



In mathematics, a stiff equation is a differential equation for which certain numerical methods for solving the equation are numerically unstable, unless the step size is taken to be extremely small. It has proven difficult to formulate a precise definition of stiffness, but the main idea is that the equation includes some terms that can lead to rapid variation in the solution.

When integrating a differential equation numerically, one would expect the requisite step size to be relatively small in a region where the solution curve displays much variation and to be relatively large where the solution curve straightens out to approach a line with slope nearly zero. For some problems this is not the case. Sometimes the step size is forced down to an unacceptably small level in a region where the solution curve is very smooth. The phenomenon being exhibited here is known as stiffness. In some cases we may have two different problems with the same solution, yet problem one is not stiff and two is stiff. problem Clearly the phenomenon cannot be a property of the exact solution, since this is the same for both problems, and must be a property of the differential system itself. It is thus appropriate to speak of stiff systems.



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²³⁸U fission case calculation : <u>10000</u> years decay time



10 000 years







$ODE \rightarrow not finished$

Option	Value	Description	Default value
N_Implant	100	number of points : Irradiation	100
N_Decay	1000	number of points : DECAY	100
AbsError	1.000e-06	absolute error tolerance	1e-11
RelError	1.000e-02	relative error tolerance	1e-03
Y_thrshld	1.000e-05	Minimum yield value	1e-10



²³⁸U fission case calculation : <u>models comparison</u>



• 2. List of isotopes to implant from file		🖆 "238U	_Coulomb Fission .radlist "	N of isotopes = 490
C 3. Select detector to obtain the list o	f isotopes stopped in	FP_PPAC0	Refresh	N of isotopes = 0
Press "Escape" to interrupt calculations	Total Irradiation Rate	17 pps	⊢Irradiation (Implantation)− IT : Irradiation Time [N of DI @ time	(IT) = 556

Option	Value	Description	Default value
N_Implant	100	number of points : Irradiation	100
N_Decay	1000	number of points : DECAY	100
AbsError	1.000e-06	absolute error tolerance	1e-11
RelError	1.000e-02	relative error tolerance	1e-03
Y_thrshld	1.000e-05	Minimum yield value	1e-10

decay time in sec	3E+07	3E+09	3E+11									
years	1	100	1000									
model	elap	elapsed calculation time, sec										
ODE	101.82	stopped	stopped									
RKF45	23.86	320.03	464.55									
NR:odeint	27.22	366.22*	532.19*									
* wrong calculation	result at the end of a	decay time (see previ	ous slides)									

Use the **RKF45** model for similar tasks!



²³⁸U fission case calculation with RKF45: <u>option comparison</u>





decay time in sec	3E+07	(1 year)										
model	RKF45	RKF45	RKF45	RKF45	RKF45	RKF45	RKF45	RKF45	RKF45	RKF45	ODE	NR: odeint
N_implant	100	5	10	1000	100	100	100	100	100	100	100	100
N_decay	1000	10	100	10000	1000	1000	1000	1000	1000	1000	1000	1000
AbsError	1E-06	1E-06	1E-06	1E-06	1E-01	1E-11	1E-16	1E-06	1E-06	1E-11	1E-11	1E-11
RelError	1E-02	1E-02	1E-02	1E-02	1E-02	1E-02	1E-02	1E-05	1E-10	1E-05	1E-05	1E-05
Y_threshold	1E-05	1E-05	1E-05	1E-05	1E+00	1E-10	1E-15	1E-05	1E-05	1E-10	1E-10	1E-10
elapsed calculation time, sec	23.86	2.76	14.56	29.43	23.55	26.61	24.13	23.74	23.52	24.01	122.55	26.84
Number of different isotopes @ FT	124	142	128	122	95	130	131	124	124	130	130	130









Option	Value	Description	Default value
N_Implant	100	number of points : Isradiation	100
N_Decay	1000	number of points : DECAY	100
AbsError	1.000e-11	absolute error tolerance	1e-11
RelError	1.000e-06	relative error tolerance	1e-03
Y_thishid	1.000e-10	Minimum yield value	1e-10

decay time in sec	3E+05	3E+07	3E+09	3E+11	3E+13	3E+15						
years	1.E-02	1.E+00	1.E+02	1.E+03	1.E+05	1.E+07						
model	elapsed calculation time, sec											
ODE	15.08	61.5	89.86	105.79	125.89	122.67						
RKF45	5.6	15.07	19.81	21.97	25.06	23.09						
NR:odeint	106.42*	108.41*	107.19*	119.02*								
* wrong calculation	result : only 3 differe	ent isotopes at the en	d instead 9									

Do not use NR:odeint for similar tasks!



Stiff problem



Stiffness occurs in a problem where there are two or more very different scales of the independent variable on which the dependent variables are changing.

Radiation Residue Calculator v.2 is two-step solution:

- 1. System from 7200 ODE with short implantation time, no decay time
- 2. LISE⁺⁺ selects ODEs of nuclei used in calculations, by another words non-zero yield

So, in the case of ²²⁹Th only 9 equations are used in the second step calculations



Number of iterations in the current calculation step. If you see for each step 50000, then it means the integrator reaches the maximum number of iterations, and did not find solution. You got stiffness. Try to increase number of steps, play with abs. & rel. errors. See the next page





1. Chose fragment to implant-



decay time in sec	1E+05	(1.2days)										
										$\overline{}$		
model	RKF45	RKF45	RKF45	RKF45	RKF45	RKF45	ODE	ODE	ODE	ODE	ODE	ODE
N_implant	100	100	100	100	100	100	100	100	100	100	100	100
N_decay	10000	1000	1000	1000	10000	100000	10000	1000	1000	1000	10000	100000
AbsError	1E-07	1E-07	1E-05	1E-15	1E-15	1E-15	1E-07	1E-07	1E-05	1E-15	1E-15	1E-15
RelError	1E-03	1E-03	1E-03	1E-05	1E-05	1E-05	1E-03	1E-03	1E-03	1E-05	1E-05	1E-05
Y_threshold	1E-06	1E-06	1E-04	1E-14	1E-14	1E-14	1E-06	1E-06	1E-04	1E-14	1E-14	1E-14
elapsed calculation time, sec	4.74	2.57	1.81	2.32	4.48	26.77	6.01	4.63	1.21	5.11	7.22	25.87
Flag max steps reached	NO	yes	yes	yes	NO	NO	NO	NO	NO	NO	NO	NO
209Bi yield	5.4E-01	5.3E-01	5.3E-01	5.2E-01	5.3E-01	5.3E-01	5.3E-01	5.3E-01	5.4E-01	5.3E-01	5.3E-01	5.3E-01
217At yield	2.7E-06	2.7E-06	0		2.7E-06	2.7E-06		2.9E-06	0	2.7E-06	2.7E-06	2.7E-06
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Do no use these settings:

Stiffness not solved

Very high Y-threshold – some isotopes have been lost

recommended





1. Chose fragment to implant-



decay time in sec	1E+06	(12days)										
											\frown	
model	RKF45	RKF45	RKF45	RKF45	RKF45	RKF45	ODE	ODE	ODE	ODE	ODE	ODE
N_implant	100	100	100	100	100	100	100	100	100	100	100	100
N_decay	10000	1000	1000	1000	10000	100000	10000	1000	1000	1000	10000	100000
AbsError	1E-07	1E-07	1E-05	1E-15	1E-15	1E-15	1E-07	1E-07	1E-05	1E-15	1E-15	1E-15
RelError	1E-03	1E-03	1E-03	1E-05	1E-05	1E-05	1E-03	1E-03	1E-03	1E-05	1E-05	1E-05
Y_threshold	1E-06	1E-06	1E-04	1E-14	1E-14	1E-14	1E-06	1E-06	1E-04	1E-14	1E-14	1E-14
elapsed calculation time, sec	18.49	6.83	6.12	6.62	18.19	39.96	46.18	27.73	FLAG=4	28.24	47.56	65.99
Flag max steps reached	yes	yes	yes	yes	yes	NO	NO	yes	FLAG=4	yes	NO	NO
209Bi yield	6.90E+02	4.20E+01	3.00E+01	4.20E+01	6.90E+02	6.90E+02	6.90E+02	1.80E+02		1.80E+02	6.90E+02	6.90E+02
217At yield	1.80E-04	3.50E-05	0	3.50E-05	1.80E-04	1.80E-04	1.80E-04	8.30E-05		8.30E-05	1.80E-04	1.80E-04
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Do no use these settings:

- Stiffness not solved
- Very high Y-threshold some isotopes have been lost
- Calculations were tot finished

recommended

Use the ODE method for tasks similar to the ²²⁹Th case !



²²⁹Th case : settings comparison \rightarrow decay time 7 seconds



decay time in sec	3E+07	(1 year)							
model	RKF45	RKF45	RKF45	RKF45	RKF45	RKF45	RKF45	RKF45	RKF45
N_implant	100	100	100	100	100	100	100	100	100
N_decay	1000	1000	1000	10000	100	10	1000	1000	100000
AbsError	1E-11	1E-11	1E-04	1E-04	1E-04	1E-04	1E+00	1E-15	1E-15
RelError	1E-05	1E-02	1E-02	1E-02	1E-02	1E-02	1E-01	1E-10	1E-05
۲_threshold	1E-10	1E-10	1E-03	1E-03	1E-03	1E-03	1E+00	1E-14	1E-14
elapsed calculation time, sec	11.07	11.72	9.97	70.52	1.69	0.69	5.81	11.14	348.8
Flag max steps reached	yes	yes	yes	yes	yes	yes	yes	yes	yes
209Bi yield	2.2E+02	2.2E+02	2.2E+02	1.3E+04	3.4E+00	7.4E-02	3.8E+04	2.2E+02	2.5E+05
217At yield			0		0	0	0	9.30E-05	1.30E-03

Do no use these settings:

Stiffness not solved

• Very high Y-threshold – some isotopes have been lost

						-							
model	ODE	ODE	ODE	ODE	ODE	ODE	ODE	ODE	ODE	ODE	ODE	ODE	ODE
N_implant	100	100	100	100	100	100	100	100	100	100	100	100	100
N_decay	1000	1000	1000	10000	10000	100	10	1000	1000	100000	300000	600000	1.00E+06
AbsError	1E-11	1E-11	1E-04	1E-15	1E-15	1E-15	1E-15	1E+00	1E-15	1E-15	1E-15	1E-15	1E-15
RelError	1E-05	1E-02	1E-02	1E-05	1E-10	1E-10	1E-10	1E-01	1E-05	1E-10	1E-10	1E-10	1E-10
Y_threshold	1E-10	1E-10	1E-03	1E-14	1E-14	1E-14	1E-14	1E+00	1E-14	1E-14	1E-14	1E-14	1E-14
elapsed calculation time, sec	57.61	58.7	42.97	FLAG=4	352.13	8.63	1.42	9.5	57.74	1296.82	1405.89	1521.6	FLAG=4
Flag max steps reached	yes	yes	yes	yes	yes	yes	yes	no/yes	yes	no/yes	NO	NO	FLAG=4
209Bi yield	1.3E+03	1.4E+03	2.8E+03		6.5E+04	3.8E+00	1.7E-03	4.6E+05	1.3E+03	3.5E+05	3.7E+05	3.7E+05	
217At yield	2.60E-04	2.80E-04	0		1.20E-03	8.20E-06	1.41E-07	0	2.6E-04	1.30E-03	1.30E-03	1.30E-03	