06-720 Advanced Process Systems Engineering Spring, 2011

Homework 9 Due: 4/18/11

1. Consider the reactor optimization problem given by:

$$\begin{aligned}
\min \quad & L - 500\int_0^L (T(t) - T_S)dt \\
s.t. \quad & \frac{dq}{dt} = 0.3(1 - q(t))exp(20(1 - 1/T(t)),\ q(0) = 0 \\
& \frac{dT}{dt} = -1.5(T(t) - T_S) + 2/3\frac{dq}{dt},\ T(0) = 1
\end{aligned}$$

where $q(t)$ and $T(t)$ are the normalized reactor conversion and temperature, respectively, and the decision variables are $T_S \in [0.5, 1]$ and $L \in [0.5, 1.25]$.

   (a) Derive the direct sensitivity equations for the DAEs in this problem.

   (b) Using MATLAB or a similar package, apply the sequential approach to find the optimum values for the decision variables.

   (c) How would you reformulate the problem so that the path constraint $T(t) \leq 1.45$ can be enforced?

2. Consider the system of differential equations:

$$\begin{aligned}
\frac{dz_1}{dt} &= z_2 \\
\frac{dz_2}{dt} &= 1600z_1 - (\pi^2 + 1600)sin(\pi t)
\end{aligned}$$

   (a) Show that the analytic solution of these differential equations are the same for the initial conditions $z_1(0) = 0, z_2(0) = \pi$ and the boundary conditions $z_1(0) = z_1(1) = 0$.

   (b) Find the analytic solution for the initial and boundary value problems. Comment on the dichotomy of each system.

3. Consider the following reactor optimization problem.

$$\begin{aligned}
\max \quad & c_2(1.0) \\
s.t. \quad & \frac{dc_1}{dt} = -k_1(T)c_1^2,\ c_1(0) = 1 \\
& \frac{dc_2}{dt} = k_1(T)c_1^2 - k_2(T)c_2,\ c_2(0) = 0
\end{aligned}$$

where $k_1 = 4000\ exp(-2500/T)$, $k_2 = 62000\ exp(-5000/T)$ and $T \in [298, 398]$. Discretize the temperature profile as piecewise constants over N_T periods and perform the following.

   (a) Derive the direct sensitivity equations for the DAEs in this problem.

   (b) Derive the adjoint sensitivity equations for the DAEs in this problem.

   (c) Solve using the sequential strategy with MATLAB or a similar package.

   (d) Solve using the multiple shooting strategy with MATLAB or a similar package.

Solution — HW 9

1\. $\text{Min } L - 500\int_0^L (T - T_s)\,dt$

$$\text{s.t.}\quad \dot{q} = 0.3(1-q)\exp(20(1-1/T))$$
$$q(0) = 0$$
$$\dot{T} = -1.5\,(T(t) - T_s) + \tfrac{2}{3}\dot{q}$$
$$T(0) = 1$$
$$L \in [0.5, 1.25];\ T_s \in [0.5, 1]$$

a) Sensitivity eqns.

- note that $t \in [0, L]$ so we need to normalize length: $t = \tau L$, $\tau \in [0,1]$

this leads to:

$$\text{Min}\quad L - 500\, z(1)$$
$$\frac{dq}{d\tau} = 0.3L(1-q)\exp(20(1-1/T)),\quad q(0) = 0$$
$$\frac{dT}{d\tau} = -1.5L(T - T_s) + 0.2L(1-q)\exp(20(1-1/T))$$
$$T(0) = 1$$
$$\frac{dz}{d\tau} = L(T - T_s),\quad z(0) = 0$$

sensitivity eqns (wrt T_s & L)

$$\dot{S}_{qL} = -0.3LS_{qL}\exp(20(1-1/T)) + 0.3(1-q)\exp(20(1-1/T)) + \frac{6}{T^2}(1-q)L\exp(20(1-1/T))\,S_{TL}$$

$$\dot{S}_{qT_s} = -0.3 L S_{qT_s} \exp(20(1-1/T)) + \frac{6}{T^2}(1-q) L \exp(20(1-1/T)) S_{TT_s}$$

$$\dot{S}_{TL} = -1.5(T-T_s) - 1.5 L S_{TL} + 0.2(1-q)\exp(20(1-1/T)) + 0.2 L \exp(20(1-1/T)) \left[\frac{20}{T^2}(1-q) S_{TL} - 0.2 S_{qL}\right]$$

$$\dot{S}_{TT_s} = -1.5 L S_{TS} + 1.5 L + 0.2 L \exp(20(1-1/T)) \left[\frac{20}{T^2}(1-q) S_{TT_s} - 0.2 S_{qT_s}\right]$$

$$S_{qL} = (T-T_s) \qquad S_{qT_s} = -L$$

$$S_{ij}(0) = 0.$$

b) solution of hot spot problem (solved w/ AMPL as a test case with profiles below.)

c) In sequential approach, it is difficult to place bounds on states. One "trick" is to define

$$\dot{z} = (\max(0, T-1.45))^2, \quad z(0) = 0$$

and to impose $z(t_f) \leq \varepsilon$ as a final time constraint. This violates LICQ but is smooth.

Profiles for $T(t) \leq 1.45$ are given on next pg.

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# Dynamic Optimization of Hot Spot
Reactor - Problem 1 in HW 9

# This file implements the dynamic
optimization of a hot spot reactor.
# It uses the simultaneous approach
but is meant to provide a solution
# requested for the sequential
approach.

# Written by  L. T. Biegler/ CMU, 4-
17-2011

param nfe;
let nfe:= 100;
set  I:= 1..nfe;
set  J:= 1..3;

param   qinit  :=0.;
param   tinit  :=1;
param   zinit  :=0;

param omega{J,J};

let omega[1,1] :=   0.19681547722366;
let omega[1,2] :=0.39442431473909;
let omega[1,3] :=0.37640306270047;
let omega[2,1] := -0.06553542585020;
let omega[2,2] :=0.29207341166523;
let omega[2,3] :=0.51248582618842;
let omega[3,1] := 0.02377097434822;
let omega[3,2] :=-0.04154875212600;
let omega[3,3] :=0.11111111111111;

param h{i in I} := 1/nfe;

# Initial guess of the decision
variables

var q{i in I,j in J} >= 0., <= 1., :=
0.5;
var t{i in I,j in J} >= 0., <=
10., := 10;
var z{i in I,j in J} >= 0., <=
10., := 1.;
var tt{i in I,j in J} >= 0., <=
10., := 1.;
var qdot{I,J};
var tdot{I,J};
var zdot{I,J};
var ts >= 0.05, <= 1.:= 0.7;
var ll >= 0.5, <= 1.25:= 0.8;
# var ll >= 0.5, <= 10.:= 0.8;
var q0{i in I} >=0, <=1, :=qinit;
var t0{i in I} >= 0, <= 10, := tinit;
var tt0{i in I} >= 0, <= 10, := 1;
var z0{i in I} >= 0, <= 1, := zinit;
var qf >= 0, <= 1, := qinit;
var tf >= 0, <= 10, := tinit;
var zf >= 0, <= 10, := zinit;
var ttf >= 0, <= 10., := 1;

minimize phi: ll - 500*zf;

FECOLc{i in I, j in J}:
q[i,j]=(q0[i]+h[i]*sum{k in J}
(omega[k,j]*qdot[i,k])) ;

FECOLt{i in I, j in J}:
t[i,j]= (t0[i]+h[i]*sum{k in J}
(omega[k,j]*tdot[i,k])) ;

FECOLz{i in I, j in J}:
z[i,j]= (z0[i]+h[i]*sum{k in J}
(omega[k,j]*zdot[i,k])) ;

FECOLtt{i in I, j in J}:
tt[i,j]= tt0[i]+h[i]*sum{k in J}
(omega[k,j]*ll) ;

CONq{i in I diff {1}}:
q0[i] = (q0[i-1] + h[i-1]*sum{j in J}
(qdot[i-1,j]*omega[j,3]));

CONt{i in I diff {1}}:
t0[i] = (t0[i-1] + h[i-1]*sum{j in J}
(tdot[i-1,j]*omega[j,3]));

CONz{i in I diff {1}}:
z0[i] = (z0[i-1] + h[i-1]*sum{j in J}
(zdot[i-1,j]*omega[j,3]));

CONtt{i in I diff {1}}:
tt0[i] = tt0[i-1] + h[i-1]*sum{j in
J} (ll*omega[j,3]);

ODEq{i in I, j in J}:
qdot[i,j] = ll*(0.3*(1-
q[i,j])*exp(20*(1-1/t[i,j])));

ODEt{i in I, j in J}:
tdot[i,j] = ll*(-1.5*(t[i,j]-ts) +
2/3*qdot[i,j]);

ODEz{i in I, j in J}:
zdot[i,j] = ll*(t[i,j]-ts);

FINq: qf = q[nfe, 3];
FINt: tf = t[nfe, 3];
FINz: zf = z[nfe, 3];
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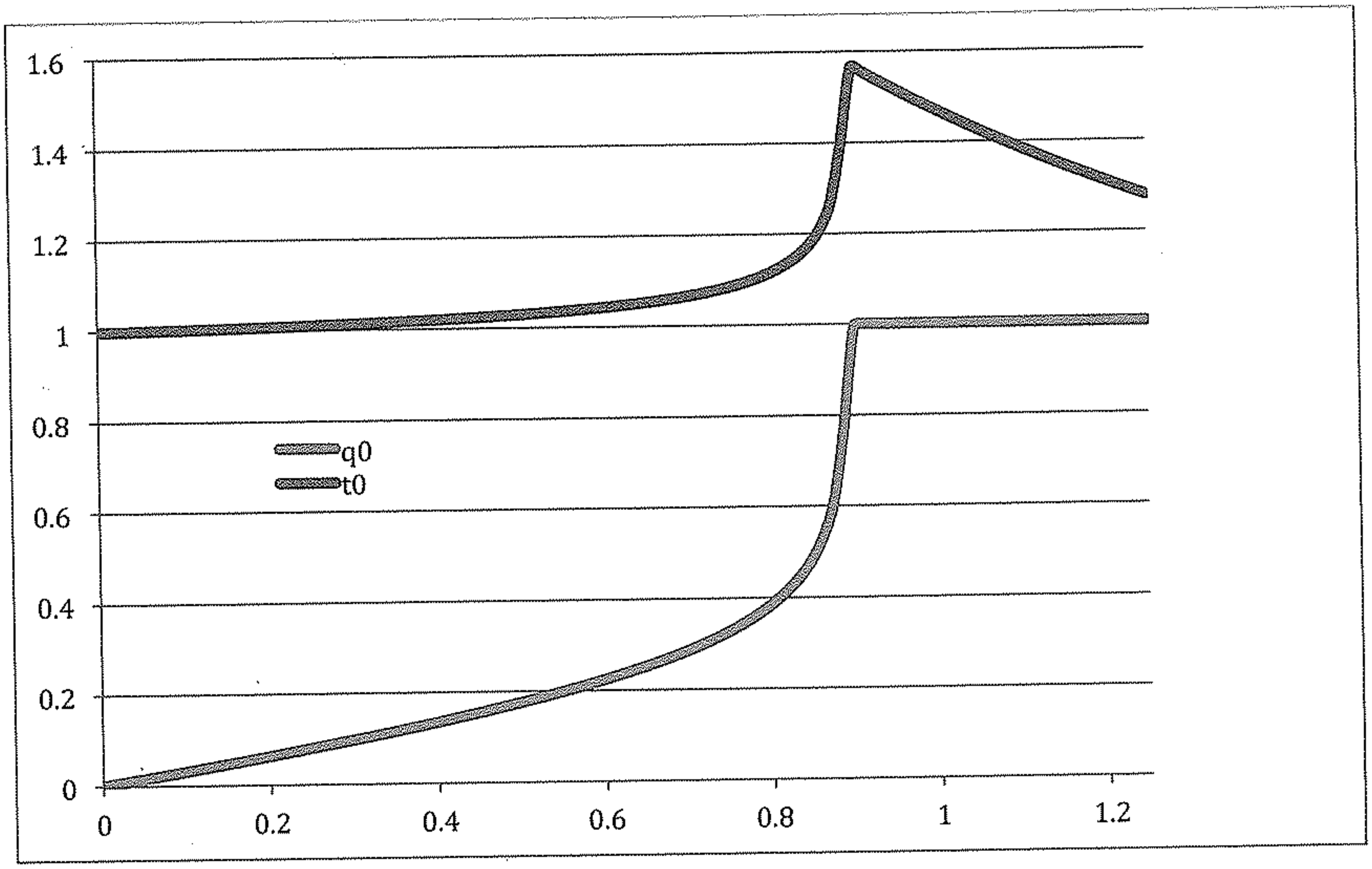
FINtt: ttf = tt[nfe, 3];

IQ: q0[1] = qinit;
IT: t0[1] = tinit;
IZ: z0[1] = zinit;

ITT: tt0[1] = 0;

option solver Ipopt;

solve;
```



add constraint

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tc{i in I, j in J}: t[i,j] <= 1.45;
solve;
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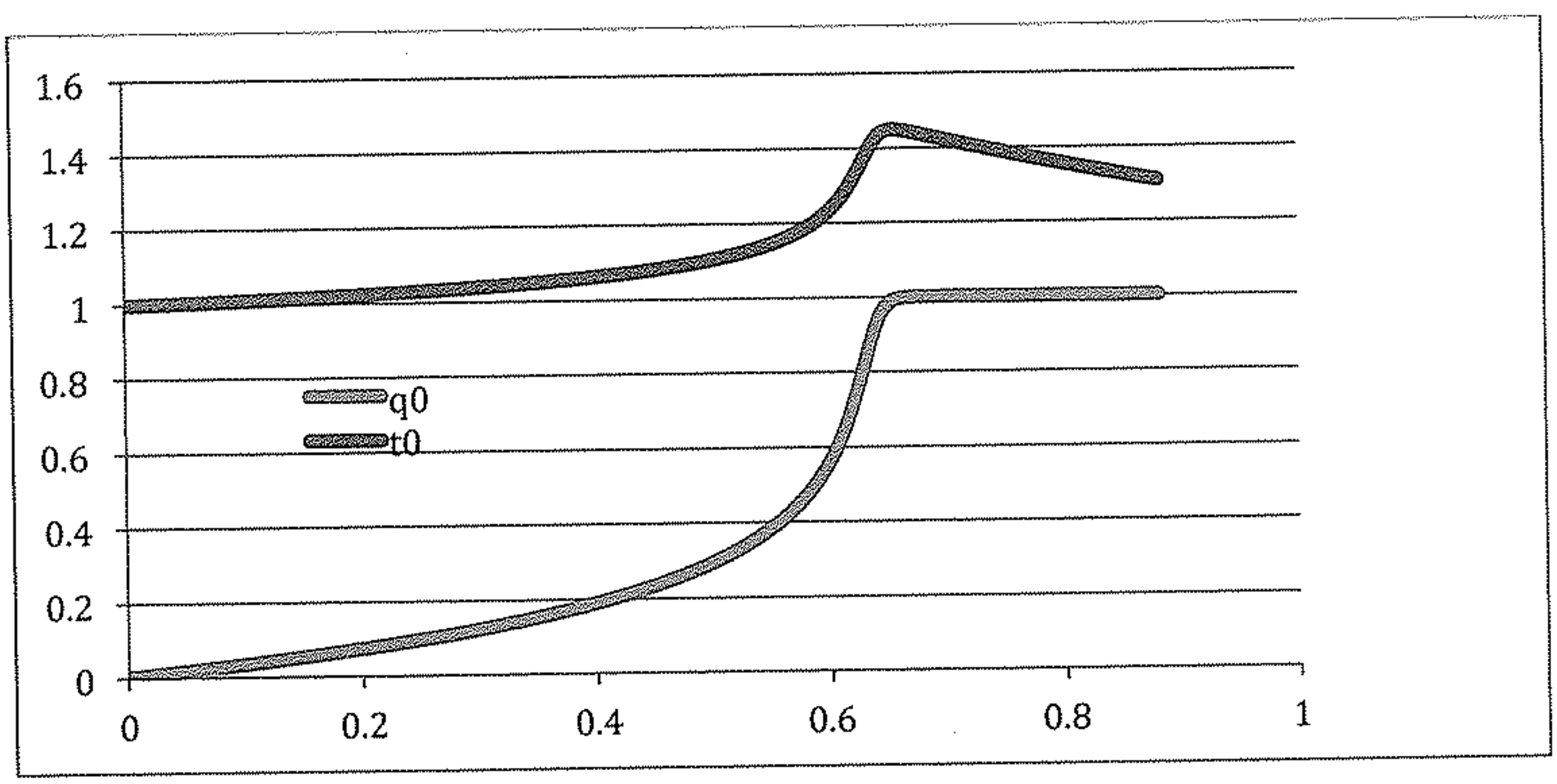


2. Bock problem

$$\dot{z}_1 = z_2$$
$$\dot{z}_2 = 1600 z_1 - (\pi^2 + 1600) \sin \pi t$$

a) $z_1(0) = 0$ has solution
$z_2(0) = \pi$
$z_1 = \sin \pi t$
$z_2 = \pi \cos \pi t$

This is same solution as:
$z_1(0) = 0$
$z_1(1) = 0$

b) For initial value problem, the unstable mode is not "pinned down" and there is no dichotomy.

For boundary value problem, both stable & unstable modes are "pinned down"

3. $\min -c_2(1.0)$

s.t.

$$\dot{c}_1 = -k_1(T)\,c_1^2, \quad c_1(0) = 1$$

$$\dot{c}_2 = k_1(T)\,c_1^2 - k_2(T)\,c_2$$

$$c_2(0) = 0$$

$$k_1 = 4000 \exp(-2500/T)$$

$$k_2 = 62000 \exp(-5000/T)$$

$$T \in [298, 398]$$

a) Sensitivity eqns wrt T_j

(1) $\dot{S}_{1j} = -2k_1(T_j)\,c_1 S_{1j}, \quad S_{1j}(0) = 0$

(2) $\dot{S}_{2j} = 2k_1(T_j)\,c_1 S_{1j} - k_2(T_j)\,S_{2j}, \quad S_{2j}(0) = 0$

for $t \notin [t_{j-1}, t_j]$

(3) $\dot{S}_{1j} = -2k_1(T_j)\,c_1 S_{1j} - \dfrac{\partial k_1}{\partial T_j} c_1^2, \quad S_{1j}(0) = 0$

(4) $\dot{S}_{2j} = 2k_1(T_j)\,c_1 S_{1j} - k_2(T_j)\,S_{2j} + 2\dfrac{\partial k_1}{\partial T_j} c_1^2 - \dfrac{\partial k_2}{\partial T_j} c_2, \quad S_{2j}(0) = 0$

$$\frac{\partial k_1}{\partial T_j} = \frac{1.6}{T^2} \exp(-2500/T)$$

$$\frac{\partial k_2}{\partial T_j} = \frac{12.4}{T^2} \exp(-5000/T)$$

$$\frac{d\phi}{dT_j} = -S_{2j}(1)$$

b) Adjoint sensitivity

$$\lambda^T f = \lambda_1(-k_1(T)c_1^2) + \lambda_2(k_1(T)c_1^2 - k_2(T)c_2)$$

$$\dot{\lambda}_1 = 2k_1(T)c_1(\lambda_1 - \lambda_2), \quad \lambda_1(1) = 0$$
$$\dot{\lambda}_2 = \lambda_2 k_2(T), \quad \lambda_2(1) = -1$$

$$\frac{d\phi}{dT_j} = \int_{t_{j-1}}^{t_j} \left((\lambda_2 - \lambda_1)\frac{\partial k_1}{\partial T_j} c_1^2 - \lambda_2 \frac{\partial k_2}{\partial T_j} c_2 \right) dt$$

c) Solution w/ sequential approach

Solve $\quad \text{Min} \; -c_2(1)$
$\quad$ s.t. $298 \le T_j \le 398$

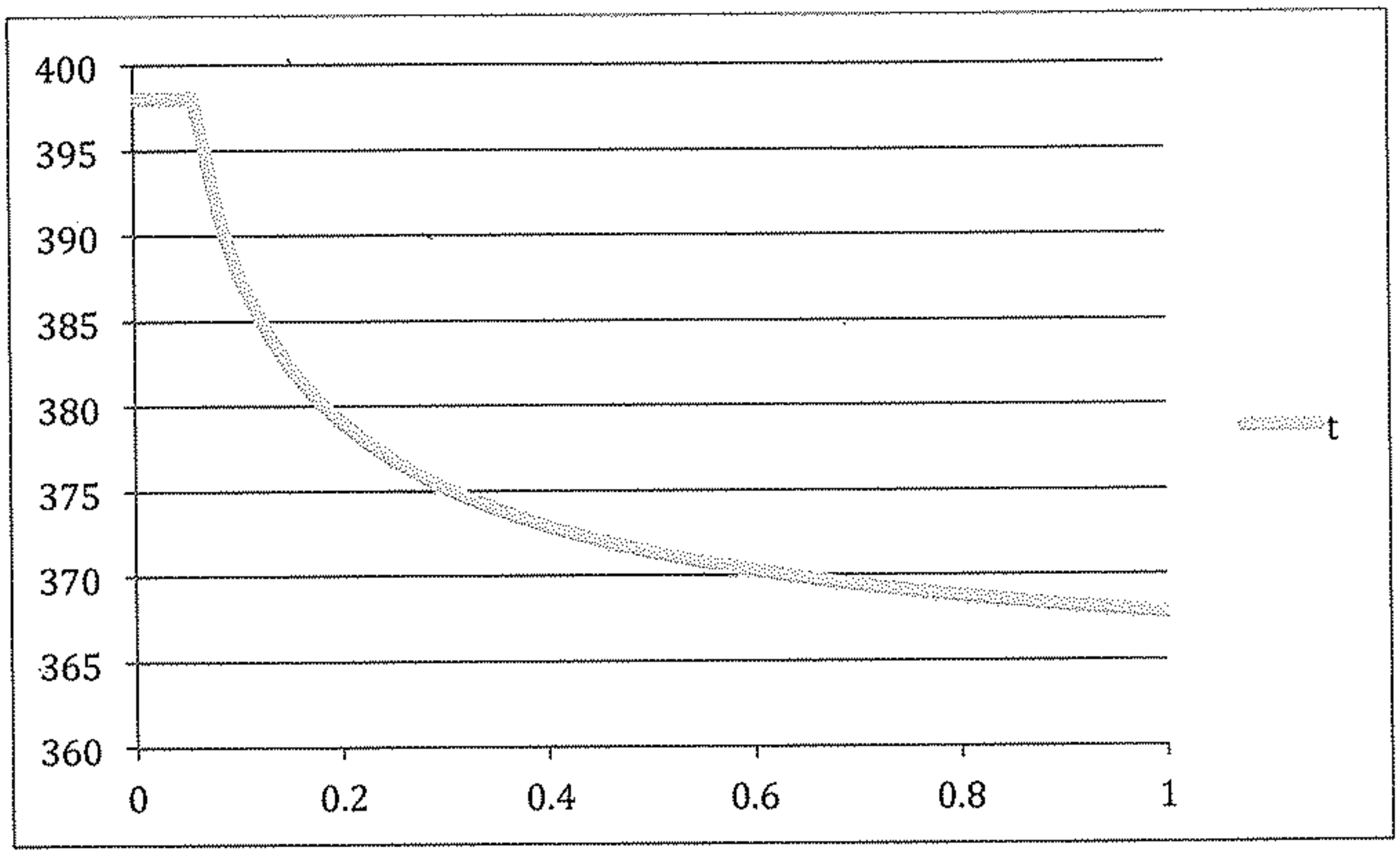
with $c_1(t)$, $c_2(t)$ and $\partial c_2 / \partial T_j$ evaluated from parts a) or b).
The solution is on next page.

d) Solution with multiple shooting

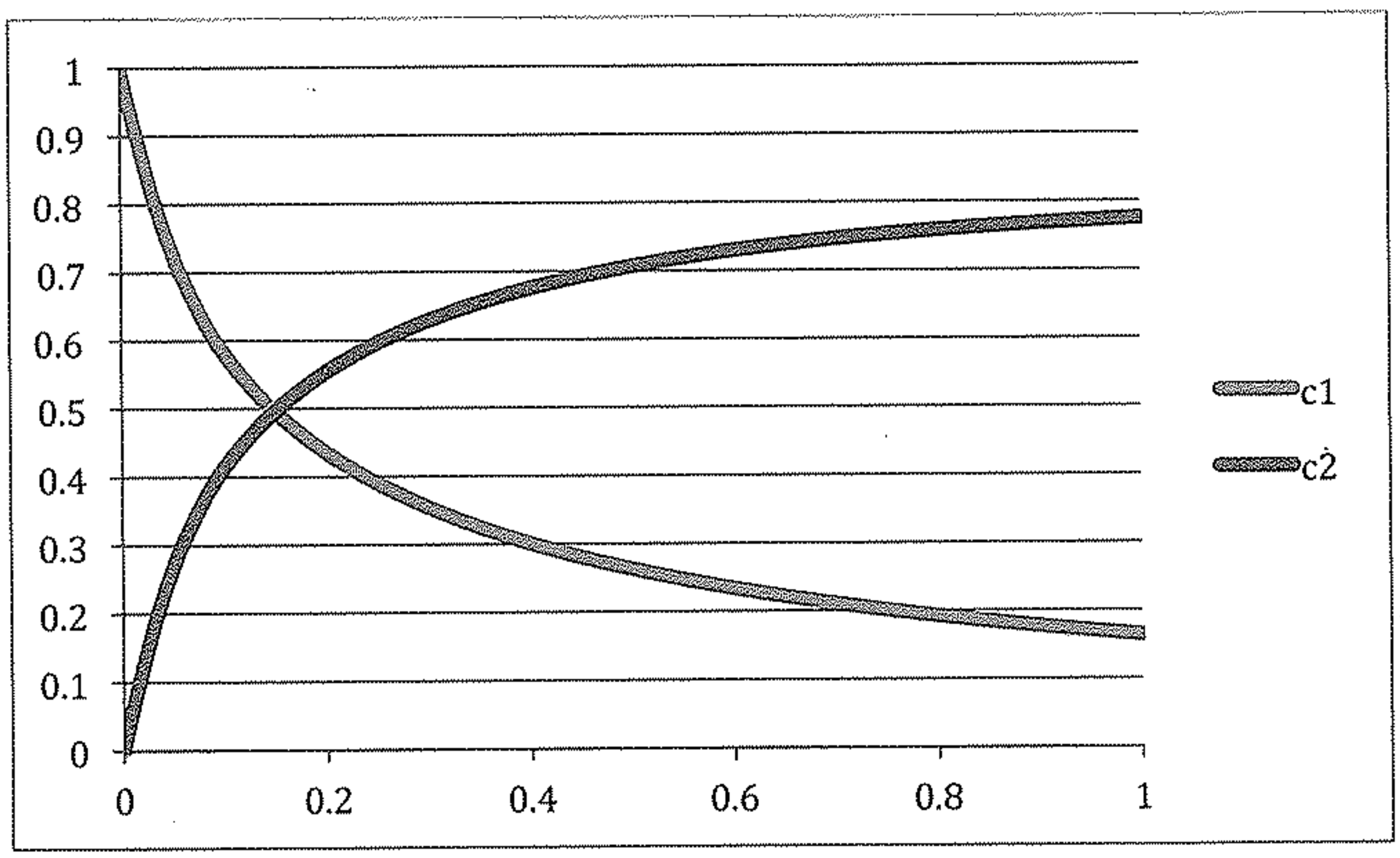
Solve $\quad \text{Min} \; -c_{2,NT}(1)$
$\quad$ s.t. $298 \le T_j \le 398$
$$c_{1j}(t_j) - \bar{c}_{1,j+1} = 0$$
$$c_{2j}(t_j) - \bar{c}_{2,j+1} = 0$$
$$j = 1, \ldots NT-1$$

where $\bar{c}_{1j}$, $\bar{c}_{2j}$ are also initial conditions for each segment of

Solution Profiles Nonisothermal Batch Reactor (Max c2(1))



Optimal Temperature Profile



Optimal Concentration Profiles

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# Dynamic Optimization of Hot
Spot Reactor - Problem 1 in HW
9

# This file implements the
dynamic optimization of a
nonisothermal
# batch reactor.  It uses the
simultaneous approach but is
meant to
# provide a solution requested
for the sequential or multiple
shooting
# approach.
```

```
# Written by  L. T. Biegler/
CMU, 4-17-2011

param nfe;
let nfe:= 20;
set  I:= 1..nfe;
set  J:= 1..3;

param   c1init  :=1.;
param   c2init  :=0.;

param omega{J,J};

let omega[1,1] :=
0.19681547722366;
let
omega[1,2] :=0.39442431473909;
let
omega[1,3] :=0.37640306270047;
let omega[2,1] := -
0.06553542585020;
let
omega[2,2] :=0.29207341166523;
let
omega[2,3] :=0.51248582618842;
let omega[3,1] :=
0.02377097434822;
let omega[3,2] :=-
0.04154875212600;
let
omega[3,3] :=0.11111111111111;

param h{i in I} := 1/nfe;

# Initial guess of the decision
variables

var c1{i in I,j in J} >= 0., <=
1., := 0.5;
var c2{i in I,j in J} >= 0., <=
1., := 0.5;
var t{i in I,j in J} >= 298.,
<= 398., := 350;
var tt{i in I,j in J} >= 0.;
var c1dot{I,J};
var c2dot{I,J};

var c10{i in I} >=0, <=1, :=
0.5;
var c20{i in I} >=0, <=1, :=
0.5;
var tt0{i in I} >= 0;
var c1f >= 0, <= 1, := 0.5;
var c2f >= 0, <= 1, := 0.5;
var ttf >= 0;

minimize phi: -c2f;

FECOLc1{i in I, j in J}:
c1[i,j]=(c10[i]+h[i]*sum{k in
J}
(omega[k,j]*c1dot[i,k])) ;

FECOLc2{i in I, j in J}:
c2[i,j]=(c20[i]+h[i]*sum{k in
J}
(omega[k,j]*c2dot[i,k])) ;

FECOLtt{i in I, j in J}:
tt[i,j]= tt0[i]+h[i]*sum{k in
J} (omega[k,j]) ;

CONc1{i in I diff {1}}:
c10[i] = (c10[i-1] + h[i-
1]*sum{j in J} (c1dot[i-
1,j]*omega[j,3]));

CONc2{i in I diff {1}}:
c20[i] = (c20[i-1] + h[i-
1]*sum{j in J} (c2dot[i-
1,j]*omega[j,3]));

CONtt{i in I diff {1}}:
tt0[i] = tt0[i-1] + h[i-
1]*sum{j in J} (omega[j,3]);

ODE1{i in I, j in J}:
c1dot[i,j] = -4000*exp(-
2500/t[i,j])*c1[i,j]*c1[i,j];

ODE2{i in I, j in J}:
c2dot[i,j] = 4000*exp(-
2500/t[i,j])*c1[i,j]*c1[i,j]
- 62000*exp(-
5000/t[i,j])*c2[i,j];

FINc1: c1f = c1[nfe, 3];
FINc2: c2f = c2[nfe, 3];
FINtt: ttf = tt[nfe, 3];

IC1: c10[1] = c1init;
IC2: c20[1] = c2init;
ITT: tt0[1] = 0;

option solver Ipopt;

solve;
```

the state equations:

$$\dot{c}_{1j} = -k_1(T_j)\, c_{1j}^2 \,, \quad c_{1j}(t_{j-1}) = \bar{c}_{1j}$$

$$\dot{c}_{2j} = k_1(T_j)\, c_{1j}^2 - k_2(T_j)\, c_{2j} \,, \quad c_{2j}(t_{j-1}) = \bar{c}_{2j}$$

Sensitivity equns for each segment are: the same as (3)-(4) for T_j, but not (1)-(2). The initial condition sensitivities are given by:

$$\dot{\bar{S}}_{1j} = -2k_1(T_j)\,\bar{S}_{1j}\,c_1 \,, \quad \bar{S}_{1j}(t_{j-1}) = 1$$

$$\dot{\bar{S}}_{2j} = 2k_1(T_j)\,c_1\,\bar{S}_{1j} - k_2(T_j)\,\bar{S}_{2j} \,, \quad \bar{S}_{2j}(t_{j-1}) = 1$$

for $t \in [t_{j-1}, t_j]$, $j = 2, \ldots NT$

The solution profiles are on the next page.