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Linear compartmental systems: II—A software to obtain the symbolic kinetic equations

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Abstract Software has been implemented in this work to take full advantage of the characteristics of current operating systems and to provide the optimized symbolic kinetic equations for the linear compartmental systems derived in part I of this series. This software, called RM-w2011, is implemented using the C# language and runs under Windows XP, Vista and 7. It is applicable to any linear compartmental system, closed or open, and with a zero input in one or more of its compartments. Apart from the optimized equations that the software provides, if so desired, non optimized equations are offered to compare the advantage of using optimized equations while using non optimized ones, whenever they do not coincide. Moreover, the software circumvents the limitations of other previous software tools that operated with non optimized symbolic equations.

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1 Introduction

Varon et al. [1] obtained general symbolic kinetic equations which gave the instantaneous amount of substance in any compartment of a linear compartmental system, open or closed, with or without traps, and with a zero input in one or more system compartments. As part of the same contribution, algorithms were established which helped obtain the expressions of the coefficients involved in symbolic equations, plus the values of the parameters involved in them, without having to invert matrices or develop determinants. In parallel, the same authors [2] have implemented a software in the BASIC language which provides the values of the parameters involved in these equations and the expression of the coefficients as a function of the fractional transfer coefficients and, whenever required, the fractional excretion coefficients.

In subsequent contributions, Garcia-Meseguer et al. [3,4] improved the above-mentioned equations so that the coefficients involved in them were always non negative. They also implemented a software, called COEFICOM, in the Visual BASIC language for MS-DOS, which obtained the expression of these coefficients as a function of the fractional transfer coefficients. All the above-mentioned contributions allow us to obtain general and symbolic kinetic equations that are valid for any linear compartmental system with a zero input and, with the help of computerized processes, to obtain the expressions and the values of the coefficients and parameters involved in them. Yet these contributions are limited in that the symbolic equations obtained refer to the entire linear compartmental system, including all the fractional transfer coefficients and zero inputs, regardless of whether or not they influence the instant amount of substance in the desired system compartment. In part I of this series [5], we named these equations general non optimized kinetic equations, as indicated in Table 1 of the aforementioned work. One limitation of this software in connection with the equations implemented in the references indicated, in addition to those inherent in the BASIC language, is that it does not offer the equation form, but the expressions of the coefficients involved in it.

Previous limitations have been overcome in this contribution as the equations used are the optimized general kinetic equations described in part I of this series: Eqs. (44), (45) and (46). These have been completely simplified, and only involve those fractional transfer coefficients and zero inputs that influence the instantaneous amount of substance in the desired compartment. This software provides the form of the equation corresponding to each case, plus the expressions of the coefficients and the values of the parameters involved in it.

The results obtained in part I of this series will be the starting point for the implementation of the RM-w2011software in the present part II, which directly provides optimized symbolic equations.

This work aims to implement a software that takes advantage of the characteristics of current operating systems and provides the optimized symbolic equations presented in part I of this series. Moreover, for comparison purposes, the non optimized general

kinetic equations for linear compartmental systems, open or closed, with a zero input in one or more of its compartments, will be implemented.

2 Material and methods

The so-called RM-w2011 computer application has been designed for MS Windows operating systems in any of the current versions: XP, Vista or 7. For this reason, we have used the Visual Studio 2008 Professional environment, provided by Microsoft, and the modern technology of Microsoft's programming .NET in language C# to create the graphical environment and to encapsulate the classes of the data structures and functions, thus facilitating program design and reusability of the generated code.

In order to cut memory requirements and computing time, we have not used any third party symbolic package, instead new specific library functions have been developed for computing Eqs. (44)–(46) of paper I of this series. Below is a list of the classes implemented for this application, without indicating the description of its functionality or file content, but with the definitions of the functions, in order to keep this work short.

The implemented classes were: cbFila.cs, cbGrafo.cs, cbLigando.cs, Clase.cs, Fi.cs, Kij.cs, listaNodos.cs, ProductoKij.cs and Ys.cs.

Coefficients $F_q(E_i)$ and $(f_{k,i})_q(E_i)$, as described in paper I of this series, were obtained using an instance of Fi.cs, where the complexity of the implemented algorithm is n_k^{2q}, and where n_k is the number of non zero $K_{i,j}$ in the corresponding class.

3 Software implemented

We describe below the characteristics and use of the computer application which has been developed to accomplish the objective of this contribution. The computer application is called RM-w2011 and it provides the analytical expressions corresponding to the general kinetic equations in any compartment of any linear compartmental system, either closed or open. This software is available free of charge either upon request from the authors or from the UCLM web server at http://oretano.iele-ab.uclm.es/~fgarcia/RM-w2011/. The equations determined by the program correspond to the general kinetic expressions optimized, as established in part I of this series (see Table 1 of paper I) for the amount of substance of compartment x_i as a function of time. Moreover, the user can instruct the program to generate, if necessary, the non optimized general kinetic equations (see Table 1 in Paper I of this series) corresponding to Eqs. (B.1)–(B.3).

For both the optimized and non optimized general kinetic equations, the fact that zero input may refer to one or more system compartments has been taken into account.

3.1 Data input

The RM-w2011 application has a designed graphical environment that allows any type of linear compartmental system (Fig. 1), even a highly complex one, to be entered easily and rapidly.
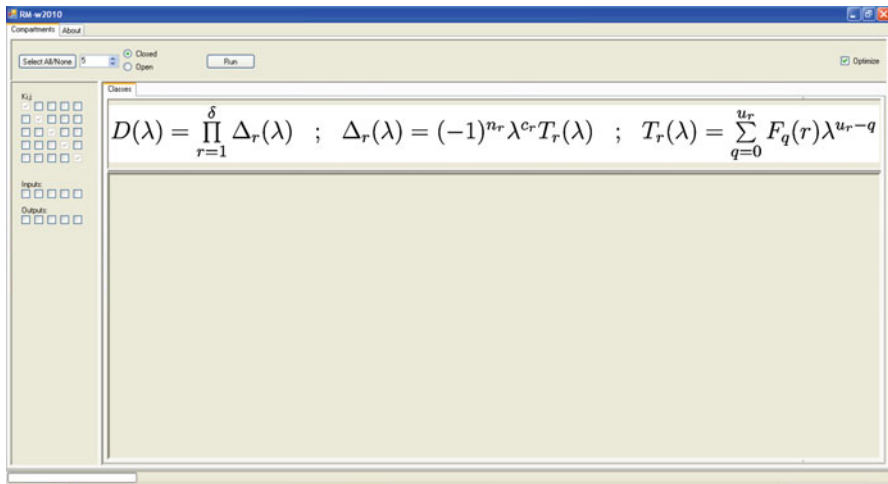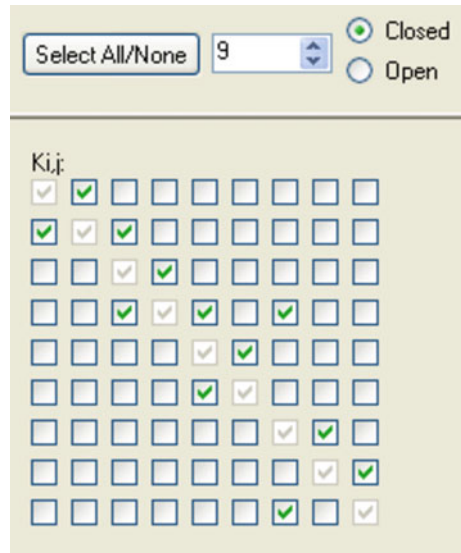
Fig. 1 Main screen of the RM-w2011 application

Fig. 2 Screen corresponding to a closed 9-compartment compartmental system in which the values of non null $K_{i,j}$ coefficients are indicated

In order to study compartmental systems, begin by indicating (Fig. 2) the number of system compartments (open or closed) by using the controls located on the top panel. Finally in the square matrix of the left panel, whose size will change according to the number of indicated compartments, the non null $K_{i,j}$ coefficients of the compartmental system in the study will appear.

3.2 Obtaining results

Once the information has been entered as described in the previous paragraph, the system input must be indicated to the program; i.e., in which compartments substance

is to be injected by marking the corresponding box of the row labeled "*Inputs*". The desired exit expressions will be indicated by marking the suitable box of the row labeled "*Outputs*".

After establishing the entries and exits, pressing "*Run*" will not only initiate the calculation of the F_i and $(f_{k,i})$ expressions for each exit and the equivalence classes in the system under study, but will generate the corresponding expressions, which will appear in an ASCII format in the text box placed to the right of the application window. To facilitate the use of these expressions, the RM-w2011 software will also show the optimized equations described in this paper corresponding to the time-concentration expressions of each exit indicated by the user.

Finally, it is to be noted that the program will offer the possibility of obtaining the expressions of the equations mentioned above, but in the non optimized form (see Table 1 of part I of this series). For this purpose, it will be necessary to deactivate the "*xOptimize*" box placed to the right of the top panel which, by default, will be activated when the program is executed. Thus, as in the examples included in "Appendix A", it is very simple to compare the results obtained by both methods and to estimate the advantage of employing the optimized equations, as already mentioned in part I of this series.

3.3 Examples

This section presents the expressions of the general kinetic equations, both optimized and non optimized, obtained using the RM-w2011 computer application for two examples of compartmental systems: one corresponding to a closed system and the other to an open system.

All the examples covered in this subsection, and those included in Appendices A and B, have been computed under MS-Windows XP using a compatible PC with Intel Core2 Duo CPU @ 2.40 GHz and 2 GB of installed memory (RAM). The CPU time in all cases was very short and never took longer than 2 s.

3.3.1 Application to an example of a closed compartmental system

To illustrate the application of the RM-w2011 software to closed compartmental systems, we will use the compartmental system whose connectivity diagram is shown in Fig. 3 by assuming that we are interested in the optimized symbolic equation that provides the instantaneous amount of matter, x_4 in compartment X_4, when a zero input is placed in compartments X_1, X_2 and X_3. This example was already solved manually without using any software in paper I of this series. Figure 4 shows a screenshot corresponding to the data input of the system under study, where it is indicated that the system is closed and consists of 9 compartments, with the matter injected into X_1, X_3 and X_6 (boxes marked as "*Inputs*"), and that we wish to know the instantaneous amount of matter in compartment X_4 ("*Outputs*").

After introducing the data entry, press "*Run*" in the program. Almost immediately, the results will be obtained for the expression of the concentration-time equation for the indicated compartment (X_4), the output generated in two tabs: the first one (Fig. 5) labeled "*Classes* ($\delta = 4$)" will contain the information of the four classes of equiva-
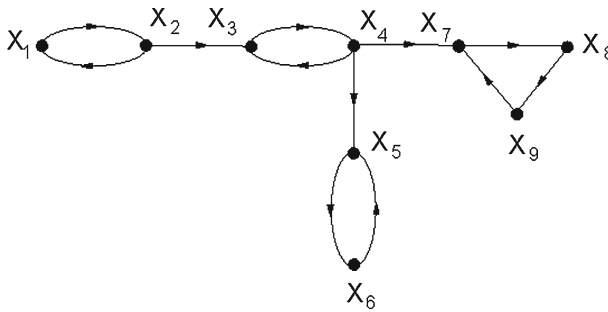
Fig. 3 Connectivity diagram corresponding to the example of a closed 9-compartment compartmental system, denoted by $X_1, \ldots, X_9$. The *arrows* indicate the direct connections among the compartments
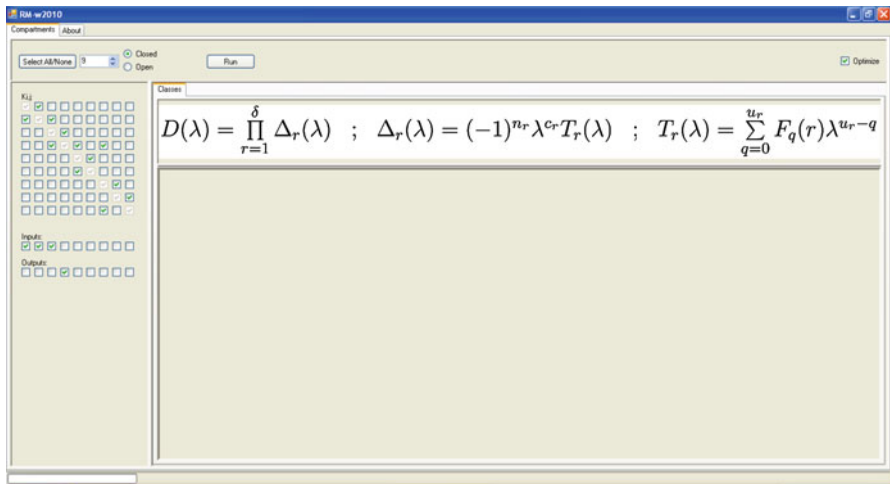

Fig. 4 Screenshot of the data entry corresponding to the compartmental diagram shown in Fig. 3

lence of the condensation diagram in the system; the second (Fig. 6), labeled "$x4$", will offer the calculated values of $(f_{k,i})_q$ and $F_{u(4)}$ corresponding to (E_4), i.e., $(f_{k,i})_q(E_4)$ and $F_{u(4)}(E_4)$, together with the optimized equations that allow us to obtain the corresponding expression for the concentration-time equation for compartment X_4.

The readings of the obtained results are shown below in Listings 1 and 2.

According to Eqs. (44)–(46) of paper I of this series, and to the equation for x_4 is:

$$x_4 = A_{4,0} + A_{4,1}e^{\lambda_1 t} + A_{4,2}e^{\lambda_2 t} + A_{4,3}e^{\lambda_3 t} + A_{4,4}e^{\lambda_4 t} \tag{1}$$

$$A_{4,0} = \frac{(f_{1,4})_4(E_4)x_1^0 + (f_{2,4})_4(E_4)x_2^0 + (f_{3,4})_4(E_4)x_3^0}{F_4(E_4)} \tag{2}$$

$$A_{4,h} = -\frac{x_1^0 \sum_{q=0}^{4}(f_{1,4})_q(E_i)\lambda_h^{4-q} + x_2^0 \sum_{q=0}^{4}(f_{2,4})_q(E_i)\lambda_h^{4-q} + x_3^0 \sum_{q=0}^{4}(f_{2,4})_q(E_i)\lambda_h^{4-q}}{\lambda_h \prod_{\substack{p=1 \\ p\neq h}}^{4}(\lambda_p - \lambda_h)}$$
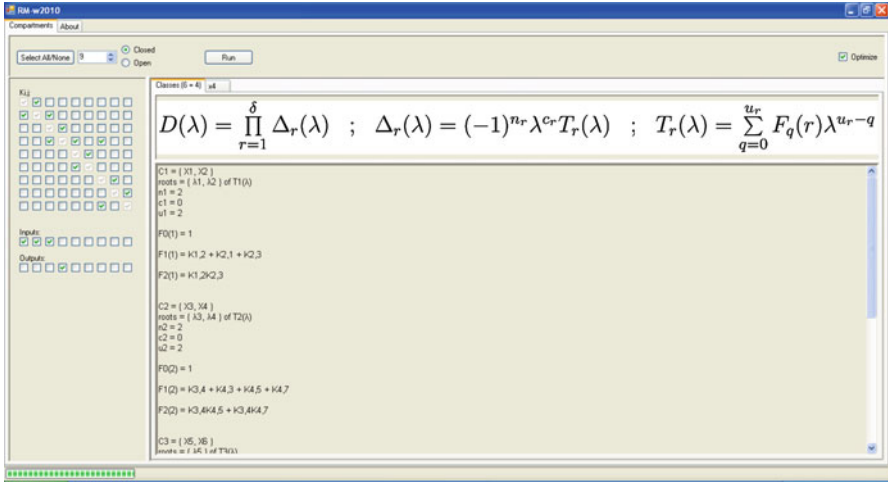
$$(h = 1, 2, 3, 4) \tag{3}$$

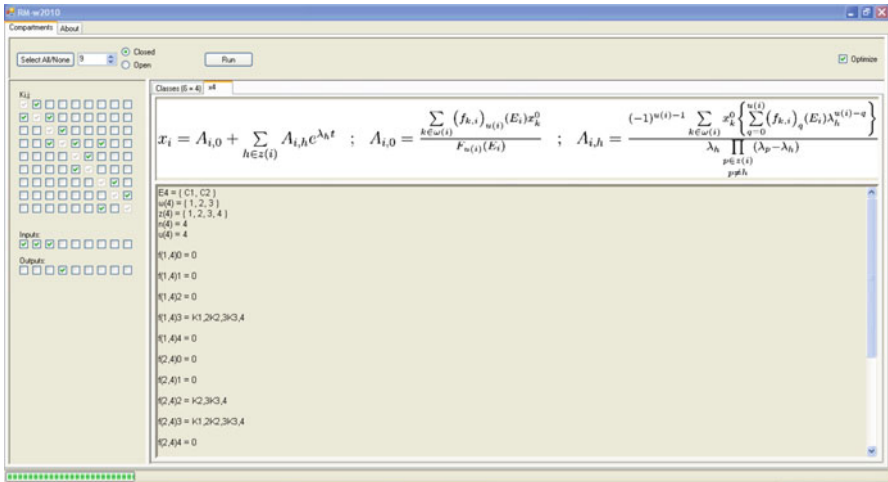**Fig. 5** Screenshot of the data output of the tab "*Classes*"

Fig. 6 Screenshot of the data output of the tab "*x4*"

In Eqs. (1) and (3), λ_1 and λ_2 are the roots of the polynomial

$$T_1(\lambda) = \lambda^2 + F_1(1)\lambda + F_2(1) \tag{4}$$

and λ_3 and λ_4 are the roots of the polynomial

$$T_2(\lambda) = \lambda^2 + F_1(2)\lambda + F_2(2) \tag{5}$$

The expressions of all the coefficients involved in Eqs. (1)–(3) are indicated in Listings 1 and 2.

Listing 1 Equivalence classes
and their associated roots for the
example in Fig. 3

```
C1 = { X1, X2 }
roots = { λ1, λ2 } of T1(λ)
n1 = 2
c1 = 0
u1 = 2

F0(1) = 1

F1(1) = K1,2 + K2,1 + K2,3

F2(1) = K1,2K2,3

C2 = { X3, X4 }
roots = { λ3, λ4 } of T2(λ)
n2 = 2
c2 = 0
u2 = 2

F0(2) = 1

F1(2) = K3,4 + K4,3 + K4,5 + K4,7

F2(2) = K3,4K4,5 + K3,4K4,7

C3 = { X5, X6 }
roots = { λ5 } of T3(λ)
n3 = 2
c3 = 1
u3 = 1

F0(3) = 1

F1(3) = K5,6 + K6,5

C4 = { X7, X8, X9 }
roots = { λ7, λ8 } of T4(λ)
n4 = 3
c4 = 1
u4 = 2

F0(4) = 1

F1(4) = K7,8 + K8,9 + K9,7

F2(4) = K7,8K8,9 + K7,8K9,7 + K8,9K9,7
```

Obtaining the non optimized equations corresponding to the same example   As indicated above, the program also allows us to obtain the expression of the concentration-time by considering the entire system as a whole, as well as the part that has no influence on outcome; i.e., using the non optimized kinetic equations. If the user deactivates "*Optimize*" and presses "*Run*", the results obtained for the non optimized expressions will be shown (as in Listings A1 and A2 in "Appendix A"); as seen, they are much more complex than the previous Listings 1 and 2.

According to Eqs. (44)–(46) of paper I of this series and to Listings 1 and 2 above, the equation for x_4 is:

$$x_4 = A_{4,0} + A_{4,1}e^{\lambda_1 t} + A_{4,2}e^{\lambda_2 t} + A_{4,3}e^{\lambda_3 t} + A_{4,4}e^{\lambda_4 t} + A_{4,5}e^{\lambda_5 t} + A_{4,6}e^{\lambda_6 t}$$
$$+ A_{4,7}e^{\lambda_7 t} \tag{6}$$

Listing 2 The expressions obtained for functions $(f_{k,4})_q(E_4)$ and $F_4(E_4)$ corresponding to the example in Fig. 3. To simplify, these functions are denoted merely as $(f_{k,4})q$ and F_4 because E_4 has been indicated at the top of the listing

```
E4 = { C1, C2 }
ω(4) = { 1, 2, 3 }
z(4) = { 1, 2, 3, 4 }
n(4) = 4
u(4) = 4

f(1,4)0 = 0

f(1,4)1 = 0

f(1,4)2 = 0

f(1,4)3 = K1,2K2,3K3,4

f(1,4)4 = 0

f(2,4)0 = 0

f(2,4)1 = 0

f(2,4)2 = K2,3K3,4

f(2,4)3 = K1,2K2,3K3,4

f(2,4)4 = 0

f(3,4)0 = 0

f(3,4)1 = K3,4

f(3,4)2 = K1,2K3,4 + K2,1K3,4 + K2,3K3,4

f(3,4)3 = K1,2K2,3K3,4

f(3,4)4 = 0

F4 = K1,2K2,3K3,4K4,5 + K1,2K2,3K3,4K4,7
```

$$A_{4,0} = \frac{(f_{1,4})_7 x_1^0 + (f_{2,4})_7 x_2^0 + (f_{3,4})_7 x_3^0}{F_7} \tag{7}$$

$$A_{4,h} = \frac{x_1^0 \sum_{q=0}^{7} (f_{1,4})_q \lambda_h^{7-q} + x_2^0 \sum_{q=0}^{7} (f_{2,4})_q (E_i) \lambda_h^{7-q} + x_3^0 \sum_{q=0}^{7} (f_{2,4})_q \lambda_h^{7-q}}{\lambda_h \prod_{\substack{p=1 \\ p \neq h}}^{7} (\lambda_p - \lambda_h)}$$

$$(h = 1, 2, \ldots, 7) \tag{8}$$

In Eqs. (6) and (8), $\lambda_1, \ldots, \lambda_7$ are the roots of the polynomial

$$T(\lambda) = \lambda^7 + F_1 \lambda^6 + F_2 \lambda^5 + F_3 \lambda^4 + F_4 \lambda^3 + F_5 \lambda^2 + F_6 \lambda + F_7 \tag{9}$$

The expressions of all the coefficients involved in Eqs. (6)–(9) above are indicated in Listings A1 and A2 in "Appendix A".
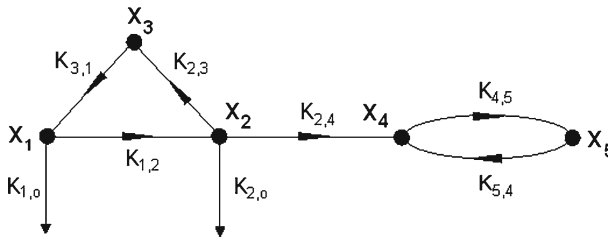
Fig 7 Connectivity diagram corresponding to the example of an open 5-compartment compartmental system, denoted by $X_1, \ldots, X_5$. $K_{i,j}$ $(i, j = 1, 2, \ldots, 5)$ indicates the flow of matter among the compartments and $K_{i,o}$ refers to the removal of matter from compartment X_i

Fig 8 The data entry corresponding to the compartmental diagram shown in Fig. 7

3.3.2 Application to an example of an open compartmental system

To show the application of the RM-w2011 software to an open compartmental system, we will use the compartmental system whose connectivity diagram is shown in Fig. 7. To do so, we will assume that we are interested in the optimized symbolic equation, which provides the quantity of matter x_4 in compartment X_4 when an input zero is placed in compartment X_3. Figure 8 represents a screenshot of the data entry of the system under study, which indicates that the system is open and consists of 5 compartments, when the matter is injected into X_3 (boxes marked as "*Inputs*") and the instantaneous amount of matter in X_4 (*Outputs*") is desired.

After completing the data entry and by clicking on the "*Run*" button, the program will almost immediately provide the results for the expression of the concentration-time equation of the indicated compartment (X_4) by generating the output in two tabs: the first (Fig. 9), labeled as "*Classes* ($\delta = 3$)" will provide the information of the three classes of equivalence of the system condensation diagram; the second
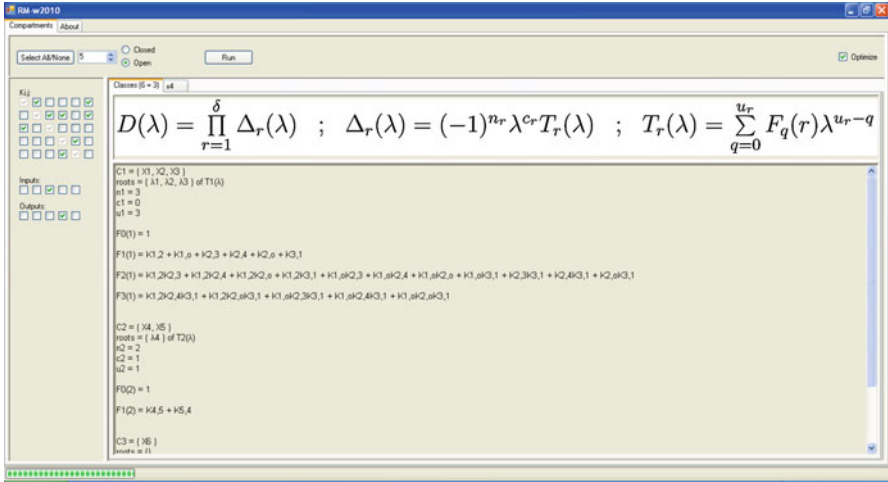
Fig 9 Screenshot corresponding to the output of the tab "*Classes*"
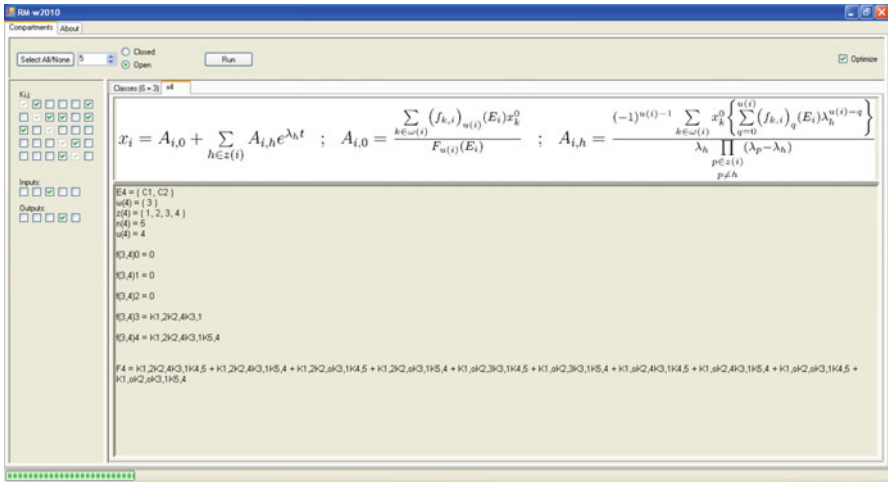
Fig 10 Screenshot corresponding to the output of the tab "*x4*"

(Fig. 10), labeled as "*x4*", will display the calculated values $(f_{k,4})_q$ and $F_{u(4)}$ for E_4; i.e., $(f_{k,4})_q(E_4)$ and $F_{u(4)}(E_4)$; together with the optimized equations used to obtain the expression of the concentration-time equation for compartment X_4.

Below we find the results for Listings 3 and 4 to facilitate their reading:

According to Eqs. (44)–(46) of paper I of this series, and to Listings 1 and 2 above, the equation for x_4 is:

$$x_4 = A_{4,0} + A_{4,1}e^{\lambda_1 t} + A_{4,2}e^{\lambda_2 t} + A_{4,3}e^{\lambda_3 t} \tag{10}$$

$$A_{4,0} = \frac{(f_{1,4})_3(E_4)x_3^0}{F_3(E_4)} \tag{11}$$

```
C1 = { X1, X2, X3 }
roots = { λ1, λ2, λ3 } of T1(λ)
n1 = 3
c1 = 0
u1 = 3

F0(1) = 1

F1(1) = K1,2 + K1,o + K2,3 + K2,4 + K2,o + K3,1

F2(1) = K1,2K2,3 + K1,2K2,4 + K1,2K2,o + K1,2K3,1 + K1,oK2,3 +
        K1,oK2,4 + K1,oK2,o + K1,oK3,1 + K2,3K3,1 + K2,4K3,1 +
        K2,oK3,1

F3(1) = K1,2K2,4K3,1 + K1,2K2,oK3,1 + K1,oK2,3K3,1 +
        K1,oK2,4K3,1 + K1,oK2,oK3,1

C2 = { X4, X5 }
roots = { λ4 } of T2(λ)
n2 = 2
c2 = 1
u2 = 1

F0(2) = 1

F1(2) = K4,5 + K5,4

C3 = { X6 }
roots = {}
n3 = 1
c3 = 1
u3 = 0
```

Listing 3 Equivalence classes and their associated roots for the example in Fig. 7

$$A_{4,h} = \frac{x_3^0 \sum_{q=0}^{3} (f_{3,4})_q (E_4) \lambda_h^{3-q}}{\lambda_h \prod_{\substack{p=1 \\ p \neq h}}^{3} (\lambda_p - \lambda_h)} \quad (h = 1, 2, 3) \tag{12}$$

In Eqs. (10) and (12), λ_1, λ_2 and λ_3 are the roots of the polynomial

$$T_1(\lambda) = \lambda^3 + F_1(1)\lambda^2 + F_2(1)\lambda + F_3(1) \tag{13}$$

The expressions of all the coefficients involved in Eqs. (10)–(13) above are indicated in Listings 3 and 4.

Obtaining non optimized equations corresponding to this same example   As indicated, the program also allows us to obtain the expressions of the concentration-time equations and, throughout the system as a whole, also the part of it that has no influence on outcome; that is, using the non optimized kinetic equations. Deactivate the box "*Optimize*" and press "*Run*" again. The results obtained for the non optimized expressions will be reflected in Listings B1 and B2 in "Appendix B". As seen, these are more complex than the corresponding Listings 3 and 4.

```
E4  =  { C1, C2 }
ω(4)  =  { 3 }
z(4)  =  { 1, 2, 3, 4 }
n(4)  =  5
u(4)  =  4

f(3,4)0  =  0

f(3,4)1  =  0

f(3,4)2  =  0

f(3,4)3  =  K1,2K2,4K3,1

f(3,4)4  =  K1,2K2,4K3,1K5,4

F4  =  K1,2K2,4K3,1K4,5 + K1,2K2,4K3,1K5,4 + K1,2K2,oK3,1K4,5 +
       K1,2K2,oK3,1K5,4 + K1,oK2,3K3,1K4,5 + K1,oK2,3K3,1K5,4 +
       K1,oK2,4K3,1K4,5 + K1,oK2,4K3,1K5,4 + K1,oK2,oK3,1K4,5 +
       K1,oK2,oK3,1K5,4
```

Listing 4 The expressions obtained for functions $(f_{3,4})_q(E_4)$ and $F_4(E_4)$ corresponding to the example in Fig. 7. To simplify, these functions are denoted merely as $(f_{3,4})q$ and F_4 because E_4 has been indicated at the top of the listing

According to Eqs. (B.1)–(B.3) of paper I of this series and to Listings 1 and 2 above, the equation for x_4 is:

$$x_4 = A_{4,0} + A_{4,1}e^{\lambda_1 t} + A_{4,2}e^{\lambda_2 t} + A_{4,3}e^{\lambda_3 t} + A_{4,4}e^{\lambda_4 t} \tag{14}$$

$$A_{4,0} = \frac{(f_{3,4})4 x_3^0}{F_4} \tag{15}$$

$$A_{4,h} = -\frac{x_3^0 \sum_{q=0}^{4} (f_{3,4})_q \lambda_h^{4-q}}{\lambda_h \prod_{\substack{p=1 \\ p \neq h}}^{4} (\lambda_p - \lambda_h)} \quad (h = 1, 2, 3, 4) \tag{16}$$

In Eqs. (14) and (16), $\lambda_1, \lambda_2, \lambda_3$ and λ_4 are the roots of the polynomial

$$T(\lambda) = \lambda^4 + F_1\lambda^3 + F_2\lambda^2 + F_3\lambda + F_4 \tag{17}$$

The expressions of all the coefficients involved in Eqs. (14)–(17) above are indicated in Listings B1 and B2 of "Appendix B".

Finally, the mathematical notation used in this paper coincides with that described in detail in the first work of this series.

4 Results

Given that the number of terms which appears in the expressions of coefficients F_q and $f(k, i)_q$ corresponding to E_i will grow quickly to increase the number of compartments and the number of non null coefficients $K_{i,j}$, this computer program has

been designed to store the intermediate data on a hard disk instead of in the main memory, thus providing the kinetic equations of the compartmental system under study. Without this strategy, the kinetic equations could not be obtained according to the memory space needed to store the intermediate data: in complex cases, this memory space would probably be greater than the RAM installed in the computer system.

The examples used in this paper are relatively simple and this program's power will be evidenced when it is applied to more complex compartmental systems. With an average desktop PC, like that described in Sect. 3.3, it should be possible to obtain the symbolic kinetic equations for a linear compartmental system of up to 60 non zero $K_{i,j}$.

Finally, the results (i.e., the kinetic equations) obtained by the program itself will be stored in the memory, unlike the intermediate data corresponding to obtaining the coefficients involved in the equations. This enables use in any other application by employing the operating system's "*copy and paste*" option. This implies a limitation to the maximum size of the string of characters that can be handled, which is 2^{31}; i.e., more than 2,147 million characters. Although it is unlikely that a real compartmental system could reach this limit, should it do so, these would be erroneous and, although the system would be resolved, the solution to this could not be generated on the screen. It is possible that this limitation, due exclusively to the operating system, could be overcome by using new versions or upgrades of it.

5 Discussion

As possible improvements to the RM-w2011 software in the near future, new features, such as those described below, could be added: (1) incorporation of the approximation of the rapid equilibrium of the reversible steps to directly generate the corresponding equations; (2) inclusion of the possibility of providing numerical values to the fractional transfer coefficients to give a numerical expression for the instantaneous quantities of matter in the system compartments involved; (3) addition to the same software the possibility of obtaining the kinetic mean parameters, which are time-independent, such as mean residence time (MRT), departure time, occupation, turnover and half-life, as recently carried out by Villalba et al. [6] independently of MRTs; (4) development of a combined environment that allows, for the system under study, both the analytical and numerical solutions corresponding to the integration of the differential equation system to be obtained by describing their kinetic behavior without having to use different applications: thus, a single environment would virtually cover all researchers' needs in this field.

6 Conclusion

In this work, a computer application, called RM-w2011, has been implemented, which provides both the optimized and non optimized kinetic equations for the linear compartmental and enzymatic systems studied in paper I of this series. This application considerably cuts the execution time if compared with that of other applications [2–4].

Appendix A

The expressions and values corresponding to the non optimized equations indicated below in Listings A1 and A2, as seen, are much more complex than their corresponding Listings 1 and 2 mentioned in the main text corresponding to the optimized equations.

```
C1 = { X1, X2, X3, X4, X5, X6, X7, X8, X9 }
roots = { λ1, λ2, λ3, λ4, λ5, λ6, λ7, λ8 } of T1(λ)
n1 = 9
c1 = 1
u1 = 8

F0(1) = 1

F1(1) = K1,2 + K2,1 + K2,3 + K3,4 + K4,3 + K4,5 + K4,7 + K5,6 +
        K6,5 + K7,8 + K8,9 + K9,7

F2(1) = K1,2K2,3 + K1,2K3,4 + K1,2K4,3 + K1,2K4,5 + K1,2K4,7 +
        K1,2K5,6 + K1,2K6,5 + K1,2K7,8 + K1,2K8,9 + K1,2K9,7 +
        K2,1K3,4 + K2,1K4,3 + K2,1K4,5 + K2,1K4,7 + K2,1K5,6 +
        K2,1K6,5 + K2,1K7,8 + K2,1K8,9 + K2,1K9,7 + K2,3K3,4 +
        K2,3K4,3 + K2,3K4,5 + K2,3K4,7 + K2,3K5,6 + K2,3K6,5 +
        K2,3K7,8 + K2,3K8,9 + K2,3K9,7 + K3,4K4,5 + K3,4K4,7 +
        K3,4K5,6 + K3,4K6,5 + K3,4K7,8 + K3,4K8,9 + K3,4K9,7 +
        K4,3K5,6 + K4,3K6,5 + K4,3K7,8 + K4,3K8,9 + K4,3K9,7 +
        K4,5K5,6 + K4,5K6,5 + K4,5K7,8 + K4,5K8,9 + K4,5K9,7 +
        K4,7K5,6 + K4,7K6,5 + K4,7K7,8 + K4,7K8,9 + K4,7K9,7 +
        K5,6K7,8 + K5,6K8,9 + K5,6K9,7 + K6,5K7,8 + K6,5K8,9 +
        K6,5K9,7 + K7,8K8,9 + K7,8K9,7 + K8,9K9,7

F3(1) = K1,2K2,3K3,4 + K1,2K2,3K4,3 + K1,2K2,3K4,5 +
        K1,2K2,3K4,7 + K1,2K2,3K5,6 + K1,2K2,3K6,5 +
        K1,2K2,3K7,8 + K1,2K2,3K8,9 + K1,2K2,3K9,7 +
        K1,2K3,4K4,5 + K1,2K3,4K4,7 + K1,2K3,4K5,6 +
        K1,2K3,4K6,5 + K1,2K3,4K7,8 + K1,2K3,4K8,9 +
        K1,2K3,4K9,7 + K1,2K4,3K5,6 + K1,2K4,3K6,5 +
        K1,2K4,3K7,8 + K1,2K4,3K8,9 + K1,2K4,3K9,7 +
        K1,2K4,5K5,6 + K1,2K4,5K6,5 + K1,2K4,5K7,8 +
        K1,2K4,5K8,9 + K1,2K4,5K9,7 + K1,2K4,7K5,6 +
        K1,2K4,7K6,5 + K1,2K4,7K7,8 + K1,2K4,7K8,9 +
        K1,2K4,7K9,7 + K1,2K5,6K7,8 + K1,2K5,6K8,9 +
        K1,2K5,6K9,7 + K1,2K6,5K7,8 + K1,2K6,5K8,9 +
        K1,2K6,5K9,7 + K1,2K7,8K8,9 + K1,2K7,8K9,7 +
        K1,2K8,9K9,7 + K2,1K3,4K4,5 + K2,1K3,4K4,7 +
        K2,1K3,4K5,6 + K2,1K3,4K6,5 + K2,1K3,4K7,8 +
        K2,1K3,4K8,9 + K2,1K3,4K9,7 + K2,1K4,3K5,6 +
        K2,1K4,3K6,5 + K2,1K4,3K7,8 + K2,1K4,3K8,9 +
```

Listing A1 Roots of the system compartment using the non optimized expressions

```
                    K2,1K4,3K9,7 + K2,1K4,5K5,6 + K2,1K4,5K6,5 +
                    K2,1K4,5K7,8 + K2,1K4,5K8,9 + K2,1K4,5K9,7 +
                    K2,1K4,7K5,6 + K2,1K4,7K6,5 + K2,1K4,7K7,8 +
                    K2,1K4,7K8,9 + K2,1K4,7K9,7 + K2,1K5,6K7,8 +
                    K2,1K5,6K8,9 + K2,1K5,6K9,7 + K2,1K6,5K7,8 +
                    K2,1K6,5K8,9 + K2,1K6,5K9,7 + K2,1K7,8K8,9 +
                    K2,1K7,8K9,7 + K2,1K8,9K9,7 + K2,3K3,4K4,5 +
                    K2,3K3,4K4,7 + K2,3K3,4K5,6 + K2,3K3,4K6,5 +
                    K2,3K3,4K7,8 + K2,3K3,4K8,9 + K2,3K3,4K9,7 +
                    K2,3K4,3K5,6 + K2,3K4,3K6,5 + K2,3K4,3K7,8 +
                    K2,3K4,3K8,9 + K2,3K4,3K9,7 + K2,3K4,5K5,6 +
                    K2,3K4,5K6,5 + K2,3K4,5K7,8 + K2,3K4,5K8,9 +
                    K2,3K4,5K9,7 + K2,3K4,7K5,6 + K2,3K4,7K6,5 +
                    K2,3K4,7K7,8 + K2,3K4,7K8,9 + K2,3K4,7K9,7 +
                    K2,3K5,6K7,8 + K2,3K5,6K8,9 + K2,3K5,6K9,7 +
                    K2,3K6,5K7,8 + K2,3K6,5K8,9 + K2,3K6,5K9,7 +
                    K2,3K7,8K8,9 + K2,3K7,8K9,7 + K2,3K8,9K9,7 +
                    K3,4K4,5K5,6 + K3,4K4,5K6,5 + K3,4K4,5K7,8 +
                    K3,4K4,5K8,9 + K3,4K4,5K9,7 + K3,4K4,7K5,6 +
                    K3,4K4,7K6,5 + K3,4K4,7K7,8 + K3,4K4,7K8,9 +
                    K3,4K4,7K9,7 + K3,4K5,6K7,8 + K3,4K5,6K8,9 +
                    K3,4K5,6K9,7 + K3,4K6,5K7,8 + K3,4K6,5K8,9 +
                    K3,4K6,5K9,7 + K3,4K7,8K8,9 + K3,4K7,8K9,7 +
                    K3,4K8,9K9,7 + K4,3K5,6K7,8 + K4,3K5,6K8,9 +
                    K4,3K5,6K9,7 + K4,3K6,5K7,8 + K4,3K6,5K8,9 +
                    K4,3K6,5K9,7 + K4,3K7,8K8,9 + K4,3K7,8K9,7 +
                    K4,3K8,9K9,7 + K4,5K5,6K7,8 + K4,5K5,6K8,9 +
                    K4,5K5,6K9,7 + K4,5K6,5K7,8 + K4,5K6,5K8,9 +
                    K4,5K6,5K9,7 + K4,5K7,8K8,9 + K4,5K7,8K9,7 +
                    K4,5K8,9K9,7 + K4,7K5,6K7,8 + K4,7K5,6K8,9 +
                    K4,7K5,6K9,7 + K4,7K6,5K7,8 + K4,7K6,5K8,9 +
                    K4,7K6,5K9,7 + K4,7K7,8K8,9 + K4,7K7,8K9,7 +
                    K4,7K8,9K9,7 + K5,6K7,8K8,9 + K5,6K7,8K9,7 +
                    K5,6K8,9K9,7 + K6,5K7,8K8,9 + K6,5K7,8K9,7 +
                    K6,5K8,9K9,7

            F4(1) = K1,2K2,3K3,4K4,5 + K1,2K2,3K3,4K4,7 +
                    K1,2K2,3K3,4K5,6 + K1,2K2,3K3,4K6,5 +
                    K1,2K2,3K3,4K7,8 + K1,2K2,3K3,4K8,9 +
                    K1,2K2,3K3,4K9,7 + K1,2K2,3K4,3K5,6 +
                    K1,2K2,3K4,3K6,5 + K1,2K2,3K4,3K7,8 +
                    K1,2K2,3K4,3K8,9 + K1,2K2,3K4,3K9,7 +
                    K1,2K2,3K4,5K5,6 + K1,2K2,3K4,5K6,5 +
                    K1,2K2,3K4,5K7,8 + K1,2K2,3K4,5K8,9 +
                    K1,2K2,3K4,5K9,7 + K1,2K2,3K4,7K5,6 +
                    K1,2K2,3K4,7K6,5 + K1,2K2,3K4,7K7,8 +
                    K1,2K2,3K4,7K8,9 + K1,2K2,3K4,7K9,7 +
                    K1,2K2,3K5,6K7,8 + K1,2K2,3K5,6K8,9 +
                    K1,2K2,3K5,6K9,7 + K1,2K2,3K6,5K7,8 +
                    K1,2K2,3K6,5K8,9 + K1,2K2,3K6,5K9,7 +
                    K1,2K2,3K7,8K8,9 + K1,2K2,3K7,8K9,7 +
                    K1,2K2,3K8,9K9,7 + K1,2K3,4K4,5K5,6 +
                    K1,2K3,4K4,5K6,5 + K1,2K3,4K4,5K7,8 +
                    K1,2K3,4K4,5K8,9 + K1,2K3,4K4,5K9,7 +
                    K1,2K3,4K4,7K5,6 + K1,2K3,4K4,7K6,5 +
                    K1,2K3,4K4,7K7,8 + K1,2K3,4K4,7K8,9 +
                    K1,2K3,4K4,7K9,7 + K1,2K3,4K5,6K7,8 +
```

Listing A1 continued

```
            K1,2K3,4K5,6K8,9 + K1,2K3,4K5,6K9,7 +
            K1,2K3,4K6,5K7,8 + K1,2K3,4K6,5K8,9 +
            K1,2K3,4K6,5K9,7 + K1,2K3,4K7,8K8,9 +
            K1,2K3,4K7,8K9,7 + K1,2K3,4K8,9K9,7 +
            K1,2K4,3K5,6K7,8 + K1,2K4,3K5,6K8,9 +
            K1,2K4,3K5,6K9,7 + K1,2K4,3K6,5K7,8 +
            K1,2K4,3K6,5K8,9 + K1,2K4,3K6,5K9,7 +
            K1,2K4,3K7,8K8,9 + K1,2K4,3K7,8K9,7 +
            K1,2K4,3K8,9K9,7 + K1,2K4,5K5,6K7,8 +
            K1,2K4,5K5,6K8,9 + K1,2K4,5K5,6K9,7 +
            K1,2K4,5K6,5K7,8 + K1,2K4,5K6,5K8,9 +
            K1,2K4,5K6,5K9,7 + K1,2K4,5K7,8K8,9 +
            K1,2K4,5K7,8K9,7 + K1,2K4,5K8,9K9,7 +
            K1,2K4,7K5,6K7,8 + K1,2K4,7K5,6K8,9 +
            K1,2K4,7K5,6K9,7 + K1,2K4,7K6,5K7,8 +
            K1,2K4,7K6,5K8,9 + K1,2K4,7K6,5K9,7 +
            K1,2K4,7K7,8K8,9 + K1,2K4,7K7,8K9,7 +
            K1,2K4,7K8,9K9,7 + K1,2K5,6K7,8K8,9 +
            K1,2K5,6K7,8K9,7 + K1,2K5,6K8,9K9,7 +
            K1,2K6,5K7,8K8,9 + K1,2K6,5K7,8K9,7 +
            K1,2K6,5K8,9K9,7 + K2,1K3,4K4,5K5,6 +
            K2,1K3,4K4,5K6,5 + K2,1K3,4K4,5K7,8 +
            K2,1K3,4K4,5K8,9 + K2,1K3,4K4,5K9,7 +
            K2,1K3,4K4,7K5,6 + K2,1K3,4K4,7K6,5 +
            K2,1K3,4K4,7K7,8 + K2,1K3,4K4,7K8,9 +
            K2,1K3,4K4,7K9,7 + K2,1K3,4K5,6K7,8 +
            K2,1K3,4K5,6K8,9 + K2,1K3,4K5,6K9,7 +
            K2,1K3,4K6,5K7,8 + K2,1K3,4K6,5K8,9 +
            K2,1K3,4K6,5K9,7 + K2,1K3,4K7,8K8,9 +
            K2,1K3,4K7,8K9,7 + K2,1K3,4K8,9K9,7 +
            K2,1K4,3K5,6K7,8 + K2,1K4,3K5,6K8,9 +
            K2,1K4,3K5,6K9,7 + K2,1K4,3K6,5K7,8 +
            K2,1K4,3K6,5K8,9 + K2,1K4,3K6,5K9,7 +
            K2,1K4,3K7,8K8,9 + K2,1K4,3K7,8K9,7 +
            K2,1K4,3K8,9K9,7 + K2,1K4,5K5,6K7,8 +
            K2,1K4,5K5,6K8,9 + K2,1K4,5K5,6K9,7 +
            K2,1K4,5K6,5K7,8 + K2,1K4,5K6,5K8,9 +
            K2,1K4,5K6,5K9,7 + K2,1K4,5K7,8K8,9 +
            K2,1K4,5K7,8K9,7 + K2,1K4,5K8,9K9,7 +
            K2,1K4,7K5,6K7,8 + K2,1K4,7K5,6K8,9 +
            K2,1K4,7K5,6K9,7 + K2,1K4,7K6,5K7,8 +
            K2,1K4,7K6,5K8,9 + K2,1K4,7K6,5K9,7 +
            K2,1K4,7K7,8K8,9 + K2,1K4,7K7,8K9,7 +
            K2,1K4,7K8,9K9,7 + K2,1K5,6K7,8K8,9 +
            K2,1K5,6K7,8K9,7 + K2,1K5,6K8,9K9,7 +
            K2,1K6,5K7,8K8,9 + K2,1K6,5K7,8K9,7 +
            K2,1K6,5K8,9K9,7 + K2,3K3,4K4,5K5,6 +
            K2,3K3,4K4,5K6,5 + K2,3K3,4K4,5K7,8 +
            K2,3K3,4K4,5K8,9 + K2,3K3,4K4,5K9,7 +
            K2,3K3,4K4,7K5,6 + K2,3K3,4K4,7K6,5 +
            K2,3K3,4K4,7K7,8 + K2,3K3,4K4,7K8,9 +
            K2,3K3,4K4,7K9,7 + K2,3K3,4K5,6K7,8 +
            K2,3K3,4K5,6K8,9 + K2,3K3,4K5,6K9,7 +
            K2,3K3,4K6,5K7,8 + K2,3K3,4K6,5K8,9 +
            K2,3K3,4K6,5K9,7 + K2,3K3,4K7,8K8,9 +
            K2,3K3,4K7,8K9,7 + K2,3K3,4K8,9K9,7 +
            K2,3K4,3K5,6K7,8 + K2,3K4,3K5,6K8,9 +
```

Listing A1   continued

```
                        K2,3K4,3K5,6K9,7 + K2,3K4,3K6,5K7,8 +
                        K2,3K4,3K6,5K8,9 + K2,3K4,3K6,5K9,7 +
                        K2,3K4,3K7,8K8,9 + K2,3K4,3K7,8K9,7 +
                        K2,3K4,3K8,9K9,7 + K2,3K4,5K5,6K7,8 +
                        K2,3K4,5K5,6K8,9 + K2,3K4,5K5,6K9,7 +
                        K2,3K4,5K6,5K7,8 + K2,3K4,5K6,5K8,9 +
                        K2,3K4,5K6,5K9,7 + K2,3K4,5K7,8K8,9 +
                        K2,3K4,5K7,8K9,7 + K2,3K4,5K8,9K9,7 +
                        K2,3K4,7K5,6K7,8 + K2,3K4,7K5,6K8,9 +
                        K2,3K4,7K5,6K9,7 + K2,3K4,7K6,5K7,8 +
                        K2,3K4,7K6,5K8,9 + K2,3K4,7K6,5K9,7 +
                        K2,3K4,7K7,8K8,9 + K2,3K4,7K7,8K9,7 +
                        K2,3K4,7K8,9K9,7 + K2,3K5,6K7,8K8,9 +
                        K2,3K5,6K7,8K9,7 + K2,3K5,6K8,9K9,7 +
                        K2,3K6,5K7,8K8,9 + K2,3K6,5K7,8K9,7 +
                        K2,3K6,5K8,9K9,7 + K3,4K4,5K5,6K7,8 +
                        K3,4K4,5K5,6K8,9 + K3,4K4,5K5,6K9,7 +
                        K3,4K4,5K6,5K7,8 + K3,4K4,5K6,5K8,9 +
                        K3,4K4,5K6,5K9,7 + K3,4K4,5K7,8K8,9 +
                        K3,4K4,5K7,8K9,7 + K3,4K4,5K8,9K9,7 +
                        K3,4K4,7K5,6K7,8 + K3,4K4,7K5,6K8,9 +
                        K3,4K4,7K5,6K9,7 + K3,4K4,7K6,5K7,8 +
                        K3,4K4,7K6,5K8,9 + K3,4K4,7K6,5K9,7 +
                        K3,4K4,7K7,8K8,9 + K3,4K4,7K7,8K9,7 +
                        K3,4K4,7K8,9K9,7 + K3,4K5,6K7,8K8,9 +
                        K3,4K5,6K7,8K9,7 + K3,4K5,6K8,9K9,7 +
                        K3,4K6,5K7,8K8,9 + K3,4K6,5K7,8K9,7 +
                        K3,4K6,5K8,9K9,7 + K4,3K5,6K7,8K8,9 +
                        K4,3K5,6K7,8K9,7 + K4,3K5,6K8,9K9,7 +
                        K4,3K6,5K7,8K9,7 + K4,5K5,6K7,8K8,9 +
                        K4,5K5,6K7,8K9,7 + K4,5K5,6K8,9K9,7 +
                        K4,5K6,5K7,8K8,9 + K4,5K6,5K7,8K9,7 +
                        K4,5K6,5K8,9K9,7 + K4,7K5,6K7,8K8,9 +
                        K4,7K5,6K7,8K9,7 + K4,7K5,6K8,9K9,7 +
                        K4,7K6,5K7,8K8,9 + K4,7K6,5K7,8K9,7 +
                        K4,7K6,5K8,9K9,7

          F5(1) = K1,2K2,3K3,4K4,5K5,6 + K1,2K2,3K3,4K4,5K6,5 +
                        K1,2K2,3K3,4K4,5K7,8 + K1,2K2,3K3,4K4,5K8,9 +
                        K1,2K2,3K3,4K4,5K9,7 + K1,2K2,3K3,4K4,7K5,6 +
                        K1,2K2,3K3,4K4,7K6,5 + K1,2K2,3K3,4K4,7K7,8 +
                        K1,2K2,3K3,4K4,7K8,9 + K1,2K2,3K3,4K4,7K9,7 +
                        K1,2K2,3K3,4K5,6K7,8 + K1,2K2,3K3,4K5,6K8,9 +
                        K1,2K2,3K3,4K5,6K9,7 + K1,2K2,3K3,4K6,5K7,8 +
                        K1,2K2,3K3,4K6,5K8,9 + K1,2K2,3K3,4K6,5K9,7 +
                        K1,2K2,3K3,4K7,8K8,9 + K1,2K2,3K3,4K7,8K9,7 +
                        K1,2K2,3K3,4K8,9K9,7 + K1,2K2,3K4,3K5,6K7,8 +
                        K1,2K2,3K4,3K5,6K8,9 + K1,2K2,3K4,3K5,6K9,7 +
                        K1,2K2,3K4,3K6,5K7,8 + K1,2K2,3K4,3K6,5K8,9 +
                        K1,2K2,3K4,3K6,5K9,7 + K1,2K2,3K4,3K7,8K8,9 +
                        K1,2K2,3K4,3K7,8K9,7 + K1,2K2,3K4,3K8,9K9,7 +
                        K1,2K2,3K4,5K5,6K7,8 + K1,2K2,3K4,5K5,6K8,9 +
                        K1,2K2,3K4,5K5,6K9,7 + K1,2K2,3K4,5K6,5K7,8 +
                        K1,2K2,3K4,5K6,5K8,9 + K1,2K2,3K4,5K6,5K9,7 +
                        K1,2K2,3K4,5K7,8K8,9 + K1,2K2,3K4,5K7,8K9,7 +
                        K1,2K2,3K4,5K8,9K9,7 + K1,2K2,3K4,7K5,6K7,8 +
```

Listing A1 continued

```
K1,2K2,3K4,7K5,6K8,9 + K1,2K2,3K4,7K5,6K9,7 +
K1,2K2,3K4,7K6,5K7,8 + K1,2K2,3K4,7K6,5K8,9 +
K1,2K2,3K4,7K6,5K9,7 + K1,2K2,3K4,7K7,8K8,9 +
K1,2K2,3K4,7K7,8K9,7 + K1,2K2,3K4,7K8,9K9,7 +
K1,2K2,3K5,6K7,8K8,9 + K1,2K2,3K5,6K7,8K9,7 +
K1,2K2,3K5,6K8,9K9,7 + K1,2K2,3K6,5K7,8K8,9 +
K1,2K2,3K6,5K7,8K9,7 + K1,2K2,3K6,5K8,9K9,7 +
K1,2K3,4K4,5K5,6K7,8 + K1,2K3,4K4,5K5,6K8,9 +
K1,2K3,4K4,5K5,6K9,7 + K1,2K3,4K4,5K6,5K7,8 +
K1,2K3,4K4,5K6,5K8,9 + K1,2K3,4K4,5K6,5K9,7 +
K1,2K3,4K4,5K7,8K8,9 + K1,2K3,4K4,5K7,8K9,7 +
K1,2K3,4K4,5K8,9K9,7 + K1,2K3,4K4,7K5,6K7,8 +
K1,2K3,4K4,7K5,6K8,9 + K1,2K3,4K4,7K5,6K9,7 +
K1,2K3,4K4,7K6,5K7,8 + K1,2K3,4K4,7K6,5K8,9 +
K1,2K3,4K4,7K6,5K9,7 + K1,2K3,4K4,7K7,8K8,9 +
K1,2K3,4K4,7K7,8K9,7 + K1,2K3,4K4,7K8,9K9,7 +
K1,2K3,4K5,6K7,8K8,9 + K1,2K3,4K5,6K7,8K9,7 +
K1,2K3,4K5,6K8,9K9,7 + K1,2K3,4K6,5K7,8K8,9 +
K1,2K3,4K6,5K7,8K9,7 + K1,2K3,4K6,5K8,9K9,7 +
K1,2K4,3K5,6K7,8K8,9 + K1,2K4,3K5,6K7,8K9,7 +
K1,2K4,3K5,6K8,9K9,7 + K1,2K4,3K6,5K7,8K8,9 +
K1,2K4,3K6,5K7,8K9,7 + K1,2K4,3K6,5K8,9K9,7 +
K1,2K4,5K5,6K7,8K8,9 + K1,2K4,5K5,6K7,8K9,7 +
K1,2K4,5K5,6K8,9K9,7 + K1,2K4,5K6,5K7,8K8,9 +
K1,2K4,5K6,5K7,8K9,7 + K1,2K4,5K6,5K8,9K9,7 +
K1,2K4,7K5,6K7,8K8,9 + K1,2K4,7K5,6K7,8K9,7 +
K1,2K4,7K5,6K8,9K9,7 + K1,2K4,7K6,5K7,8K8,9 +
K1,2K4,7K6,5K7,8K9,7 + K1,2K4,7K6,5K8,9K9,7 +
K2,1K3,4K4,5K5,6K7,8 + K2,1K3,4K4,5K5,6K8,9 +
K2,1K3,4K4,5K5,6K9,7 + K2,1K3,4K4,5K6,5K7,8 +
K2,1K3,4K4,5K6,5K8,9 + K2,1K3,4K4,5K6,5K9,7 +
K2,1K3,4K4,5K7,8K8,9 + K2,1K3,4K4,5K7,8K9,7 +
K2,1K3,4K4,5K8,9K9,7 + K2,1K3,4K4,7K5,6K7,8 +
K2,1K3,4K4,7K5,6K8,9 + K2,1K3,4K4,7K5,6K9,7 +
K2,1K3,4K4,7K6,5K7,8 + K2,1K3,4K4,7K6,5K8,9 +
K2,1K3,4K4,7K6,5K9,7 + K2,1K3,4K4,7K7,8K8,9 +
K2,1K3,4K4,7K7,8K9,7 + K2,1K3,4K4,7K8,9K9,7 +
K2,1K3,4K5,6K7,8K8,9 + K2,1K3,4K5,6K7,8K9,7 +
K2,1K3,4K5,6K8,9K9,7 + K2,1K3,4K6,5K7,8K8,9 +
K2,1K3,4K6,5K7,8K9,7 + K2,1K3,4K6,5K8,9K9,7 +
K2,1K4,3K5,6K7,8K8,9 + K2,1K4,3K5,6K7,8K9,7 +
K2,1K4,3K5,6K8,9K9,7 + K2,1K4,3K6,5K7,8K8,9 +
K2,1K4,3K6,5K7,8K9,7 + K2,1K4,3K6,5K8,9K9,7 +
K2,1K4,5K5,6K7,8K8,9 + K2,1K4,5K5,6K7,8K9,7 +
K2,1K4,5K5,6K8,9K9,7 + K2,1K4,5K6,5K7,8K8,9 +
K2,1K4,5K6,5K7,8K9,7 + K2,1K4,5K6,5K8,9K9,7 +
K2,1K4,7K5,6K7,8K8,9 + K2,1K4,7K5,6K7,8K9,7 +
K2,1K4,7K5,6K8,9K9,7 + K2,1K4,7K6,5K7,8K8,9 +
K2,1K4,7K6,5K7,8K9,7 + K2,1K4,7K6,5K8,9K9,7 +
K2,3K3,4K4,5K5,6K7,8 + K2,3K3,4K4,5K5,6K8,9 +
K2,3K3,4K4,5K5,6K9,7 + K2,3K3,4K4,5K6,5K7,8 +
K2,3K3,4K4,5K6,5K8,9 + K2,3K3,4K4,5K6,5K9,7 +
K2,3K3,4K4,5K7,8K8,9 + K2,3K3,4K4,5K7,8K9,7 +
K2,3K3,4K4,5K8,9K9,7 + K2,3K3,4K4,7K5,6K7,8 +
K2,3K3,4K4,7K5,6K8,9 + K2,3K3,4K4,7K5,6K9,7 +
K2,3K3,4K4,7K6,5K7,8 + K2,3K3,4K4,7K6,5K8,9 +
K2,3K3,4K4,7K6,5K9,7 + K2,3K3,4K4,7K7,8K8,9 +
```

Listing A1 continued

```
                    K2,3K3,4K4,7K7,8K9,7 + K2,3K3,4K4,7K8,9K9,7 +
                    K2,3K3,4K5,6K7,8K8,9 + K2,3K3,4K5,6K7,8K9,7 +
                    K2,3K3,4K5,6K8,9K9,7 + K2,3K3,4K6,5K7,8K8,9 +
                    K2,3K3,4K6,5K7,8K9,7 + K2,3K3,4K6,5K8,9K9,7 +
                    K2,3K4,3K5,6K7,8K8,9 + K2,3K4,3K5,6K7,8K9,7 +
                    K2,3K4,3K5,6K8,9K9,7 + K2,3K4,3K6,5K7,8K8,9 +
                    K2,3K4,3K6,5K7,8K9,7 + K2,3K4,3K6,5K8,9K9,7 +
                    K2,3K4,5K5,6K7,8K8,9 + K2,3K4,5K5,6K7,8K9,7 +
                    K2,3K4,5K5,6K8,9K9,7 + K2,3K4,5K6,5K7,8K8,9 +
                    K2,3K4,5K6,5K7,8K9,7 + K2,3K4,5K6,5K8,9K9,7 +
                    K2,3K4,7K5,6K7,8K8,9 + K2,3K4,7K5,6K7,8K9,7 +
                    K2,3K4,7K5,6K8,9K9,7 + K2,3K4,7K6,5K7,8K8,9 +
                    K2,3K4,7K6,5K7,8K9,7 + K2,3K4,7K6,5K8,9K9,7 +
                    K3,4K4,5K5,6K7,8K8,9 + K3,4K4,5K5,6K7,8K9,7 +
                    K3,4K4,5K5,6K8,9K9,7 + K3,4K4,5K6,5K7,8K8,9 +
                    K3,4K4,5K6,5K7,8K9,7 + K3,4K4,5K6,5K8,9K9,7 +
                    K3,4K4,7K5,6K7,8K8,9 + K3,4K4,7K5,6K7,8K9,7 +
                    K3,4K4,7K5,6K8,9K9,7 + K3,4K4,7K6,5K7,8K8,9 +
                    K3,4K4,7K6,5K7,8K9,7 + K3,4K4,7K6,5K8,9K9,7

F6(1) = K1,2K2,3K3,4K4,5K5,6K7,8 + K1,2K2,3K3,4K4,5K5,6K8,9 +
                    K1,2K2,3K3,4K4,5K5,6K9,7 + K1,2K2,3K3,4K4,5K6,5K7,8 +
                    K1,2K2,3K3,4K4,5K6,5K8,9 + K1,2K2,3K3,4K4,5K6,5K9,7 +
                    K1,2K2,3K3,4K4,5K7,8K8,9 + K1,2K2,3K3,4K4,5K7,8K9,7 +
                    K1,2K2,3K3,4K4,5K8,9K9,7 + K1,2K2,3K3,4K4,7K5,6K7,8 +
                    K1,2K2,3K3,4K4,7K5,6K8,9 + K1,2K2,3K3,4K4,7K5,6K9,7 +
                    K1,2K2,3K3,4K4,7K6,5K7,8 + K1,2K2,3K3,4K4,7K6,5K8,9 +
                    K1,2K2,3K3,4K4,7K6,5K9,7 + K1,2K2,3K3,4K4,7K7,8K8,9 +
                    K1,2K2,3K3,4K4,7K7,8K9,7 + K1,2K2,3K3,4K4,7K8,9K9,7 +
                    K1,2K2,3K3,4K5,6K7,8K8,9 + K1,2K2,3K3,4K5,6K7,8K9,7 +
                    K1,2K2,3K3,4K5,6K8,9K9,7 + K1,2K2,3K3,4K6,5K7,8K8,9 +
                    K1,2K2,3K3,4K6,5K7,8K9,7 + K1,2K2,3K3,4K6,5K8,9K9,7 +
                    K1,2K2,3K4,3K5,6K7,8K8,9 + K1,2K2,3K4,3K5,6K7,8K9,7 +
                    K1,2K2,3K4,3K5,6K8,9K9,7 + K1,2K2,3K4,3K6,5K7,8K8,9 +
                    K1,2K2,3K4,3K6,5K7,8K9,7 + K1,2K2,3K4,3K6,5K8,9K9,7 +
                    K1,2K2,3K4,5K5,6K7,8K8,9 + K1,2K2,3K4,5K5,6K7,8K9,7 +
                    K1,2K2,3K4,5K5,6K8,9K9,7 + K1,2K2,3K4,5K6,5K7,8K8,9 +
                    K1,2K2,3K4,5K6,5K7,8K9,7 + K1,2K2,3K4,5K6,5K8,9K9,7 +
                    K1,2K2,3K4,7K5,6K7,8K8,9 + K1,2K2,3K4,7K5,6K7,8K9,7 +
                    K1,2K2,3K4,7K5,6K8,9K9,7 + K1,2K2,3K4,7K6,5K7,8K8,9 +
                    K1,2K2,3K4,7K6,5K7,8K9,7 + K1,2K2,3K4,7K6,5K8,9K9,7 +
                    K1,2K2,3K4,4K5,5K6,7K7,8K8,9 + K1,2K2,3K4,4K5,5K6,7K8,9 +
                    K1,2K2,3K4,4K5,5K6,8K9,7 + K1,2K2,3K4,4K5,6K5,7K8,9 +
                    K1,2K2,3K4,4K5,6K5,7K8,9,7 + K1,2K2,3K4,4K5,6K5,8K9,7 +
                    K1,2K2,3K4,4K7,5K6,7K8,9 + K1,2K2,3K4,4K7,5K6,7K9,7 +
                    K1,2K2,3K4,4K7,5K6,8K9,7 + K1,2K2,3K4,4K7,6K5,7K8,9 +
                    K1,2K2,3K4,4K7,6K5,7K9,7 + K1,2K2,3K4,4K7,6K5,8K9,7 +
                    K2,1K3,4K4,5K5,6K7,8K8,9 + K2,1K3,4K4,5K5,6K7,8K9,7 +
                    K2,1K3,4K4,5K5,6K8,9K9,7 + K2,1K3,4K4,5K6,5K7,8K8,9 +
                    K2,1K3,4K4,5K6,5K7,8K9,7 + K2,1K3,4K4,5K6,5K8,9K9,7 +
                    K2,1K3,4K4,7K5,6K7,8K8,9 + K2,1K3,4K4,7K5,6K7,8K9,7 +
                    K2,1K3,4K4,7K5,6K8,9K9,7 + K2,1K3,4K4,7K6,5K7,8K8,9 +
                    K2,1K3,4K4,7K6,5K7,8K9,7 + K2,1K3,4K4,7K6,5K8,9K9,7 +
                    K2,3K3,4K4,5K5,6K7,8K8,9 + K2,3K3,4K4,5K5,6K7,8K9,7 +
                    K2,3K3,4K4,5K5,6K8,9K9,7 + K2,3K3,4K4,5K6,5K7,8K8,9 +
                    K2,3K3,4K4,5K6,5K7,8K9,7 + K2,3K3,4K4,5K6,5K8,9K9,7 +
                    K2,3K3,4K4,7K5,6K7,8K8,9 + K2,3K3,4K4,7K5,6K7,8K9,7 +
                    K2,3K3,4K4,7K5,6K8,9K9,7 + K2,3K3,4K4,7K6,5K7,8K8,9 +
                    K2,3K3,4K4,7K6,5K7,8K9,7 + K2,3K3,4K4,7K6,5K8,9K9,7

F7(1) = K1,2K2,3K3,4K4,5K5,6K7,8K8,9 +
                    K1,2K2,3K3,4K4,5K5,6K7,8K9,7 +
                    K1,2K2,3K3,4K4,5K5,6K8,9K9,7 +
                    K1,2K2,3K3,4K4,5K6,5K7,8K8,9 +
                    K1,2K2,3K3,4K4,5K6,5K7,8K9,7 +
                    K1,2K2,3K3,4K4,5K6,5K8,9K9,7 +
                    K1,2K2,3K3,4K4,7K5,6K7,8K8,9 +
                    K1,2K2,3K3,4K4,7K5,6K7,8K9,7 +
                    K1,2K2,3K3,4K4,7K5,6K8,9K9,7 +
                    K1,2K2,3K3,4K4,7K6,5K7,8K8,9 +
                    K1,2K2,3K3,4K4,7K6,5K7,8K9,7 +
                    K1,2K2,3K3,4K4,7K6,5K8,9K9,7

F8(1) = 0
```

Listing A1   continued

```
E4 = { C1 }
ω(4) = { 1, 2, 3 }
z(4) = { 1, 2, 3, 4, 5, 6, 7, 8 }
n(4) = 9
u(4) = 8

f(1,4)0 = 0

f(1,4)1 = 0

f(1,4)2 = 0

f(1,4)3 = K1,2K2,3K3,4

f(1,4)4 = K1,2K2,3K3,4K5,6 + K1,2K2,3K3,4K6,5 + K1,2K2,3K3,4K7,8 +
          K1,2K2,3K3,4K8,9 + K1,2K2,3K3,4K9,7

f(1,4)5 = K1,2K2,3K3,4K5,6K7,8 + K1,2K2,3K3,4K5,6K8,9 +
          K1,2K2,3K3,4K5,6K9,7 + K1,2K2,3K3,4K6,5K7,8 +
          K1,2K2,3K3,4K6,5K8,9 + K1,2K2,3K3,4K6,5K9,7 +
          K1,2K2,3K3,4K7,8K8,9 + K1,2K2,3K3,4K7,8K9,7 +
          K1,2K2,3K3,4K8,9K9,7

f(1,4)6 = K1,2K2,3K3,4K5,6K7,8K8,9 + K1,2K2,3K3,4K5,6K7,8K9,7 +
          K1,2K2,3K3,4K5,6K8,9K9,7 + K1,2K2,3K3,4K6,5K7,8K8,9 +
          K1,2K2,3K3,4K6,5K7,8K9,7 + K1,2K2,3K3,4K6,5K8,9K9,7

f(1,4)7 = 0

f(2,4)0 = 0

f(2,4)1 = 0

f(2,4)2 = K2,3K3,4

f(2,4)3 = K1,2K2,3K3,4 + K2,3K3,4K5,6 + K2,3K3,4K6,5 +
          K2,3K3,4K7,8 + K2,3K3,4K8,9 + K2,3K3,4K9,7

f(2,4)4 = K1,2K2,3K3,4K5,6 + K1,2K2,3K3,4K6,5 + K1,2K2,3K3,4K7,8 +
          K1,2K2,3K3,4K8,9 + K1,2K2,3K3,4K9,7 + K2,3K3,4K5,6K7,8 +
          K2,3K3,4K5,6K8,9 + K2,3K3,4K5,6K9,7 + K2,3K3,4K6,5K7,8 +
          K2,3K3,4K6,5K8,9 + K2,3K3,4K6,5K9,7 + K2,3K3,4K7,8K8,9 +
          K2,3K3,4K7,8K9,7 + K2,3K3,4K8,9K9,7

f(2,4)5 = K1,2K2,3K3,4K5,6K7,8 + K1,2K2,3K3,4K5,6K8,9 +
          K1,2K2,3K3,4K5,6K9,7 + K1,2K2,3K3,4K6,5K7,8 +
          K1,2K2,3K3,4K6,5K8,9 + K1,2K2,3K3,4K6,5K9,7 +
          K1,2K2,3K3,4K7,8K8,9 + K1,2K2,3K3,4K7,8K9,7 +
          K1,2K2,3K3,4K8,9K9,7 + K2,3K3,4K5,6K7,8K8,9 +
          K2,3K3,4K5,6K7,8K9,7 + K2,3K3,4K5,6K8,9K9,7 +
          K2,3K3,4K6,5K7,8K8,9 + K2,3K3,4K6,5K7,8K9,7 +
          K2,3K3,4K6,5K8,9K9,7
```

Listing A2 The expressions of coefficients $(f_{k,4})_q$ in Fig. 3 using the non optimized equations

```
f(2,4)6 = K1,2K2,3K3,4K5,6K7,8K8,9 + K1,2K2,3K3,4K5,6K7,8K9,7 +
          K1,2K2,3K3,4K5,6K8,9K9,7 + K1,2K2,3K3,4K6,5K7,8K8,9 +
          K1,2K2,3K3,4K6,5K7,8K9,7 + K1,2K2,3K3,4K6,5K8,9K9,7

f(2,4)7 = 0

f(3,4)0 = 0

f(3,4)1 = K3,4

f(3,4)2 = K1,2K3,4 + K2,1K3,4 + K2,3K3,4 + K3,4K5,6 + K3,4K6,5 +
          K3,4K7,8 + K3,4K8,9 + K3,4K9,7

f(3,4)3 = K1,2K2,3K3,4 + K1,2K3,4K5,6 + K1,2K3,4K6,5 +
          K1,2K3,4K7,8 + K1,2K3,4K8,9 + K1,2K3,4K9,7 +
          K2,1K3,4K5,6 + K2,1K3,4K6,5 + K2,1K3,4K7,8 +
          K2,1K3,4K8,9 + K2,1K3,4K9,7 + K2,3K3,4K5,6 +
          K2,3K3,4K6,5 + K2,3K3,4K7,8 + K2,3K3,4K8,9 +
          K2,3K3,4K9,7 + K3,4K5,6K7,8 + K3,4K5,6K8,9 +
          K3,4K5,6K9,7 + K3,4K6,5K7,8 + K3,4K6,5K8,9 +
          K3,4K6,5K9,7 + K3,4K7,8K8,9 + K3,4K7,8K9,7 +
          K3,4K8,9K9,7

f(3,4)4 = K1,2K2,3K3,4K5,6 + K1,2K2,3K3,4K6,5 + K1,2K2,3K3,4K7,8 +
          K1,2K2,3K3,4K8,9 + K1,2K2,3K3,4K9,7 + K1,2K3,4K5,6K7,8 +
          K1,2K3,4K5,6K8,9 + K1,2K3,4K5,6K9,7 + K1,2K3,4K6,5K7,8 +
          K1,2K3,4K6,5K8,9 + K1,2K3,4K6,5K9,7 + K1,2K3,4K7,8K8,9 +
          K1,2K3,4K7,8K9,7 + K1,2K3,4K8,9K9,7 + K2,1K3,4K5,6K7,8 +
          K2,1K3,4K5,6K8,9 + K2,1K3,4K5,6K9,7 + K2,1K3,4K6,5K7,8 +
          K2,1K3,4K6,5K8,9 + K2,1K3,4K6,5K9,7 + K2,1K3,4K7,8K8,9 +
          K2,1K3,4K7,8K9,7 + K2,1K3,4K8,9K9,7 + K2,3K3,4K5,6K7,8 +
          K2,3K3,4K5,6K8,9 + K2,3K3,4K5,6K9,7 + K2,3K3,4K6,5K7,8 +
          K2,3K3,4K6,5K8,9 + K2,3K3,4K6,5K9,7 + K2,3K3,4K7,8K8,9 +
          K2,3K3,4K7,8K9,7 + K2,3K3,4K8,9K9,7 + K3,4K5,6K7,8K8,9 +
          K3,4K5,6K7,8K9,7 + K3,4K5,6K8,9K9,7 + K3,4K6,5K7,8K8,9 +
          K3,4K6,5K7,8K9,7 + K3,4K6,5K8,9K9,7

f(3,4)5 = K1,2K2,3K3,4K5,6K7,8 + K1,2K2,3K3,4K5,6K8,9 +
          K1,2K2,3K3,4K5,6K9,7 + K1,2K2,3K3,4K6,5K7,8 +
          K1,2K2,3K3,4K6,5K8,9 + K1,2K2,3K3,4K6,5K9,7 +
          K1,2K2,3K3,4K7,8K8,9 + K1,2K2,3K3,4K7,8K9,7 +
          K1,2K2,3K3,4K8,9K9,7 + K1,2K3,4K5,6K7,8K8,9 +
          K1,2K3,4K5,6K7,8K9,7 + K1,2K3,4K5,6K8,9K9,7 +
          K1,2K3,4K6,5K7,8K8,9 + K1,2K3,4K6,5K7,8K9,7 +
          K1,2K3,4K6,5K8,9K9,7 + K2,1K3,4K5,6K7,8K8,9 +
          K2,1K3,4K5,6K7,8K9,7 + K2,1K3,4K5,6K8,9K9,7 +
          K2,1K3,4K6,5K7,8K8,9 + K2,1K3,4K6,5K7,8K9,7 +
          K2,1K3,4K6,5K8,9K9,7 + K2,3K3,4K5,6K7,8K8,9 +
          K2,3K3,4K5,6K7,8K9,7 + K2,3K3,4K5,6K8,9K9,7 +
          K2,3K3,4K6,5K7,8K8,9 + K2,3K3,4K6,5K7,8K9,7 +
          K2,3K3,4K6,5K8,9K9,7

f(3,4)6 = K1,2K2,3K3,4K5,6K7,8K8,9 + K1,2K2,3K3,4K5,6K7,8K9,7 +
          K1,2K2,3K3,4K5,6K8,9K9,7 + K1,2K2,3K3,4K6,5K7,8K8,9 +
          K1,2K2,3K3,4K6,5K7,8K9,7 + K1,2K2,3K3,4K6,5K8,9K9,7

f(3,4)7 = 0

F7 = K1,2K2,3K3,4K4,5K5,6K7,8K8,9 + K1,2K2,3K3,4K4,5K5,6K7,8K9,7 +
     K1,2K2,3K3,4K4,5K5,6K8,9K9,7 + K1,2K2,3K3,4K4,5K6,5K7,8K8,9 +
     K1,2K2,3K3,4K4,5K6,5K7,8K9,7 + K1,2K2,3K3,4K4,5K6,5K8,9K9,7 +
     K1,2K2,3K3,4K4,7K5,6K7,8K8,9 + K1,2K2,3K3,4K4,7K5,6K7,8K9,7 +
     K1,2K2,3K3,4K4,7K5,6K8,9K9,7 + K1,2K2,3K3,4K4,7K6,5K7,8K8,9 +
     K1,2K2,3K3,4K4,7K6,5K7,8K9,7 + K1,2K2,3K3,4K4,7K6,5K8,9K9,7
```

Listing A2 continued

Appendix B

The expressions and values corresponding to the non optimized equations indicated below in Listings B1 and B2 which, as seen, are much more complex than their corresponding Listings 3 and 4 corresponding to the optimised equations.

```
C1 = { X1, X2, X3, X4, X5, X6 }
roots = { λ1, λ2, λ3, λ4, λ5 } of T1(λ)
n1 = 6
c1 = 1
u1 = 5


F0(1) = 1

F1(1) = K1,2 + K1,o + K2,3 + K2,4 + K2,o + K3,1 + K4,5 + K5,4

F2(1) = K1,2K2,3 + K1,2K2,4 + K1,2K2,o + K1,2K3,1 + K1,2K4,5 +
        K1,2K5,4 + K1,oK2,3 + K1,oK2,4 + K1,oK2,o + K1,oK3,1 +
        K1,oK4,5 + K1,oK5,4 + K2,3K3,1 + K2,3K4,5 + K2,3K5,4 +
        K2,4K3,1 + K2,4K4,5 + K2,4K5,4 + K2,oK3,1 + K2,oK4,5 +
        K2,oK5,4 + K3,1K4,5 + K3,1K5,4

F3(1) = K1,2K2,3K4,5 + K1,2K2,3K5,4 + K1,2K2,4K3,1 +
        K1,2K2,4K4,5 + K1,2K2,4K5,4 + K1,2K2,oK3,1 +
        K1,2K2,oK4,5 + K1,2K2,oK5,4 + K1,2K3,1K4,5 +
        K1,2K3,1K5,4 + K1,oK2,3K3,1 + K1,oK2,3K4,5 +
        K1,oK2,3K5,4 + K1,oK2,4K3,1 + K1,oK2,4K4,5 +
        K1,oK2,4K5,4 + K1,oK2,oK3,1 + K1,oK2,oK4,5 +
        K1,oK2,oK5,4 + K1,oK3,1K4,5 + K1,oK3,1K5,4 +
        K2,3K3,1K4,5 + K2,3K3,1K5,4 + K2,4K3,1K4,5 +
        K2,4K3,1K5,4 + K2,oK3,1K4,5 + K2,oK3,1K5,4

F4(1) = K1,2K2,4K3,1K4,5 + K1,2K2,4K3,1K5,4 + K1,2K2,oK3,1K4,5 +
        K1,2K2,oK3,1K5,4 + K1,oK2,3K3,1K4,5 + K1,oK2,3K3,1K5,4 +
        K1,oK2,4K3,1K4,5 + K1,oK2,4K3,1K5,4 + K1,oK2,oK3,1K4,5 +
        K1,oK2,oK3,1K5,4

F5(1) = 0
```

Listing B1 Roots of the compartmental system using the non optimized expressions

```
E4 = { C1 }
ω(4) = { 3 }
z(4) = { 1,2,3,4,5 }
n(4) = 6
u(4) = 5


f(3,4)0 = 0

f(3,4)1 = 0

f(3,4)2 = 0

f(3,4)3 = K1,2K2,4K3,1

f(3,4)4 = K1,2K2,4K3,1K5,4


F4 = K1,2K2,4K3,1K4,5 + K1,2K2,4K3,1K5,4 + K1,2K2,oK3,1K4,5 +
     K1,2K2,oK3,1K5,4 + K1,oK2,3K3,1K4,5 + K1,oK2,3K3,1K5,4 +
     K1,oK2,4K3,1K4,5 + K1,oK2,4K3,1K5,4 + K1,oK2,oK3,1K4,5 +
     K1,oK2,oK3,1K5,4
```

Listing B2 The expressions of coefficients $(f_{3,4})_q$ from the example in Fig. 7 using the non optimized equations

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