Nonisothermal Multifluid Transition to Equilibrium

Processes of interest to the simulation of CH_4 production from gas hydrates in porous media include multifluid flow and heat transport along with complex phase transitions, including hydrate dissociation and formation. Before executing problems with the additional complexities involved with the gas hydrate phase, a base case problem has been designed to examine the numerical simulation of multifluid flow and heat transport processes with a single phase transition from aqueous saturated to unsaturated conditions for a water-CH_4 system outside the stability region for gas hydrate formation. The problem involves a horizontal one-dimensional closed domain (no flow boundary conditions), initialized with gradients in aqueous pressure, gas pressure, and temperature that yield aqueous saturated conditions on half of the domain and aqueous unsaturated conditions on the other half of the domain. The simulation then proceeds to an equilibrium condition in pressure and temperature. The results of numerical simulations of CH_4 hydrate formations in geologic media largely depend on the computation of thermodynamic and transport properties. Therefore, a portion of this problem involves reporting property data for selected temperatures and pressures.

After execution and comparison of simulator results for this base case problem, a companion problem will be defined that includes a methane hydrate phase and associated phase transitions as the problem evolves to an equilibrium state.

Base Case Problem Description

Gradients in aqueous pressure, gas pressure, and temperature are imposed across a 20-m one-dimensional horizontal domain, discretized using uniformly spaced 1-m grid cells. A horizontal domain is used to eliminate gravitational body forces from the problem, as an additional simplification. The pressure and temperature gradients are specified to yield aqueous saturation conditions in the first 10 grid cells and aqueous unsaturated conditions in the remaining 10 grid cells. The simulation then proceeds to equilibrium conditions in pressure, phase saturations, and temperature. Variable time stepping should be used to capture the flow and transport processes at early and late times during simulation. A schematic of the initial conditions for the problem are shown in Figure 1 and problem parameters and specifications are provided in Table 1. The list of processes simulated in this problem include:

1. aqueous-gas multifluid flow subject to relative permeability, capillary effects, and phase transition from aqueous saturated to unsaturated
2. heat transport across multifluid porous media with phase advection and component diffusion
3. change in CH_4 solubility in water with pressure and temperature
4. change in thermodynamic and transport properties with pressure and temperature

Table 1. Problem Parameters and Specifications

Parameter	Value
Porosity	0.3
Bulk Density	1855 kg/m^3
Grain Density	2650 kg/m^3
Bulk Specific Heat	525 J/kg K
Grain Specific Heat	750 J/kg K
Hydraulic Conductivity	0.1 Darcy
Dry Thermal Conductivity	2.0 W/m K
Water-Saturated Thermal Conductivity	2.18 W/m K
Pore Compressibility	5.0 x 10^{-10} Pa^{-1}
Capillary Pressure Model	van Genuchten, see Equation (1)
α parameter	0.132 m^{-1}
n parameter	2.823
β_{gl} parameter	1.0
s_{lr} parameter	0.0
Aqueous Relative Permeability Model	Mualem, see Equation (2)
m parameter	0.6458
Gas Relative Permeability Model	Mualem, see Equation (3)
m parameter	0.6458

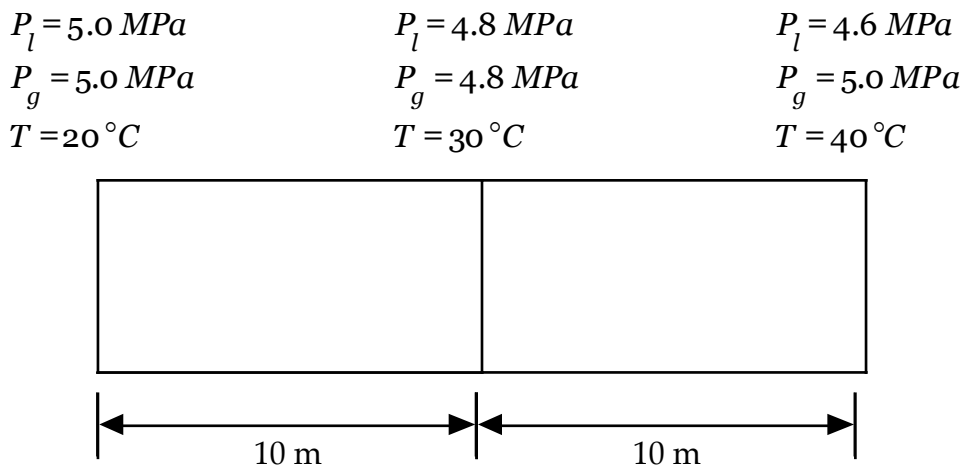

Figure 1. Problem Schematic

The van Genuchten capillary pressure model expresses the relationship between gas-aqueous capillary pressure head and the aqueous saturation (van Genuchten, 1981):

$$\bar{s}_l = \frac{s_l - s_{lr}}{1 - s_{lr}} = \left[1 + \left(\alpha\, \beta_{gl}\, h_{gl}\right)^n\right]^{-m} ;\ where\ m = 1 - \frac{1}{n} \tag{1}$$

where, $\bar{s}_l$ is the effective aqueous saturation, s_l is the aqueous saturation, s_{lr} is the residual aqueous saturation, β_{gl} is the interfacial tension scaling factor, and h_{gl} is the gas-aqueous capillary pressure head. A plot of the van Genuchten function for the parameters in Table 1 is shown in Figure A.1, and tabular data for this function is provided in Table A.1. The Mualem (1964) porosity distribution function, when combined with the van Genuchten capillary pressure relationship yields the following functions for aqueous and gas phase relative permeability:

$$k_{rl} = \left(\bar{s}_l\right)^{1/2}\left[1 - \left(1 - \left(\bar{s}_l\right)^{1/m}\right)^m\right]^2 \tag{2}$$

$$k_{rg} = \left(1 - \bar{s}_l\right)^{1/2}\left[\left(1 - \left(\bar{s}_l\right)^{1/m}\right)^m\right]^2 \tag{3}$$

where, k_{rl} is the aqueous-phase relative permeability and k_{rg} is the gas-phase relative permeability. Plots of the Mualem functions of relative permeability for the parameters in Table 1 are shown in Figure A.1, and tabular data for these functions are provide in Table A.1.

Simulation Results

Profiles of temperature, aqueous saturation, dissolved CH_4 mass fraction and aqueous pressure at selected times (i.e., 0, 1, 10, 100, 1,000, and 10,000 days) are shown in Figures 2 through 5, respectively. The profile plots show equilibrium conditions are achieved by 10,000 days. Aqueous pressure and according saturation reach equilibrium conditions by 1,000 days indicating the faster response of the hydrologic system compared against the thermal system; where, the temperature does not reach equilibrium conditions until 10,000 days. Transition to thermal equilibrium progresses rapidly until the hydrologic system reaches equilibrium by 1,000 days. From here, progress toward thermal equilibrium is dependent on low gradients and diffusive heat transfer. Likewise, transition to equilibrium for the dissolved CH_4 proceeds rapidly until 1,000 days; where, advances toward equilibrium are controlled by aqueous and gas diffusion processes. Equilibrium conditions are listed in Table 2. As a check on CH_4 mass balance the integrated amount of total- and dissolved-CH_4 mass was output during the simulation. As expected, the total-CH_4 mass remained unchanged at

72.1257 kg, but the dissolved-CH_4 mass changed from an initial value of 3.792 kg to an equilibrium value of 3.578 kg.

Table 2. Equilibrium Conditions

Parameter	Value
Temperature	28.83 C
Aqueous Pressure	4.7242 MPa
Gas Pressure	4.7964 MPa
Aqueous Saturation	0.655
Aqueous Relative Permeability	0.115
Aqueous CH_4 Mass Fraction	0.913×10^{-3}
Gas CH_4 Mass Fraction	0.999148

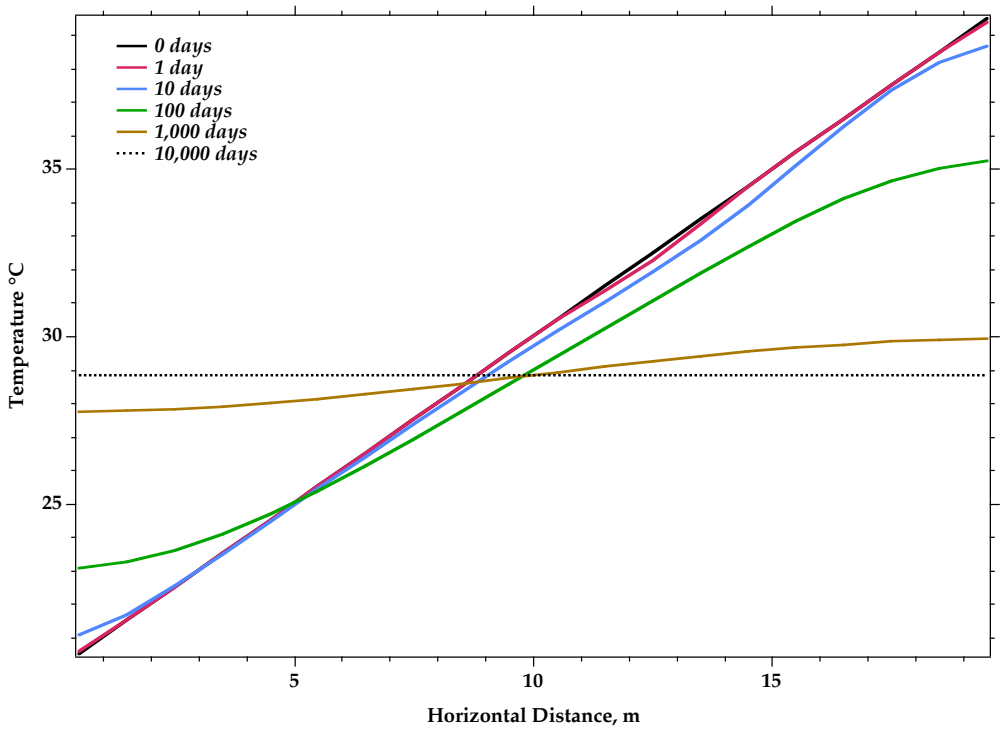

Figure 2. Simulated Temperature Profiles

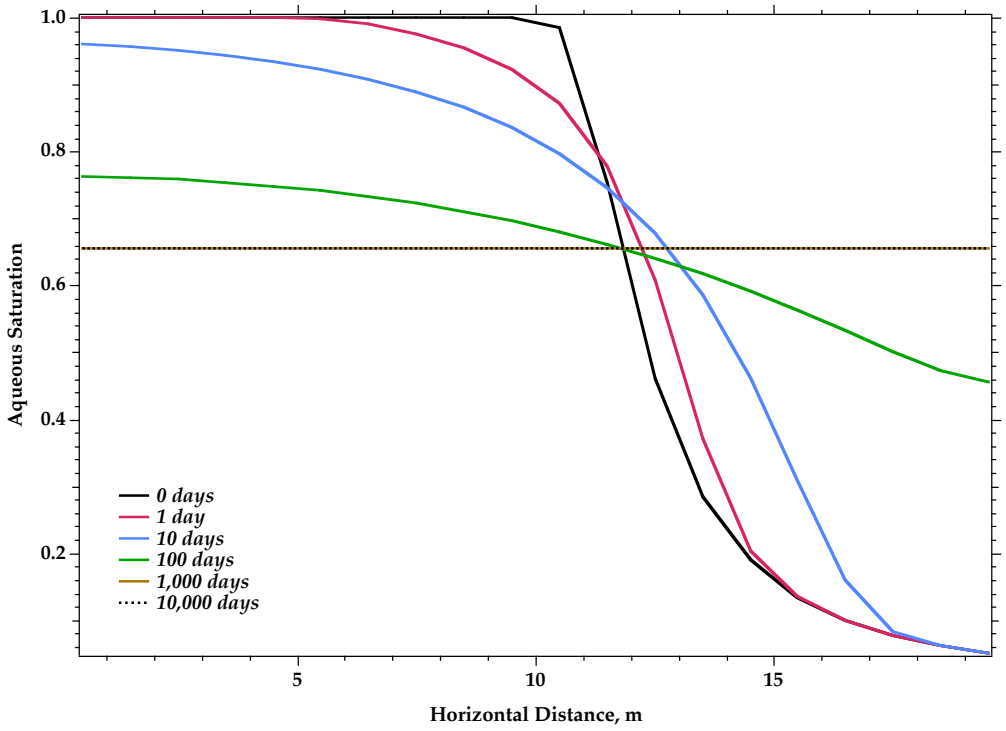

Figure 3. Simulated Aqueous Saturation Profiles

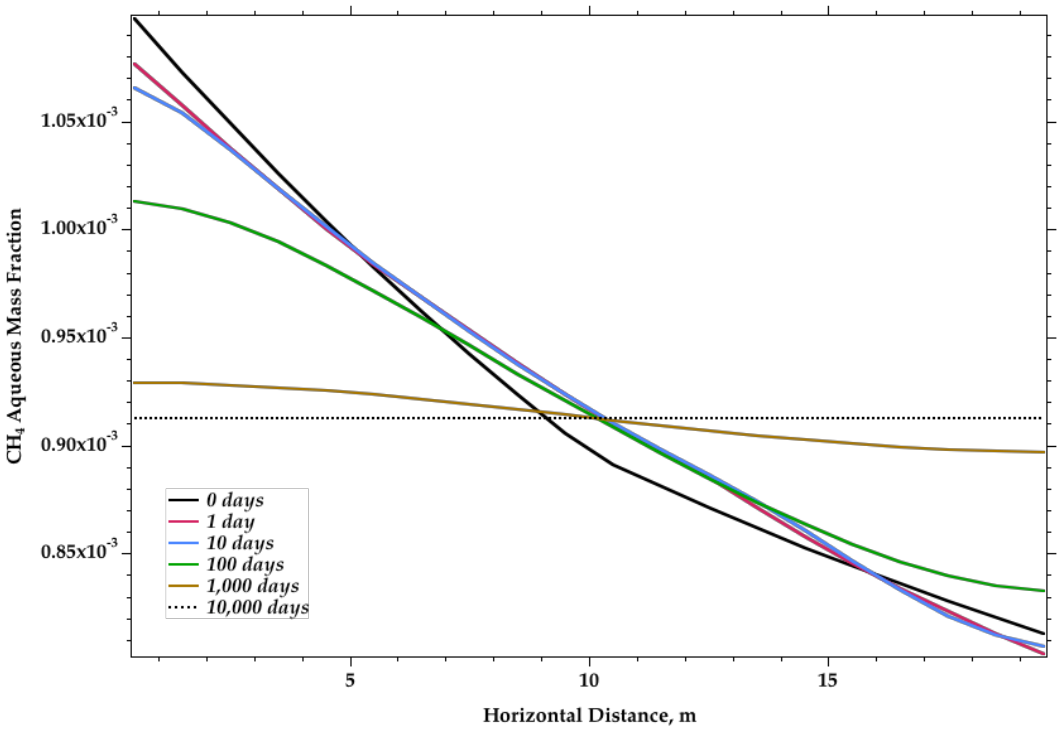

Figure 4. Simulated Aqueous CH_4 Mass Fraction Profiles

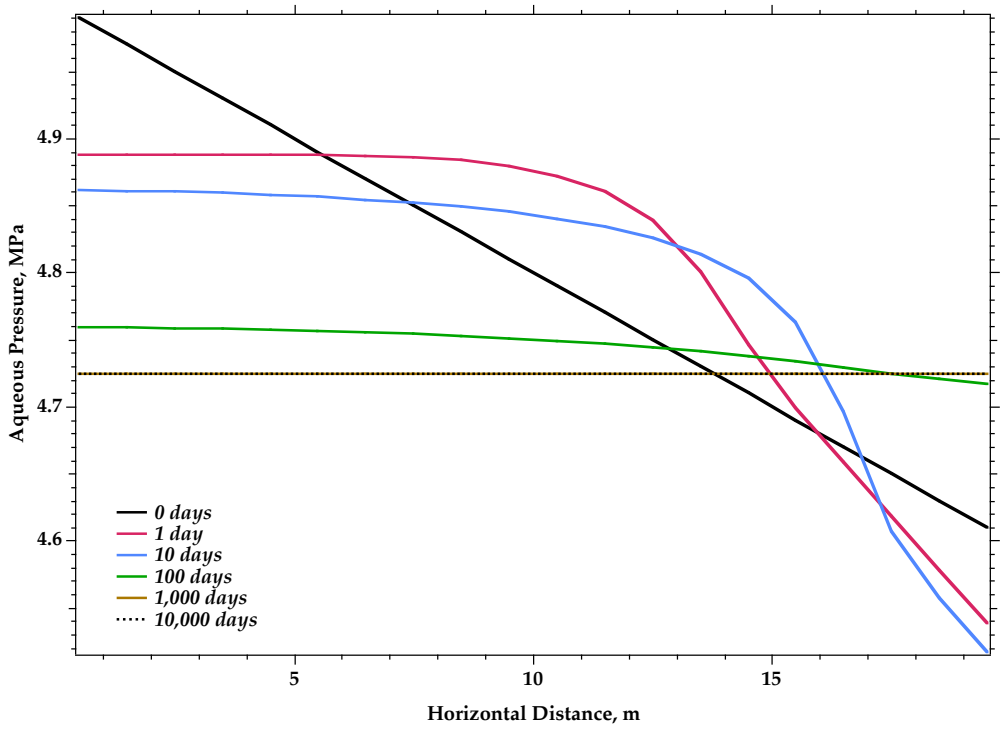

Figure 5. Simulated Aqueous Pressure Profiles

References

Mualem, Y. 1976. "A new model for predicting the hydraulic conductivity of unsaturated porous media." *Water Resources Research*. 12:513-522.

van Genuchten, M. T. A. 1980. "A closed-form equation for predicting the hydraulic conductivity of unsaturated soils." *Soil Sci. Soc. Am. J.* 44:892-898.

Appendix

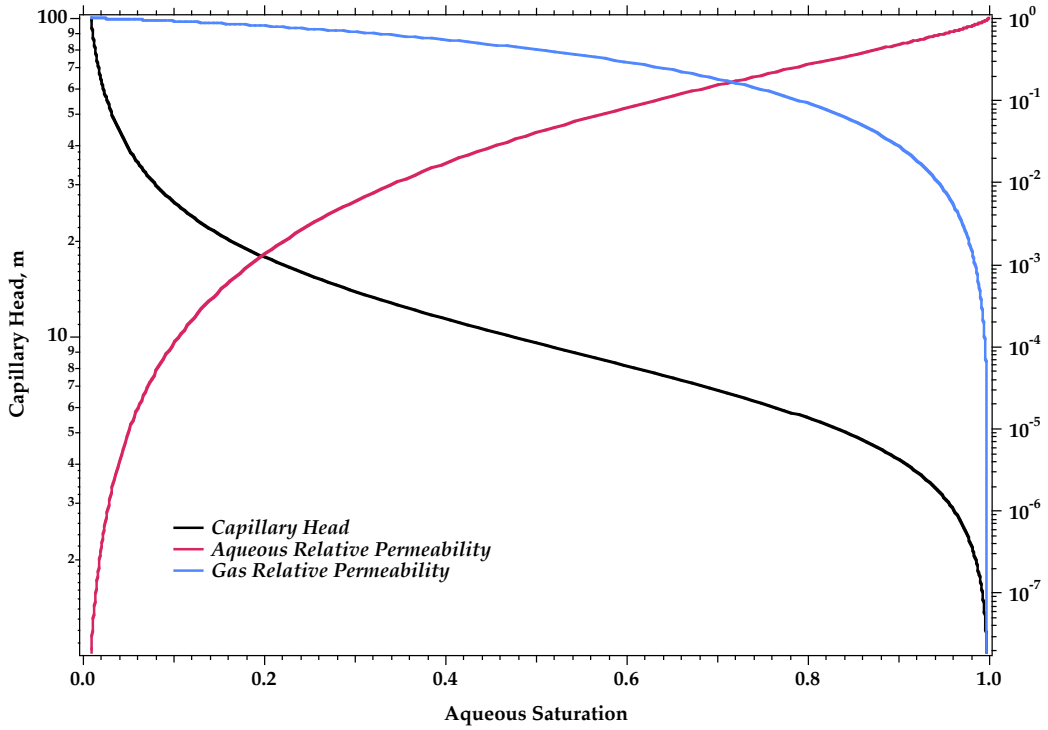

Figure A.1. van Genuchten and Mualem Functions

Table A.1 van Genuchten and Mualem Functions

Aqueous Saturation	Capillary Head, m	Aqu. Rel. Perm.	Gas Rel. Perm.
1	0	1	0
0.99777	1.01822	0.948178	3.12211e-05
0.997653	1.03678	0.946455	3.41961e-05
0.997531	1.05567	0.944675	3.74549e-05
0.997402	1.07491	0.942837	4.10224e-05
0.997267	1.0945	0.940938	4.49304e-05
0.997125	1.11445	0.938979	4.9208e-05
0.996975	1.13475	0.936955	5.38936e-05
0.996817	1.15543	0.934865	5.90233e-05
0.996651	1.17649	0.932708	6.46395e-05
0.996477	1.19793	0.93048	7.07881e-05
0.996294	1.21976	0.928181	7.75207e-05
0.996101	1.24199	0.925807	8.48929e-05
0.995898	1.26462	0.923357	9.29598e-05
0.995684	1.28767	0.920828	0.000101793
0.99546	1.31113	0.918218	0.000111461
0.995224	1.33503	0.915524	0.000122046
0.994976	1.35936	0.912745	0.000133629
0.994715	1.38413	0.909877	0.000146308
0.99444	1.40935	0.906917	0.000160183

0.994152	1.43504	0.903864	0.000175371
0.993848	1.46119	0.900714	0.000191988
0.993529	1.48782	0.897466	0.000210172
0.993194	1.51493	0.894115	0.000230066
0.992841	1.54254	0.89066	0.000251832
0.99247	1.57065	0.887097	0.000275644
0.99208	1.59927	0.883423	0.000301692
0.99167	1.62841	0.879635	0.000330188
0.991239	1.65809	0.875731	0.000361352
0.990786	1.68831	0.871707	0.000395431
0.99031	1.71907	0.86756	0.000432703
0.98981	1.7504	0.863287	0.000473452
0.989285	1.7823	0.858885	0.000518006
0.988732	1.81478	0.854351	0.00056671
0.988152	1.84785	0.84968	0.000619949
0.987542	1.88152	0.844871	0.000678132
0.986901	1.91581	0.83992	0.000741714
0.986228	1.95073	0.834823	0.000811186
0.985521	1.98627	0.829578	0.000887087
0.984778	2.02247	0.82418	0.000969995
0.983998	2.05933	0.818628	0.00106054
0.983179	2.09686	0.812916	0.00115942
0.982319	2.13507	0.807044	0.00126738
0.981416	2.17398	0.801006	0.00138522
0.980468	2.21359	0.794801	0.00151383
0.979473	2.25393	0.788425	0.00165418
0.978429	2.29501	0.781875	0.00180728
0.977333	2.33683	0.775149	0.00197428
0.976183	2.37942	0.768243	0.00215639
0.974977	2.42278	0.761156	0.00235492
0.973712	2.46693	0.753885	0.00257131
0.972385	2.51189	0.746427	0.0028071
0.970994	2.55766	0.73878	0.00306398
0.969536	2.60427	0.730943	0.00334371
0.968007	2.65173	0.722914	0.00364826
0.966405	2.70005	0.714691	0.00397974
0.964726	2.74926	0.706274	0.00434039
0.962967	2.79936	0.697661	0.00473264
0.961126	2.85037	0.688853	0.00515913
0.959197	2.90232	0.679848	0.00562264
0.957179	2.95521	0.670646	0.00612621
0.955066	3.00906	0.66125	0.00667307
0.952856	3.0639	0.651658	0.0072667
0.950544	3.11973	0.641874	0.00791076
0.948127	3.17659	0.631899	0.00860925
0.9456	3.23448	0.621735	0.00936638
0.942959	3.29342	0.611385	0.0101866
0.940201	3.35344	0.600852	0.0110749

0.93732	3.41455	0.590141	0.0120361
0.934313	3.47677	0.579257	0.0130757
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0.927902	3.60465	0.556989	0.0154135
0.924488	3.67034	0.545618	0.016724
0.920931	3.73722	0.534098	0.0181378
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0.881707	4.39681	0.425276	0.0367806
0.876472	4.47693	0.412823	0.0396685
0.871047	4.55852	0.400346	0.0427545
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0.023496	59.231	5.7667e-07	0.984353
0.0227372	60.3104	5.12417e-07	0.984925
0.0220029	61.4095	4.55316e-07	0.985475
0.0212921	62.5286	4.04573e-07	0.986005
0.0206043	63.6681	3.5948e-07	0.986514
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0.0186707	67.2126	2.52161e-07	0.987931
0.0180672	68.4375	2.24046e-07	0.988368
0.0174832	69.6847	1.99063e-07	0.988789
0.016918	70.9546	1.76864e-07	0.989194
0.0163711	72.2476	1.57139e-07	0.989584
0.0158417	73.5642	1.39613e-07	0.989959
0.0153295	74.9048	1.24041e-07	0.99032
0.0148338	76.2699	1.10204e-07	0.990668
0.014354	77.6598	9.79106e-08	0.991003
0.0138898	79.075	8.69877e-08	0.991325
0.0134405	80.516	7.72828e-08	0.991636
0.0130057	81.9833	6.86603e-08	0.991935
0.012585	83.4773	6.09993e-08	0.992223
0.0121779	84.9986	5.41929e-08	0.9925
0.0117839	86.5476	4.81456e-08	0.992767
0.0114026	88.1248	4.2773e-08	0.993024
0.0110337	89.7307	3.79997e-08	0.993272
0.0106767	91.3659	3.37589e-08	0.993511
0.0103312	93.031	2.99912e-08	0.99374
0.00999686	94.7263	2.66439e-08	0.993962
0.00967334	96.4526	2.36702e-08	0.994175
0.00936029	98.2103	2.10282e-08	0.994381
0.00905735	100	1.8681e-08	0.994579