ChE 400: Applied Chemical Engineering Calculations
Tutorial 5: Use of Matlab to Calculate Laplace Transforms

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This handout contains information about:
- How to calculate Laplace transform using Matlab
- How to calculate Inverse Laplace transform using Matlab
- Example of application of the Laplace transform method for the solution of chemical engineering problems

1. Calculation of Laplace Transforms and Inverse Laplace Transforms using Matlab:
The operations can be calculated symbolically by using the commands:

1. laplace(fun): where "fun" represents the function for which the Laplace transform is going to be calculated
2. ilaplace(fun): where "fun" represents the function for which the inverse Laplace transform is going to be calculated

Reminders:
3. Remember to use "*syms*" to specify that the variable is symbolic
4. Sometimes the function calculated (laplace or inverse of laplace) is too long and it is hard to write from the Matlab command window. To have a much nicer representation of the solution found the command "*pretty*" can be used as shown: pretty(fun), where "fun" represents the function that we want to express in a more legible way.

2. Exercises:

2.1 Calculate the Laplace transform of the following functions using Matlab:
$$x^3 + 3\cos 2x$$


```
>> syms x
>> Laplace(x^3+3*cos(2*x))

ans =

6/s^4+3*s/(s^2+4)

>>
```

$$x^2 \sin(4x)$$

2.2 Reproduce the following example: Calculate the inverse Laplace transform o $F(s) = \dfrac{1}{(s^2+1)(s^2+4s+8)}$

3. Series of continuous stirred tank reactors (transient response):

A chemical reaction takes place in a series of three continuous stirred tank reactors arrange as shown in the figure. A chemical engineer is interested in studying the transient response of the system. The initial concentration of A in each of the reactors is $C_{a,i}=1$ mol/l.
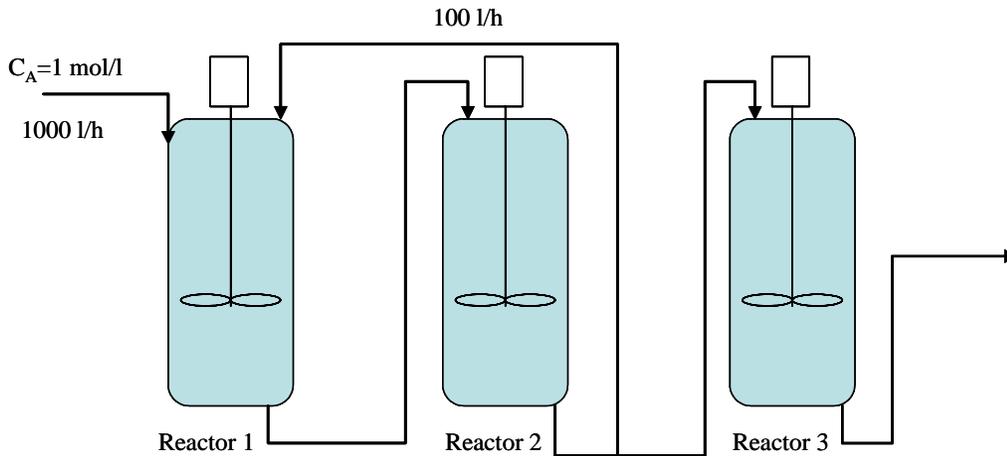
The chemical reaction is a first order irreversible reaction of the type:

$$A \xrightarrow{\ k_i\ } B$$

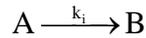The conditions of temperature in each reactor are such that the value of the rate constant k_i is different in each reactor. Also, the volume of each reactor V_i is different. The values of k_i and V_i are given below:

Reactor	Vi (l)	ki (h-1)
1	1000	0.1
2	1500	0.2
3	100	0.4

Develop a set of equations (model) to solve for the concentration of A in each of the reactors as a function of time.

Solution of set of ODE

As explained in class after the assumptions are considered and performing a component balance and a total balance in each of the reactors we can develop the set of equations to solve for modeling the concentration of A (c_{Ai}) as a function of time in each of the reactors. This solution only explains how to solve the set of equations obtained from the material balance when using Laplace transform. The other steps previous to the ones explained here have been extensively considered in class. The symbols and nomenclature used here are the same used in class.

The equations that need to be solved to model the concentration of A in each of the reactors are given by:

$$R1: \quad \frac{dc_{A1}}{dt} = \frac{1}{V_1}\left[1000 + 100c_{A2} - 1100c_{A1} - k_1 V_1 c_{A1}\right] \tag{1}$$

$$R2: \quad \frac{dc_{A2}}{dt} = \frac{1}{V_2}\left[1100c_{A1} - 1100c_{A2} - k_2 V_2 c_{A2}\right] \tag{2}$$

$$R3: \quad \frac{dc_{A3}}{dt} = \frac{1}{V_3}\left[1000c_{A2} - 1000c_{A3} - k_3 V_3 c_{A3}\right] \tag{3}$$

Eqs. (1), (2), and (3) apply for reactors 1, 2, and 3, respectively. They need to be solved simultaneously along with the following initial values (boundary conditions):

$$\text{at } t = 0 \ \ c_{A1} = c_{A2} = c_{A3} = 1 \ \frac{\text{mol}}{\text{l}} \tag{4}$$

Because the equations are linear with constant coefficients, they can be solved using the Laplace transform method. In order to do that, the first step is to take the Laplace transform of each of the equations. As an exercise you should be able to obtain the following equations after taking Laplace transform (you need to use the Laplace transform table along with some of the properties discussed in class):

$$R1: \quad sC_{A1} - 1 = \frac{1}{V_1}\left[\frac{1000}{s} + 100C_{A2} - 1100C_{A1} - k_1 V_1 C_{A1}\right] \tag{5}$$

$$R2: \quad sC_{A2} - 1 = \frac{1}{V_2}\left[1100C_{A1} - 1100C_{A2} - k_2 V_2 C_{A2}\right] \tag{6}$$

$$R3: \quad C_{A3} - 1 = \frac{1}{V_3}\left[1000C_{A2} - 1000C_{A3} - k_3 V_3 C_{A3}\right] \tag{7}$$

Notice that the initial values have already been integrated to Eqs. (5)-(7). Another important point is to notice that $c_{Ai} \neq C_{Ai}$. The capital letter indicates the Laplace transform of the concentration function (we said in class that we will use the capital letter to express Laplace transforms). In detail the Laplace transform of the concentration at any reactor is given by:

$$\mathcal{L}\{c_{Ai}\} = C_{Ai}(s) = C_{Ai}$$

As mentioned in class instead of keep writing $C_{Ai}(s)$ all the time we can just write down C_{Ai}.

Eqs. (5)-(7) can be rearranged as:

$$\left(sV_1 + 1100 + k_1 V_1\right)C_{A1} - 100C_{A2} = \frac{1000}{s} + V_1 \tag{8}$$

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$$-1100C_{A1} + \left(sV_2 + 1100 + k_2V_2\right)C_{A2} = V_2 \tag{9}$$

$$-1000C_{A2} + \left(sV_3 + 1000 + k_3V_3\right)C_{A3} = V_3 \tag{10}$$

The equations given above are a set of linear algebraic equations (LAE), which can be represented in matrix form as:

$$\begin{bmatrix} sV_1 + 1100 + k_1V_1 & -100 & 0 \\ -1100 & sV_2 + 1100 + k_2V_2 & 0 \\ 0 & -1000 & sV_3 + 1000 + k_3V_3 \end{bmatrix}\begin{bmatrix} C_{A1} \\ C_{A2} \\ C_{A3} \end{bmatrix} = \begin{bmatrix} \dfrac{1000}{s} + V_1 \\ V_2 \\ V_3 \end{bmatrix} \tag{11}$$

That is: $[A][C_A] = [b]$

The set of LAE can be solved using Cramer's rule. Once the vector $[C_A]$ is found, the inverse Laplace transform can be calculated and the final concentration of A in each of the reactors is obtained. All these steps were done in Matlab. The program code and the solution shown in the command window are given below. As an exercise you are encourage to practice this exercise by writing your own code in Matlab. All the calculations shown in Matlab are symbolic (*syms*). The use of the command "*pretty*" is also shown.

PROGRAM CODE:

```
% This program solves for system of algebraic equations using cramer's rule
% It also calculate the inverse laplace transform, providing the equation for
% the concentration of A in each of the reactors.
% The command pretty have been used to better understand the printout of the equations
%
% ALL THE CALCULATIONS DONE IN THIS PROGRAM ARE SYMBOLIC
% Developed by G.G.B. on 10/31/02 last modified on 11/07/02
%------------------------------------------------------------------------------
clc
syms Ca1 Ca2 Ca3 s       % Definition of the symbolic variables
%----------------------------------------------------------------------
% Definition of constants used in the program
%----------------------------------------------------------------------
k1=0.1;              % kinetics constant for Reactor 1 in h-1
k2=0.2;              % kinetics constant for Reactor 2 in h-1
k3=0.4;              % kinetics constant for Reactor 3 in h-1
v1=1000;              % Volume of Reactor 1 in l
v2=1500;              % Volume of Reactor 2 in l
v3=100;              % Volume of Reactor 3 in l
%------------------------------------------------------------------------
%   COEFFICIENT MATRIX: A
%------------------------------------------------------------------------
A=[s*v1+1100+k1*v1 -100 0; -1100 s*v2+1100+k2*v2 0; 0 -1000 s*v3+1000+k3*v3]; % This is the coefficient matrix given in
the handout
%------------------------------------------------------------------------
%   solution of LAE using Cramer's rule
%------------------------------------------------------------------------
%fprintf(1,'This is the determinant A\n');
%pretty(A)
fprintf(1,'This is the variable Ca1\n');
Ca1=det([1000/s+v1 -100 0; v2 s*v2+1100+k2*v2 0; v3 -1000 s*v3+1000+k3*v3])/det(A);
pretty(Ca1)
fprintf(1,'This is the variable Ca2\n');
```

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```
Ca2=det([s*v1+1100+k1*v1 1000/s+v1 0; -1100 v2 0; 0 v3 s*v3+1000+k3*v3])/det(A);
pretty(Ca2)
fprintf(1,'This is the variable Ca3\n');
Ca3=det([s*v1+1100+k1*v1 -100 1000/s+v1; -1100 s*v2+1100+k2*v2 v2; 0 -1000 v3])/det(A);
pretty(Ca3)
%------------------------------------------------------------------------------
%          Calculation of inverse Laplace Transform
%------------------------------------------------------------------------------
ca1=ilaplace(Ca1);
fprintf(1,'This is after inverse then ca1\n');
pretty(ca1)
ca2=ilaplace(Ca2);
fprintf(1,'This is after inverse then ca2\n');
pretty(ca2)
ca3=ilaplace(Ca3);
fprintf(1,'This is after inverse then ca3\n');
pretty(ca3)
```

RESULTS:

The solution has been separated in two windows for presentation purposes.

```
Command Window                                                    _ □ ×
File  Edit  View  Web  Window  Help

>> This is the variable Ca1

                             2                           3
                    1865 s  + 3312 s + 1456 + 150 s
       1000000 ------------------------------------------------------------
                      3                2
              s (150000000 s  + 1880000000 s  + 3485000000 s + 1632800000)
This is the variable Ca2

                                        2
                        (52 + 5 s) (15 s  + 29 s + 11)
       2000000 ------------------------------------------------------------
                      3                2
              s (150000000 s  + 1880000000 s  + 3485000000 s + 1632800000)
This is the variable Ca3

                             3          2
                      150 s  + 1820 s  + 3057 s + 1100
       1000000 ------------------------------------------------------------
                      3                2
              s (150000000 s  + 1880000000 s  + 3485000000 s + 1632800000)
This is after inverse then cal

Ready
```

```
Command Window                                                    _ □ ×
File  Edit  View  Web  Window  Help

This is after inverse then cal

  140   17        16                   1/2
  --- + --- exp(- -- t) cosh(1/30 82    t)
  157   157       15

            73         16      1/2                1/2
         + ----- exp(- -- t) 82     sinh(1/30 82    t)
           12874       15
This is after inverse then ca2

  110   47        16                   1/2
  --- + --- exp(- -- t) cosh(1/30 82    t)
  157   157       15

            281        16     1/2               1/2
         + ---- exp(- -- t) 82     sinh(1/30 82    t)
           6437        15
This is after inverse then ca3

  1375    3214                  3837650       16      1/2           1/2
  ---- + ------ exp(- 52/5 t) + -------- exp(- -- t) 82     sinh(1/30 82    t)
  2041   169689                 84022161       15

           629900       16                1/2
         + ------- exp(- -- t) cosh(1/30 82    t)
           2049321       15
>>

Ready
```

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