Approximate Analytic Solution of a problem of diffusion, using Intelligent CAS

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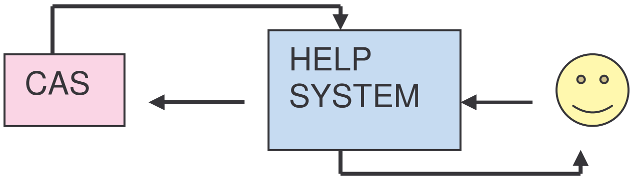
Abstract: Using a help system to make easier the CAS-user connection, we propose the problem of solving the equation of diffusion with variable coefficients. We transform the problem at the Laplace domain and we use the Bromwich integral and the residue theorem in order to do the inverse Laplace transform and then explicit solution is obtained.

Keywords: Help system, CAS, diffusion equation, Residue Theorem, Laplace transformed.

1. Introduction



Despite the advantages that the CAS systems *[2],[8]* provides to make high level mathematical developments, it becomes a serious problem when various different commands are used to solve mathematical expressions, because it may take more time to learn how to use the CAS, than making the operation manually.

These kind of problems could be easily solved by an Intelligent help system *[1]* that could interpret the characters that the user writes on a TOUCHPAD (like the ones used in tablet pc, palm pilots, laptops, etc), so that, the help system requires a software able to translate this characters into commands.

This kind of help makes much easier and faster the general manipulation of the CAS, not only CAS give us the possibility of taking advantage of the highly speed computers, but also we may avoid the whole process of learning the software.

Another advantage is that we will be able to solve differential equations as the one shown in this paper.

Concretely in this work we presented a method of symbolic solution with CAS for the following diffusion-reaction with reaction memory integral-differential equation [4], [5], [6]

(1)

$$\left(\frac{\partial}{\partial t} C(r,t)\right) - \frac{\xi(t)\left(\left(\frac{\partial}{\partial r} C(r,t)\right) + r\left(\frac{\partial^2}{\partial r^2} C(r,t)\right)\right)}{r} - \delta(t)\, C(r,t) \qquad -\delta_1(t)\int_0^t M(t-\tau)\, C(r,\tau)\, d\tau = 0$$

with the initial condition

$$C(r,0) = 0 \tag{2}$$

and with the boundary conditions

$$C(r,a) = C_b\, \mathbf{e}^{(\beta t)} \tag{3}$$

Where C(r,t) represents the concentration of a determined substance at a circle of radius r at time t.
The equation (1) represents a chemical or nuclear reactor in which a determined substance is produced to a variable rate in the time denoted δ(t), being δ_1(t) the parameter of the reaction memory, corresponding to a function of memory denoted M(t); and being ξ(t) the diffusivity of the substance, assumed to be time dependant. The equation (2) expresses that initially there is no substance present in the reactor and the equation (3) indicates that the substance reactivates is spread from the boundary of the reactor towards the center, being C_b the concentration of the substance in the border and β it is the growth or decrease rate of the boundary concentration.
The question here is analytically to solve the equation (1) with the conditions (2) and (3) using symbolic computation assisted by CAS, with the object of describe the concentration of substances in a circular reactor.

2. Methods

Given the equation (1) we try to solve it, but first we have to solve the equation with constants coefficients and when we got it, just do the substitution of the coefficients. Like the equation with the variable coefficients can not be solved analytically despite to be linear, we use here an approximate analytical method that consist in the application of the Laplace transform technique to (4) assuming constant parameters and afterward the effect of variable coefficients is incorporated.

$$\left(\frac{\partial}{\partial t} C(r,t)\right) - \frac{\xi\left(\left(\frac{\partial}{\partial r} C(r,t)\right) + r\left(\frac{\partial^2}{\partial r^2} C(r,t)\right)\right)}{r} - \delta\, C(r,t) \qquad -\delta_1\int_0^t M(t-\tau)\, C(r,\tau)\, d\tau = 0 \tag{4}$$

The Laplace transformed solution of (4) with (2) and (3) is

$$\Gamma_1(r,s) = -\frac{C_0\, J_0(\lambda(s)\, r)}{J_0(\lambda(s)\, a)\,(-s+\beta)} \tag{5}$$

Where the function λ(s) is given by:

$$\sqrt{\frac{-s+\delta+\delta_1\,\mu(s)}{\xi}} = \lambda(s) \tag{6}$$

being μ(s) the Laplace transform of the reaction memory function.

Now to consider the time dependency of the coefficients of (1), we do the substitutions on (6) by the form

$$\begin{aligned} \delta &= \Delta(s) \\ \delta_1 &= \Delta_1(s) \\ \xi &= \Xi(s) \end{aligned} \tag{7}$$

We get $\Delta(s)$, $\Delta_1(s)$ and $\Xi(s)$ after applying the Laplace transform to the coefficients $\delta(t)$, $\delta_1(t)$ and $\zeta(t)$ respectively

we obtain the following kernel

$$\sqrt{\frac{-s + \Delta(s) + \Delta_1(s)\,\mu(s)}{\Xi(s)}} = \Lambda(s) \tag{8}$$

now having (8) we can replace it in (5) and obtain the Laplace transformed solution with the coefficients variables

$$\Gamma_1(r, s) = -\frac{C_0\, J_0(\Lambda(s)\, r)}{J_0(\Lambda(s)\, a)\,(-s + \beta)} \tag{9}$$

Finally, in the CAS we apply the Bromwich integral and the residues theorem **[7]** to obtain the inverse Laplace transform of (5) and (9)

3. Results

We consider now the solution of (4) with conditions (2) and (3)

$$\mathrm{C}(r, t) = \frac{C_0\, J_0(\lambda(\beta)\, r)\, \mathrm{e}^{(\beta t)}}{J_0(\lambda(\beta)\, a)} + \left(\sum_{n=1}^{\infty} \left(\sum_{i=1}^{m} \left(-\frac{C_0\, J_0\!\left(\frac{\alpha_n r}{a}\right) \mathrm{e}^{(S_{i,n} t)}}{(S_{i,n} - \beta)\, J_1(\alpha_n) \left(\frac{d}{dS_{i,n}} \lambda(S_{i,n}) \right) a} \right) \right) \right) \tag{10}$$

where $S_{i,n}$ are the roots f the following equation

$$\lambda(s)\, a = \alpha_n \tag{11}$$

and being *m* the degree of (11) and α_n the zeroes of Bessel function $J_0(x)$ [3].

The solution for the case of the variable coefficients is given by:

$$\mathrm{C}(r, t) = \frac{C_0\, J_0(\Lambda(\beta)\, r)\, \mathrm{e}^{(\beta t)}}{J_0(\Lambda(\beta)\, a)} + \left(\sum_{n=1}^{\infty} \left(\sum_{i=1}^{M} \left(-\frac{C_0\, J_0\!\left(\frac{\alpha_n r}{a}\right) \mathrm{e}^{(S_{i,n} t)}}{(S_{i,n} - \beta)\, J_1(\alpha_n) \left(\frac{d}{dS_{i,n}} \Lambda(S_{i,n}) \right) a} \right) \right) \right) \quad 12$$

where now $S_{i,n}$ are the roots f the equation

$$\Lambda(s)\, a = \alpha_n \tag{13}$$

and being *M* the degree of (13).

4. Analysis of results

The solution (10) shows explosive behavior only when $S_{i,n}>0$, it means that, according to (11) and (6) when the equation

$$\sqrt{\frac{-s + \delta + \delta_1\, \mu(s)}{\xi}}\; a = \alpha_n \tag{14}$$

has a positive and real solution.

Similarly, the solution (12) shows explosive behavior only when $S_{i,n}>0$, it means that, according to (8) and (13) when the equation

$$\sqrt{\frac{-s + \Delta(s) + \Delta_1(s)\, \mu(s)}{\Xi(s)}}\; a = \alpha_n \tag{15}$$

has a positive and real solution.

5. Discussion and conclusions

We have presented and proposed in this work a method for approximate solution to reaction-diffusion equation with memory and transport coefficients variable on time. Such method is implemented using a general design of a help system for aid the users of Computer Algebra Systems.
The reason for to use *Help system* is that the user is able to do calculations easily.
For example, if it is necessary to calculate the diffusion equation solution, the user first would have to type the equation and then give the instruction to do the Laplace transform, after that, the equation is solved in Laplace domain and finally realize the inverse transform to obtain the solution.

References

[1] SANTOS, Renato P., and ROQUE, Waldir L., *An Expert Help System for Computer Algebra Systems*, internal report, Institut für Algorithmen und Kognitive Systeme, Universität Karlsruhe, 1990.
[2] www.maplesoft.com
[3] Frank Bowman, Introduction to Bessel Functions, Dover Publications Inc, New York, 1958
[4] Bird R.B., Stewart W.E., and Lightfoot E. N., Transport Phenomena, 2nd edition, John Wiley, New York, 2002.
[5] Problem Solutions in Transport Phenomena: Heat Transfer Problems. www.syvum.com/eng/heat/
[6] Problem Solutions in Transport Phenomena:Mass Transfer Problems. www.syvum.com/eng/mass
[7] Apostol T., *Análisis matemático*, Editorial Reverté, 1988
[8] en www.wikipedia.org/wiki/Computer_algebra_system