

# Schematic Symbolic Solution of a Reaction-Diffusion Equation with Memory inside a Circular Reactor

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*Abstract:* - Certain work about symbolic computational mass transfer is realized. Using computer algebra, the explicit solution for a reaction-diffusion equation with memory and boundary conditions for a circular reactor, is derived. The method of solution is the Laplace Transform Technique with inverse by residues. The solution is obtained by means of certain algorithm for computer algebra. As a result we obtain the basic reproductive number for the reactor. We conclude that the transport problem that was considered, to despite to be linear, is symbolically non-computable due to the effects of the memory.

*Key-Words:* - Reaction-diffusion equation, Residue Theorem, Computer Algebra, Memory, Amplification, Basic Reproductive Number, Threshold, Bessel Functions, non-computable problem

## 1 Introduction

We consider certain reaction-transport process with memory for the case a circular reactor. The mathematical model that we use, is a linear reaction-diffusion equation with memory and external sources. The effective transport equation considered here, is a linear and in-homogeneous integral-differential equation subjected to determined boundary condition of the Dirichlet kind. Such equation to despite to be linear, is very complicated and its solution is very hard to obtain when the only way is using pen and paper. From other side, such equation can not be solved using the method of separation of variables.

Here we show that the solution of our linear model can be obtained at symbolical form, when we use certain relatively simple algorithm for computer algebra.

Our algorithm is based on the Laplace transform technique, jointly with the realization of the inverse transform by mean of residue theorem of the theory of functions of complex variable.

From the solution that is obtained, the basic reproductive rate for the reactor is derived.

Is remarkable that our problem, to despite to be linear and with algorithmic solution, is after all non-computable symbolically is only computable numerically. We have an example of non-computable linear problem.

## 2 The Mathematical Problem

Here we consider certain “chemical” reaction of the form



We assume that we have a solid disk of radius  $a$  which is made of the substance A. Then we attach at the boundary of disk, certain ring of substance B, and the reaction (1) starts. Our problem is to obtain a mathematical formula for the evolution on time of the concentration of substance B inside the solid disk, and to derive the threshold condition for the reaction (1) effectively occurs.

We consider here, the following transport equation for the substance B [1, 2, 3]

$$\left(\frac{\partial}{\partial t} u(r, t)\right) - \delta \Delta^2 u(r, t) - \kappa u(r, t) - M_1(r, t) + M_2(r, t) + F(r) = 0 \quad (2)$$

where the mass transport of substance B, is realized within a circular region of radius  $a$  with polar coordinates  $(r, \theta)$ ; and  $u(r, t)$  denotes the concentration of the substance B, at place  $r$  at time  $t$ . The Laplacian operator for polar coordinates reads

$$\Delta^2 u(r, t) = \frac{\left(\frac{\partial}{\partial r} u(r, t)\right) + r \left(\frac{\partial^2}{\partial r^2} u(r, t)\right)}{r} \quad (3)$$

for the case of axial symmetry, which is assumed. The constant  $\kappa$  is the effective rate of production of the substance B, and has the following structure:

$$\kappa = \beta_1 S_0 - \gamma_1 \tag{4}$$

where  $\beta_1$  is reactivity of substance A,  $S_0$  is the initial density of the solid disk of substance A and  $\gamma_1$  is rate of decaying of substance B that produces substance C.

We assume that the reaction (1) has memory and this memory is of two kinds to know:  $M_1(r,t)$  denotes the memory of reactivity of substance A relative to the substance B, and is given by

$$M_1(r, t) = \beta_2 S_0 \int_0^t u(r, \tau) (t - \tau) e^{(-\epsilon_1(t-\tau))} d\tau \tag{5}$$

where  $\beta_2$  is the intensity of the memory of reactivity and  $\epsilon_1$  is the factor of attenuation of such memory. From the other side  $M_2(r,t)$  denotes the memory of production of substance C, relative to the substance B, and is given by

$$M_2(r, t) = \gamma_2 \int_0^t u(r, \tau) (t - \tau) e^{(-\epsilon_2(t-\tau))} d\tau \tag{6}$$

where  $\gamma_2$  is the intensity of the memory of production of substance C and  $\epsilon_2$  is the factor of attenuation of this memory.

We also assume that apart of the ring of substance B attached to the boundary of the solid disk of substance A, we have a permanent source of substance B, denoted  $F(r)$ , inside the disk with the distribution:

$$F(r) = a_1 + a_3 r^2 \tag{7}$$

where  $a_1$  and  $a_3$  are certain constants.

The initial condition is the corresponding to the case when initially the solid disk only contains substance A, it is to say:

$$u(r, 0) = 0 \tag{8}$$

The boundary condition is the corresponding to the presence of the ring of substance B and reads

$$u(a, t) = \mu_b e^{(-\eta t)} \tag{9}$$

where  $\mu_b$  is the density of the ring and  $\eta$  is constant of decay of the substance B on the ring.

The mathematical that is proposed here, is the solution of the equation (2) with (3)-(7), subjected to the initial condition (8) and to the boundary condition (9).

### 3 Problem Solution

Our problem is a linear problem analytically soluble, but our problem can not be solved by means of the

method of separation of variables. It is necessary to apply the Laplace Transform method, and to make the inverse transform by means of the theorem of residues [4]. Since the equations (2)-(9) are too voluminous like being solved by hand with pencil and paper, it is necessary to apply some type of system of computer algebra that allows symbolic computation [5,6].

#### 3.1. Method of Solution

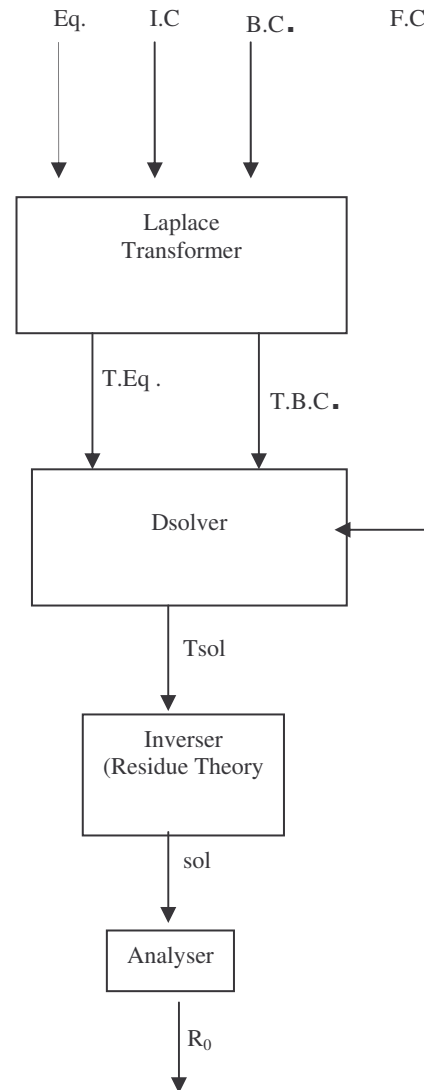


Figure 1. sketch of the algorithm

Figure 1 shows a sketch of the algorithm that we have used to solve (2)-(9). As it is observed, the inputs of the algorithm are: Eq, that represents the equation (2) with (3)-(7); I.C. that represents the initial conditions (8); B.C. that represents the boundary condition (9); and F.C. that represents a certain finitude condition for the solutions.

The output for the algorithm is the basic reproductive rate of the substance B inside the solid disk of substance A, denoted  $R_0$ . The algorithm operates as it follows.

The inputs Eq., I.C., and B.C, by means of a Laplace Transformer are turned into a transformed equation denoted T.Eq. and a transformed boundary condition denoted T.B.C. Then, T.Eq, T.B.C. and F.C. are processed by a certain Dsolver that generates the transformed solution denoted Tsol. Next, Tsol is processed by means of an inverser with residue theorem, and we obtain the explicit form of the solution, denote sol. Finally using a stability analyzer, we deduce the explicit form of  $R_0$  and the algorithm is finished.

### 3.2. Results of Computations

Using our algorithm for computer algebra, the solution of the equations (2)-(9), that is obtained, is given by

$$u(r, t) = u_1(r, t) + u_2(r) + u_3(r, t) \tag{10}$$

where

$$u_1(r, t) = \frac{J_0(\sqrt{\lambda(-\eta)} r) \mu_b e^{(-\eta t)}}{J_0(\sqrt{\lambda(-\eta)} a)} \tag{11}$$

$$u_2(r) = u_{2,1}(r) + u_{2,2}(r) \tag{12}$$

$$u_{2,1}(r) = -\frac{-a_1 \lambda(0) - \lambda(0) a_3 r^2 + 4 a_3}{\lambda(0)^2 \delta} \tag{13}$$

$$u_{2,2}(r) = -\frac{(-4a_3 + \lambda(0)a_3 a^2 + a_1 \lambda(0)) J_0\left(\lambda(0) \left(\frac{1}{2}\right) r\right)}{J_0\left(\lambda(0) \left(\frac{1}{2}\right) a\right) \lambda(0)^2 \delta} \tag{14}$$

$$u_3(r, t) = \sum_{i=1}^5 \left( \sum_{n=1}^{\infty} G_{i,n}(r, t) \right) \tag{15}$$

$$G_{i,n}(r, t) = \frac{G_{1,i,n}(r, t)}{G_{2,i,n}(r, t)} \tag{16}$$

$$G_{1,i,n} = -2 e^{(S_{i,n} t)} J_0\left(\frac{\alpha_n r}{a}\right) (K_1 a_3 + K_2 a_1 + K_3) \tag{17}$$

$$K_1 = -a^4 (\alpha_n - 2) (\alpha_n + 2) (S_{i,n} + \eta) \tag{18}$$

$$K_2 = -a^2 \alpha_n^2 (S_{i,n} + \eta) \tag{19}$$

$$K_3 = \mu_b \alpha_n^4 \delta S_{i,n} \tag{20}$$

$$G_{2,i,n}(r, t) = a^2 \alpha_n^3 \delta S_{i,n} (S_{i,n} + \eta) J_1(\alpha_n) \left( \lim_{s \rightarrow S_{i,n}} \frac{d}{ds} \lambda(s) \right) \tag{21}$$

with

$$\lambda(s) = \frac{L(s)}{\delta (s + \varepsilon_1)^2 (s + \varepsilon_2)^2} \tag{22}$$

$$L(s) = -s^5 + A_1 s^4 + A_2 s^3 + A_3 s^2 + A_4 s + A_5 \tag{23}$$

where the coefficients A are given at Table 1 (up); and being  $S_{i,n}$  the roots of the equation of fifth degree

$$s^5 + B_1 s^4 + B_2 s^3 + B_3 s^2 + B_4 s + B_5 = 0 \tag{24}$$

with the coefficients B are given at Table 1 (down), Finally,  $J_m(x)$  is the Bessel function of order  $m$  of the first kind,  $a$  is the radius of the circular reactor and  $\alpha_n$  are the zeroes of  $J_0$ , namely [7]

$$J_0(\alpha_n) = 0 \tag{25}$$

### 3.3 Analysis of Results

As is evident from the equations (10)-(25), the solution of (2)-(9) is very formidable as for to be manipulated by hand using pen and paper. The great advantage of computer algebra is protuberant.

As it is observed at the equation (10), the solution of (2)-(9), consists of three summands. The first one is given at (11), the second is given at (12)-(14) and the third is given at (15)-(21) with the specifications (22)-(25). For  $\eta > 0$ , the first summand (11), decays exponentially with the time and it does not represent any amplification of the concentration of substance B inside the circular reactor..

The second summand (12)-(14) does not depend on time and represents the stationary concentration profile of substance B, that is established within the reactor and again, it does not give any kind of amplification of the concentration of substance B.

The third summand (15)-(21) is also a sum of terms with exponential dependence on time and some of such terms can be exponentially increasing with the time and then an amplification of the concentration of the substance B inside the circular reactor, would be had. The condition so that a such amplification is generated is that (24) admits a positive real solution, it is to say that  $B_5 < 0$ , where  $B_5$  is given at the Table 1. This last condition can be rewritten as the threshold condition for the triggered of the amplification of the concentration of the substance B inside the circular reactor,, namely,  $R_{0,n} > 1$ , where

$$R_{0,n} = \frac{(\varepsilon_2^2 \beta_2 + \varepsilon_2^2 \beta_1 \varepsilon_1^2) S_0}{\varepsilon_1^2 \gamma_2 + \varepsilon_1^2 \gamma_1 \varepsilon_2^2 + \frac{\varepsilon_1^2 \alpha_n^2 \delta \varepsilon_2^2}{a^2}} \quad (26)$$

The critical parameter  $R_{0,n}$  will be named the basic reproductive number for the substance B and measures the effective tendency of the circular reactor to amplify the concentration of the substance B. The fundamental or ground value of the reproductive number (26), corresponds to  $n=1$ , with  $\alpha_1=2.405$ , namely

$$R_{0,1} = \frac{\varepsilon_2^2 (\beta_2 + \beta_1 \varepsilon_1^2) S_0 a^2}{(\gamma_2 a^2 + \gamma_1 a^2 \varepsilon_2^2 + 5.784025\delta \varepsilon_2^2) \varepsilon_1^2} \quad (27)$$

The equation (27) can be rewritten as

$$R_{0,1} = \frac{R_0}{\frac{5.784025000 \delta \varepsilon_2^2}{\gamma_2 a^2 + \gamma_1 a^2 \varepsilon_2^2} + 1} \quad (28)$$

where  $R_0$  is the basic reproductive number when  $a \rightarrow \infty$ , and is given by

$$R_0 = \frac{S_0 \varepsilon_2^2 (\beta_2 + \beta_1 \varepsilon_1^2)}{\varepsilon_1^2 (\gamma_2 + \gamma_1 \varepsilon_2^2)} \quad (29)$$

Now, for the case when  $\eta = 0$ , the equation (11) lost its dependence on time and can be considered as certain stationary concentration profile of substance B inside the circular reactor, jointly with the terms (12)-(14). The condition for (11)-(14) be really genuine stationary concentration profiles of substance B inside the reactor is

$$0 < \lambda(0) \quad (30)$$

which is equivalent to  $L(0) > 0$  with  $L(s)$  being given at (23), and this last is equivalent to  $A_5 > 0$ , where  $A_5$  is given at the Table 1. This condition can be rewritten as  $R_0 > 1$ , where  $R_0$  is given at (29). Finally, when  $\eta < 0$ , then (11) has exponential increasing with time and corresponds to the irruption of the global amplification of the concentration of the substance B inside the reactor, without necessity of any kind of reaction threshold

We can see from (28) and (29) that

$$R_{0,1} < R_0 \quad (31)$$

Now, from the perspective of the possibility of to control the reaction (1), we have that the percentage

of decreasing of the initial density of the substance A inside the circular reactor, denoted  $S_0$ , both to prevent the stationary concentration profiles (11)-(14) as to obstruct the exponential amplification of the concentration of the substance B according with (15)-(21), are given, respectively by

$$P_{st} = 1 - \frac{1}{R_0} \quad (32)$$

$$P_A = 1 - \frac{1}{R_{0,1}} \quad (33)$$

From (31)-(33) we deduce that

$$P_A < P_{st} \quad (34)$$

it is to say the percentage of decreasing of the initial concentration of the substance A inside the reactor, to prevent the stationary concentration profiles of substance B, denote  $P_{st}$  is greater than the percentage of decreasing the initial concentration of substance A for to prevent the global amplification of the concentration of substance B, denoted  $P_A$ . In other words is more expedite to avoid the amplification of the concentration of the substance B that to avoid the presence of stationary concentration profiles of B. Finally, from the solution that was obtained we can to derive the formula for the total mass of substance B at every time  $t$  inside the reactor, which is given at the Fig. 3, and it is defined as

$$U(t) = \int_0^a u(r, t) r dr \quad (35)$$

## 4 Conclusion

The problem that was considered here, is a linear problem, whose solution can be obtained symbolically using certain algorithm and then the basic reproductive rate for the reaction can be derived. From this perspective the considered linear problem is fully computable. But to say the truth, the solution (24) is non-computable symbolically, is just only numerically computable. This implies that our linear transport problem is truly non-computable symbolically, and then the solution that was provided here, is a schematic solution that can not be specified symbolically with more details given the non-computable character of (24).

In all case, the algorithm that was used can be applied for others linear problems with boundary conditions, both computable as non-computable. Computer algebra is very useful to study transport phenomena.

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Table 1. Coefficients of equations (23) and (24)

**Coefficients of equation (23)**

$$\begin{aligned}
 A_1 &= \beta_1 S_0 - 2 \varepsilon_2 - \gamma_1 - 2 \varepsilon_1 \\
 A_2 &= -4 \varepsilon_1 \varepsilon_2 + 2 \beta_1 S_0 \varepsilon_2 - 2 \gamma_1 \varepsilon_1 - \varepsilon_2^2 + 2 \beta_1 S_0 \varepsilon_1 - \varepsilon_1^2 - 2 \gamma_1 \varepsilon_2 \\
 A_3 &= -\gamma_1 \varepsilon_2^2 - 2 \varepsilon_1 \varepsilon_2^2 + \beta_2 S_0 - \gamma_2 + 4 \beta_1 S_0 \varepsilon_1 \varepsilon_2 + \beta_1 S_0 \varepsilon_1^2 + \beta_1 S_0 \varepsilon_2^2 - 4 \gamma_1 \varepsilon_1 \varepsilon_2 - \gamma_1 \varepsilon_1^2 \\
 &\quad - 2 \varepsilon_1^2 \varepsilon_2 \\
 A_4 &= -2 \gamma_2 \varepsilon_1 + 2 \beta_1 S_0 \varepsilon_1^2 \varepsilon_2 - \varepsilon_1^2 \varepsilon_2^2 + 2 \beta_1 S_0 \varepsilon_1 \varepsilon_2^2 - 2 \gamma_1 \varepsilon_1^2 \varepsilon_2 - 2 \gamma_1 \varepsilon_1 \varepsilon_2^2 + 2 \beta_2 S_0 \varepsilon_2 \\
 A_5 &= -\gamma_1 \varepsilon_1^2 \varepsilon_2^2 + \beta_1 S_0 \varepsilon_1^2 \varepsilon_2^2 + \beta_2 S_0 \varepsilon_2^2 - \gamma_2 \varepsilon_1^2
 \end{aligned}$$

**Coefficients of equation (24)**

$$\begin{aligned}
 B_1 &= 2 \varepsilon_1 + 2 \varepsilon_2 - \beta_1 S_0 + \gamma_1 + \frac{\alpha_n^2 \delta}{a^2} \\
 B_2 &= 4 \varepsilon_1 \varepsilon_2 + \frac{2 \alpha_n^2 \delta \varepsilon_2}{a^2} + \frac{2 \alpha_n^2 \delta \varepsilon_1}{a^2} + 2 \gamma_1 \varepsilon_2 + \varepsilon_2^2 - 2 \beta_1 S_0 \varepsilon_1 - 2 \beta_1 S_0 \varepsilon_2 + 2 \gamma_1 \varepsilon_1 + \varepsilon_1^2 \\
 B_3 &= \gamma_1 \varepsilon_2^2 + \frac{\alpha_n^2 \delta \varepsilon_1^2}{a^2} - \beta_2 S_0 + 2 \varepsilon_1^2 \varepsilon_2 + \gamma_1 \varepsilon_1^2 + \frac{4 \alpha_n^2 \delta \varepsilon_1 \varepsilon_2}{a^2} + 2 \varepsilon_1 \varepsilon_2^2 - \beta_1 S_0 \varepsilon_2^2 + \gamma_2 \\
 &\quad - \beta_1 S_0 \varepsilon_1^2 - 4 \beta_1 S_0 \varepsilon_1 \varepsilon_2 + \frac{\alpha_n^2 \delta \varepsilon_2^2}{a^2} + 4 \gamma_1 \varepsilon_1 \varepsilon_2 \\
 B_4 &= \frac{2 \alpha_n^2 \delta \varepsilon_1 \varepsilon_2^2}{a^2} + \varepsilon_1^2 \varepsilon_2^2 - 2 \beta_2 S_0 \varepsilon_2 + 2 \gamma_2 \varepsilon_1 - 2 \beta_1 S_0 \varepsilon_1^2 \varepsilon_2 + \frac{2 \alpha_n^2 \delta \varepsilon_1^2 \varepsilon_2}{a^2} \\
 &\quad - 2 \beta_1 S_0 \varepsilon_1 \varepsilon_2^2 + 2 \gamma_1 \varepsilon_1^2 \varepsilon_2 + 2 \gamma_1 \varepsilon_1 \varepsilon_2^2 \\
 B_5 &= \gamma_2 \varepsilon_1^2 + \gamma_1 \varepsilon_1^2 \varepsilon_2^2 + \frac{\alpha_n^2 \delta \varepsilon_1^2 \varepsilon_2^2}{a^2} - \beta_2 S_0 \varepsilon_2^2 - \beta_1 S_0 \varepsilon_1^2 \varepsilon_2^2
 \end{aligned}$$

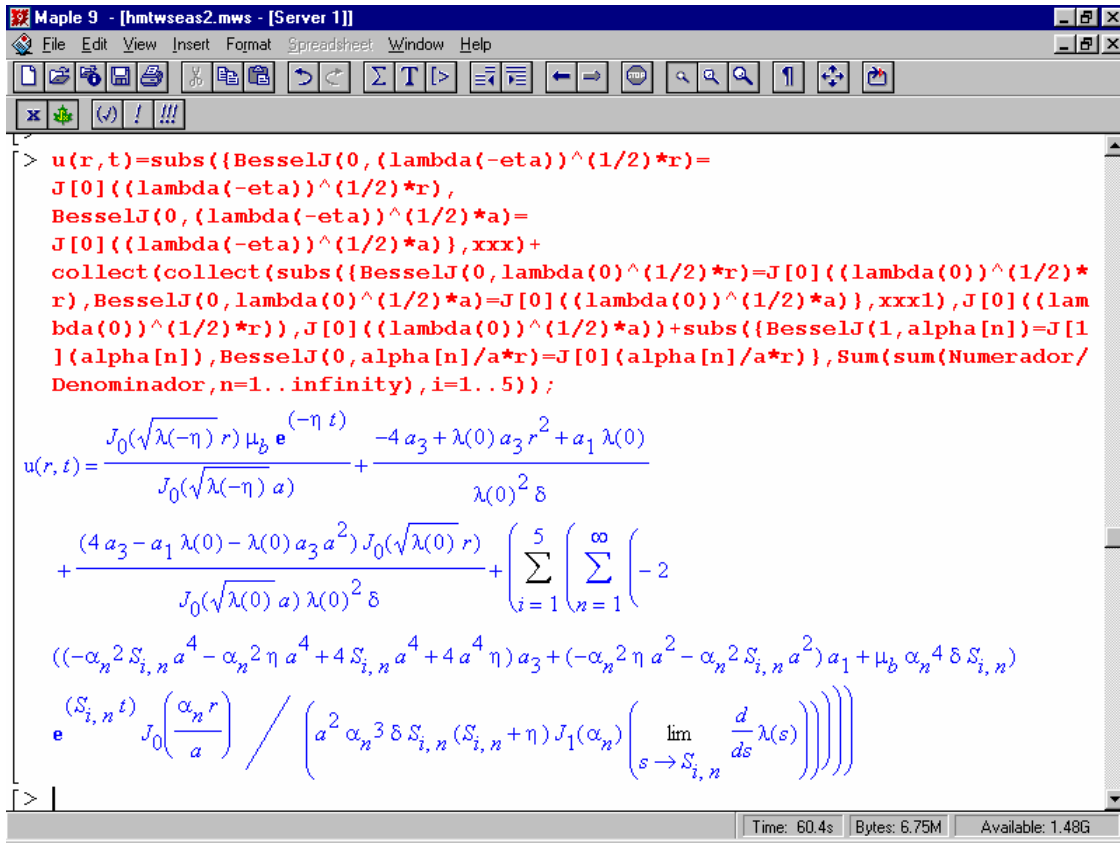


Figure 2. Full analytical solution of the problem (2)-(9)

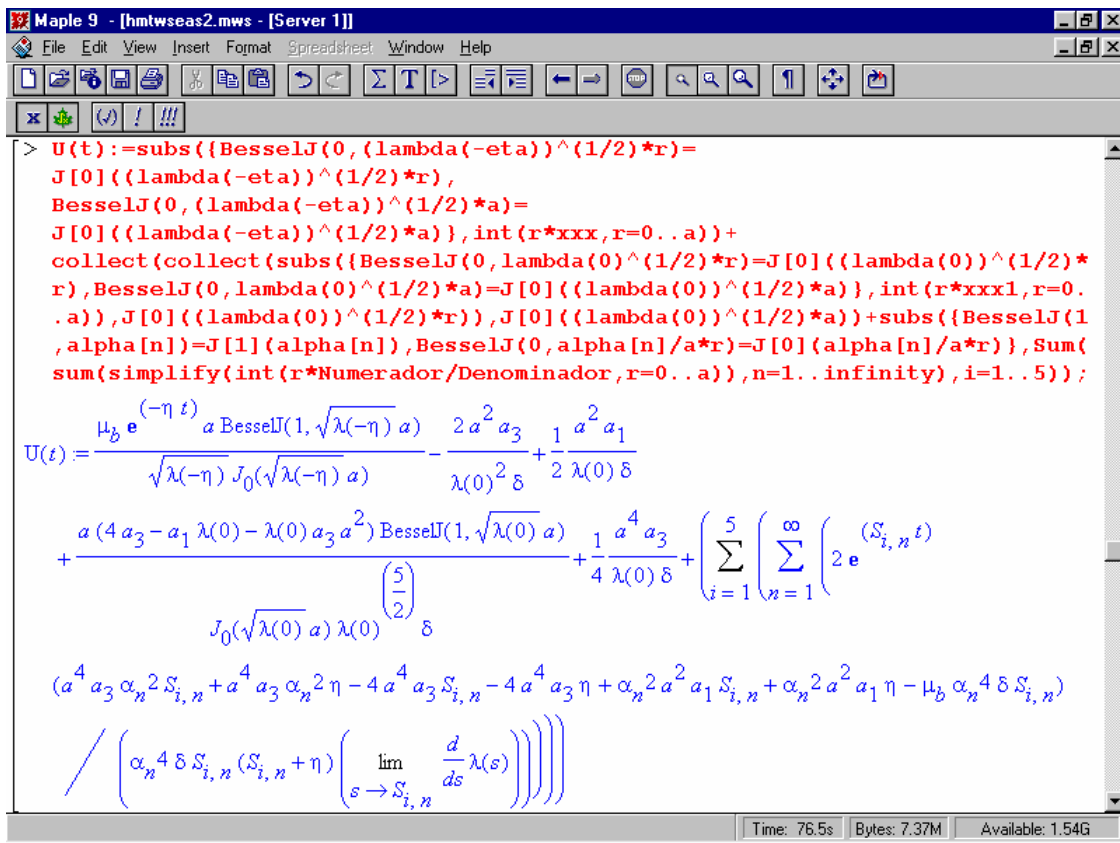


Figure 3. Explicit form of the equation (35)