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Thermal Analysis of Chemical Reactions with Exponential Heat Generation using Double Interpolation process

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Abstract: This study focuses on the thermal analysis of chemical reactions characterized by exponential heat generation, modeled using a reaction-diffusion equation. The non-linear nature of the heat generation, driven by temperature, reflects the rapid acceleration of reaction rates at higher temperatures. A double interpolation process is used to improve the precision of temperature distribution solutions over space and time. Starting from the classical heat equation with a reaction term, the analysis employs Dirichlet boundary conditions and a Gaussian initial temperature profile. The double interpolation method enhances solution accuracy, particularly in capturing steep temperature gradients caused by exponential heat generation. This approach is especially valuable for high-temperature chemical reactions, such as combustion, where precise thermal control is essential. The study's results provide insights into the thermal behavior of reactive systems, making it useful for applications like industrial reactors and heat-sensitive processes.

Keywords: Thermal analysis, chemical reactions, exponential heat generation, double interpolation process, reaction kinetics

I. INTRODUCTION

Thermal analysis of chemical reactions with exponential heat generation is a critical area of study in reaction kinetics and heat transfer. This process examines how chemical reactions generate heat and how that heat impacts the overall thermal behavior of the system. In many chemical processes, the rate of heat generation follows an exponential pattern, especially in reactions with strong temperature dependence, such as combustion or decomposition reactions. Understanding this thermal behavior is essential for controlling the reaction and preventing dangerous thermal runaway scenarios. The double interpolation process is a numerical technique used to approximate solutions in such complex systems, providing more accurate results by interpolating values at two stages of the computational grid. This method helps capture the non-linearities in heat generation and temperature distribution, ensuring a more precise analysis of transient thermal profiles. By applying this technique, researchers can better model the diffusion of heat, reaction rates, and energy conservation principles, offering a deeper understanding of thermal stability and process control in chemical reactions.

Jafari et al. (2016) demonstrated how this method could efficiently handle complex nonlinear systems, providing accurate and rapid convergence results. Their research focused on unsteady flow, particularly in scenarios involving chemical reactions and boundary conditions, contributing to a better understanding of how heat and mass transfer processes evolve in confined geometries. **Sobamowo (2016)** focused on heat transfer through extended surfaces, taking into account the non-linear nature of temperature dependency. Sobamowo's approach offered enhanced accuracy in predicting the thermal performance of fins, particularly under conditions where the heat generation rate varied with temperature. **Arbabi et al. (2017)** introduced a two-dimensional Haar wavelet method for solving systems of partial differential equations (PDEs). This method, known for its precision in numerical analysis, was applied to complex heat transfer and fluid dynamics problems. By using Haar wavelets, Arbabi and colleagues were able to efficiently approximate solutions to PDEs that describe the behavior of systems with varying boundary and initial conditions, enhancing computational efficiency in solving thermal and fluid flow equations. **Turkyilmazoglu (2018)**

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provided an efficient method to address heat conduction issues, particularly in finned surfaces, which are often used to improve heat dissipation in various applications. The paper showed that the decomposition method could be applied to a wide range of problems, including those with complex geometries and non-linear heat transfer properties. **Pasha et al. (2019)** applied to heat and mass transfer problems, focusing on overcoming the challenges of non-linearity and discontinuities in system behavior. This modification improved the convergence and accuracy of solutions, making the method applicable to a wider range of practical engineering problems. **Turkyilmazoglu (2019)** focused on overcoming the limitations of traditional decomposition techniques by introducing modifications that significantly improved the rate of convergence. This advancement is particularly useful in heat transfer problems where computational efficiency is paramount. **Nawaz and Arif (2020)** enhanced the capability of FEM to handle unsteady and reactive systems, offering a robust tool for solving complex fluid dynamics problems where both chemical reactions and heat transfer play a crucial role. **Waqas et al. (2020)** focused on analyzing how fluid properties, such as viscosity and thermal conductivity, change within the flow field, significantly affecting heat and mass transfer. The work introduced improvements in the double diffusion model, contributing to the understanding of chemically reactive non-Newtonian fluid systems.n **Nawaz et al. (2021)** addressed the challenges of modeling heat transfer in MHD flows, particularly in radiative and reactive environments. Their approach offered a higher-order accurate method to tackle complex interactions between heat, mass, and electromagnetic fields in such systems. **Nawaz et al. (2021)** additionally fostered an unequivocal fourth-request smaller mathematical plan to concentrate on the intensity move of limit layer stream. This high-order method allowed for more accurate resolution of boundary layer dynamics, crucial in applications involving high-temperature gradients and rapid fluid motion near surfaces. **Hayat et al. (2021)** used finite difference methods (FDM) to investigate nonlinear blended convective nanofluid stream with entropy age. In nanofluids, which are fluids containing nanoparticles, the interaction between fluid flow, heat transfer, and entropy production was the subject of this investigation. The study shed light on the thermal and energy efficiency of nanofluids in engineering systems. **Yang et al. (2021)** improved the accuracy and stability of numerical solutions for time-dependent heat conduction, especially in systems with complex geometries and boundary conditions. This work contributed to the field of heat transfer by offering a more precise method for handling transient heat conduction scenarios.

These studies collectively represent significant advancements in numerical methods and their applications to heat transfer, mass transfer, and fluid dynamics problems. Each approach provides valuable insights and tools for solving increasingly complex systems in engineering and physical sciences.

II. CHEMICAL REACTION WITH EXPONENTIAL HEAT GENERATION

In problems involving reaction-diffusion non-linearity where chemical reactions or heat generation depend on the temperature, we modify the classical heat equation to account for the non-linear effects. The general form of the reaction-diffusion equation is:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + f(u) \quad (1)$$

where:

$u(x,t)$ is the temperature at position x and time t,

α is the thermal diffusivity,

$\frac{\partial^2 u}{\partial x^2}$ is the Laplacian (representing spatial diffusion of heat),

$f(u)$ is the reaction term or heat generation term, which depends non-linearly on u. Here we consider exponential linearity e^u i.e. $f(u) = e^u$ (2)

This represents scenarios where the heat generation rate increases exponentially with temperature, often applicable in chemical reactions where higher temperatures lead to rapid increases in reaction rates.

Initial condition: If there is a localized heat source or reaction center, the initial temperature might be Gaussian:

$$u(x,0) = Ae^{-\frac{(x-x_0)^2}{2\sigma^2}} \quad (3)$$

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where A is the peak temperature, x_0 is the center of the heat source, and σ determines the spread of the temperature distribution.

Dirichlet Boundary Condition (fixed temperature at the boundaries):

$$u(0,t) = u(1,t) = 0 \quad (4)$$

This would represent a situation where the boundaries are held at a fixed temperature (e.g., 0).

III. IMPLEMENTATION OF DOUBLE INTERPOLATION PROCESS

Using the double interpolation method, we may now solve equation (1) in addition to conditions (2) and (3), and we obtain

The difference interval of x as *0.2*, denoted as $h = 0.2$
Calculating the duration of t

$$k = \frac{h^2}{2c^2} = \frac{(0.2)^2}{2} = 0.02 \quad (5)$$

Thus $x_0 = 0, x_1 = 0.2, x_2 = 0.4, x_3 = 0.6, x_4 = 0.8, x_5 = 1$
$t_0 = 0, t_1 = 0.02, t_2 = 0.04, t_3 = 0.06, t_4 = 0.08, t_5 = 0.1$
Initially we solve the proposed using the Crank Nicolson method, we discretize both the time and space variables.

Let $x_i = i\Delta x$ (6)

where $i = \Delta x$, where $i = 0,1,2, \ldots N$ and $\Delta x = \frac{1}{N}$

$t^n = n\Delta t$, where $n = 0,1,2 \ldots$ (7)

The Crank-Nicolson method is a combination of the implicit and explicit methods. The temporal derivative $\frac{\partial u}{\partial t}$ at time $t_{n+1/2}$ (midpoint) is approximated as:

$$\frac{\partial u}{\partial t} \approx \frac{u_i^{n+1} - u_i^n}{\Delta t} \quad (8)$$

The second spatial derivative $\frac{\partial^2 u}{\partial x^2}$ is approximated using a central difference scheme, and the average at n and $n+1$ time steps is used:

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{(\Delta x)^2} + \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \quad (9)$$

Thus, the Crank-Nicolson scheme for the reaction-diffusion equation (1) becomes:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha\left[\frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{(\Delta x)^2} + \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}\right] + \frac{1}{2}\left[e^{u_i^{n+1}} + e^{u_i^n}\right] \quad (10)$$

Rearrange the equation so that terms involving u_i^{n+1} are on one side and terms involving u_i^n are on the other. This results in a system of linear equations that can be written in matrix form as:

$$Au^{n+1} = Bu^n + F \quad (11)$$

Where:

A is a tridiagonal matrix with coefficients from the Crank-Nicolson scheme for the u_i^{n+1} terms.

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B is a tridiagonal matrix with coefficients from the u_i^n terms.

u^n is the vector of temperatures at time step n.

F accounts for the nonlinear term e^u.

For the boundary conditions: $u_0^n = u_N^n = 0$ for all n (12)

For the initial condition: $u_i^0 = \mathrm{Ae}^{-\frac{(x_i - x_0)^2}{2\sigma^2}}$ (13)

Assuming $A = 1$, $x_0 = 0.5$, and $\sigma = 0.1$

Table 1

	x=0.0	x=0.2	x=0.4	x=0.6	x=0.8	x=1.0
t=0.00	0	0.011108997	0.60653066	0.60653066	0.011108997	0
t=0.02	0	0.181035887	0.417019832	0.417019832	0.181035887	0
t=0.04	0	0.194066978	0.337371933	0.337371933	0.194066978	0
t=0.06	0	0.176986143	0.287843865	0.287843865	0.176986143	0
t=0.08	0	0.156609081	0.250093756	0.250093756	0.156609081	0
t=0.10	0	0.138231843	0.219297605	0.219297605	0.138231843	0

Table 2

u_{1i}	$\Delta^{0+1}u_{1i}$	$\Delta^{0+2}u_{1i}$	$\Delta^{0+3}u_{1i}$	$\Delta^{0+4}u_{1i}$	$\Delta^{0+5}u_{1i}$
0.011108997	0.16992689	-0.156895799	0.126783873	-0.099968174	0.078448526
0.181035887	0.013031091	-0.030111926	0.026815699	-0.021519648	
0.194066978	-0.017080835	-0.003296227	0.005296051		
0.176986143	-0.020377062	0.001999824			
0.156609081	-0.018377238				
0.138231843					

Table 3

u_{2i}	$\Delta^{0+1}u_{2i}$	$\Delta^{0+2}u_{2i}$	$\Delta^{0+3}u_{2i}$	$\Delta^{0+4}u_{2i}$	$\Delta^{0+5}u_{2i}$
0.60653066	-0.189510828	0.109862929	-0.079743098	0.061401226	-0.047883355
0.417019832	-0.079647899	0.030119831	-0.018341872	0.013517871	
0.337371933	-0.049528068	0.011777959	-0.004824001		
0.287843865	-0.037750109	0.006953958			
0.250093756	-0.030796151				
0.219297605					

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Table 4

u_{3i}	$\Delta^{0+1}u_{3i}$	$\Delta^{0+2}u_{3i}$	$\Delta^{0+3}u_{3i}$	$\Delta^{0+4}u_{3i}$	$\Delta^{0+5}u_{3i}$
0.60653066	-0.189510828	0.109862929	-0.079743098	0.061401226	-0.047883355
0.417019832	-0.079647899	0.030119831	-0.018341872	0.013517871	
0.337371933	-0.049528068	0.011777959	-0.004824001		
0.287843865	-0.037750109	0.006953958			
0.250093756	-0.030796151				
0.219297605					

Table 5

u_{4i}	$\Delta^{0+1}u_{4i}$	$\Delta^{0+2}u_{4i}$	$\Delta^{0+3}u_{4i}$	$\Delta^{0+4}u_{4i}$	$\Delta^{0+5}u_{4i}$
0.011108997	0.16992689	-0.156895799	0.126783873	-0.099968174	0.078448526
0.181035887	0.013031091	-0.030111926	0.026815699	-0.021519648	
0.194066978	-0.017080835	-0.003296227	0.005296051		
0.176986143	-0.020377062	0.001999824			
0.156609081	-0.018377238				
0.138231843					

Table 6

u_{i0}	$\Delta^{1+0}u_{i0}$	$\Delta^{2+0}u_{i0}$	$\Delta^{3+0}u_{i0}$	$\Delta^{4+0}u_{i0}$	$\Delta^{5+0}u_{i0}$
0	0.011108997	0.584312666	-1.179734329	1.179734329	0
0.011108997	0.595421663	-0.595421663	0	1.179734329	
0.60653066	0	-0.595421663	1.179734329		
0.60653066	-0.595421663	0.584312666			
0.011108997	-0.011108997				
0					

Table 7

u_{i1}	$\Delta^{1+0}u_{i1}$	$\Delta^{2+0}u_{i1}$	$\Delta^{3+0}u_{i1}$	$\Delta^{4+0}u_{i1}$	$\Delta^{5+0}u_{i1}$
0	0.181035887	0.054948058	-0.290932003	0.290932003	0
0.181035887	0.235983945	-0.235983945	0	0.290932003	
0.417019832	0	-0.235983945	0.290932003		
0.417019832	-0.235983945	0.054948058			
0.181035887	-0.181035887				
0					

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Table 8

u_{i2}	$\Delta^{1+0}u_{i2}$	$\Delta^{2+0}u_{i2}$	$\Delta^{3+0}u_{i2}$	$\Delta^{4+0}u_{i2}$	$\Delta^{5+0}u_{i2}$
0	0.194066978	-0.050762023	-0.092542932	0.092542932	0
0.194066978	0.143304955	-0.143304955	0	0.092542932	
0.337371933	0	-0.143304955	0.092542932		
0.337371933	-0.143304955	-0.050762023			
0.194066978	-0.194066978				
0					

Table 9

u_{i3}	$\Delta^{1+0}u_{i3}$	$\Delta^{2+0}u_{i3}$	$\Delta^{3+0}u_{i3}$	$\Delta^{4+0}u_{i3}$	$\Delta^{5+0}u_{i3}$
0	0.176986143	-0.066128421	-0.044729301	0.044729301	0
0.176986143	0.110857722	-0.110857722	0	0.044729301	
0.287843865	0	-0.110857722	0.044729301		
0.287843865	-0.110857722	-0.066128421			
0.176986143	-0.176986143				
0					

Table 10

u_{i4}	$\Delta^{1+0}u_{i4}$	$\Delta^{2+0}u_{i4}$	$\Delta^{3+0}u_{i4}$	$\Delta^{4+0}u_{i4}$	$\Delta^{5+0}u_{i4}$
0	0.156609081	-0.063124406	-0.030360269	0.030360269	0
0.156609081	0.093484675	-0.093484675	0	0.030360269	
0.250093756	0	-0.093484675	0.030360269		
0.250093756	-0.093484675	-0.063124406			
0.156609081	-0.156609081				
0					

Table 11

u_{i5}	$\Delta^{1+0}u_{i5}$	$\Delta^{2+0}u_{i5}$	$\Delta^{3+0}u_{i5}$	$\Delta^{4+0}u_{i5}$	$\Delta^{5+0}u_{i5}$
0	0.138231843	-0.057166081	-0.023899681	0.023899681	0
0.138231843	0.081065762	-0.081065762	0	0.023899681	
0.219297605	0	-0.081065762	0.023899681		
0.219297605	-0.081065762	-0.057166081			
0.138231843	-0.138231843				
0					

Since both the First and the Last Column of Table 1 contain 0, this means that

$\Delta^{0+1}u_{00} = \Delta^{0+2}u_{00} = \Delta^{0+3}u_{00} = \Delta^{0+4}u_{00} = \Delta^{0+5}u_{00} = 0$

And $\Delta^{0+1}u_{50} = \Delta^{0+2}u_{50} = \Delta^{0+3}u_{50} = \Delta^{0+4}u_{50} = \Delta^{0+5}u_{50} = 0$

From Table 2, we get

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$\Delta^{0+1}u_{10} = 0.16992689, \Delta^{0+2}u_{10} = -0.1568958, \Delta^{0+3}u_{10} = 0.126783873, \Delta^{0+4}u_{10} = -0.09996817, \Delta^{0+5}u_{10} = 0.078448526$

From Table 3

$\Delta^{0+1}u_{20} = -0.18951083, \Delta^{0+2}u_{20} = 0.109862929, \Delta^{0+3}u_{20} = -0.0797431, \Delta^{0+4}u_{20} = 0.061401226, \Delta^{0+5}u_{20} = -0.047883355$

From Table 4

$\Delta^{0+1}u_{30} = -0.18951083, \Delta^{0+2}u_{30} = 0.109862929, \Delta^{0+3}u_{30} = -0.0797431, \Delta^{0+4}u_{30} = 0.061401226, \Delta^{0+5}u_{30} = -0.047883355$

From Table 5

$\Delta^{0+1}u_{40} = 0.16992689, \Delta^{0+2}u_{40} = -0.1568958, \Delta^{0+3}u_{40} = 0.126783873, \Delta^{0+4}u_{40} = -0.09996817, \Delta^{0+5}u_{40} = 0.078448526$

From Table 6

$\Delta^{1+0}u_{00} = 0.011108997, \Delta^{2+0}u_{00} = 0.584312666, \Delta^{3+0}u_{00} = -1.17973433, \Delta^{4+0}u_{00} = 1.179734329, \Delta^{5+0}u_{00} = 0$

From Table 7

$\Delta^{1+0}u_{01} = 0.181035887, \Delta^{2+0}u_{01} = 0.054948058, \Delta^{3+0}u_{01} = -0.290932003, \Delta^{4+0}u_{01} = 0.290932003, \Delta^{5+0}u_{01} = 0$

From Table 8

$\Delta^{1+0}u_{02} = 0.194066978, \Delta^{2+0}u_{02} = -0.05076202, \Delta^{3+0}u_{02} = -0.092542932, \Delta^{4+0}u_{02} = 0.092542932, \Delta^{5+0}u_{02} = 0$

From Table 9

$\Delta^{1+0}u_{03} = 0.176986143, \Delta^{2+0}u_{03} = -0.06612842, \Delta^{3+0}u_{03} = -0.0447293, \Delta^{4+0}u_{03} = 0.044729301, \Delta^{5+0}u_{03} = 0$

From Table 10

$\Delta^{1+0}u_{04} = 0.156609081, \Delta^{2+0}u_{04} = -0.06312441, \Delta^{3+0}u_{04} = -0.03036027, \Delta^{4+0}u_{04} = 0.030360269, \Delta^{5+0}u_{04} = 0$

From Table 11

$\Delta^{1+0}u_{05} = 0.138231843, \Delta^{2+0}u_{05} = -0.05716608, \Delta^{3+0}u_{05} = -0.023899968, \Delta^{4+0}u_{05} = 0.023899681, \Delta^{5+0}u_{05} = 0$

$\Delta^{1+1}u_{00} = \Delta^{1+0}u_{01} - \Delta^{1+0}u_{00} = 0.16992689$

$\Delta^{1+2}u_{00} = \Delta^{1+0}u_{02} - 2\Delta^{1+0}u_{01} + \Delta^{1+0}u_{00} = -0.1568958$

$\Delta^{2+1}u_{00} = \Delta^{2+0}u_{01} - \Delta^{2+0}u_{00} = -0.529364608$

$\Delta^{3+1}u_{00} = \Delta^{3+0}u_{01} - \Delta^{3+0}u_{00} = 0.888802327$

$\Delta^{1+3}u_{00} = \Delta^{1+0}u_{03} - 3\Delta^{1+0}u_{02} + 3\Delta^{1+0}u_{01} - \Delta^{1+0}u_{00} = 0.126783873$

$\Delta^{2+2}u_{00} = \Delta^{2+0}u_{02} - 2\Delta^{2+0}u_{01} + \Delta^{2+0}u_{00} = 0.42365453$

$\Delta^{1+4}u_{00} = \Delta^{1+0}u_{04} - 4\Delta^{1+0}u_{03} + 6\Delta^{1+0}u_{02} - 4\Delta^{1+0}u_{01} + \Delta^{1+0}u_{00} = -0.09996817$

$\Delta^{4+1}u_{00} = \Delta^{4+0}u_{01} - \Delta^{4+0}u_{00} = -0.888802326$

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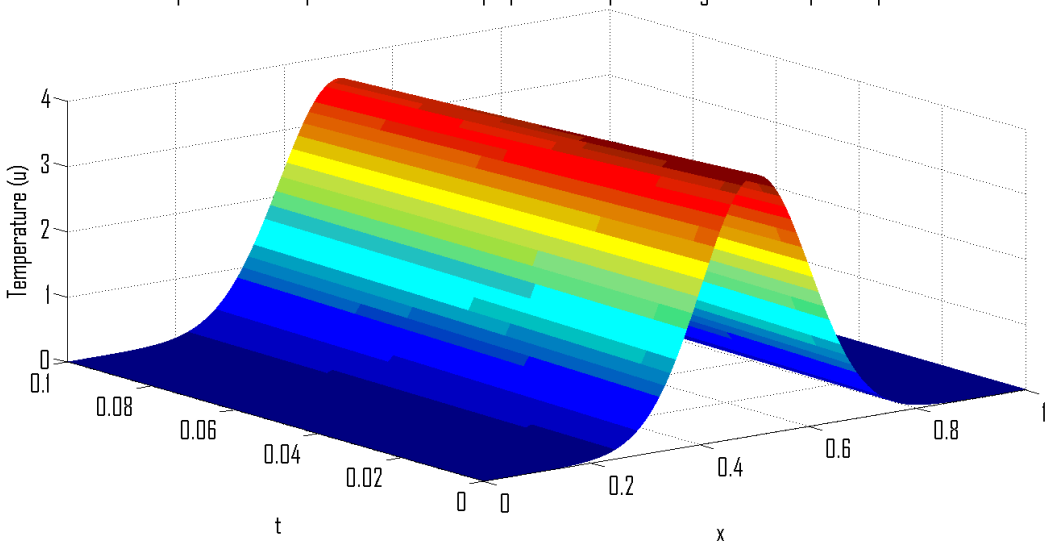
$$\Delta^{3+2}u_{00} = \Delta^{3+0}u_{02} - 2\Delta^{3+0}u_{01} + \Delta^{3+0}u_{00} = -0.690413256$$

$$\Delta^{2+3}u_{00} = \Delta^{2+0}u_{03} - 3\Delta^{2+0}u_{02} + 3\Delta^{2+0}u_{01} - \Delta^{2+0}u_{00} = -0.333310852$$

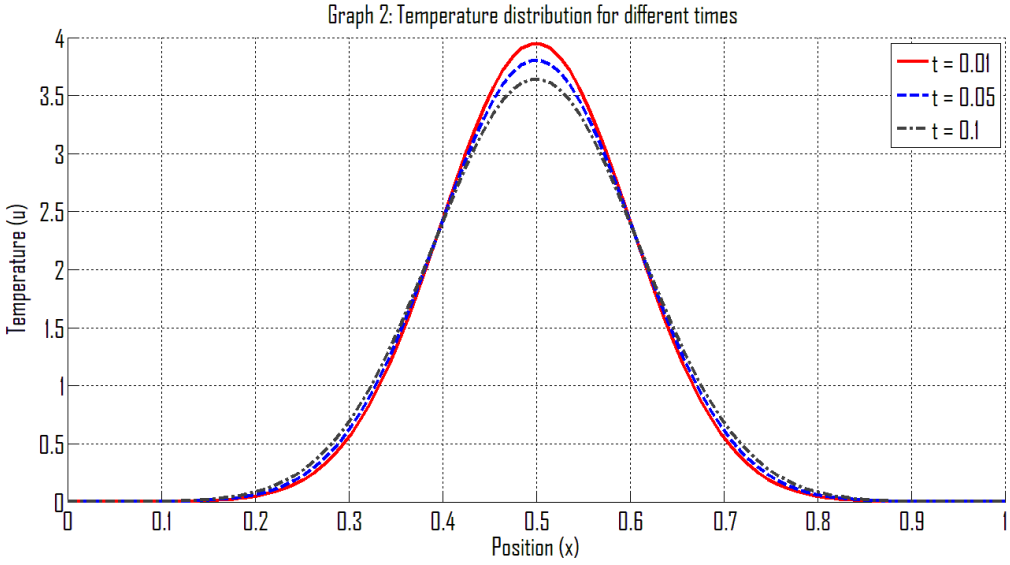
$$u(x,t) = 0.055544985\,x + 8.4963445t + 7.303908325x(x-0.2) + 42.48111375xt - 196.11975t(t-0.02) - 24.57779854x(x-0.2)(x-0.4) - 33.085288xt(x-0.2) - 98.059875xt(t-0.02) + 2641.434854t(t-0.02)(t-0.04) \quad (14)$$

IV. RESULTS AND DISCUSSION

Graph 1: 3D surface plot of the solution of propsed heat equation using double interpolation process



Graph 2: Temperature distribution for different times



The graph (1) depicts a 3D surface plot showing the solution of a heat equation using a double interpolation process. The axes represent position (x), time (t), and temperature (u). The surface plot illustrates how the temperature evolves over time across the spatial domain. The initial heat distribution, shown by higher temperature values near the middle of the spatial domain at earlier times, gradually diffuses outward, lowering the peak temperature as time progresses. This diffusion effect aligns with the behavior of solutions to heat equations, where thermal energy spreads over time due to the heat conduction process. The double interpolation method used in this solution helps to improve the smoothness and accuracy of the temperature distribution over both space and time, as evidenced by the gradient in the surface colors, which transition smoothly from high temperatures (red) to lower ones (blue). The plot effectively

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demonstrates how temperature decreases and spreads over the spatial domain as time increases, consistent with the heat diffusion phenomenon.

The three curves in graph (2), each corresponding to a different time, show the evolution of the temperature profile. Initially, at $t = 0.01$ (red solid line), the temperature distribution has a sharp peak near the center of the domain, indicating a high concentration of heat at that location. As time progresses, for $t = 0.05$ (blue dashed line) and $t = 0.1$ (black dash-dotted line), the temperature distribution broadens and the peak temperature decreases. This behavior is typical in heat diffusion processes, where the heat spreads out over time, causing the central peak to flatten and the temperature to equilibrate across the domain. The graph effectively demonstrates the spreading of heat and the reduction of peak temperature over time.

V. CONCLUDING REMARKS

In conclusion, the thermal analysis of chemical reactions with exponential heat generation, utilizing the double interpolation process, provides significant insights into the complex interplay between heat generation, reaction kinetics, and thermal behavior. By applying the double interpolation technique, more accurate and stable numerical solutions can be achieved, enabling precise modeling of temperature distribution and heat transfer in systems where reactions are highly sensitive to temperature changes. This approach is particularly valuable for understanding and preventing thermal runaway in exothermic reactions, improving process safety and efficiency. The ability to capture non-linear thermal behaviors and accurately simulate the dynamic evolution of temperature profiles further enhances the reliability of this method in practical applications. Ultimately, this analysis offers a robust framework for optimizing chemical processes, ensuring thermal stability, and advancing the design of safer and more efficient reaction systems.

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