Report on Chemical

Generated by MTT using :
(mtt -u -q -q Chemical rep pdf)

Tue Aug 19 14:42:48 BST 2003

Contents

List of Figures

Part I

Chemical

Chapter 1

Reactor

1.1 Reactor_abg.tex

MTT command:

```
mtt Reactor abg tex
```

Figure 1.2 (on page 11) is the schematic diagram od a chemical reactor. The acausal bond graph of system **Reactor** is displayed in Figure 1.1 (on page 10) and its label file is listed in Section 1.1.1 (on page 14). The subsystems are listed in Section 1.1.2 (on page 18).

This example of a (nonlinear) chemical reactor is due to Trickett and Bogle[1] is used in this section. The reactor has two reaction mechanisms: A $\longrightarrow$ B $\longrightarrow$ C and 2A $\longrightarrow$ D. The reactor mass inflow and outflow f_r are identical. q represents the heat inflow to the reactor.

This is a two input, two-output unstable nonlinear system with unstable zero dynamics. The following figures illustrate the properties of the *linearised* system.

- Figures 1.3 (on page 12) and 1.4 (on page 12) show the three poles of the *linearised* system as the steady-state flow varies.

- Figure 1.5 (on page 13) shows the system zero (when t and c_a are the two system outputs) as the *linearised* system as the steady-state flow varies.

- Figure 1.6 (on page 14) shows the system zero (when t and c_b are the two system outputs) as the *linearised* system as the steady-state flow varies.

[1] K. J. Tricket, *Quantification of Inverse Responses for Controllability Assessment of Nonlinear Processes*, PhD Thesis, University College London, 1994

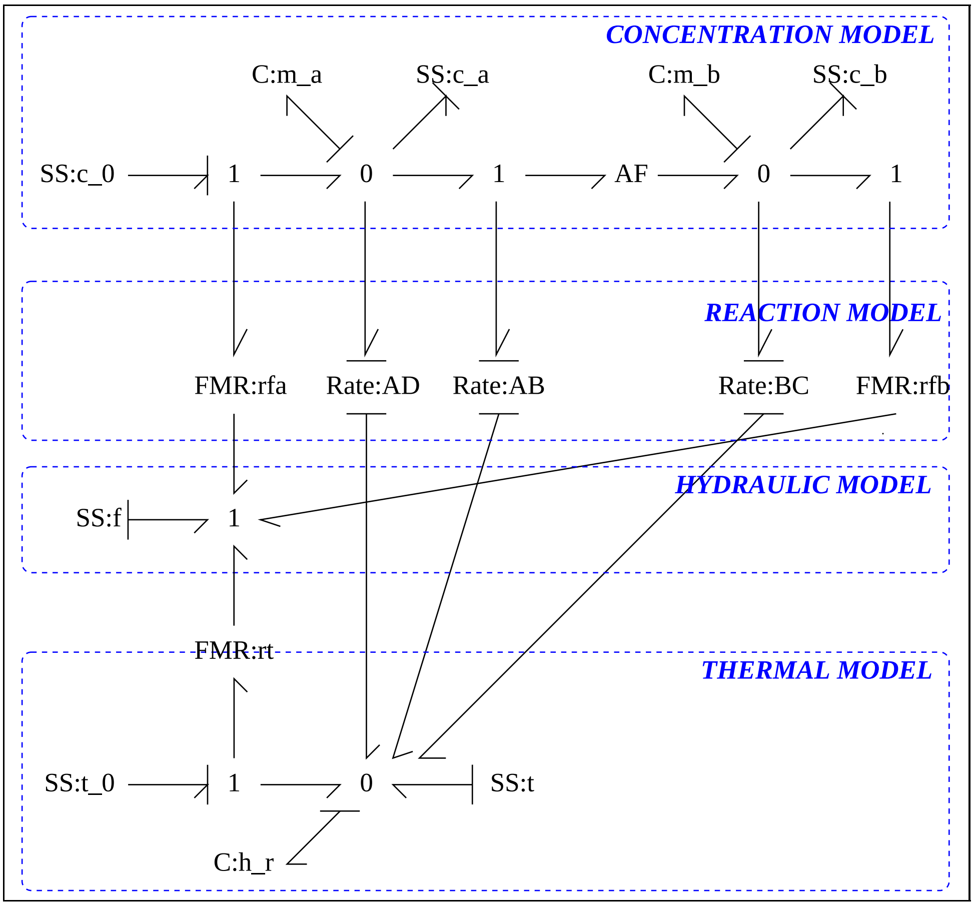


Figure 1.1: System **Reactor**: acausal bond graph

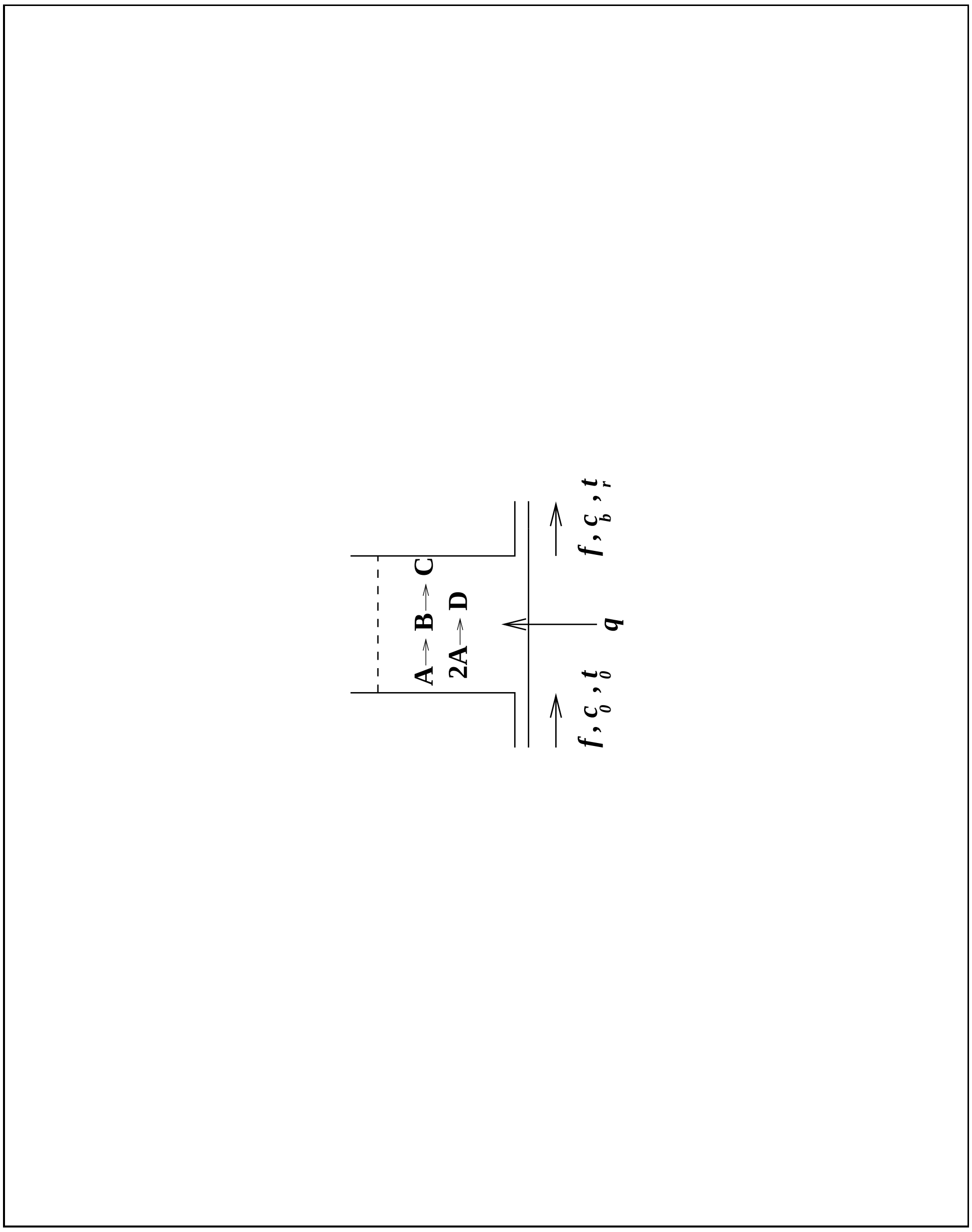


Figure 1.2: System **Reactor**, Schematic

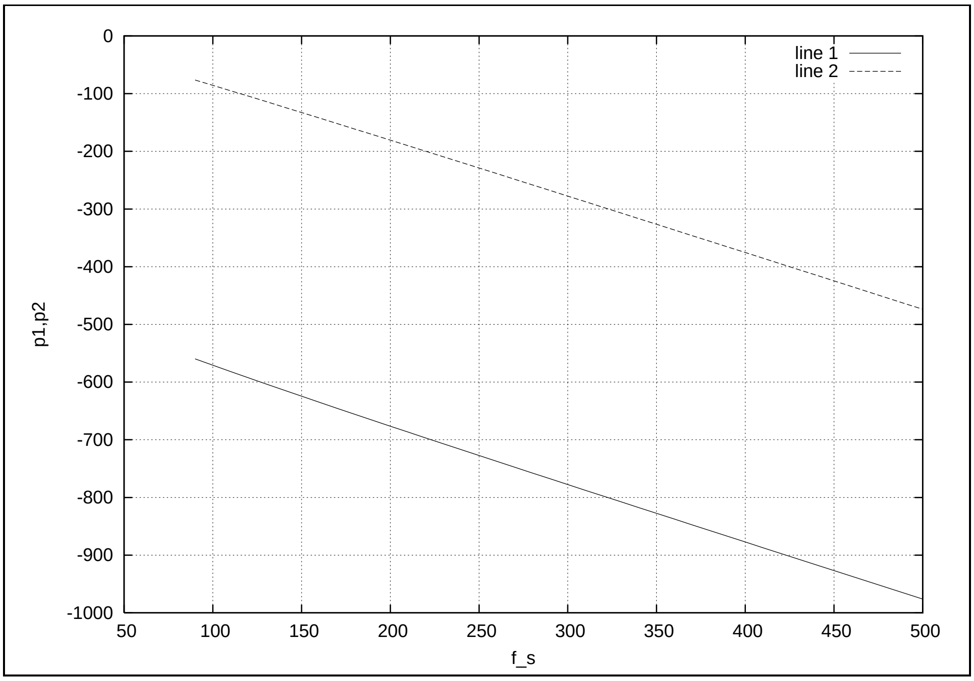


Figure 1.3: System **Reactor**: poles 1 and 2 v. steady-state flow f_s

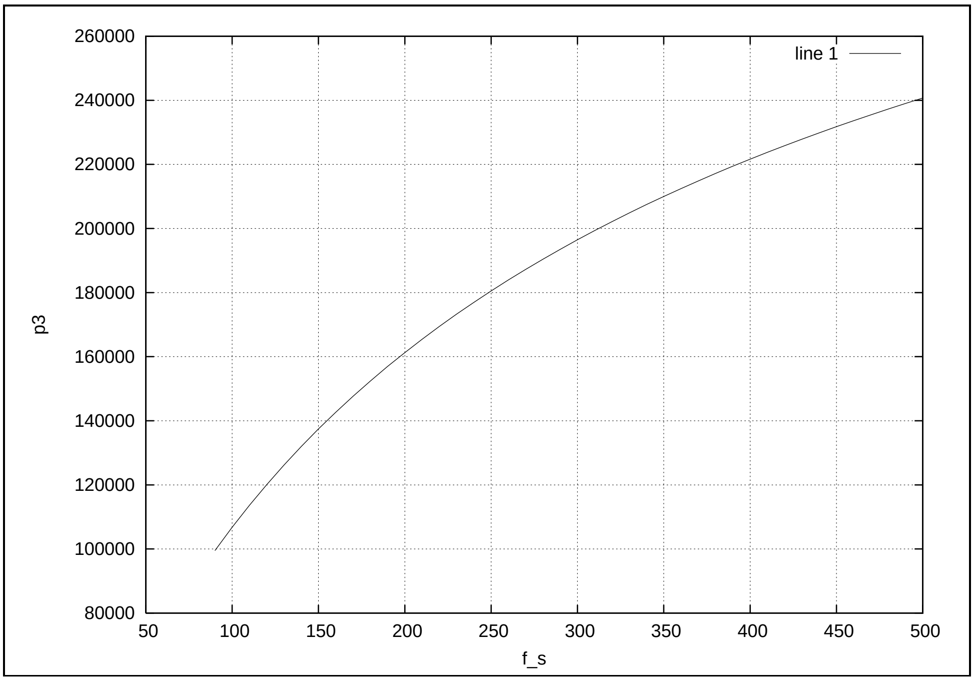


Figure 1.4: System **Reactor**: pole 3 v. steady-state flow f_s

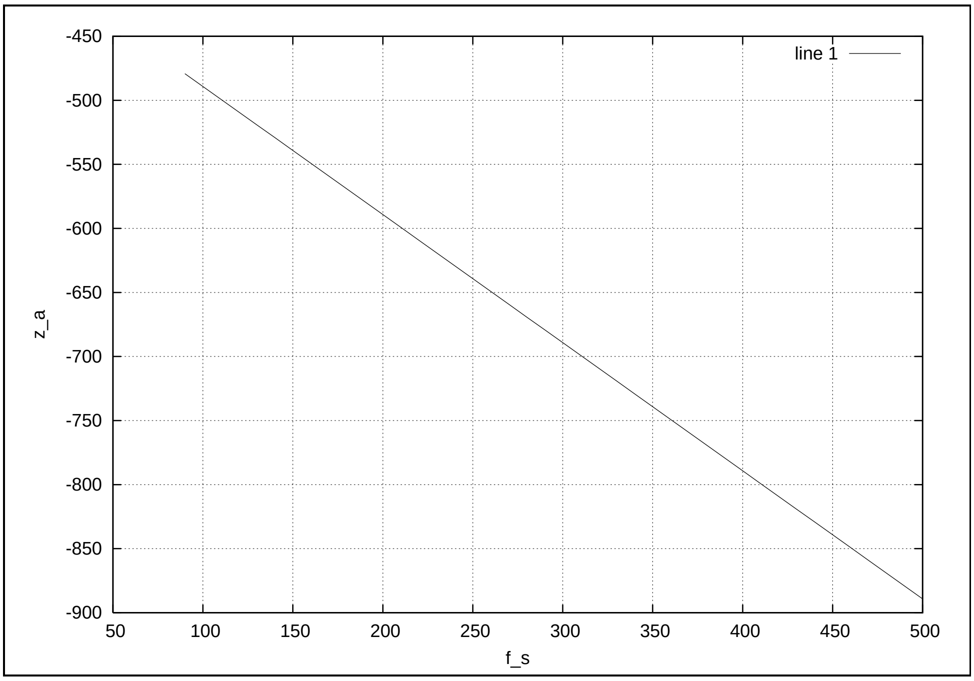


Figure 1.5: System **Reactor**: zero of system with t and c_a as output v. steady-state flow f_s

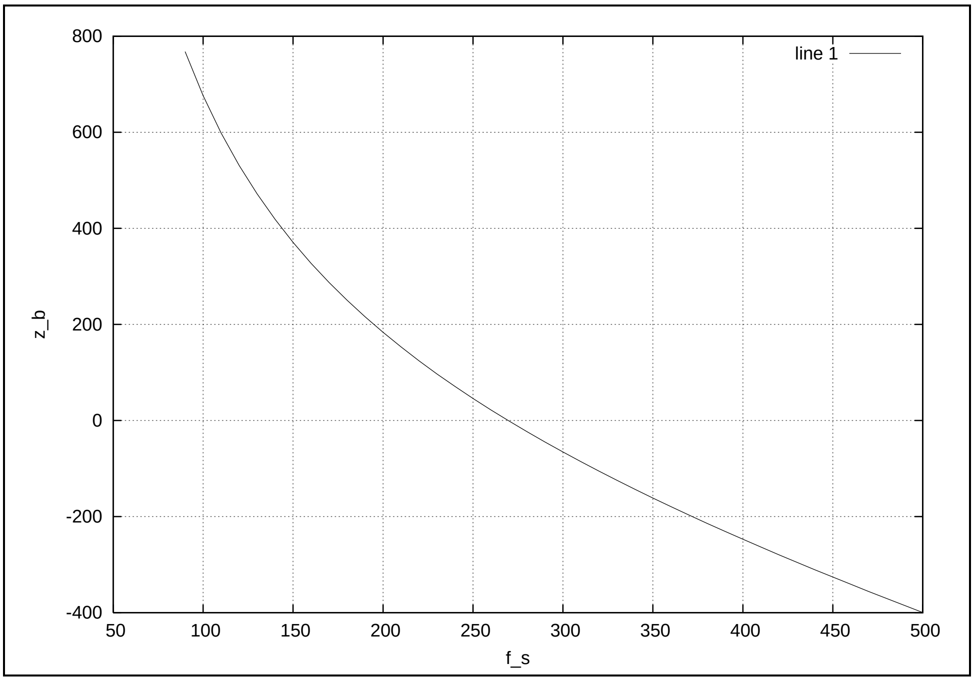


Figure 1.6: System **Reactor**: pole 3 v. steady-state flow f_s

1.1.1 Summary information

System Reactor::Simple reactor model Pseudo bond graph reactor model (based on ancient version)

Interface information:

Component Rate is in library **Chemical/Rate**

Variable declarations:

a

b

c

c_0

c_A

c_B

e_1

e_2

e_3

f_s

h

k

n

q

q_S

rho

t_0

t_s

u1

u2

v_r

x1

x2

x3

Units declarations:

This component has no UNITs declarations

The label file: Reactor_lbl.txt

```
%% Label file for system Reactor (Reactor_lbl.txt)
%SUMMARY Reactor: Simple reactor model
%DESCRIPTION Pseudo bond graph reactor model (based on ancient ver

% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% %% Version control history
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% %% $Id: Reactor_lbl.txt,v 1.2 2003/06/06 06:38:09 gawthrop Exp $
% %% $Log: Reactor_lbl.txt,v $
% %% Revision 1.2  2003/06/06 06:38:09  gawthrop
% %% Made compatible with current MTT.
% %%
% %% Revision 1.1  2000/12/28 17:09:55  peterg
% %% To RCS
% %%
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


%ALIAS Rate Chemical/Rate

% Extra variables
%VAR t_s
%VAR f_s
%VAR t_0
%VAR c_0
%VAR rho
%VAR v_r
%VAR e_1
%VAR e_2
%VAR e_3
%VAR a
%VAR b
%VAR c
%VAR c_A
%VAR c_B
%VAR x1
%VAR x2
%VAR x3
%VAR q_S
```

```
%VAR h
%VAR k
%VAR n
%VAR q

%VAR u1
%VAR u2

% Port aliases

% Argument aliases

%% each line should be of one of the following forms:
%      a comment (ie starting with %)
%      component-name cr_name arg1,arg2,..argn
%      blank

% ---- Component labels ----
% Component type C
m_a lin effort,1
m_b lin effort,1
h_r lin effort,c_p

% Component type FMR
rfa lin effort,1
rfb lin effort,1
rt lin effort,c_p

% Component type Rate
        AB Rate k_1,q_1,h_1,1
BC Rate k_2,q_2,h_2,1
AD Rate k_3,q_3,h_3,2

% Component type SS
c_0 SS c_0,internal
c_a SS external,0
c_b SS external,0
f SS internal,external
t SS external,external
t_0 SS t_0,internal
```

1.1.2 Subsystems

- Rate (3) No subsystems.

1.1.3 Rate

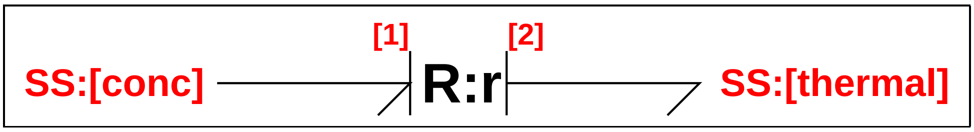


Figure 1.7: System **Rate**: acausal bond graph

The acausal bond graph of system **Rate** is displayed in Figure 3.4 (on page 63) and its label file is listed in Section 3.1.3 (on page 64). The subsystems are listed in Section 3.1.3 (on page 65).

This component represents rate of reaction equations corresponding to the chemical reaction:

$$\text{nA} \longrightarrow \text{B} \tag{1.1}$$

The relevant equations are

$$\begin{aligned} \frac{dc_a}{dt} &= k_a c_a^n e^{-\frac{q_a}{T}} \\ Q &= h_a k_a c_a^n e^{-\frac{q_a}{T}} \end{aligned} \tag{1.2}$$

where $\frac{dc_a}{dt}$ is the rate of change of concentration of species A and Q is the corresponding heat generated.

Summary information

System Rate:

Interface information:

Parameter $1 represents actual parameter **k,q,h,n**

Port in represents actual port **conc**

Port out represents actual port **thermal**

Variable declarations:

This component has no PAR declarations

Units declarations:

This component has no UNITs declarations

The label file: Rate_lbl.txt

```
%% Label file for system Rate (Rate_lbl.txt)
%SUMMARY Rate
%DESCRIPTION

% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% %% Version control history
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% %% $Id: Rate_lbl.txt,v 1.1 2000/05/19 19:54:15 peterg Exp $
% %% $Log: Rate_lbl.txt,v $
% %% Revision 1.1  2000/05/19 19:54:15  peterg
% %% Initial revision
% %%
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


% Port aliases
%ALIAS in conc
%ALIAS out thermal

% Argument aliases
%ALIAS $1 k,q,h,n

%% Each line should be of one of the following forms:
%      a comment (ie starting with %)
%      component-name cr_name arg1,arg2,..argn
%      blank

% ---- Component labels ----
r  Rate k,q,h,n

% Component type SS
[conc] SS external,external
[thermal] SS external,external
```

Subsystems

No subsystems.

1.2 Reactor_cbg.ps

MTT command:

```
mtt Reactor cbg ps
```

This representation is given as Figure 1.8 (on page 20).

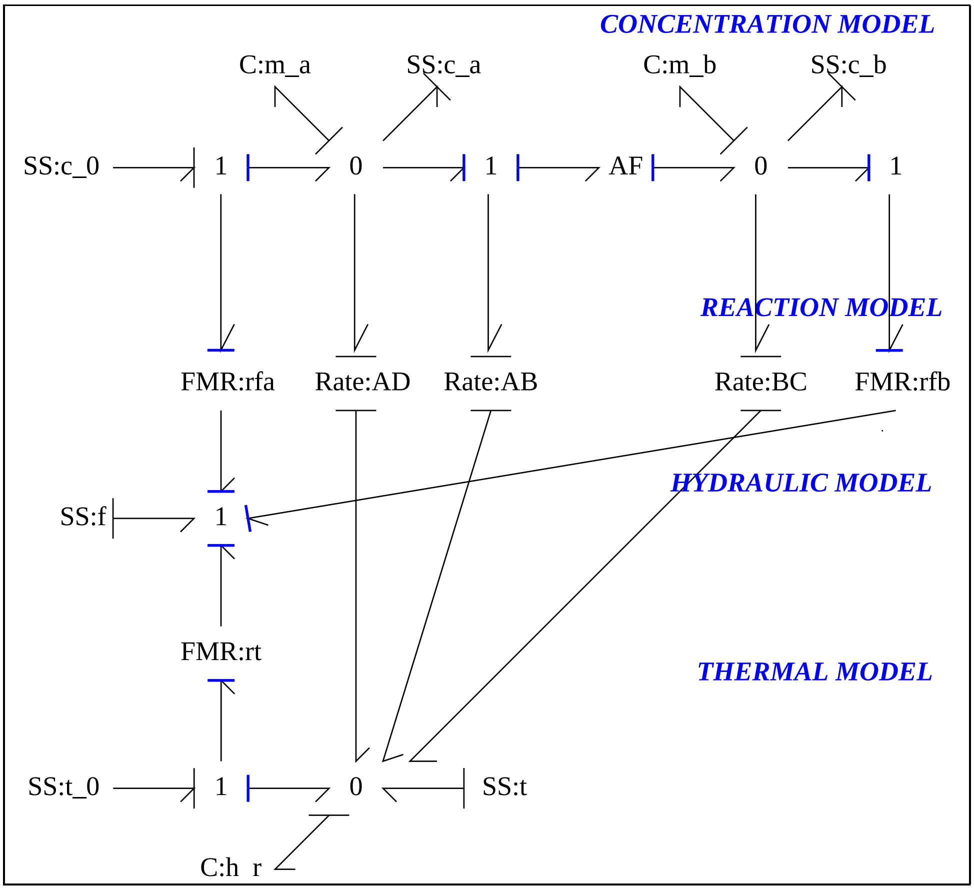


Figure 1.8: System **Reactor**, representation cbg (-noargs)

1.3 Reactor_struc.tex

MTT command:

```
mtt Reactor struc tex
```

List of inputs for system Reactor			
	Component	System	Repetition
1	f	Reactor__f	1
2	t	Reactor__t	1

List of outputs for system Reactor			
	Component	System	Repetition
1	c_a	Reactor__c_a	1
2	c_b	Reactor__c_b	1
3	t	Reactor__t	1

List of states for system Reactor			
	Component	System	Repetition
1	m_a	Reactor__m_a	1
2	m_b	Reactor__m_b	1
3	h_r	Reactor__h_r	1

1.4 Reactor_ode.tex

MTT command:

```
mtt Reactor ode tex
```

$$\begin{aligned} \dot{x}_1 &= -x_1^2\varepsilon_3 k_3 - x_1(\varepsilon_1 k_1 + u_1) + c_0 u_1 \\ \dot{x}_2 &= x_1\varepsilon_1 k_1 - x_2(\varepsilon_2 k_2 + u_1) \\ \dot{x}_3 &= x_1^2\varepsilon_3 h_3 k_3 + x_1\varepsilon_1 h_1 k_1 + x_2\varepsilon_2 h_2 k_2 + c_p u_1 t_0 - u_1 x_3 + u_2 \end{aligned} \tag{1.3}$$

$$\begin{aligned} y_1 &= x_1 \\ y_2 &= x_2 \\ y_3 &= \frac{x_3}{c_p} \end{aligned} \tag{1.4}$$

1.5 Reactor_sspar.tex

MTT command:

```
mtt Reactor sspar tex
```

```
%% Reduce steady-state parameter file (Reactor_sspar.r)
%% as siso_sspar ecxept that inputs/states have different meaning
%% Steady state for constant c_a, c_b and t=t_s and f=f_s

%% Unit volume Reactor:
v_r := 1;

%% Do the inputs first -- this avoids problems with reduce not
%% recognising that complicated expressions are zero

%% The exponentials.
e_1 := e^(-q_1/t_s);
e_2 := e^(-q_2/t_s);
e_3 := e^(-q_3/t_s);

%Steady-state input q needed to achieve steady-state t_s
q_s := -(
        + (t_0-t_s)*c_p*f_s
        + e_1*h_1*k_1*x1
        + e_2*h_2*k_2*x2
        + e_3*h_3*k_3*x1^2
       );

%% The two inputs at steady-state
MTTu1 := f_s;
MTTu2 := q_s;

%States (masses)
x1 := c_a*v_r;
x2 := c_b*v_r;

%Thermal state
x3 := c_p*t_s*v_r;

%Load up the vectors
MTTx1 := x1;
```

```
MTTx2 := x2;
MTTx3 := x3;

MTTy1 := c_b;
MTTy2 := t_s;

%% Finally, solve for the steady-state concentrations
%% Solve for ca - a quadratic.
a  := k_3*e_3; %caˆ2
b  := k_1*e_1 + f_s; %caˆ1
c  := -c_0*f_s;

c_a := (-b + sqrt(bˆ2 - 4*a*c))/(2*a);

%% solve for c_b
c_b  := c_a*k_1*e_1/(f_s+k_2*e_2);


END;
```

1.6 Reactor_ss.tex

MTT command:

```
mtt Reactor ss tex
```

$$x = \begin{pmatrix} \frac{\left(\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}-\varepsilon_1 k_1-f_s\right)}{(2\varepsilon_3 k_3)} \\ \frac{\left(\varepsilon_1 k_1\left(\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}-\varepsilon_1 k_1-f_s\right)\right)}{(2\varepsilon_3 k_3(\varepsilon_2 k_2+f_s))} \\ c_p t_s \end{pmatrix} \tag{1.5}$$

$$u = \left(\frac{\left(-4|\varepsilon_1|^2 c_0\varepsilon_2\varepsilon_3 f_s h_3 k_2 k_3-4abs(\varepsilon_1)^2 c_0\varepsilon_3 f_s^2 h_3 k_3-|\varepsilon_1|^2\varepsilon_1^2\varepsilon_2 h_3 k_1^2 k_2-|\varepsilon_1|^2\varepsilon_1^2 f_s h_3 k_1^2-2abs(\varepsilon_1)^2\varepsilon_1\varepsilon_2 f_s h_3 k_1 k_2-2|\varepsilon_1|^2\varepsilon_1 f_s^2 h_3 k_1-|\varepsilon_1|^2\varepsilon_2 f\right.}{} \right. \tag{1.6}$$

$$y = \begin{pmatrix} \frac{\left(\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}-\varepsilon_1 k_1-f_s\right)}{(2\varepsilon_3 k_3)} \\ \frac{\left(\varepsilon_1 k_1\left(\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}-\varepsilon_1 k_1-f_s\right)\right)}{(2\varepsilon_3 k_3(\varepsilon_2 k_2+f_s))} \\ t_s \end{pmatrix} \tag{1.7}$$

$$\dot{x} = \begin{pmatrix} \frac{\left(-4|\varepsilon_1|^2 c_0\varepsilon_3 f_s k_3-|\varepsilon_1|^2\varepsilon_1^2 k_1^2-2|\varepsilon_1|^2\varepsilon_1 f_s k_1-|\varepsilon_1|^2 f_s^2+4c_0\varepsilon_1^2\varepsilon_3 f_s k_3+\varepsilon_1^4 k_1^2+2\varepsilon_1^3 f_s k_1+\varepsilon_1^2 f_s^2\right)}{\left(4\varepsilon_1^2\varepsilon_3 k_3\right)} \\ 0 \\ 0 \end{pmatrix} \tag{1.8}$$

1.7 Reactor_sm.tex

MTT command:

```
mtt Reactor sm tex
```

$$A = \begin{pmatrix} -\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)} & 0 & \\ \varepsilon_1 k_1 & -(\varepsilon_2 k_2+f_s) & \\ \sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}h_3+\varepsilon_1 h_1 k_1-\varepsilon_1 h_3 k_1-f_s h_3 & \varepsilon_2 h_2 k_2 & \frac{\left(4|\varepsilon_1|^2 c_0\varepsilon_2\varepsilon_3\right.}{} \end{pmatrix} \tag{1.9}$$

$$B = \begin{pmatrix} \frac{\left(-\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}+2c_0\varepsilon_3 k_3+\varepsilon_1 k_1+f_s\right)}{(2\varepsilon_3 k_3)} & 0 \\ \frac{\left(\varepsilon_1 k_1\left(-\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}+\varepsilon_1 k_1+f_s\right)\right)}{(2\varepsilon_3 k_3(\varepsilon_2 k_2+f_s))} & 0 \\ c_p(t_0-t_s) & 1 \end{pmatrix} \tag{1.10}$$

$$C = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{1}{c_p} \end{pmatrix} \tag{1.11}$$

$$D = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \tag{1.12}$$

1.8 Reactor_simpar.tex

MTT command:

```
mtt Reactor simpar tex
```

```
# -*-octave-*- Put Emacs into octave-mode
# Simulation parameters for system Reactor (Reactor_simpar.txt)
# Generated by MTT on Fri Mar 3 12:11:48 GMT 2000.
###############################################################
## Version control history
###############################################################
## $Id: Reactor_simpar.txt,v 1.1 2000/12/28 17:09:55 peterg Exp $
## $Log: Reactor_simpar.txt,v $
## Revision 1.1  2000/12/28 17:09:55  peterg
## To RCS
##
## Revision 1.1  2000/08/24 12:32:25  peterg
## Initial revision
##
###############################################################


LAST        = 0.1;       # Last time in simulation
DT          = 0.0002;        # Print interval
STEPFACTOR  = 1;          # Integration steps per print interval
WMIN        = -1;         # Minimum frequency = 10^WMIN
WMAX        = 2;          # Maximum frequency = 10^WMAX
WSTEPS      = 100;        # Number of frequency steps
INPUT       = 1;          # Index of the input
```

1.9 Reactor_numpar.tex

MTT command:

```
mtt Reactor numpar tex
```

```
# -*-octave-*- Put Emacs into octave-mode
# Numerical parameter file (Reactor_numpar.txt)
# Generated by MTT at Fri Mar  3 09:22:56 GMT 2000
# %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
# %% Version control history
# %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
# %% $Id: Reactor_numpar.txt,v 1.2 2003/06/06 06:38:18 gawthrop Ex
# %% $Log: Reactor_numpar.txt,v $
# %% Revision 1.2  2003/06/06 06:38:18  gawthrop
# %% Made compatible with current MTT.
# %%
# %% Revision 1.1  2000/12/28 17:09:55  peterg
# %% To RCS
# %%
# %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

## Dummies
a = 0; # Dummy
b = 0; # Dummy
c = 0; # Dummy
c_0 = 0; # Dummy
c_a = 0; # Dummy
c_b = 0; # Dummy
c_p = 0; # Dummy
e_1 = 0; # Dummy
e_2 = 0; # Dummy
e_3 = 0; # Dummy
f_s = 0; # Dummy
h = 0; # Dummy
h_1 = 0; # Dummy
h_2 = 0; # Dummy
h_3 = 0; # Dummy
k = 0; # Dummy
k_1 = 0; # Dummy
k_2 = 0; # Dummy
k_3 = 0; # Dummy
n = 0; # Dummy
q = 0; # Dummy
q_1 = 0; # Dummy
q_2 = 0; # Dummy
q_3 = 0; # Dummy
q_s = 0; # Dummy
rho = 0; # Dummy
t_0 = 0; # Dummy
```

```
t_s = 0; # Dummy
v_r = 0; # Dummy
x1 = 0; # Dummy
x2 = 0; # Dummy
x3 = 0; # Dummy

## The bulk liquid
rho = 900; # Density
c_p = 5.0; # Specific heat

## Substance A
k_1 = 2.5e10; # Reaction rate constant
q_1 = 1e4; # Exotherm constant
h_1 = 1e4; # Heat of reaction

## Substance B
k_2 = 2.65e12; # Reaction rate constant
q_2 = 1.2e4; # Exotherm constant
h_2 = 1.2e4; # Heat of reaction

## Substance C
k_3 = 6e7; # Reaction rate constant
q_3 = 8e3; # Exotherm constant
h_3 = 3e4; # Heat of reaction

## Inflow parameters
c_0 = 10; # Inflow conc
t_0 = 530; # Inflow temp

## Steady-state values
t_s = 530; # Steady-state temp
f_s = 100; # Steady-state flow








u1 = 1.0; # Added by MTT on Thu Jun 05 12:45:35 BST 2003
```

```
u2 = 1.0; # Added by MTT on Thu Jun 05 12:45:35 BST 2003
```

1.10 Reactor_input.tex

MTT command:

```
mtt Reactor input tex
```

```
# -*-octave-*- Put Emacs into octave-mode
# Input specification (Reactor_input.txt)
# Generated by MTT at Fri Mar  3 11:52:23 GMT 2000
###############################################################
## Version control history
###############################################################
## $Id: Reactor_input.txt,v 1.3 2003/06/06 06:38:02 gawthrop Exp $
## $Log: Reactor_input.txt,v $
## Revision 1.3  2003/06/06 06:38:02  gawthrop
## Made compatible with current MTT.
##
## Revision 1.2  2000/12/28 18:52:24  peterg
## Updated for new formats
##
## Revision 1.1  2000/12/28 17:09:55  peterg
## To RCS
##
###############################################################

## Reduce steady-state parameter file (Reactor_sspar.r)
## as siso_sspar ecxept that inputs/states have different meaning
## Steady state for constant c_a, c_b and t=t_s and f=f_s

## Unit volume Reactor:
v_r = 1;


## The exponentials.
e_1 = exp(-q_1/t_s);
e_2 = exp(-q_2/t_s);
e_3 = exp(-q_3/t_s);

## Solve for the steady-state concentrations
## Solve for ca - a quadratic.
a  = k_3*e_3; #caˆ2
b  = k_1*e_1 + f_s; #caˆ1
c  = -c_0*f_s;

c_a = (-b + sqrt(bˆ2 - 4*a*c))/(2*a);

## solve for c_b
c_b  = c_a*k_1*e_1/(f_s+k_2*e_2);


#States (masses)
x1 = c_a*v_r;
x2 = c_b*v_r;

#Thermal state
x3 = c_p*t_s*v_r;


#Steady-state input q needed to achieve steady-state t_s
q_s = -( (t_0-t_s)*c_p*f_s + e_1*h_1*k_1*x1 + e_2*h_2*k_2*x2 + e_3*h_3*k

## The two inputs at steady-state
u1 = f_s;
u2 = q_s;


# Set the inputs
## Removed by MTT on Thu Dec 28 18:44:39 GMT 2000: mttu(1) = u1 + 0.1*u1
## Removed by MTT on Thu Dec 28 18:44:39 GMT 2000: mttu(2) = u2 + 0.1*u2



## Removed by MTT on Thu Jun  5 12:48:41 BST 2003: reactor_f
= u1 + 0.1*u1*(t>0.01); # Added by MTT on Thu Dec 28 18:44:47 GMT 2000
## Removed by MTT on Thu Jun  5 12:48:41 BST 2003: reactor_t
= u2 + 0.1*u2*(t>0.05); # Added by MTT on Thu Dec 28 18:44:47 GMT 2000
reactor__f = u1 + 0.1*u1*(t>0.01); # f (Reactor)
reactor__t = u2 + 0.1*u2*(t>0.05) ; # t (Reactor)
```

1.11 Reactor_state.tex

MTT command:

```
mtt Reactor state tex
```

```
# -*-octave-*- Put Emacs into octave-mode
# State specification (Reactor_state.txt)
# Generated by MTT at Fri Mar  3 11:52:23 GMT 2000
###############################################################
## Version control history
###############################################################
## $Id: Reactor_state.txt,v 1.3 2003/06/06 06:38:31 gawthrop Exp $
## $Log: Reactor_state.txt,v $
## Revision 1.3  2003/06/06 06:38:31  gawthrop
## Made compatible with current MTT.
##
## Revision 1.2  2000/12/28 18:52:25  peterg
## Updated for new formats
##
## Revision 1.1  2000/12/28 17:09:55  peterg
## To RCS
##
###############################################################

## Reduce steady-state parameter file (Reactor_sspar.r)
## as siso_sspar ecxept that states/states have different meaning
## Steady state for constant c_a, c_b and t=t_s and f=f_s

## Unit volume Reactor:
v_r = 1;


## The exponentials.
e_1 = exp(-q_1/t_s);
e_2 = exp(-q_2/t_s);
e_3 = exp(-q_3/t_s);

## Solve for the steady-state concentrations
## Solve for ca - a quadratic.
a  = k_3*e_3; #ca^2
b  = k_1*e_1 + f_s; #ca^1
```

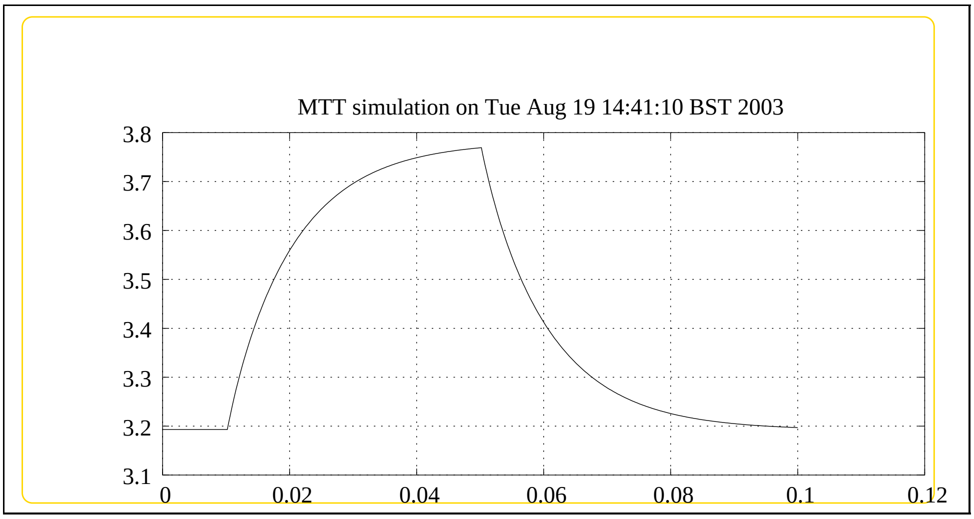
```
c  = -c_0*f_s;

c_a = (-b + sqrt(b^2 - 4*a*c))/(2*a);

## solve for c_b
c_b  = c_a*k_1*e_1/(f_s+k_2*e_2);


#States (masses)
x1 = c_a*v_r;
x2 = c_b*v_r;

#Thermal state
x3 = c_p*t_s*v_r;


#Steady-state state q needed to achieve steady-state t_s
q_s = -((t_0-t_s)*c_p*f_s + e_1*h_1*k_1*x1 + e_2*h_2*k_2*x2 + e_3*h_3*k_

## The two inputs at steady-state
u1 = f_s;
u2 = q_s;

## Load up the states
## Removed by MTT on Thu Dec 28 18:46:20 GMT 2000: mttx(1) = x1;
## Removed by MTT on Thu Dec 28 18:46:20 GMT 2000: mttx(2) = x2;
## Removed by MTT on Thu Dec 28 18:46:20 GMT 2000: mttx(3) = x3;




## Removed by MTT on Thu Jun  5 12:47:23 BST 2003: reactor_h_r
= x3; # Added by MTT on Thu Dec 28 18:46:25 GMT 2000
## Removed by MTT on Thu Jun  5 12:47:23 BST 2003: reactor_m_a
= x1; # Added by MTT on Thu Dec 28 18:46:25 GMT 2000
## Removed by MTT on Thu Jun  5 12:47:23 BST 2003: reactor_m_b
= x2; # Added by MTT on Thu Dec 28 18:46:25 GMT 2000
reactor__h_r = x3;
reactor__m_a = x1;
reactor__m_b = x2;
```

1.12 Reactor_odeso.ps *(-Reactor__c_a)*

MTT command:

```
mtt Reactor odeso ps 'Reactor__c_a'
```

This representation is given as Figure 1.9 (on page 32).



1.13 Reactor_odeso.ps *(-Reactor__c_b)*

MTT command:

```
mtt Reactor odeso ps 'Reactor__c_b'
```

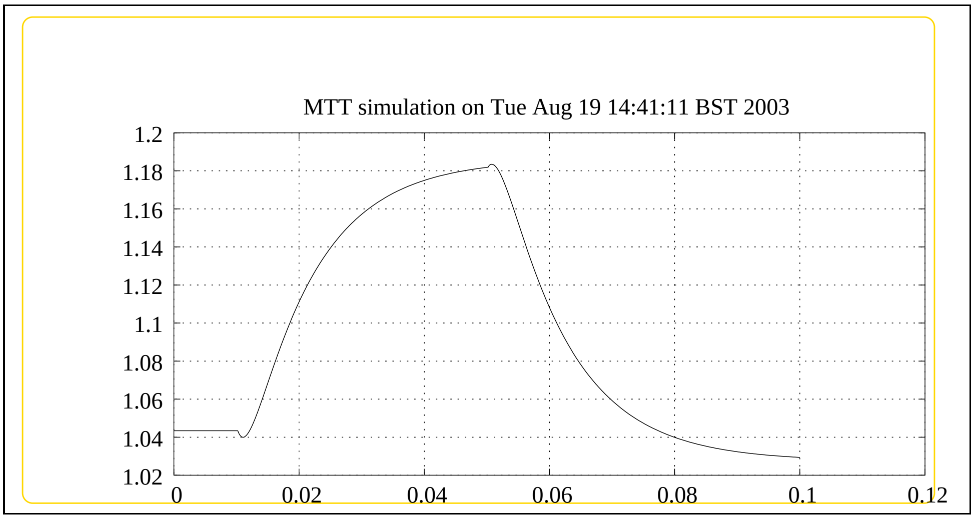
This representation is given as Figure 1.10 (on page 33).

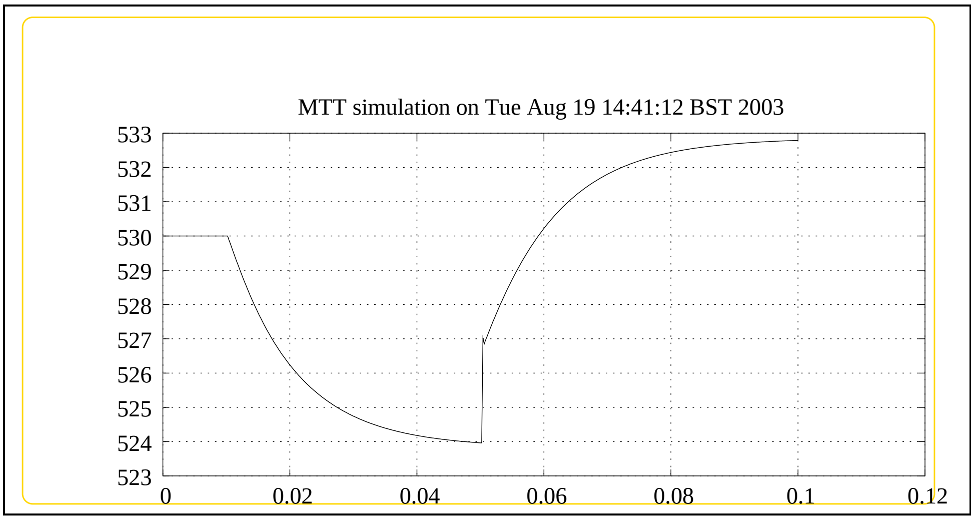
1.14 Reactor_odeso.ps *(-Reactor__t)*

MTT command:

```
mtt Reactor odeso ps 'Reactor__t'
```

This representation is given as Figure 1.11 (on page 33).


MTT simulation on Tue Aug 19 14:41:11 BST 2003
1.2
1.18
1.16
1.14
1.12
1.1
1.08
1.06
1.04
1.02
0
0.02
0.04
0.06
0.08
0.1
0.12


MTT simulation on Tue Aug 19 14:41:12 BST 2003
533
532
531
530
529
528
527
526
525
524
523
0
0.02
0.04
0.06
0.08
0.1
0.12

Chapter 2

ReactorTF

2.1 ReactorTF_abg.tex

MTT command:

```
mtt ReactorTF abg tex
```

Figure 2.2 (on page 37) is the schematic diagram of a chemical reactor.

The acausal bond graph of system **ReactorTF** is displayed in Figure 2.1 (on page 36) and its label file is listed in Section 2.1.1 (on page 35). The subsystems are listed in Section 2.1.2 (on page 42).

This example of a (nonlinear) chemical reactor is due to Trickett and Bogle[1] is used in this section. The reactor has two reaction mechanisms: $\mathrm{A} \to \mathrm{B} \to \mathrm{C}$ and $2\mathrm{A} \to \mathrm{D}$. The reactor mass inflow and outflow f_r are identical. q represents the heat inflow to the reactor.

The control loop t/f has been inverted. The resulting SISO system has two interpretations:

1. the *dynamics* of the c_b/q loop when the t/f loop is under perfect control and

2. the *inverse* dynamics of the t/f loop.

Figures 2.3 (on page 38) and 2.4 (on page 38) shows the poles of the linearised system as the steady-state flow varies: these are the *zeros* of the t/f control-loop when the c_b/q loop is *open*.

2.1.1 Summary information

System ReactorTF::Simple reactor model – TF loop inverted Pseudo bond graph reactor model (based on ancient version)

[1] K. J. Tricket, *Quantification of Inverse Responses for Controllability Assessment of Nonlinear Processes*, PhD Thesis, University College London, 1994

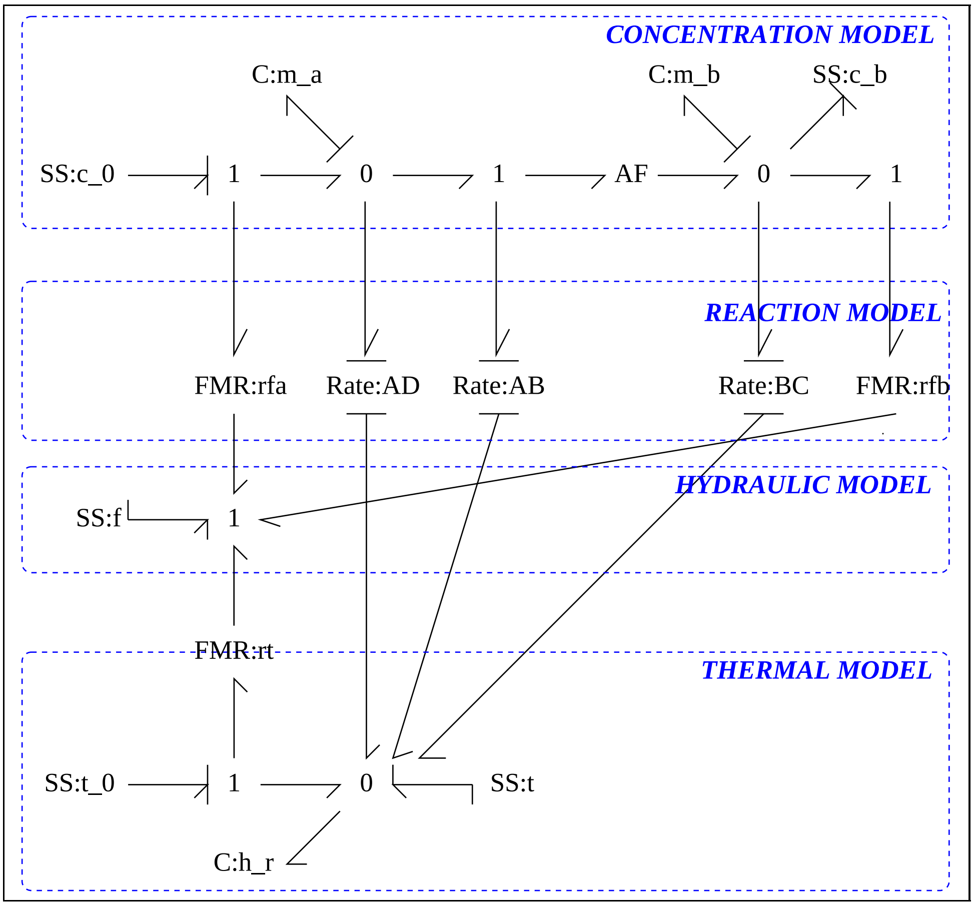


Figure 2.1: System **ReactorTF**: acausal bond graph

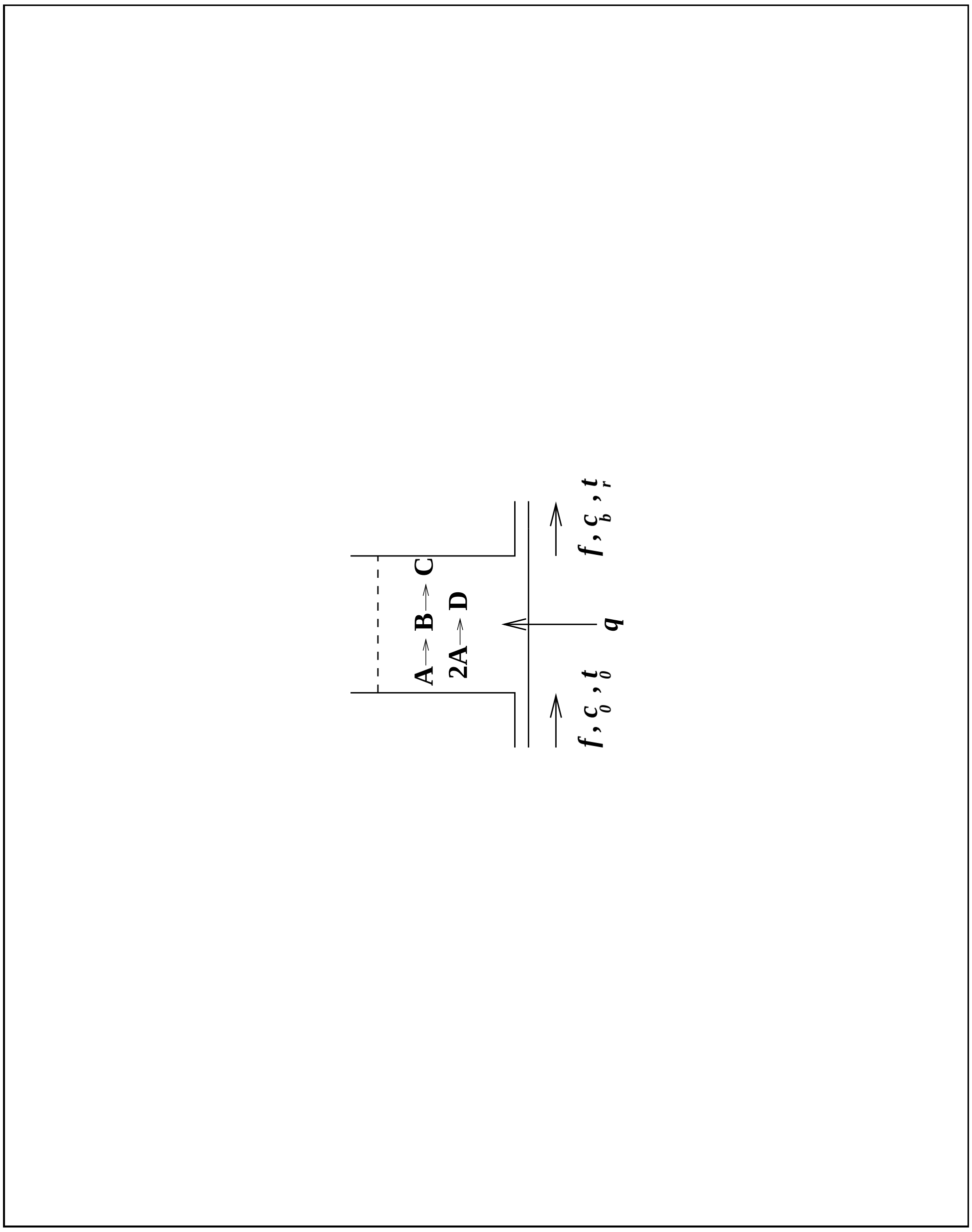


Figure 2.2: System **ReactorTF**, Schematic

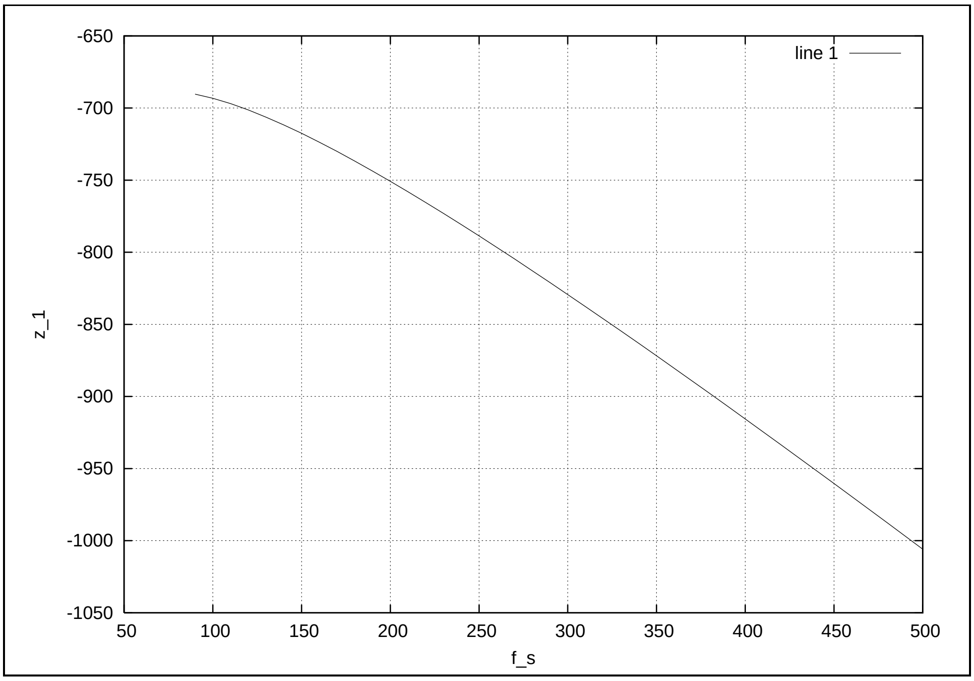


Figure 2.3: System**ReactorTF**: zero 1 v flow

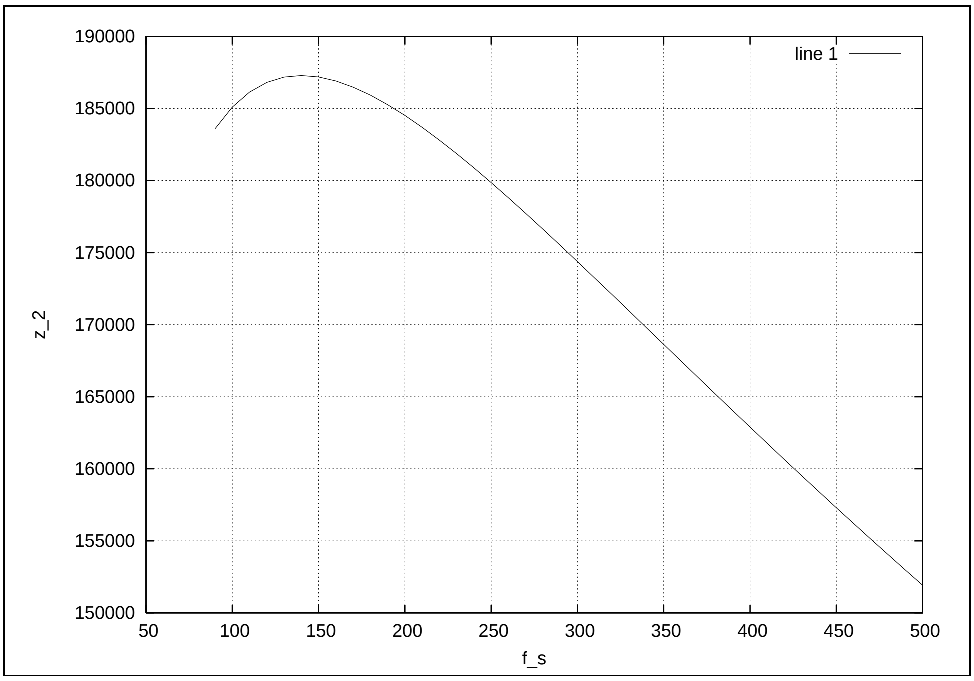


Figure 2.4: System**ReactorTF**: zero 2 v flow

Interface information:

Component Rate is in library **Chemical/Rate**

Variable declarations:

a

b

c

c_0

c_A

c_B

e_1

e_2

e_3

f_s

h

k

n

q

q_S

rho

t_0

t_s

v_r

x1

x2

x3

Units declarations:

This component has no UNITs declarations

The label file: ReactorTF_lbl.txt

```
%% Label file for system ReactorTF (ReactorTF_lbl.txt)
%SUMMARY ReactorTF: Simple reactor model -- TF loop inverted
%DESCRIPTION Pseudo bond graph reactor model (based on ancient ver

% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% %% Version control history
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% %% $Id: ReactorTF_lbl.txt,v 1.2 2003/06/06 06:38:51 gawthrop Exp
% %% $Log: ReactorTF_lbl.txt,v $
% %% Revision 1.2  2003/06/06 06:38:51  gawthrop
% %% Made compatible with current MTT.
% %%
% %% Revision 1.1  2000/12/28 17:12:57  peterg
% %% To RCS
% %%
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


%ALIAS Rate Chemical/Rate

% Extra variables
%VAR t_s
%VAR f_s
%VAR t_0
%VAR c_0
%VAR rho
%VAR v_r
%VAR e_1
%VAR e_2
%VAR e_3
%VAR a
%VAR b
%VAR c
%VAR c_A
%VAR c_B
```

```
%VAR x1
%VAR x2
%VAR x3
%VAR q_S

%VAR h
%VAR k
%VAR n
%VAR q


% Port aliases

% Argument aliases

%% each line should be of one of the following forms:
%       a comment (ie starting with %)
%       component-name cr_name arg1,arg2,..argn
%       blank

% ---- Component labels ----
% Component type C
m_a lin effort,1
m_b lin effort,1
h_r lin effort,c_p

% Component type FMR
rfa lin effort,1
rfb lin effort,1
rt lin effort,c_p

% Component type Rate
        AB Rate k_1,q_1,h_1,1
BC Rate k_2,q_2,h_2,1
AD Rate k_3,q_3,h_3,2

% Component type SS
c_0 SS c_0,internal
c_b SS external,0
f SS internal,internal
t SS t_s,external
```

```
t_0 SS t_0,internal
```

2.1.2 Subsystems

- Rate (3) No subsystems.

2.1.3 Rate

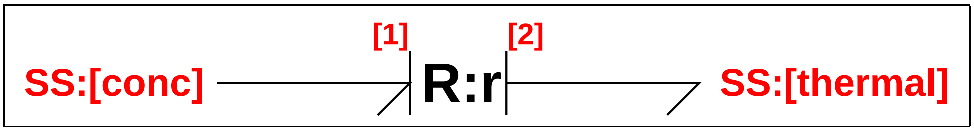


Figure 2.5: System **Rate**: acausal bond graph

The acausal bond graph of system **Rate** is displayed in Figure 3.4 (on page 63) and its label file is listed in Section 3.1.3 (on page 64). The subsystems are listed in Section 3.1.3 (on page 65).
This component represents rate of reaction equations corresponding to the chemical reaction:

$$\mathrm{nA} \longrightarrow \mathrm{B} \tag{2.1}$$

The relevant equations are

$$\begin{aligned} \frac{dc_a}{dt} &= k_a c_a^n e^{-\frac{q_a}{T}} \\ Q &= h_a k_a c_a^n e^{-\frac{q_a}{T}} \end{aligned} \tag{2.2}$$

where $\frac{dc_a}{dt}$ is the rate of change of concentration of species A and Q is the corresponding heat generated.

Summary information

System Rate:

Interface information:

Parameter $1 represents actual parameter **k,q,h,n**

Port in represents actual port **conc**

Port out represents actual port **thermal**

Variable declarations:

This component has no PAR declarations

Units declarations:

This component has no UNITs declarations

The label file: Rate_lbl.txt

```
%% Label file for system Rate (Rate_lbl.txt)
%SUMMARY Rate
%DESCRIPTION

% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% %% Version control history
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% %% $Id: Rate_lbl.txt,v 1.1 2000/05/19 19:54:15 peterg Exp $
% %% $Log: Rate_lbl.txt,v $
% %% Revision 1.1  2000/05/19 19:54:15  peterg
% %% Initial revision
% %%
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


% Port aliases
%ALIAS in conc
%ALIAS out thermal

% Argument aliases
%ALIAS $1 k,q,h,n

%% Each line should be of one of the following forms:
%      a comment (ie starting with %)
%       component-name cr_name arg1,arg2,..argn
%       blank

% ---- Component labels ----
r  Rate k,q,h,n

% Component type SS
[conc] SS external,external
[thermal] SS external,external
```

Subsystems

No subsystems.

2.2 ReactorTF_cbg.ps

MTT command:

```
mtt ReactorTF cbg ps
```

This representation is given as Figure 2.6 (on page 45).

2.3 ReactorTF_struc.tex

MTT command:

```
mtt ReactorTF struc tex
```

List of inputs for system ReactorTF			
	Component	System	Repetition
1	t	ReactorTF__t	1

List of nonstates for system ReactorTF			
	Component	System	Repetition
1	h_r	ReactorTF__h_r	1

List of outputs for system ReactorTF			
	Component	System	Repetition
1	c_b	ReactorTF__c_b	1

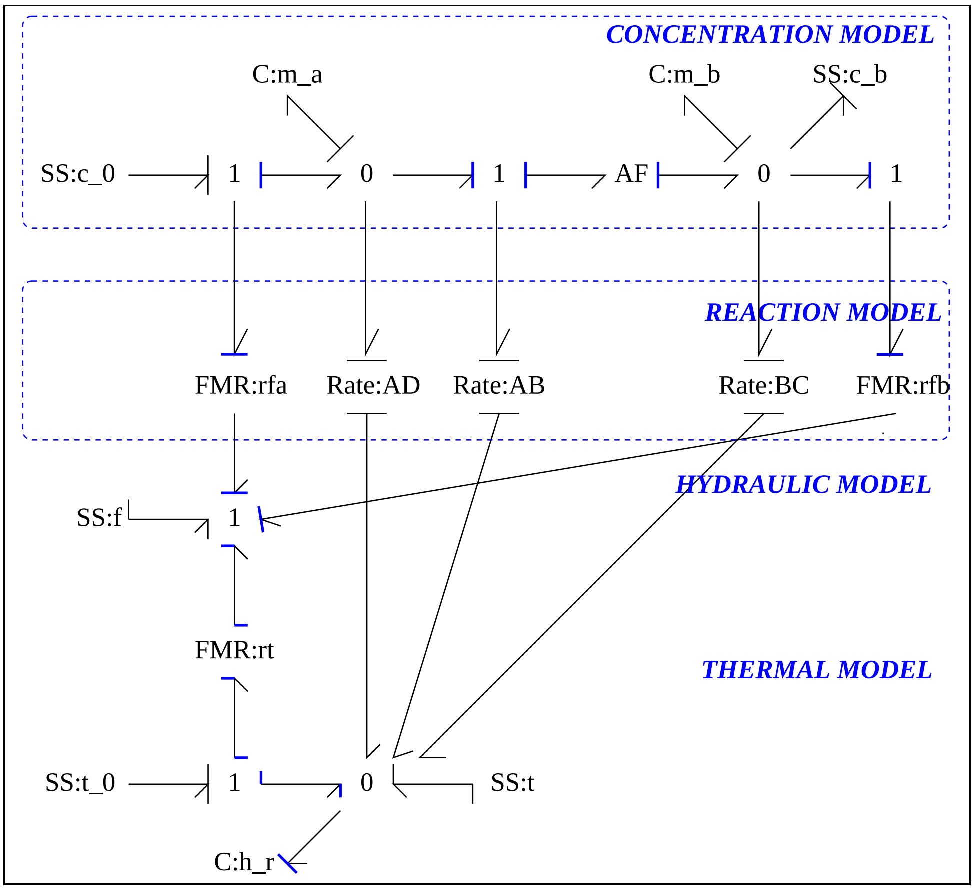


Figure 2.6: System **ReactorTF**, representation cbg (-noargs)

List of states for system ReactorTF			
	Component	System	Repetition
1	m_a	ReactorTF__m_a	1
2	m_b	ReactorTF__m_b	1

2.4 ReactorTF_ode.tex

MTT command:

```
mtt ReactorTF ode tex
```

$$\begin{aligned}\dot{x}_1 &= \frac{\bigl(x_1^3\varepsilon_3h_3k_3+x_1^2(-c_0\varepsilon_3h_3k_3-c_p\varepsilon_3k_3t_0+c_p\varepsilon_3k_3t_s+\varepsilon_1h_1k_1)+x_1x_2\varepsilon_2h_2k_2+x_1(-c_0\varepsilon_1h_1k_1-c_p}{(c_p(t_0-t_s))}\\ \dot{x}_2 &= \frac{\bigl(x_1^2x_2\varepsilon_3h_3k_3+x_1x_2\varepsilon_1h_1k_1+x_1c_p\varepsilon_1k_1(t_0-t_s)+x_2^2\varepsilon_2h_2k_2+x_2(-c_p\varepsilon_2k_2t_0+c_p\varepsilon_2k_2t_s+u_1)\bigr)}{(c_p(t_0-t_s))}\end{aligned} \tag{2.3}$$

$$y_1 = x_2 \tag{2.4}$$

2.5 ReactorTF_sspar.tex

MTT command:

```
mtt ReactorTF sspar tex

%% Reduce steady-state parameter file (ReactorTF_sspar.r)
%% as siso_sspar ecxept that inputs/states have different meaning
%% Steady state for constant c_a, c_b and t=t_s and f=f_s

%% Unit volume ReactorTF:
v_r := 1;

%% Do the inputs first -- this avoids problems with reduce not
%% recognising that complicated expressions are zero

%% The exponentials.
e_1 := eˆ(-q_1/t_s);
```

```
e_2 := eˆ(-q_2/t_s);
e_3 := eˆ(-q_3/t_s);

%Steady-state input q needed to achieve steady-state t_s
q_s := -(
        + (t_0-t_s)*c_p*f_s
        + e_1*h_1*k_1*x1
        + e_2*h_2*k_2*x2
        + e_3*h_3*k_3*x1ˆ2
       );

%% The input at steady-state
MTTu1 := q_s;

%States (masses)
x1 := c_a*v_r;
x2 := c_b*v_r;

%Thermal state
x3 := c_p*t_s*v_r;

%Load up the vectors
MTTx1 := x1;
MTTx2 := x2;

MTTy1 := c_b;
%MTTy2 := t_s;

%% Finally, solve for the steady-state concentrations
%% Solve for ca - a quadratic.
a  := k_3*e_3; %caˆ2
b  := k_1*e_1 + f_s; %caˆ1
c  := -c_0*f_s;

c_a := (-b + sqrt(bˆ2 - 4*a*c))/(2*a);

%% solve for c_b
c_b  := c_a*k_1*e_1/(f_s+k_2*e_2);


END;
```

2.6 ReactorTF_ss.tex

MTT command:

```
mtt ReactorTF ss tex
```

$$x = \begin{pmatrix} \frac{\left(\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}-\varepsilon_1 k_1-f_s\right)}{(2\varepsilon_3 k_3)} \\ \frac{\left(\varepsilon_1 k_1\left(\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}-\varepsilon_1 k_1-f_s\right)\right)}{(2\varepsilon_3 k_3(\varepsilon_2 k_2+f_s))} \end{pmatrix} \tag{2.5}$$

$$u = (\frac{(-4|\varepsilon_1|^2 c_0\varepsilon_2\varepsilon_3 f_s h_3 k_2 k_3-4abs(\varepsilon_1)^2 c_0\varepsilon_3 f_s^2 h_3 k_3-|\varepsilon_1|^2\varepsilon_1^2\varepsilon_2 h_3 k_1^2 k_2-|\varepsilon_1|^2\varepsilon_1^2 f_s h_3 k_1^2-2abs(\varepsilon_1)^2\varepsilon_1\varepsilon_2 f_s h_3 k_1 k_2-2|\varepsilon_1|^2\varepsilon_1 f_s^2 h_3 k}{} \tag{2.6}$$

$$y = \begin{pmatrix} \frac{\left(\varepsilon_1 k_1\left(\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}-\varepsilon_1 k_1-f_s\right)\right)}{(2\varepsilon_3 k_3(\varepsilon_2 k_2+f_s))} \end{pmatrix} \tag{2.7}$$

$$\dot{x} = \begin{pmatrix} \frac{\left(-4|\varepsilon_1|^2 c_0\varepsilon_3 f_s k_3-|\varepsilon_1|^2\varepsilon_1^2 k_1^2-2|\varepsilon_1|^2\varepsilon_1 f_s k_1-|\varepsilon_1|^2 f_s^2+4c_0\varepsilon_1^2\varepsilon_3 f_s k_3+\varepsilon_1^4 k_1^2+2\varepsilon_1^3 f_s k_1+\varepsilon_1^2 f_s^2\right)}{\left(4\varepsilon_1^2\varepsilon_3 k_3\right)} \\ 0 \end{pmatrix} \tag{2.8}$$

2.7 ReactorTF_sm.tex

MTT command:

```
mtt ReactorTF sm tex
```

$$A = (\frac{(4|\varepsilon_1|^2 c_0\varepsilon_3 f_s h_3 k_3+|\varepsilon_1|^2\varepsilon_1^2 h_3 k_1^2+2|\varepsilon_1|^2\varepsilon_1 f_s h_3 k_1+|\varepsilon_1|^2 f_s^2 h_3-2\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}c_0\varepsilon_1^2\varepsilon_3 h_3 k_3-2\sqrt{(4c_0\varepsilon_3}}{(k_1(4|\varepsilon_1|^2 c_0\varepsilon_3 f_s h_3 k_3+|\varepsilon_1|^2\varepsilon_1^2 h_3 k_1^2+2|\varepsilon_1|^2\varepsilon_1 f_s h_3 k_1+abs(\varepsilon_1)} \tag{2.9}$$

$$B = \begin{pmatrix} \frac{\left(\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}-2c_0\varepsilon_3 k_3-\varepsilon_1 k_1-f_s\right)}{\left(2c_p\varepsilon_3 k_3(t_0-t_s)\right)} \\ \frac{\left(\varepsilon_1 k_1\left(\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}-\varepsilon_1 k_1-f_s\right)\right)}{\left(2c_p\varepsilon_3 k_3(\varepsilon_2 k_2 t_0-\varepsilon_2 k_2 t_s+f_s t_0-f_s t_s)\right)} \end{pmatrix} \tag{2.10}$$

$$C = \begin{pmatrix} 0 & 1 \end{pmatrix} \tag{2.11}$$

$$D = \begin{pmatrix} 0 \end{pmatrix} \tag{2.12}$$

2.8 ReactorTF_simpar.tex

MTT command:

```
mtt ReactorTF simpar tex
```

```
# -*-octave-*- Put Emacs into octave-mode
# Simulation parameters for system ReactorTF (ReactorTF_simpar.txt)
# Generated by MTT on Fri Mar 3 12:11:48 GMT 2000.
###############################################################
## Version control history
###############################################################
## $Id: ReactorTF_simpar.txt,v 1.1 2000/12/28 17:12:57 peterg Exp $
## $Log: ReactorTF_simpar.txt,v $
## Revision 1.1  2000/12/28 17:12:57  peterg
## To RCS
##
###############################################################


LAST        = 0.05;       # Last time in simulation
DT          = 0.0002;        # Print interval
STEPFACTOR  = 1;          # Integration steps per print interval
WMIN        = -1;         # Minimum frequency = 10^WMIN
WMAX        = 2;          # Maximum frequency = 10^WMAX
WSTEPS      = 100;        # Number of frequency steps
INPUT       = 1;          # Index of the input
```

2.9 ReactorTF_numpar.tex

MTT command:

```
mtt ReactorTF numpar tex
```

```
# -*-octave-*- Put Emacs into octave-mode
# Numerical parameter file (ReactorTF_numpar.txt)
# Generated by MTT at Fri Mar  3 09:22:56 GMT 2000

# %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
# %% Version control history
# %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
# %% $Id: ReactorTF_numpar.txt,v 1.1 2000/12/28 17:12:57 peterg Ex
# %% $Log: ReactorTF_numpar.txt,v $
# %% Revision 1.1  2000/12/28 17:12:57  peterg
# %% To RCS
# %%
# %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

## Dummies
a = 0; # Dummy
b = 0; # Dummy
c = 0; # Dummy
c_0 = 0; # Dummy
c_a = 0; # Dummy
c_b = 0; # Dummy
c_p = 0; # Dummy
e_1 = 0; # Dummy
e_2 = 0; # Dummy
e_3 = 0; # Dummy
f_s = 0; # Dummy
h = 0; # Dummy
h_1 = 0; # Dummy
h_2 = 0; # Dummy
h_3 = 0; # Dummy
k = 0; # Dummy
k_1 = 0; # Dummy
k_2 = 0; # Dummy
k_3 = 0; # Dummy
n = 0; # Dummy
q = 0; # Dummy
```

```
q_1 = 0; # Dummy
q_2 = 0; # Dummy
q_3 = 0; # Dummy
q_s = 0; # Dummy
rho = 0; # Dummy
t_0 = 0; # Dummy
t_s = 0; # Dummy
v_r = 0; # Dummy
x1 = 0; # Dummy
x2 = 0; # Dummy
x3 = 0; # Dummy

## The bulk liquid
rho = 900; # Density
c_p = 5.0; # Specific heat

## Substance A
k_1 = 2.5e10; # Reaction rate constant
q_1 = 1e4; # Exotherm constant
h_1 = 1e4; # Heat of reaction

## Substance B
k_2 = 2.65e12; # Reaction rate constant
q_2 = 1.2e4; # Exotherm constant
h_2 = 1.2e4; # Heat of reaction

## Substance C
k_3 = 6e7; # Reaction rate constant
q_3 = 8e3; # Exotherm constant
h_3 = 3e4; # Heat of reaction

## Inflow parameters
c_0 = 10; # Inflow conc
t_0 = 500; # Inflow temp

## Steady-state values
t_s = 530; # Steady-state temp
f_s = 100; # Steady-state flow
```

2.10 ReactorTF_input.tex

MTT command:

```
mtt ReactorTF input tex
```

```
# -*-octave-*- Put Emacs into octave-mode
# Input specification (ReactorTF_input.txt)
# Generated by MTT at Fri Mar  3 11:52:23 GMT 2000
###############################################################
## Version control history
###############################################################
## $Id: ReactorTF_input.txt,v 1.2 2003/06/06 06:38:44 gawthrop Exp
## $Log: ReactorTF_input.txt,v $
## Revision 1.2  2003/06/06 06:38:44  gawthrop
## Made compatible with current MTT.
##
## Revision 1.1  2000/12/28 17:12:57  peterg
## To RCS
##
###############################################################

## Reduce steady-state parameter file (ReactorTF_sspar.r)
## as siso_sspar ecxept that inputs/states have different meaning
## Steady state for constant c_a, c_b and t=t_s and f=f_s

## Unit volume ReactorTF:
v_r = 1;


## The exponentials.
e_1 = exp(-q_1/t_s);
e_2 = exp(-q_2/t_s);
e_3 = exp(-q_3/t_s);
```

```
## Solve for the steady-state concentrations
## Solve for ca - a quadratic.
a  = k_3*e_3; #caˆ2
b  = k_1*e_1 + f_s; #caˆ1
c  = -c_0*f_s;

c_a = (-b + sqrt(bˆ2 - 4*a*c))/(2*a);

## solve for c_b
c_b  = c_a*k_1*e_1/(f_s+k_2*e_2);


#States (masses)
x1 = c_a*v_r;
x2 = c_b*v_r;

#Thermal state
#x3 = c_p*t_s*v_r;


#Steady-state input q needed to achieve steady-state t_s
q_s = -( (t_0-t_s)*c_p*f_s + e_1*h_1*k_1*x1 + e_2*h_2*k_2*x2 + e_3*h_3*k

# Set the inputs
## Removed by MTT on Thu Jun  5 14:13:24 BST 2003: mttu(1) = q_s + 0.1*q
reactortf__t =  q_s + 0.1*q_s*(t>0.01); # q (ReactorTF)
```

2.11 ReactorTF_state.tex

MTT command:

```
mtt ReactorTF state tex
```

```
# -*-octave-*- Put Emacs into octave-mode
# State specification (ReactorTF_state.txt)
# Generated by MTT at Fri Mar  3 11:52:23 GMT 2000
###############################################################
## Version control history
###############################################################
## $Id: ReactorTF_state.txt,v 1.2 2003/06/06 06:39:05 gawthrop Exp $
## $Log: ReactorTF_state.txt,v $
## Revision 1.2  2003/06/06 06:39:05  gawthrop
## Made compatible with current MTT.
##
## Revision 1.1  2000/12/28 17:12:57  peterg
## To RCS
##
###############################################################

## Reduce steady-state parameter file (ReactorTF_sspar.r)
## as siso_sspar ecxept that states/states have different meaning
## Steady state for constant c_a, c_b and t=t_s and f=f_s

## Unit volume ReactorTF:
v_r = 1;


## The exponentials.
e_1 = exp(-q_1/t_s);
e_2 = exp(-q_2/t_s);
e_3 = exp(-q_3/t_s);

## Solve for the steady-state concentrations
## Solve for ca - a quadratic.
a  = k_3*e_3; #caˆ2
b  = k_1*e_1 + f_s; #caˆ1
c  = -c_0*f_s;

c_a = (-b + sqrt(bˆ2 - 4*a*c))/(2*a);

## solve for c_b
c_b  = c_a*k_1*e_1/(f_s+k_2*e_2);


#States (masses)
x1 = c_a*v_r;
x2 = c_b*v_r;

#Thermal state
#x3 = c_p*t_s*v_r;

## Load up the states
## Removed by MTT on Thu Jun  5 14:14:18 BST 2003: mttx(1) = x1;
## Removed by MTT on Thu Jun  5 14:14:18 BST 2003: mttx(2) = x2;
## Removed by MTT on Thu Jun  5 14:14:18 BST 2003: mttx(3) = x3;




reactortf__m_a = x1;
reactortf__m_b = x2;
```

2.12 ReactorTF_odeso.ps

MTT command:

```
mtt ReactorTF odeso ps
```

This representation is given as Figure 2.7 (on page 55).

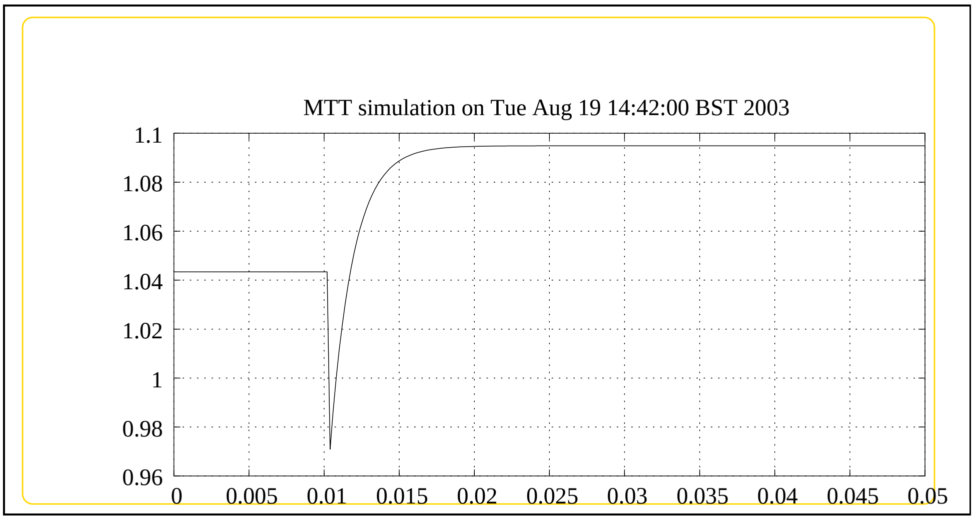


Figure 2.7: System **ReactorTF**, representation odeso (-noargs)

Chapter 3

ReactorTQ

3.1 ReactorTQ_abg.tex

MTT command:

```
mtt ReactorTQ abg tex
```

Figure 3.2 (on page 59) is the schematic diagram of a chemical reactor.

The acausal bond graph of system **ReactorTQ** is displayed in Figure 3.1 (on page 58) and its label file is listed in Section 3.1.1 (on page 57). The subsystems are listed in Section 3.1.2 (on page 63).

This example of a (nonlinear) chemical reactor is due to Trickett and Bogle[1] is used in this section. The reactor has two reaction mechanisms: A → B → C and 2A → D. The reactor mass inflow and outflow f_r are identical. q represents the heat inflow to the reactor.

The control loop t/q has been inverted. The resulting SISO system has two interpretations:

1. the *dynamics* of the c_b/f loop when the t/q loop is under perfect control and
2. the *inverse* dynamics of the t/q loop.

Figure 3.3 (on page 60) shows the poles of the linearised system as the steady-state flow varies: these are the *zeros* of the c_b/f control-loop when the t/q loop is *open*.

3.1.1 Summary information

System ReactorTQ::Simple reactor model - with TQ loop inverted Pseudo bond graph reactor model (based on ancient version)

[1] K. J. Tricket, *Quantification of Inverse Responses for Controllability Assessment of Nonlinear Processes*, PhD Thesis, University College London, 1994

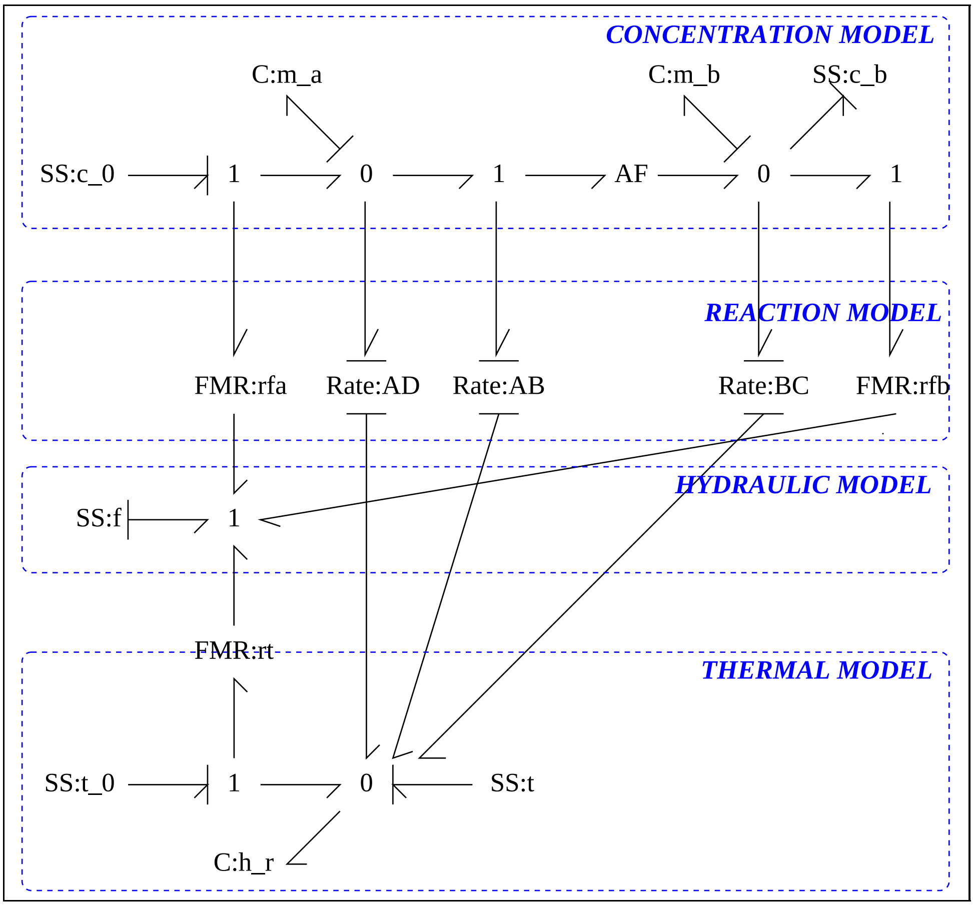


Figure 3.1: System **ReactorTQ**: acausal bond graph

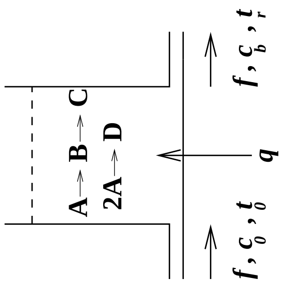


Figure 3.2: System **ReactorTQ**, Schematic

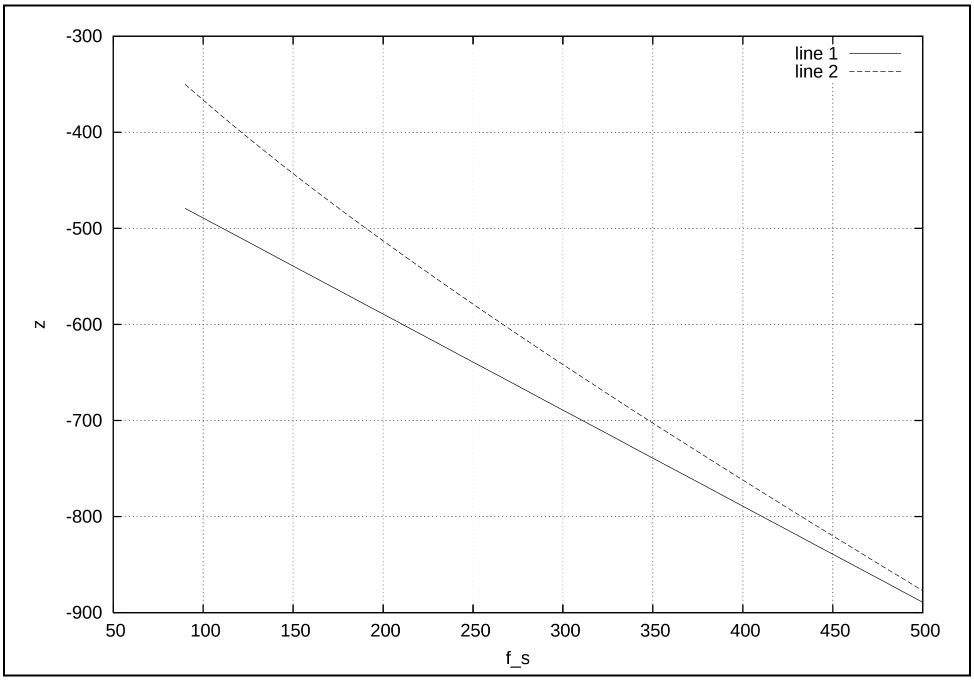


Figure 3.3: System**ReactorTQ**: zeros v flow

Interface information:

Component Rate is in library **Chemical/Rate**

Variable declarations:

a

b

c

c_0

c_A

c_B

e_1

e_2

e_3

f_s

h

k

n

q

q_S

rho

t_0

t_s

v_r

x1

x2

x3

Units declarations:

This component has no UNITs declarations

The label file: ReactorTQ_lbl.txt

```
%% Label file for system ReactorTQ (ReactorTQ_lbl.txt)
%SUMMARY ReactorTQ: Simple reactor model - with TQ loop inverted
%DESCRIPTION Pseudo bond graph reactor model (based on ancient version)

% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% %% Version control history
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% %% $Id: ReactorTQ_lbl.txt,v 1.2 2003/06/06 06:39:27 gawthrop Exp $
% %% $Log: ReactorTQ_lbl.txt,v $
% %% Revision 1.2  2003/06/06 06:39:27  gawthrop
% %% Made compatible with current MTT.
% %%
% %% Revision 1.1  2000/12/28 17:19:08  peterg
% %% To RCS
% %%
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


%ALIAS Rate Chemical/Rate

% Extra variables
%VAR t_s
%VAR f_s
%VAR t_0
%VAR c_0
%VAR rho
%VAR v_r
%VAR e_1
%VAR e_2
%VAR e_3
%VAR a
%VAR b
%VAR c
%VAR c_A
%VAR c_B
%VAR x1
%VAR x2
%VAR x3
%VAR q_S

%VAR h
%VAR k
%VAR n
%VAR q


% Port aliases

% Argument aliases

%% each line should be of one of the following forms:
%       a comment (ie starting with %)
%       component-name cr_name arg1,arg2,..argn
%       blank
% ---- Component labels ----
% Component type C
m_a lin effort,1
m_b lin effort,1
h_r lin effort,c_p

% Component type FMR
rfa lin effort,1
rfb lin effort,1
rt lin effort,c_p

% Component type Rate
        AB Rate k_1,q_1,h_1,1
BC Rate k_2,q_2,h_2,1
AD Rate k_3,q_3,h_3,2

% Component type SS
c_0 SS c_0,internal
c_b SS external,0
f SS internal,external
t SS t_s,internal
t_0 SS t_0,internal
```

3.1.2 Subsystems

- Rate (3) No subsystems.

3.1.3 Rate

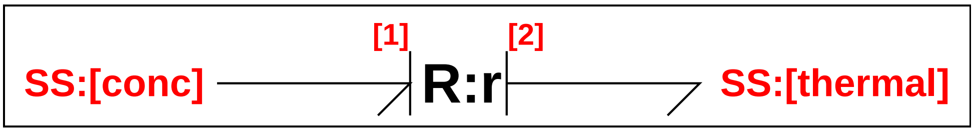


Figure 3.4: System **Rate**: acausal bond graph

The acausal bond graph of system **Rate** is displayed in Figure 3.4 (on page 63) and its label file is listed in Section 3.1.3 (on page 64). The subsystems are listed in Section 3.1.3 (on page 65).

This component represents rate of reaction equations corresponding to the chemical reaction:

$$\text{nA} \rightarrow \text{B} \tag{3.1}$$

The relevant equations are

$$\begin{aligned} \frac{dc_a}{dt} &= k_a c_a^n e^{-\frac{q_a}{T}} \\ Q &= h_a k_a c_a^n e^{-\frac{q_a}{T}} \end{aligned} \tag{3.2}$$

where $\frac{dc_a}{dt}$ is the rate of change of concentration of species A and Q is the corresponding heat generated.

Summary information

System Rate:

Interface information:

Parameter $1 represents actual parameter **k,q,h,n**

Port in represents actual port **conc**

Port out represents actual port **thermal**

Variable declarations:

This component has no PAR declarations

Units declarations:

This component has no UNITs declarations

The label file: Rate_lbl.txt

```
%% Label file for system Rate (Rate_lbl.txt)
%SUMMARY Rate
%DESCRIPTION

% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% %% Version control history
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% %% $Id: Rate_lbl.txt,v 1.1 2000/05/19 19:54:15 peterg Exp $
% %% $Log: Rate_lbl.txt,v $
% %% Revision 1.1  2000/05/19 19:54:15  peterg
% %% Initial revision
% %%
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


% Port aliases
%ALIAS in conc
%ALIAS out thermal

% Argument aliases
%ALIAS $1 k,q,h,n

%% Each line should be of one of the following forms:
%      a comment (ie starting with %)
%      component-name cr_name arg1,arg2,..argn
%      blank

% ---- Component labels ----
r  Rate k,q,h,n

% Component type SS
[conc] SS external,external
[thermal] SS external,external
```

Subsystems

No subsystems.

3.2 ReactorTQ_cbg.ps

MTT command:

```
mtt ReactorTQ cbg ps
```

This representation is given as Figure 3.5 (on page 66).

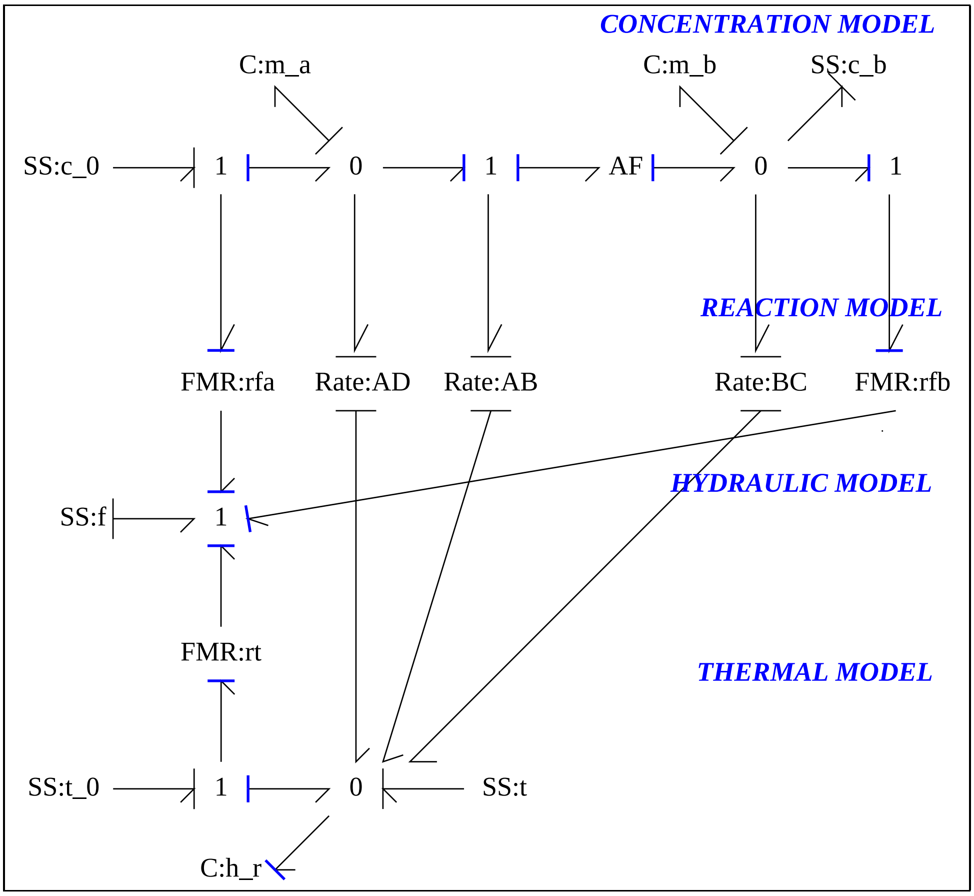


Figure 3.5: System **ReactorTQ**, representation cbg (-noargs)

3.3 ReactorTQ_struc.tex

MTT command:

```
mtt ReactorTQ struc tex
```

List of inputs for system ReactorTQ			
	Component	System	Repetition
1	f	ReactorTQ__f	1

List of nonstates for system ReactorTQ			
	Component	System	Repetition
1	h_r	ReactorTQ__h_r	1

List of outputs for system ReactorTQ			
	Component	System	Repetition
1	c_b	ReactorTQ__c_b	1

List of states for system ReactorTQ			
	Component	System	Repetition
1	m_a	ReactorTQ__m_a	1
2	m_b	ReactorTQ__m_b	1

3.4 ReactorTQ_ode.tex

MTT command:

```
mtt ReactorTQ ode tex
```

$$\begin{aligned} \dot{x}_1 &= -x_1^2\epsilon_3 k_3 - x_1(\epsilon_1 k_1 + u_1) + c_0 u_1 \\ \dot{x}_2 &= x_1\epsilon_1 k_1 - x_2(\epsilon_2 k_2 + u_1) \end{aligned} \tag{3.3}$$

$$y_1 = x_2 \tag{3.4}$$

3.5 ReactorTQ_sm.tex

MTT command:

```
mtt ReactorTQ sm tex
```

$$A = \begin{pmatrix} -\sqrt{\left(4c_0\varepsilon_3 f_s k_3 + \varepsilon_1^2 k_1^2 + 2\varepsilon_1 f_s k_1 + f_s^2\right)} & 0 \\ \varepsilon_1 k_1 & -(\varepsilon_2 k_2 + f_s) \end{pmatrix} \tag{3.5}$$

$$B = \begin{pmatrix} \frac{\left(-\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}+2c_0\varepsilon_3 k_3+\varepsilon_1 k_1+f_s\right)}{(2\varepsilon_3 k_3)} \\ \frac{\left(\varepsilon_1 k_1\left(-\sqrt{\left(4c_0\varepsilon_3 f_s k_3+\varepsilon_1^2 k_1^2+2\varepsilon_1 f_s k_1+f_s^2\right)}+\varepsilon_1 k_1+f_s\right)\right)}{(2\varepsilon_3 k_3(\varepsilon_2 k_2+f_s))} \end{pmatrix} \tag{3.6}$$

$$C = \begin{pmatrix} 0 & 1 \end{pmatrix} \tag{3.7}$$

$$D = \begin{pmatrix} 0 \end{pmatrix} \tag{3.8}$$

3.6 ReactorTQ_simpar.tex

MTT command:

```
mtt ReactorTQ simpar tex
```

```
# -*-octave-*- Put Emacs into octave-mode
# Simulation parameters for system ReactorTQ (ReactorTQ_simpar.txt
# Generated by MTT on Fri Mar 3 12:11:48 GMT 2000.
###############################################################
## Version control history
###############################################################
## $Id: ReactorTQ_simpar.txt,v 1.1 2000/12/28 17:19:08 peterg Exp
## $Log: ReactorTQ_simpar.txt,v $
## Revision 1.1  2000/12/28 17:19:08  peterg
## To RCS
##
###############################################################


LAST        = 0.05;       # Last time in simulation
DT          = 0.0002;        # Print interval
STEPFACTOR  = 1;          # Integration steps per print interval
WMIN        = -1;         # Minimum frequency = 10^WMIN
WMAX        = 2;          # Maximum frequency = 10^WMAX
WSTEPS      = 100;        # Number of frequency steps
INPUT       = 1;          # Index of the input
```

3.7 ReactorTQ_numpar.tex

MTT command:

```
mtt ReactorTQ numpar tex
```

```
# -*-octave-*- Put Emacs into octave-mode
# Numerical parameter file (ReactorTQ_numpar.txt)
# Generated by MTT at Fri Mar  3 09:22:56 GMT 2000

# %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
# %% Version control history
# %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
# %% $Id: ReactorTQ_numpar.txt,v 1.1 2000/12/28 17:19:08 peterg Exp $
# %% $Log: ReactorTQ_numpar.txt,v $
# %% Revision 1.1  2000/12/28 17:19:08  peterg
# %% To RCS
# %%
# %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

## Dummies
a = 0; # Dummy
b = 0; # Dummy
c = 0; # Dummy
c_0 = 0; # Dummy
c_a = 0; # Dummy
c_b = 0; # Dummy
c_p = 0; # Dummy
e_1 = 0; # Dummy
e_2 = 0; # Dummy
e_3 = 0; # Dummy
f_s = 0; # Dummy
h = 0; # Dummy
h_1 = 0; # Dummy
h_2 = 0; # Dummy
h_3 = 0; # Dummy
k = 0; # Dummy
k_1 = 0; # Dummy
k_2 = 0; # Dummy
k_3 = 0; # Dummy
n = 0; # Dummy
q = 0; # Dummy
```

```
q_1 = 0; # Dummy
q_2 = 0; # Dummy
q_3 = 0; # Dummy
q_s = 0; # Dummy
rho = 0; # Dummy
t_0 = 0; # Dummy
t_s = 0; # Dummy
v_r = 0; # Dummy
x1 = 0; # Dummy
x2 = 0; # Dummy
x3 = 0; # Dummy

## The bulk liquid
rho = 900; # Density
c_p = 5.0; # Specific heat

## Substance A
k_1 = 2.5e10; # Reaction rate constant
q_1 = 1e4; # Exotherm constant
h_1 = 1e4; # Heat of reaction

## Substance B
k_2 = 2.65e12; # Reaction rate constant
q_2 = 1.2e4; # Exotherm constant
h_2 = 1.2e4; # Heat of reaction

## Substance C
k_3 = 6e7; # Reaction rate constant
q_3 = 8e3; # Exotherm constant
h_3 = 3e4; # Heat of reaction

## Inflow parameters
c_0 = 10; # Inflow conc
t_0 = 530; # Inflow temp

## Steady-state values
t_s = 530; # Steady-state temp
f_s = 100; # Steady-state flow
```

3.8 ReactorTQ_input.tex

MTT command:

```
mtt ReactorTQ input tex
```

```
# -*-octave-*- Put Emacs into octave-mode
# Input specification (ReactorTQ_input.txt)
# Generated by MTT at Fri Mar  3 11:52:23 GMT 2000
###############################################################
## Version control history
###############################################################
## $Id: ReactorTQ_input.txt,v 1.2 2003/06/06 06:39:20 gawthrop Exp $
## $Log: ReactorTQ_input.txt,v $
## Revision 1.2  2003/06/06 06:39:20  gawthrop
## Made compatible with current MTT.
##
## Revision 1.1  2000/12/28 17:19:08  peterg
## To RCS
##
###############################################################

## Reduce steady-state parameter file (ReactorTQ_sspar.r)
## as siso_sspar ecxept that inputs/states have different meaning
## Steady state for constant c_a, c_b and t=t_s and f=f_s

## Unit volume ReactorTQ:
v_r = 1;


## The exponentials.
e_1 = exp(-q_1/t_s);
e_2 = exp(-q_2/t_s);
e_3 = exp(-q_3/t_s);
```

```
## Solve for the steady-state concentrations
## Solve for ca - a quadratic.
a  = k_3*e_3; #caˆ2
b  = k_1*e_1 + f_s; #caˆ1
c  = -c_0*f_s;

c_a = (-b + sqrt(bˆ2 - 4*a*c))/(2*a);

## solve for c_b
c_b  = c_a*k_1*e_1/(f_s+k_2*e_2);


#States (masses)
x1 = c_a*v_r;
x2 = c_b*v_r;

#Thermal state
x3 = c_p*t_s*v_r;

# Set the inputs
## Removed by MTT on Thu Jun  5 14:27:42 BST 2003: mttu(1) = f_s +
reactortq__f =  f_s + 0.1*f_s*(t>0.01); # f (ReactorTQ)
```

3.9 ReactorTQ_state.tex

MTT command:

```
mtt ReactorTQ state tex
```

```
# -*-octave-*- Put Emacs into octave-mode
# State specification (ReactorTQ_state.txt)
# Generated by MTT at Fri Mar  3 11:52:23 GMT 2000
###############################################################
## Version control history
###############################################################
## $Id: ReactorTQ_state.txt,v 1.2 2003/06/06 06:39:39 gawthrop Exp
## $Log: ReactorTQ_state.txt,v $
## Revision 1.2  2003/06/06 06:39:39  gawthrop
## Made compatible with current MTT.
##
## Revision 1.1  2000/12/28 17:19:08  peterg
## To RCS
##
###############################################################

## Reduce steady-state parameter file (ReactorTQ_sspar.r)
## as siso_sspar ecxept that states/states have different meaning
## Steady state for constant c_a, c_b and t=t_s and f=f_s

## Unit volume ReactorTQ:
v_r = 1;


## The exponentials.
e_1 = exp(-q_1/t_s);
e_2 = exp(-q_2/t_s);
e_3 = exp(-q_3/t_s);

## Solve for the steady-state concentrations
## Solve for ca - a quadratic.
a  = k_3*e_3; #caˆ2
b  = k_1*e_1 + f_s; #caˆ1
c  = -c_0*f_s;

c_a = (-b + sqrt(bˆ2 - 4*a*c))/(2*a);

## solve for c_b
c_b  = c_a*k_1*e_1/(f_s+k_2*e_2);


#States (masses)
x1 = c_a*v_r;
x2 = c_b*v_r;


## The two inputs at steady-state
##mttu(1) = f_s;

## Load up the states
## Removed by MTT on Thu Jun  5 14:25:48 BST 2003: mttx(1) = x1;
## Removed by MTT on Thu Jun  5 14:25:48 BST 2003: mttx(2) = x2;
reactortq__m_a = x1;
```

```
reactortq__m_b = x2;
```

3.10 ReactorTQ_odeso.ps

MTT command:

```
mtt ReactorTQ odeso ps
```

This representation is given as Figure 3.6 (on page 74).

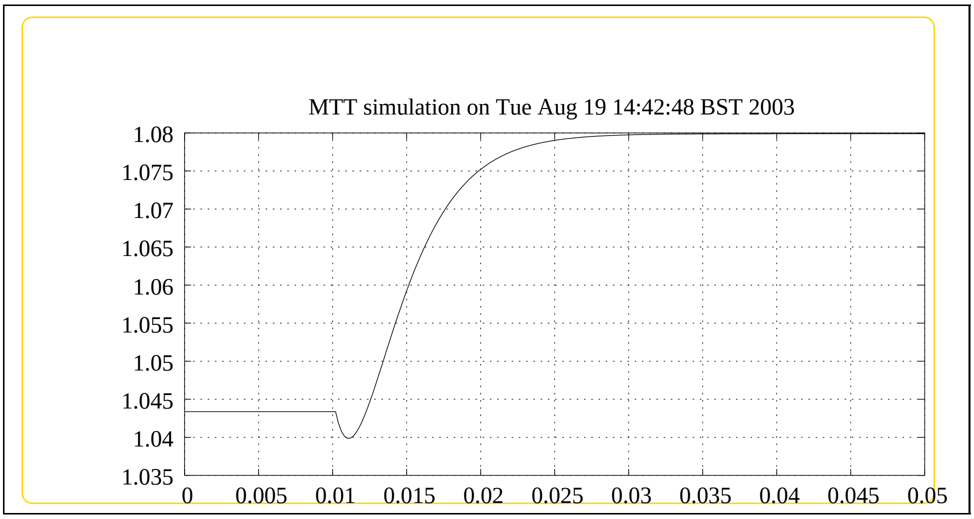


Figure 3.6: System **ReactorTQ**, representation odeso (-noargs)

Index