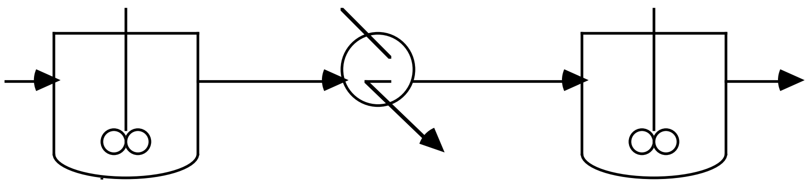
06-606 **Computational Methods** **Fall, 2011**

Due: 11/2/11

1. The reaction $A \rightarrow B$ takes place at steady state in two CSTR reactors in series as shown below in the figure. Obtain the concentrations C_{A0} and C_{A1} as a function of time given that the outlet concentration C_{A2} is given as a function of time: $C_{A2} = 0.1 - 0.005t$. Plot your results for the first 10 minutes by solving the problem analytically.

Feed = 100 ft^3/min



$V_1 = 500\ ft^3$
$k_1 = 0.05\ min^{-1}$
(Isothermal)

$V_2 = 20\ ft^3$
$k_2 = 38\ min^{-1}$
(Isothermal)

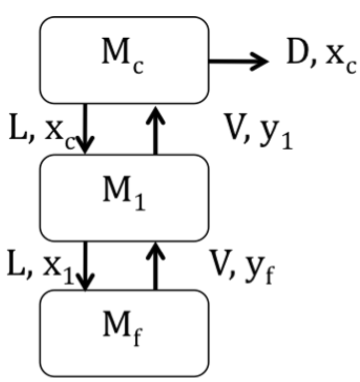
2. Find a consistent initial condition for this system and solve this problem (as stated) using DASSL.

3. What is the index of the above problem? Using the structure of these equations, reformulate the system to index 1 and solve for the first 10 minutes with your favorite integrator.

4. Formulate this problem using an index two (intermediate form) from problem 3. Choose initial conditions that are not consistent and solve the system using DASSL.

5. For problems 2. to 4., comment on the performance of DASSL for each solution. Compare your results to the analytic solution in problem 1.

6 . Consider the model for the binary 2-stage distillation system given below, where α is the relative volatility. The mass balance equations can be written as:



$M_f' = L - V$
$(M_f x_f)' = L\, x_1 - V\, y_f$
$(M_1 x_1)' = L\,(x_c - x_1) + V\,(y_f - y_1)$
$(M_c)' = V - (L + D)$
$(M_c x_c)' = V\, y_1 - (L+D)\, x_c$
$y_1 - \alpha\, x_1 / [1 + (\alpha - 1)\, x_1] = 0$
$y_f - \alpha\, x_f / [1 + (\alpha - 1)\, x_f] = 0$
$M_f = f_0(t)$, $M_1 = f_1(t)$
$L - 1.5\, D = 0$
$V = g(t)$

a) Formulate this problem as a semi-explicit DAE system. What is its index?
b) Reformulate this problem to an index 1 system.

45/45

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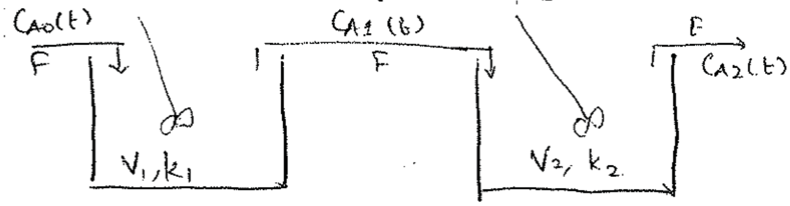
Assignment 6

1.



$$V_1 \frac{dC_{A1}}{dt} = F(C_{A0} - C_{A1}) - V_1 k_1 C_{A1}$$

$$V_2 \frac{dC_{A2}}{dt} = F(C_{A1} - C_{A2}) - V_2 k_2 C_{A2}$$

(1)

Given, $C_{A2}(t) = 0.1 - 0.005t$

$$\Rightarrow C_{A1}(t) = \frac{V_2}{F}\frac{dC_{A2}}{dt} + \left(1 + \frac{V_2 k_2}{F}\right) C_{A2} = 0.859 - 0.043t$$

(10)

$$C_{A0}(t) = \frac{V_1}{F}\frac{dC_{A1}}{dt} + \left(1 + \frac{V_1 k_1}{F}\right) C_{A1} = 0.85875 - 0.05375t$$

Using this Analytical solution, the above was plotted in MATLAB. The code and plots are attached.

2. The problem to be solved is (1).

2. The initial conditions may be found as follows,

$C_{A2}(0) = 0.1$

$\frac{dC_{A2}}{dt}(0) = -0.005$

$$C_{A1}(0) = \frac{V_2}{F}\frac{dC_{A2}}{dt}(0) + \left(1 + \frac{V_2 k_2}{F}\right) C_{A2}(0) = 0.859$$

$$\frac{dC_{A1}}{dt}(0) = \frac{V_2}{F}\frac{d^2 C_{A2}}{dt^2}(0) + \left(1 + \frac{V_2 k_2}{F}\right)\frac{dC_{A2}}{dt}(0) = -0.043$$

$$C_{A0}(0) = \frac{V_1}{F}\frac{dC_{A1}}{dt}(0) + \left(1 + \frac{V_1 k_1}{F}\right) C_{A1}(0) = 0.85875$$

~~So, the resulting system~~
Now, we need to differentiate once more to get an ODE for C_{A0}.

So, we needed 3 differentiations

Hence, the system is index-3. ✓

The resulting equations after replacing ODE for C_{A0} by the algebraic equation is,

$$C_{A2} = 0.1 - 0.005t$$

$$C_{A1} = 0.859 - 0.043t$$

$$C_{A0} = 0.85875 - 0.05375t.$$

✓

The above system is index-1. One differentiation of the algebraic equations gives ~~an~~ ODEs for all the variables.

(10/10) These are nothing but the analytical solutions plotted in question 1. The plots are already attached. ~~on~~

4. The Index-2 form is,

$$\frac{dC_{A1}}{dt} = \frac{F}{V_1} C_{A0} - \left(k_1 + \frac{F}{V_1}\right) C_{A1} = 0.2\, C_{A0} - 0.25\, C_{A1}$$

$$C_{A2} = 0.1 - 0.005t \quad ✓$$

$$C_{A1} = 0.859 - 0.043t.$$

The initial values in problem 2 were used. The above was coded in FORTRAN and solved using DASSL. The output

In the code the method uses variable order BDF method with max. order = 5. This is the default value and has not been changed.

The step size used was, $h = 0.05$.

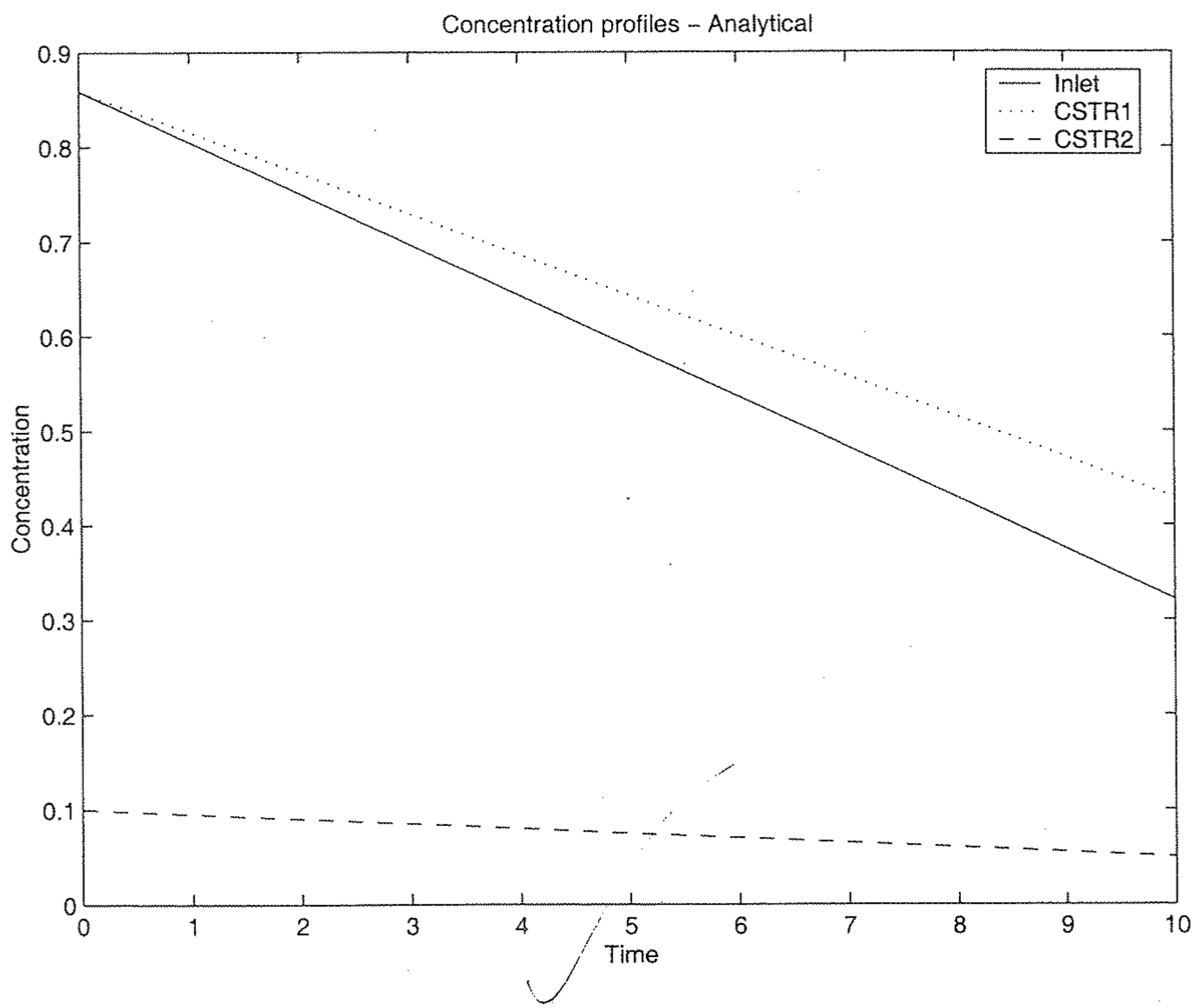
So, error $\sim O((0.05)^5)$ (assuming it used 5th order BDF)

$\sim O(5^5 \times 10^{-10})$

$\sim O(10^{-7})$

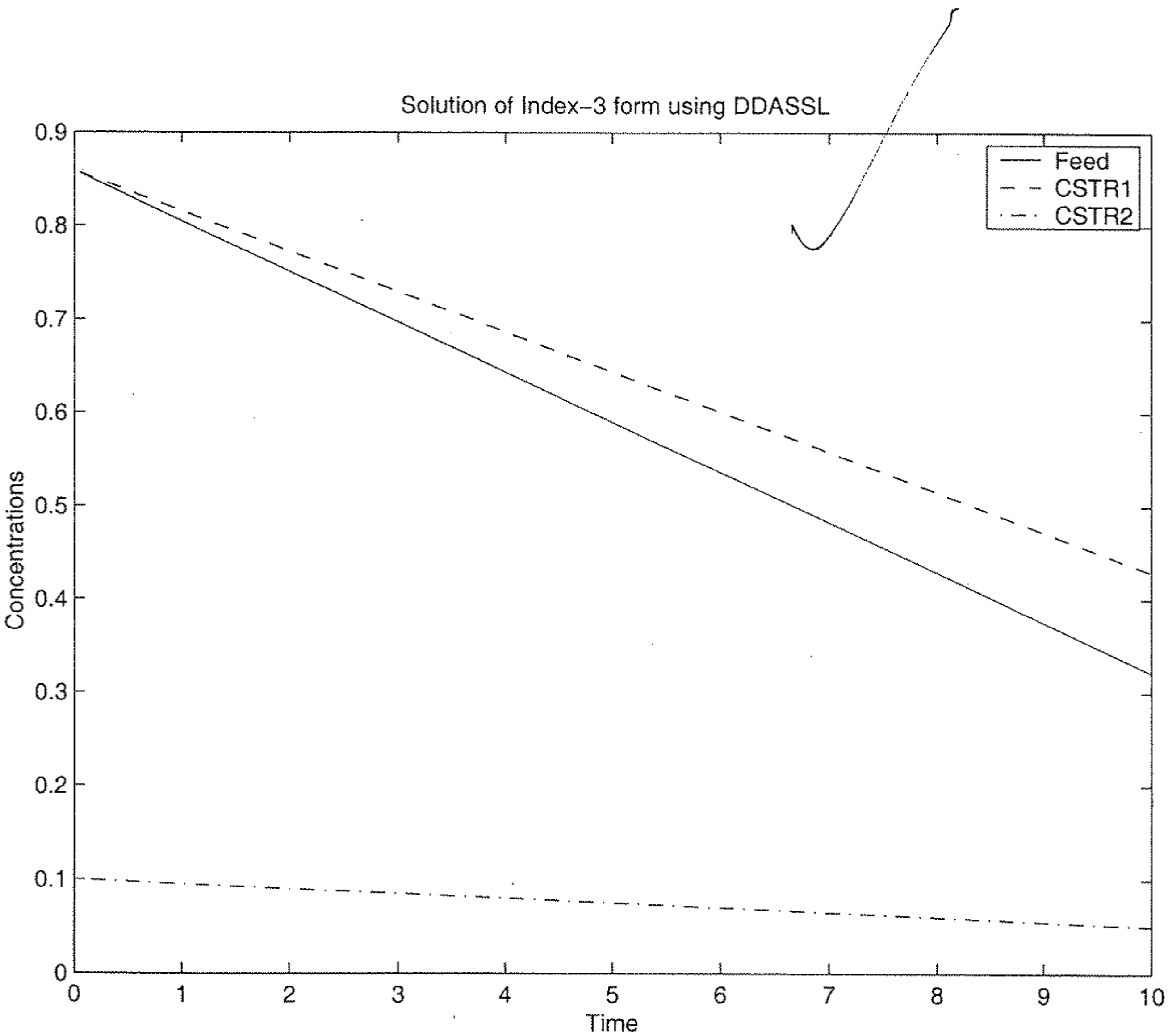
5/5

```
%Problem 1 of Hwk 5

format long e

V1 = 500 ;
V2 = 20 ;
k1 = 0.05 ;
k2 = 38 ;
F = 100 ;

data = [] ;
h = 0.1 ;
a = 0.859 ;
b = -0.05375 ;
t1 = a/(F/V1+k1) ;
t2 = b/(F/V1+k1) ;
t3 = b/(F/V1+k1)^2 ;
t4 = (F/V1+k1) ;
CA10 = 0.85875 ;

for i = 1:((10/h)+1)

  t = (i-1)*h ;
  CA2 = 0.1 - 0.005*t ;
  CA2dot = -0.005 ;
  CA1 = (V2/F)*CA2dot + ((k2*V2/F)+1)*CA2 ;
  CA1dot = ((k2*V2/F)+1)*CA2dot ;
  CA0 = (V1/F)*CA1dot + ((k1*V1/F)+1)*CA1 ;
  CA11 = (F/V1)*((t1-t3)*(1-exp(-t4*t))+t2*t)+CA10*exp(-t4*t) ;
  data = [ data ; t CA0 CA1 CA2 CA11 ] ;

end

plot(data(:,1),data(:,2),data(:,1),data(:,3),':',data(:,1),data(:,4),'--') ;
legend('Inlet','CSTR1','CSTR2',0) ;
xlabel('Time') ;
ylabel('Concentration') ;
title('Concentration profiles - Analytical') ;
```


Concentration profiles - Analytical
Inlet
CSTR1
CSTR2
Concentration
Time
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
1
2
3
4
5
6
7
8
9
10

```
c     Problem 2 of Assignment 6. Solve DAE as an Index - 3 system.

      external f , jac
      integer neq , i , iwork , idid , ipar , info
      double precision atol , rtol , rwork , rpar , t , tout , y , dy
      dimension y(3) , dy(3) , info(15) , rwork(80) , iwork(23)

      neq = 3

c     Initialize the values
      t = 0.0d0
      h = 0.05d0
      tout = h
      y(1) = 0.85875
      y(2) = 0.859
      y(3) = 0.1
      dy(1) = -0.05375
      dy(2) = -0.043
      dy(3) = -0.005

c     Assigning the code parameters
      atol = 1.0d-7
      rtol = 1.0d-6
      info(1) = 0
      info(2) = 0
      info(3) = 0
      info(4) = 0
      info(5) = 1
      info(6) = 0
      info(7) = 0
      info(8) = 0
      info(9) = 0
      info(10) = 0
      info(11) = 0
      lrw = 80
      liw = 23

c     Main program
      do 20 i = 1,200
 5       call ddassl(f,neq,t,y,dy,tout,info,rtol,atol,idid,rwork,lrw,
     *        iwork,liw,rpar,ipar,jac)
         write(6,10)t,y(1),y(2),y(3)
 10      format(e12.4,e14.6,e14.6,e14.6)

         if ( idid .eq. ( 1 .or. 2 .or. 3 ) )  then
            go to 20

               elseif ( idid .eq. -1 ) then
                  info(1) = 1
                  go to 5

                  else
                     go to 40
                  endif

 20      tout = tout + h
         stop
 40      write(6,50)idid
 50      format(///22herror halt....idid = ,i3)
         stop
```

```
      end

      subroutine f (t,y,dy,delta,ires,rpar,ipar)
      integer ires , j
      double precision t , y , dy , delta
      dimension y(3) , dy(3) , delta(3)

      ires = 0
      do 60 j = 1,3
60       if ( y(j) .lt. 0 ) ires = -1
      delta(1) = dy(2) - 0.2*y(1) + 0.25*y(2)
      delta(2) = dy(3) - 5*y(2) + 43*y(3)
      delta(3) = y(3) - 0.1 + 0.005*t
      return
      end

      subroutine jac (t,y,dy,pd,cj,rpar,ipar)
      double precision t , y , dy , pd
      dimension y(3) , dy(3) , pd(3,3)

      pd(1,1) = -0.2
      pd(1,2) = 0.25 + cj
      pd(2,2) = -5
      pd(2,3) = 43 + cj
      pd(3,3) = 1
      return
      end
```



Solution of Index-3 form using DDASSL
Concentrations
Time
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0
1
2
3
4
5
6
7
8
9
10
Feed
CSTR1
CSTR2

```
c     Problem 4 of Assignment 6. Solve DAE as an Index - 2 system.
      external f , jac
      integer neq , i , iwork , idid , ipar , info
      double precision atol , rtol , rwork , rpar , t , tout , y , dy
      dimension y(3) , dy(3) , info(15) , rwork(80) , iwork(23)

      neq = 3

c     Initialize the values
      t = 0.0d0
      h = 0.05d0
      tout = h
      y(1) = 0.85875
      y(2) = 0.859
      y(3) = 0.1
      dy(1) = -0.05375
      dy(2) = -0.043
      dy(3) = -0.005

c     Assigning the code parameters
      atol = 1.0d-7
      rtol = 1.0d-6
      info(1) = 0
      info(2) = 0
      info(3) = 0
      info(4) = 0
      info(5) = 1
      info(6) = 0
      info(7) = 0
      info(8) = 0
      info(9) = 0
      info(10) = 0
      info(11) = 0
      lrw = 80
      liw = 23

c     Main program
      do 20 i = 1,200
 5       call ddassl(f,neq,t,y,dy,tout,info,rtol,atol,idid,rwork,lrw,
     *        iwork,liw,rpar,ipar,jac)
         write(6,10)t,y(1),y(2),y(3)
 10      format(e12.4,e14.6,e14.6,e14.6)

         if ( idid .eq. ( 1 .or. 2 .or. 3 ) )  then
            go to 20

               elseif ( idid .eq. -1 ) then
                  info(1) = 1
                  go to 5

                  else
                     go to 40
                  endif

 20      tout = tout + h
         stop
 40      write(6,50)idid
 50      format(///22herror halt....idid = ,i3)
         stop
         end
```

```
      subroutine f (t,y,dy,delta,ires,rpar,ipar)
      integer ires , j
      double precision t , y , dy , delta
      dimension y(3) , dy(3) , delta(3)

      ires = 0
      do 60 j = 1,3
60       if ( y(j) .lt. 0 ) ires = -1
      delta(1) = dy(2) - 0.2*y(1) + 0.25*y(2)
      delta(2) = y(2) - 0.859 + 0.043*t
      delta(3) = y(3) - 0.1 + 0.005*t
      return
      end

      subroutine jac (t,y,dy,pd,cj,rpar,ipar)
      double precision t , y , dy , pd
      dimension y(3) , dy(3) , pd(3,3)

      pd(1,1) = -0.2
      pd(1,2) = 0.25 + cj
      pd(2,2) = 1
      pd(3,3) = 1
      return
      end
```

6)

$$M_f' = L - V$$
$$(M_f x_f)' = L x_1 - V y_f$$
$$(M_1 x_1)' = L(x_c - x_1) + V(y_f - y_1)$$

$$M_c' = V - (L+D)$$
$$(M_c x_c)' = V y_1 - (L+D) x_c$$

$$y_1 - \alpha x_1 / (1 + (\alpha - 1) x_1) = 0$$
$$y_f - \alpha x_f / (1 + (\alpha - 1) x_f) = 0$$

$$M_f = f_0(t), \quad M_1 = f_1(t)$$
$$L - 1.5D = 0$$
$$V = g(t)$$

a) Reformulate $(Mx)'$ terms leading to:

$$M_f' = L - V$$
$$x_f' = \frac{1}{M_f}\left(L(x_1 - x_f) - V(y_f - x_f)\right)$$
$$x_1' = \frac{1}{M_1}\left(L(x_c - x_1) + V(y_f - y_1) - f_1'(t) x_1\right)$$
$$M_c' = V - (L+D)$$
$$x_c' = \frac{1}{M_c}\left(V(y_1 - x_c)\right)$$
$$y_1 - \alpha x_1 / ((1 + (\alpha - 1) x_1) = 0$$
$$y_f - \alpha x_f / ((1 + (\alpha - 1) x_f) = 0$$
$$M_f = f_0(t), \quad M_1 = f_1(t)$$
$$1.5 D = L$$
$$V = g(t)$$

index 2 — recover L

b) $M_f = f_0(t)$

$M_f' = f_0'(t) = L - V$

drop first ODE and make M_f an algebraic variable. The index 1 formulation is:

$$x_f' = \frac{1}{M_f}\left(L(x_1 - x_f) - V(y_f - x_f)\right)$$

$$x_1' = \frac{1}{M_1}\left(L(x_c - x_1) + V(y_f - y_1) - f_1'(t)\, x_1\right)$$

$$M_c' = V - (L + D)$$

$$x_c' = \frac{1}{M_c}\left(V(y_1 - x_c)\right)$$

$$y_1 - \alpha x_1 / (1 + (\alpha - 1)x_1) = 0$$

$$y_f - \alpha x_f / (1 + (\alpha - 1)x_f) = 0$$

$$M_f = f_0(t)$$

$$f_0'(t) = L - V$$

$$M_1 = f_1(t)$$

$$1.5 D - L = 0$$

$$V - g(t) = 0$$