SOLUTION OF THE REACTOR POINT KINETICS EQUATIONS BY MATLAB COMPUTING

by

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The numerical solution of the point kinetics equations in the presence of Newtonian temperature feedback has been a challenging issue for analyzing the reactor transients. Reactor point kinetics equations are a system of stiff ordinary differential equations which need special numerical treatments. Although a plethora of numerical intricacies have been introduced to solve the point kinetics equations over the years, some of the simple and straightforward methods still work very efficiently with extraordinary accuracy. As an example, it has been shown recently that the fundamental backward Euler finite difference algorithm with its simplicity has proven to be one of the most effective legacy methods. Complementing the backward Euler finite difference scheme, the present work demonstrates the application of ordinary differential equation suite available in the MATLAB software package to solve the stiff reactor point kinetics equations with Newtonian temperature feedback effects very effectively by analyzing various classic benchmark cases. Fair accuracy of the results implies the efficient application of MATLAB ordinary differential equation suite for solving the reactor point kinetics equations as an alternate method for future applications.

Key words: point kinetics equation, backward Euler finite difference, MATLAB, ODE suite, NDF

INTRODUCTION

The numerical solution of the point kinetics equations (PKE) in the presence of Newtonian feedback has been a challenging issue for analyzing reactor transients. Recently a very interesting paper highlighting the various old and modern algorithms for the solution of the reactor point kinetics equations has been published by B. D. Ganapol [1]. In his seminal work Ganapol has brought out the notable historic attempts made to provide the original and efficient numerical schemes for the solution of the point kinetics equations. In addition, he has also cited the improved solution techniques, which has evolved over time.

Dated back in 1958, Akcasu [2] had given a general solution of the reactor kinetics equations without feedback by transfer function approach. In 1960, Keepin and Cox [3] had given a general solution of the reactor kinetics equations by reducing them to an integral form convenient for explicit numerical solution. Subsequently in the 1960's there were several attempts to develop numerical methods based on Runge-Kutta methods [4, 5], Euler integration schemes [6, 7], finite difference methods [8] and methods based on integral equation formulations with the slowly varying factor in each integrand represented by an assumed functional form [9-13]. A method based on analytic continuation was proposed by Vigil [14], which was well suited for fast digital application during that time. In order to avoid smaller time steps and long computing times by Runge-Kutta methods, Izumi and Noda [15] developed a new extrapolated implicit method. This method not only assured stability and accuracy but also estimated the truncation error at a particular time and could control the time interval by adjusting the magnitude of the estimated truncation error.

There were several attempts made by applying Pade and Chebyshev types of approximations, Hermite polynomials and power series solution methods for solving the point kinetics equations for various reactivity insertions [16-18]. Accurate solution of the reactor kinetics equations was obtained by Basken and Lewins [19] by applying straightforward power series recurrence relation in a lumped model with time varying reactivity. During the past one-decade many novel numerical methods, to name a few, the analytical inversion method [20], the analytical exponential method [21, 22], fourth order Rosenbrock method [23] with an automatic step size control, an integral method based on better basis function [24], have been adopted to find the accurate, efficient and stable solutions of the point kinetics equations. More recently in an inter-

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esting work Nahla [25] has introduced an efficient technique for solving the non-linear point kinetics equations in presence of the adiabatic temperature feedback effects. In this work, the predicted values of reactivity are determined using backward Euler in conjunction with the Crank Nicholson approximation scheme. The predicted value of reactivity is required later to change the nonlinear differential system to linear system.

At this point our attention is drawn to the remarks made by Ganapol [1] that although so many numerical intricacies have been introduced to solve the point kinetics equations over years, arguably the backward Euler finite difference (BEFD) algorithm with its simplicity has proven to be one of the most effective legacy methods. Complementing the proposition of Ganapol, in the present work ordinary differential equation suite (ODE suite) available in the MATLAB software package has been applied to solve the stiff reactor point kinetics equations with Newtonian temperature feedback effects very effectively by avoiding the over complicated schemes proposed in the previous works.

APPLICATION OF MATLAB FOR SOLUTION OF POINT KINETICS EQUATIONS

The basic space independent reactor point kinetics equations with m group of delayed neutrons can be written as follows

$$\frac{\mathrm{d}N(t)}{\mathrm{d}t} = \frac{\rho(t,N) - \beta}{\Lambda} N(t) + \sum_{i=1}^{m} \lambda_i C_i(t) + q(t) \quad (1)$$

$$\frac{\mathrm{d}C_i(t)}{\mathrm{d}t} = \frac{\beta_i}{\Lambda} N(t) - \lambda_i C_i(t) \text{ where, } i = 1,2,3\ldots m \quad (2)$$

by introducing the Newtonian feedback, reactivity can be represented as

$$\rho(t,N) = \rho_0(t) + B\int_0^t \mathrm{d}t\, N(t) \quad (3)$$

Here $N(t)$ is the neutron density or reactor power at time t, ρ – the reactivity, β – the total delayed neutron fraction, β_i – the fraction of the i-group of delayed neutrons, Λ – the prompt neutron generation time, Λ_i – the precursor decay constant of the i^{th} group, q – the external source, ρ_0 – the initial reactivity, and B – the absolute value of the temperature coefficient of reactivity. The above stiff non-linear ordinary differential equations are solved by MATLAB for five benchmark problems with step, ramp and sinusoidal reactivity insertions with and without temperature feedback. These benchmark problems are the same, which were solved by Ganapol and Nahla [1, 25].

MATLAB ODE suite for solving stiff differential equations

For scientific computing MATLAB software has inbuilt solvers to handle different classes of ordinary differential equations (ODE). A broad overview on the MATLAB ODE solvers along with the numerical procedures is given by Shampine and Reichelt [26]. In an initial value problem, the solution of interest is for $y' = F(t, y)$ which satisfies a specific initial condition $y = y_0$ at a given initial time t_0. The solvers for stiff problems allow the more general form $M(t)\,y' = f(t, y)$ with a mass matrix $M(t)$ that is non-singular and usually sparse. There are four special solvers designed dedicatedly to solve the stiff problems namely ODE15s, ODE23s, ODE23t, and ODE23tb. In this work the ODE15s solver has been used for solving the point kinetics equations. It is a variable order solver based on the numerical differentiation formulas (NDF), which is a modified form of the backward differentiation formulas (BDF). The various options used in the solver are mentioned in the following sections while dealing with the individual benchmark problems.

NUMERICAL RESULTS OF BENCHMARK PROBLEMS

As mentioned earlier, to substantiate the accuracy of the MATLAB ODE solver, five benchmarks are analyzed and the numerical results are compared mainly with those obtained by Ganapol through BEFD method. The results of Ganapol (hence forward referred to as BEFD results) are of specific interest as the numerical values are of very high precision (in some cases up to 19 decimal places for neutron density prediction). The basic kinetics data used in the five-benchmark cases pertaining to the three reactor systems are presented in tab. 1.

Benchmark-1: step reactivity insertion without feedback

In the first benchmark the variation of neutron density starting with an initial equilibrium value

Table 1. Reactor kinetics parameters used in the benchmarks

	Reactor-I		Reactor-II		Reactor-III	
i	β_i	λ_i [s^{-1}]	β_i	λ_i [s^{-1}]	β_i	λ_i [s^{-1}]
1	0.000285	0.0127	0.000266	0.0127	0.00021	0.0124
2	0.0015975	0.0317	0.001491	0.0317	0.00141	0.0305
3	0.001410	0.115	0.001316	0.115	0.00127	0.111
4	0.0030525	0.311	0.002849	0.311	0.00255	0.301
5	0.00096	1.40	0.000896	1.40	0.00074	1.13
6	0.000195	3.87	0.000182	3.87	0.00027	3.00
β	0.0075		0.007		0.00645	
Λ	$5\ 10^{-4}$ s		$2\ 10^{-5}$ s		$5\ 10^{-5}$ s	

Table 2. Neutron density for step reactivity insertions

Time [s]	ρ = –1 $		ρ = –0.5 $		ρ = +0.5 $	
	BEFD	MATLAB	BEFD	MATLAB	BEFD	MATLAB
1.0E–01	5.205642866E-01	5.205642866E-01	6.989252256E-01	6.989252256E-01	1.533112646E+00	1.533112646E+00
1.0E+00	4.333334453E-01	4.333334453E-01	6.070535656E-01	6.070535656E-01	2.511494291E+00	2.511494291E+00
1.0E+01	2.361106508E-01	2.361106508E-01	3.960776907E-01	3.960776907E-01	1.421502524E+01	1.421502524E+01
1.0E+02	2.866764245E-02	2.866764245E-02	7.158285444E-02	7.158285444E-02	8.006143562E+07	8.006143562E+07

Table 3. Neutron density for step reactivity insertion ρ = 1 $

Time [s]	BEFD	MATLAB
1.0E-01	2.5157661414043723001E+00	2.515766141404372E+00
5.0E-01	1.0362533810640214680E+01	1.036253381064022E+01
1.0E+00	3.2183540945534212174E+01	3.218354094553435E+01
1.0E+01	3.2469788980305281366E+09	3.246978898030739E+09
1.0E+02	2.5964846465508730749E+89	2.596484646556433E+89

N_0 = 1.0 is determined with time. The neutron density variation with time for 100 seconds in case of Reactor-I is calculated for step reactivity insertions of –1 $, –0.5 $, +0.5 $, and +1 $. It may be recalled here that, when reactivity ρ is expressed in units of effective delayed neutron fraction (β_{eff}) the unit is called "dollar" ($). Thus as per the SI unit, one dollar (1 $) of reactivity is equivalent to the effective delayed neutron fraction.

The results obtained by MATLAB are compared with the BEFD values in tabs. 2 and 3. It can be observed that for reactivity insertions of –1 $, –0.5 $, +0.5 $, the neutron densities calculated by MATLAB match exactly (up to 9 decimal places) with the BEFD results (tab. 2). In the case of reactivity insertion of 1 $, the results by BEFD method have been produced up to 19 decimal places by quadruple precision calculation. Due to limitations, in the present study the calculations are carried out by double precision only. Therefore, the results match up to 11-15 decimal places (emboldened in tab. 3). The relative and absolute tolerances considered in the MATLAB calculations are 10^{-12} and 10^{-8}, respectively.

Benchmark-2: ramp reactivity insertion without feedback

In the second benchmark a comparison is made for ramp reactivity insertion rate of 0.1 $/s without feedback in Reactor-II. The variation of neutron density with time, starting from N_0 = 1.0 are presented in tab. 4. In this case also a fair matching is observed between the MATLAB and BEFD results. Only at t = 11 s the MATLAB result differs at the 9$^{\text{th}}$ decimal place.

Benchmark-3: sinusoidal reactivity insertion without feedback

The third benchmark deals with a sinusoidal reactivity insertion without feedback in a fast reactor with β = 0.0079 (one delayed group), λ = 0.077 s^{-1}, Λ = = 10^{-8} s and a sinusoidal reactivity ρ τ ρ sin(t/T . In this benchmark, two cases are analysed. In the first case the neutron density with an initial value of N_0 = = 1.0 is calculated for ρ_0 = 0.0053333 and T = 50 s, the results of which are given in tab. 5. For comparison, the emboldened digits indicate the matching between the BEFD and MATLAB calculations. The second case is designed to determine accurately the time to the first peak (t_p) and the peak neutron density (N_p) for four different sinusoidal reactivity insertions given in tab. 6. In addition to BEFD and MATLAB methods, the results obtained by Nahla [25] through an efficient technique (referred to as ET in tab. 6) and also by power series solution (referred to as PWS in tab. 6) in an earlier work of Aboanber and Hamada [27] are also compared. Interestingly the peak neutron density values calculated by MATLAB match exactly with the BEFD values and the time to attain the first peak also matches fairly well *vis- a-vis* other methods. The variation of neutron densities over 1000 seconds for all the four values of T are shown in fig. 1 which was also posed as a challenge by Ganapol.

Table 4. Ramp reactivity insertion of 0.1 $/s

Time [s]	Neutron density	
	BEFD	MATLAB
2.0E+00	1.338200050E+00	1.338200050E+00
4.0E+00	2.228441897E+00	2.228441897E+00
6.0E+00	5.582052449E+00	5.582052449E+00
8.0E+00	4.278629573E+01	4.278629573E+01
1.0E+01	4.511636239E+05	4.511636239E+05
1.1E+01	1.792213607E+16	1.792213608E+16

Table 5. Neutron densities for sinusoidal reactivity variation

Time [s]	BEFD	MATLAB
10.0	2.065383519E+00	2.065383519E+00
20.0	8.854133921E+00	8.854133925E+00
30.0	4.064354222E+01	4.064354222E+01
40.0	6.135607517E+01	6.135607517E+01
50.0	4.610628770E+01	4.610628771E+01
60.0	2.912634840E+01	2.912634841E+01
70.0	1.895177042E+01	1.895177053E+01
80.0	1.393829211E+01	1.393829229E+01
90.0	1.253353406E+01	1.253353422E+01
100.0	1.544816514E+01	1.544816534E+01

Table 6. Time to first peak and peak densities

T [s]	$\rho_0\ 10^3$	BEFD		MATLAB		ET		PWS	
		t_p [s]	N_p	t_p [s]	N_p	t_p [s]	N_p	t_p [s]	N_p
50	5.3333	3.910712E+01	6.153015E+01	3.910719E+01	6.153015E+01	3.9111E+01	6.1531E+01	3.9112E+01	6.1530E+01
150	3.2327	1.373198E+02	9.581150E+01	1.373197E+02	9.581150E+01	1.3732E+02	9.5811E+01	1.3729E+02	9.5811E+01
250	2.3193	2.371265E+02	1.134679E+02	2.371265E+02	1.134679E+02	2.3712E+02	1.1346E+02	2.3715E+02	1.1346E+02
350	1.8083	3.370713E+02	1.238209E+02	3.370714E+02	1.238209E+02	3.3707E+02	1.2382E+02	3.3705E+02	1.2382E+02

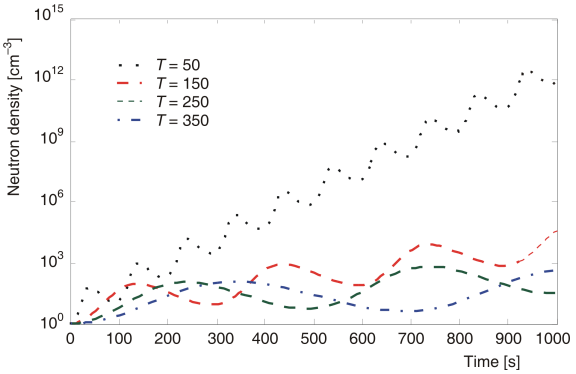

Figure 1. Neutron density variation for various values of *T*

Benchmark-4: step reactivity insertion with feedback

In the fourth benchmark, step reactivity insertion with temperature feedback is considered for Reactor-III. Like the previous cases, here the neutron density variation with time in steps of 10 s is determined for three step reactivity additions of 1.0 \$, 1.5 \$, and 2 \$ with a negative reactivity feedback (B = = 2.5 10^{-6}) as given in eq. 3. The results are compared in tab. 7. Further, the peak neutron density along with the time to attain the peak density for several step insertions with the same feedback is given in tab. 8. It may be noted that for ρ_0 = 0.1 \$, 0.2 \$, and 0.5 \$ the maximum time step taken is 10^{-5} s, where as for ρ_0 = = 1.0 \$, 1.2 \$, 1.5 \$, and 2 \$ the maximum time step taken is 10^{-6} s. As a completeness of the benchmark problem, the neutron density trace for several step reactivity insertions with feedback is also displayed in fig. 2. The more or less exact matching of the MATLAB results with that of BEFD is also observed in this benchmark.

Table 8. Time to first peak and peak density

ρ[\$]	t_p [s]		N_p	
	BEFD	MATLAB	BEFD	MATLAB
0.1	1.089694E+02	1.089694E+02	2.110490E+00	2.110490E+00
0.2	9.236818E+01	9.236818E+01	5.699818E+00	5.699818E+00
0.5	2.829469E+01	2.829469E+01	4.575243E+01	4.575243E+01
1.0	9.534776E-01	9.534770E-01	8.078681E+02	8.078681E+02
1.2	3.165970E-01	3.165970E-01	8.021025E+03	8.021025E+03
1.5	1.682894E-01	1.682890E-01	4.302461E+04	4.302460E+04
2.0	9.839055E-02	9.839040E-02	1.678457E+05	1.678457E+05

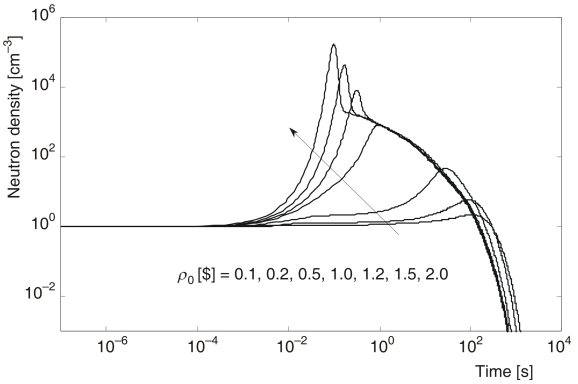

Figure 2. Neutron density variation for step reactivity insertions with feedback

Benchmark-5: ramp reactivity insertion with feedback

Benchmark-5 deals with a special case of reactivity feedback called power excursions with compen-

Table 7. Neutron density with reactivity feedback (B = 2.5 10^{-6})

Time [s]	N (for ρ = 1 \$)		N (for ρ = 1.5 \$)		N (for ρ = 2 \$)	
	BEFD	MATLAB	BEFD	MATLAB	BEFD	MATLAB
10	132.0385964	132.0385964	107.9116832	107.9116830	103.3808535	103.3808534
20	51.69986094	41.60428128	41.60428123	39.13886903	39.13886899	39.13886899
30	28.17468536	28.17468536	23.29893150	23.29893148	22.00377721	22.00377719
40	18.14633000	18.14632999	15.30342749	15.30342749	14.49367193	14.49367192
50	12.77957703	12.77957703	10.89014315	10.89014314	10.31861108	10.31861108
60	9.474932501	9.474932501	8.101031859	8.101031856	7.663319203	7.663319201
70	7.244477494	7.244477494	6.182690459	6.182690457	5.829395378	5.829395376
80	5.646289700	5.646289700	4.793307820	4.793307818	4.499427073	4.499427071
90	4.456834255	4.456834255	3.755614629	3.755614628	3.507422663	3.507422662
100	3.550102766	3.550102766	2.966074952	2.966074951	2.755126886	2.755126886

Table 9. Time to peak and peak neutron density for ramp initiated adiabatic compensation with Doppler

a [s^{-1}]	B [cm^3s^{-1}]	t_{peak} [s]		N_{peak}	
		BEFD	MATLAB	BEFD	MATLAB
0.1	10^{-11}	2.2466344E-01	2.2466300E-01	2.4203815E+11	2.4203803E+11
	10^{-13}	2.3890693E-01	2.3890700E-01	2.8986741E+13	2.8986728E+13
0.01	10^{-11}	1.1060774E+00	1.1060769E+00	2.0123519E+10	2.0123513E+10
	10^{-13}	1.1551476E+00	1.1551479E+00	2.4911782E+12	2.4911777E+12
0.003	10^{-11}	2.9105821E+00	2.9105820E+00	5.1141599E+09	5.1141589E+09
	10^{-13}	3.0076015E+00	3.0076010E+00	6.5344738E+11	6.5344729E+11
0.001	10^{-11}	7.4887663E+00	7.4887660E+00	1.2740752E+09	1.2740750E+09
	10^{-13}	7.6835876E+00	7.6835880E+00	1.7210080E+11	1.7210078E+11

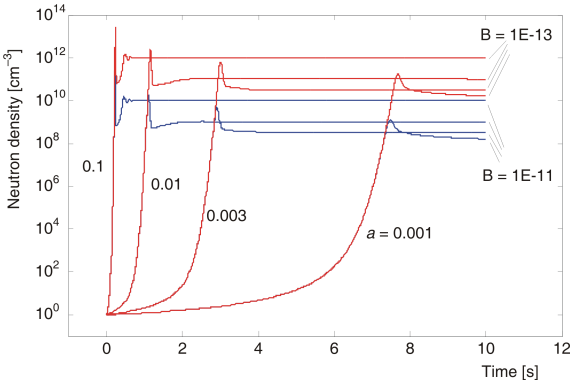

Figure 3. Compensated reactor shutdown by various ramp reactivity

sated response. This is a famous example of compensated reactor shutdown as demonstrated by Keepin [3, 28]. In this case a transient is initiated by ramp reactivity insertion with a ramp rate "*a*" where the reactivity compensation originates from strong Doppler feedback and thermal expansion. Using the kinetics data for Reactor-III, comprehensive feedback of a compensated reactor shutdown is analysed. The transient is initiated by ramp reactivity insertion with a ramp rate of "*a*" and strong Doppler shutdown "*B*". The peak neutron density and time to reach the peak neutron density is compared in tab. 9. The neutron density profiles for different ramp rates and reactivity feedback coefficients are shown in fig. 3 that perfectly match with the same obtained by the BEFD scheme. For determining the time to peak density accurately, the maximum time step considered in the calculation is 10^{-6} s. While analysing this benchmark Ganapol has pointed out the poor agreements between the BEFD results and that obtained by the PWS method in the work of Aboanber and Hamada [27]. As compared to the PWS method, a fair agreement of the BEFD and MATLAB results are observed in this work.

CONCLUSIONS

Although a plethora of numerical methods have been introduced to solve the point kinetics equations over the years, some of the simple and straightforward methods still work very efficiently with extraordinary accuracy. As an example, it has been shown recently that the fundamental BEFD algorithm with its simplicity has proven to be one of the most effective legacy methods. Complementing the BEFD scheme, in the present work advanced ordinary differential equation solvers based on the NDF available in the MATLAB software package are applied to solve the stiff reactor point kinetics equations with Newtonian temperature feedback effects. Five classical benchmark cases involving step, ramp and sinusoidal reactivity insertion have been analyzed and the results are compared with the earlier published BEFD results. Fair accuracy of the results implies the efficient application of MATLAB ODE suite for solving the reactor point kinetics equations as an alternate method for future applications.

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AUTHOR CONTRIBUTIONS

The research idea was originated by D. Mohapatra. The computational part was carried out by S. S. Singh. Both the authors together discussed and analyzed the results presented in the paper. The manuscript was written by D. Mohapatra and the figures were prepared by S. S. Singh.

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РЕШАВАЊЕ ЈЕДНАЧИНА ТАЧКАСТЕ КИНЕТИКЕ РЕАКТОРА СОФТВЕРСКИМ ПАКЕТОМ MATLAB

Нумеричко решавање једначина тачкасте кинетике са њутновском топлотном повратном спрегом изазовно је питање у анализи реакторских прелазних стања. Једначине тачкасте кинетике реактора представљају систем строгих ординарних диференцијалних једначина које захтевају посебне нумеричке поступке. Мада је током година уведено обиље сложених нумеричких поступака ради решавања једначина тачкасте кинетике, још увек су неке једноставне и директне методе делотворне са изузетном тачношћу. На пример, у скорије време показано је да једноставан фундаментални Ојлеров алгоритам коначних разлика представља један од најефикаснијих наслеђених метода. Допуњујући овај алгоритам, у овом раду се анализом различитих класичних тест случајева демонстрира изузетна применљивост процедуре за обичне диференцијалне једначине (ODE Suite), расположиве у софтверском пакету MATLAB, на решавање строгих једначина тачкасте кинетике реактора са утицајима њутновске топлотне повратне спреге. Прилична тачност резултата указује на ефикасну употребу MATLAB пакета за решавање једначина тачкасте кинетике реактора као алтернативне методе за будуће примене.

Кључне речи: једначина тачкасте кинетике, Ојлеров алгоритам коначних разлика, MATLAB, нумеричка диференцијација