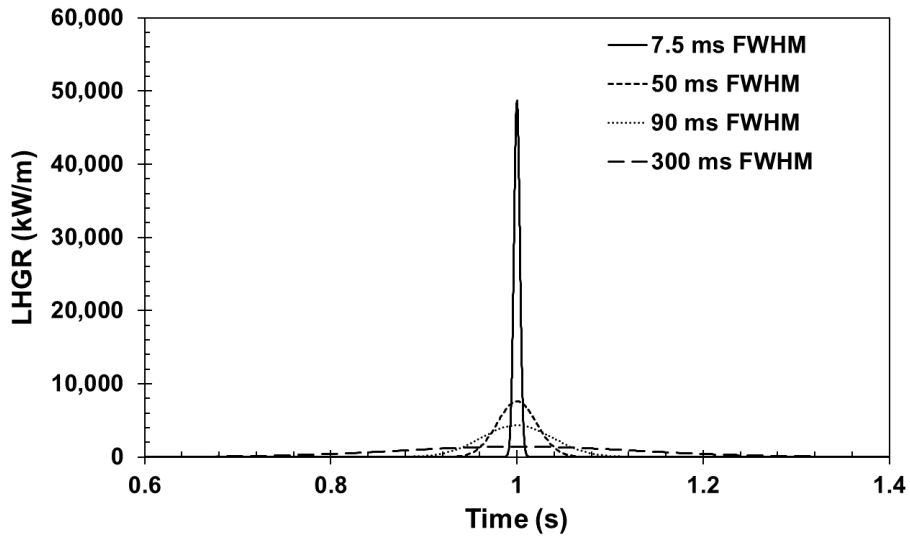


Figure 5. Representative power distributions for the range of FWHM pulse width in the M&S exercise based on equation 1.

The tabulated linear heat generation rates vs. time for each pulse width and enthalpy target are provided in supporting files. The axial and radial power profiles are assumed uniform for the Part I exercise.

3.5 Parameters to be calculated

3.5.1 List of parameters

The target output parameters to be calculated are defined in the following tables. Parameters are specified as primary or secondary to denote their priority for the exercise. Table 4 provides a list of requested output parameters for each case in Table 1.

Unless otherwise specified, each parameter should be reported as:

- a function of time with a final reported value at 200 seconds;
- at the axial mid height $z = h/2$.

Table 4. Requested output parameters. Primary outputs are bolded while secondary are regular font.

Parameter	Unit	Description
CFP	n/a	Cladding failure prediction defined as $CFP(t) = \max(X(t)/X_{critical}(t))$. X is any cladding failure parameter used by the participant and $X_{critical}$ is the critical value for predicted failure.
RAE	J/g	Variation of radial average enthalpy with respect to initial conditions of the transient in the rodlet (note that: $RAE(t=0)=0$)
TCO	°C	Temperature of cladding outer surface
SIF	MPa\sqrt{m}	Apparent stress intensity factor (see Section 3.1); if other relevant parameter is calculated by a code, it can also be added as a new column in the results file
CFR	%	Cladding final hoop strain at cooled state ($t = 200s$), permanent hoop strain as function of z where $z=0$ is fuel stack bottom
TDE	J/g	Total energy deposited per unit mass of fuel
TFC	°C	Temperature of fuel centerline
TFO	°C	Temperature of fuel outer surface
TCI	°C	Temperature of cladding inner surface
ECMH	%	Cladding mechanical (elastic + inelastic) hoop strain at the outer radius
ECMZ	%	Cladding mechanical (elastic + inelastic) axial strain at the outer radius
ECTH	%	Cladding total (thermal + elastic + inelastic) hoop strain at the outer radius
ECTZ	%	Cladding total (thermal + elastic + inelastic) axial strain at the outer radius
ECT	mm	Cladding total axial elongation
EFT	mm	Fuel column total axial elongation
SCH	MPa	Cladding hoop stress at outer radius
SCZ	MPa	Cladding axial stress at outer radius
RFO	mm	Fuel outer radius
RCI	mm	Cladding inner radius
HFC	W/m ² /K	Fuel to cladding heat transfer coefficient
HCW	W/m ² /K	Cladding to water heat transfer coefficient
PG	MPa	Free volume pressure
VOL	cc	Free volume

3.5.2 Results Formatting and Submission

- One formatted csv file is expected for each case (see attached file ‘org_HERA_case#.xlsx’ for template). Please change file name to include the specific case number reported in the file and the organization. For example, case 1 should be labeled as ‘INL_HERA_case1.csv’

Please note that each parameter only allows a maximum of 5000 points.

- If a performer is unable to provide a specific parameter output, please indicate by including “-1” in the column corresponding to that parameter.
- With the results, a simple written description of key models used in the calculations is requested. Key models include those related to the primary exercise targets noted by the bolded lines in Table 4. These include pellet-cladding contact, plasticity, failure, hydride related, etc., models and others deemed relevant to the performer. No formatting for submitting this information is specified. A simple list in a text file with relevant description and/or reference is sufficient, and brevity is recommended.

3.6 Schedule

The following schedule will be used for the HERA M&S Part I. Exact day is subject to change. The participants will be kept up to date of schedule specifics.

- June 22, 2022 – HERA M&S Exercise Kickoff: Part I
- July 15, 2022 – Participation notification and feedback on provided problem description
- November 9, 2022 – HERA M&S Phase I interim meeting for updates, preliminary individual participant results presentation and discussion.
- January 20, 2023 – Virtual meeting for pre-submission Q&A as needed
- January 27, 2023 – Participant submission of M&S Phase I results
- March 24, 2023 – Final submission of M&S Phase I results *in case of needed revision*
- Late Spring 2023 – HERA M&S Virtual Workshop, Summary of Part I results
- Late Spring 2023 – HERA M&S Part II Kickoff
- Fall 2023 – HERA M&S Part II Interim Meeting
- 2024 – HERA 2021-2024 M&S completion and summary paper(s)

4. REFERENCES

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1.123	20106.7993	1.123	23793.0458	1.123	27479.2923	1.123	0.3843
1.124	18476.7131	1.124	21864.1105	1.124	25251.5079	1.124	0.2922
1.125	16967.1608	1.125	20077.8069	1.125	23188.4531	1.125	0.2217
1.126	15570.2764	1.126	18424.8271	1.126	21279.3777	1.126	0.1678
1.127	14278.6173	1.127	16896.3638	1.127	19514.1103	1.127	0.1268
1.128	13085.149	1.128	15484.093	1.128	17883.037	1.128	0.0955
1.129	11983.2296	1.129	14180.155	1.129	16377.0804	1.129	0.0718
1.13	10966.5941	1.13	12977.1364	1.13	14987.6787	1.13	0.0539
1.131	10029.3399	1.131	11868.0522	1.131	13706.7645	1.131	0.0404
1.132	9165.9105	1.132	10846.3275	1.132	12526.7444	1.132	0.0301
1.133	8371.0814	1.133	9905.7797	1.133	11440.4779	1.133	0.0225
1.134	7639.9445	1.134	9040.601	1.134	10441.2575	1.134	0.0167
1.135	6967.8939	1.135	8245.3411	1.135	9522.7883	1.135	0.0124
1.136	6350.6114	1.136	7514.8901	1.136	8678.1689	1.136	0.0092
1.137	5784.0526	1.137	6844.4622	1.137	7904.8719	1.137	0.0068
1.138	5264.4332	1.138	6229.5793	1.138	7194.7253	1.138	0.005
1.139	4788.2155	1.139	5666.055	1.139	6543.8945	1.139	0.0037
1.14	4352.0958	1.14	5149.98	1.14	5947.8642	1.14	0.0027
1.141	3952.9915	1.141	4677.7067	1.141	5402.4218	1.141	0.002
1.142	3588.0296	1.142	4245.835	1.142	4903.6404	1.142	0.0014
1.143	3254.5341	1.143	3851.1987	1.143	4447.8633	1.143	0.0011
1.144	2950.0157	1.144	3490.852	1.144	4031.6882	1.144	0.0008
1.145	2672.1604	1.145	3162.0564	1.145	3651.9525	1.145	0.0006
1.146	2418.8191	1.146	2862.2693	1.146	3305.7195	1.146	0.0004
1.147	2187.9982	1.147	2589.1312	1.147	2990.2642	1.147	0.0003
1.148	1977.8493	1.148	2340.455	1.148	2703.0607	1.148	0.0002
1.149	1786.6609	1.149	2114.2154	1.149	2441.7699	1.149	0.0002
1.15	1612.8492	1.15	1908.5382	1.15	2204.2272	1.15	0.0001
1.151	1454.95	1.151	1721.6908	1.151	1988.4316	1.151	0.0001
1.152	1311.611	1.152	1552.073	1.152	1792.5351	1.152	0.0001
1.153	1181.5844	1.153	1398.2082	1.153	1614.832	1.153	0
1.154	1063.7195	1.154	1258.7347	1.154	1453.7499	1.154	0
1.155	956.9564	1.155	1132.3984	1.155	1307.8404	1.155	0
1.156	860.3198	1.156	1018.045	1.156	1175.7703	1.156	0
1.157	772.9125	1.157	914.6131	1.157	1056.3137	1.157	0
1.158	693.9105	1.158	821.1274	1.158	948.3443	1.158	0
1.159	622.5572	1.159	736.6928	1.159	850.8281	1.159	0
1.16	558.1587	1.16	660.4878	1.16	762.8169	1.16	0
1.161	500.0793	1.161	591.7605	1.161	683.4417	1.161	0
1.162	447.7368	1.162	529.8218	1.162	611.9069	1.162	0
1.163	400.5985	1.163	474.0415	1.163	547.4846	1.163	0
1.164	358.1777	1.164	423.8436	1.164	489.5095	1.164	0
1.165	320.0298	1.165	378.7019	1.165	437.3741	1.165	0
1.166	285.7492	1.166	338.1366	1.166	390.5239	1.166	0
1.167	254.966	1.167	301.7098	1.167	348.4536	1.167	0
1.168	227.3434	1.168	269.023	1.168	310.7026	1.168	0
1.169	202.5746	1.169	239.7133	1.169	276.8519	1.169	0
1.17	180.3808	1.17	213.4506	1.17	246.5204	1.17	0
1.171	160.5086	1.171	189.9352	1.171	219.3618	1.171	0
1.172	142.728	1.172	168.8948	1.172	195.0616	1.172	0
1.173	126.8301	1.173	150.0823	1.173	173.3345	1.173	0
1.174	112.626	1.174	133.2741	1.174	153.9222	1.174	0
1.175	99.9441	1.175	118.2672	1.175	136.5903	1.175	0
1.176	88.6296	1.176	104.8784	1.176	121.1271	1.176	0
1.177	78.5422	1.177	92.9416	1.177	107.341	1.177	0
1.178	69.5552	1.178	82.307	1.178	95.0588	1.178	0
1.179	61.5544	1.179	72.8394	1.179	84.1244	1.179	0
1.18	54.4367	1.18	64.4167	1.18	74.3968	1.18	0
1.181	48.109	1.181	56.929	1.181	65.749	1.181	0
1.182	42.4678	1.182	50.2772	1.182	58.0666	1.182	0
1.183	37.4977	1.183	44.3722	1.183	51.2468	1.183	0
1.184	33.071	1.184	39.134	1.184	45.197	1.184	0
1.185	29.1469	1.185	34.4905	1.185	39.8341	1.185	0
1.186	25.6709	1.186	30.3772	1.186	35.0836	1.186	0
1.187	22.594	1.187	26.7362	1.187	30.8784	1.187	0
1.188	19.8722	1.188	23.5154	1.188	27.1587	1.188	0
1.189	17.4664	1.189	20.6685	1.189	23.8707	1.189	0
1.19	15.3413	1.19	18.1538	1.19	20.9664	1.19	0
1.191	13.4655	1.191	15.9342	1.191	18.4029	1.191	0
1.192	11.611	1.192	13.9764	1.192	16.1417	1.192	0
1.193	10.3527	1.193	12.2507	1.193	14.1487	1.193	0
1.194	9.0683	1.194	10.7308	1.194	12.3933	1.194	0
1.195	7.9377	1.195	9.393	1.195	10.8483	1.195	0
1.196	6.9434	1.196	8.2164	1.196	9.4893	1.196	0
1.197	6.0695	1.197	7.1622	1.197	8.2949	1.197	0
1.198	5.3019	1.198	6.2739	1.198	7.2459	1.198	0
1.199	4.6282	1.199	5.4767	1.199	6.3252	1.199	0
1.2	4.0374	1.2	4.7776	1.2	5.5178	1.2	0
1.21	0.9222	1.21	1.1741	1.21	1.356	1.25	0
1.22	0.2277	1.22	0.2695	1.22	0.3112	1.5	0
1.23	0.0488	1.23	0.0577	1.23	0.0667	2	0
1.24	0.0098	1.24	0.0116	1.24	0.0133	3	0
1.25	0.0018	1.25	0.0022	1.25	0.0025	4.00E+00	0.00E+00
1.26	0.0003	1.26	0.0004	1.26	0.0004	5.00E+00	0.00E+00
1.27	0.0001	1.27	0.0001	1.27	0.0001	1.00E+01	0.00E+00
1.28	0	1.28	0	1.28	0		

1.29	0	1.29	0	1.29	0
1.3	0	1.3	0	1.3	0
1.31	0	1.31	0	1.31	0
1.32	0	1.32	0	1.32	0
1.33	0	1.33	0	1.33	0
1.34	0	1.34	0	1.34	0
1.35	0	1.35	0	1.35	0
1.36	0	1.36	0	1.36	0
1.37	0	1.37	0	1.37	0
1.38	0	1.38	0	1.38	0
1.39	0	1.39	0	1.39	0
1.4	0	1.4	0	1.4	0
1.5	0	1.5	0	1.5	0
2	0	2	0	2	0
3	0	3	0	3	0
4	0	4	0	4	0
5	0	5	0	5	0
10	0	10	0	10	0