Original CSTR

I. Continuous Stirred Tank Reactor (CSTR)

The object of study is a sophisticated simulator of a jacketed chemical reactor where an exothermic reaction takes place, shown in fig. 1. It was used as a benchmark for an expert system like diagnosis environment in two doctoral theses in Chemical Engineering at the Massachusetts Institute of Technology [1], [2], from now called the MIT-CSTR. The motivation to use this process is its high non-linearity, that it has interacting control loops, that it has multiple causal pathways with opposing tendencies between variables, thus making the process an appropriate candidate for causal analysis. Another aspect of the CSTR process is the complete availability of its analytic description. The highly popular Tennessee-Eastman (TE) chemical process [3], [4], is frequently used as the experimental benchmark for complex data-driven process condition detection techniques [5], [6], [7], [8], [9]. However, it deliberately lacks the underlying description of the mass and heat balances, the control algorithms and the simulation framework. The TE source code is available, however in an obfuscated way. On the other hand, the complete transparency of the MIT-CSTR allows the researcher a deeper understanding of the process dynamics, leading to more consolidated affirmations about his fault diagnosis methods.

A. Process Model

A reactant A with concentration c_{A0} at temperature T_1 is flowing at rate F_1 into a Continuous Stirred Tank Reactor (CSTR) where two parallel, first-order reactions $A \to B$ and $A \to C$ take place[1]. The first, dominating reaction is exothermic, the second endothermic, the overall heat balance is exothermic, raising the tank temperature to T_2. The products B, C and the remaining reactant A are leaving the tank, and pumped out with flow rate F_2 and concentrations c_A and c_B which are measured (the concentration of the byproduct c_C is ignored). A leak fault at flow rate F_3 might occur. In this case, the leak flow F_3 is subtracted from the flow F_2 after the pump to form the final effluent flow F_4. The level L of the tank is kept at the set point SP_1 which is controlled by a PI controller LC (Level controller) that sends its control signal CNT_1 to the control valve V_1.

Since the reaction is exothermic, a cooling mechanism is necessary. A coolant fluid with flow rate F_5 at temperature T_3 is entering the reactor jacket and leaving with flow rate F_8. The temperature within the jacket is T_4, higher than the original coolant temperature due to the heat exchange with the CSTR which operates at temperature T_2. Two leaks related to the coolant circuit are possible, one leak from the jacket to the exterior at flow rate F_7 and one leak from within the jacket to within the CSTR at flow rate F_6. The temperature T_2 within the CSTR is kept constant by a cascade controller. The primary controller (Temperature controller) has as the set point SP_2 the reactor temperature and delivers its output CNT_2 as the input set point SP_3 to the secondary controller (Flow controller). The coolant flow F_5 is measured and the control signal CNT_2 is sent to the control valve V_2.

Generally, the heuristic concept of resistance 'R' is used in the work of [1] for the hydraulic model. The flow F is related to a pressure drop (or gain) ΔP and a 'flow resistance' R as

$$F = \frac{\sqrt{\Delta P}}{R}, \tag{1}$$

in an analogy to Ohm's law in electricity. Serial and parallel flows model the resistances in an analogy to Kirchhoff's laws as

$$R_{\text{serial}} = R_1 + R_2, \qquad R_{\text{parallel}} = \frac{1}{\frac{1}{R_1} + \frac{1}{R_2}}. \tag{2}$$

In fig. 1 the use of resistances can be observed for several hydraulic components and also faults, R_1, R_4, R_5, R_{10} are pipe resistances that diminish the pressure of the liquid, R_3, R_6 are valve resistances, R_9 is a jacket blockage fault and R_2, R_7, R_8 are model leaks, i.e. when a leak resistance diminishes, the leak flow augments. A more detailed description of the CSTR simulator can be found in appendix A.

B. Process Faults

Table I shows 14 measured variables plus four constraints that can be additionally used for the fault diagnosis, assembled into the feature vector $\mathbf{x}$ of dimension $14 + 4 = 18$, reflecting the complete description of the process state. The considered fault classes (besides the normal class) are listed in table II. There are 21 faults that affect the process dynamics. Additionally sensor faults are simulated by modifying the 14 measured variables from table I directly.

The speed of evolution of each fault is essentially controlled by a time parameter $\tau = 10^p, p = -2, \ldots, 2$. This parameter has a decisive influence on the discernability of process states. A low value of τ means a gradual transition between normal and faulty states. A high value is equivalent

[1] The acronyms of the variables were generally chosen in accordance with the Fortran source code of the simulator and the model of fig. 1.

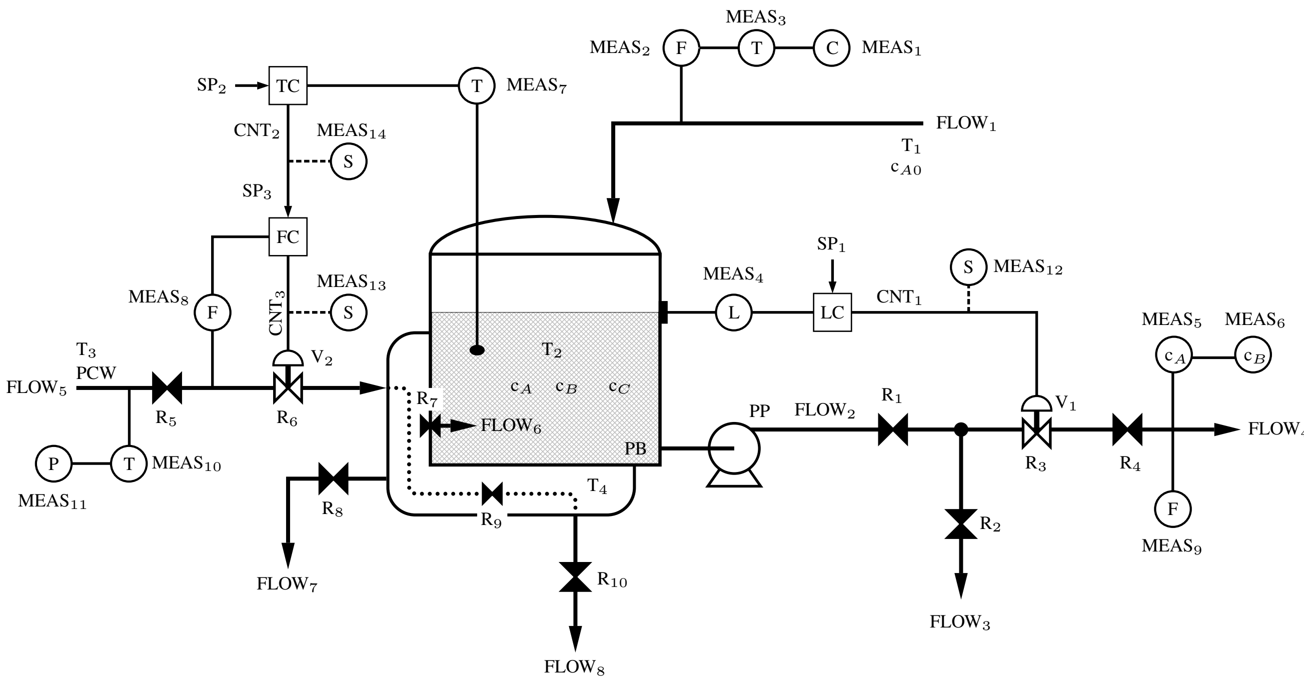

Figure 1. The CSTR simulator defined in [1], [2]. Flow rates 'FLOW' are abbreviated as 'F' in the text. All sensed variables 'MEAS' are circled.

Table I
SENSED VARIABLES AND CONSTRAINTS OF THE CSTR SIMULATOR

#	Variable/Constraint name	Acronym	Nominal value	Units
1	Feed concentration	c_{A0}	20.0	mol/m^3
2	Feed flowrate	F_1	0.25	m^3/s
3	Feed temperature	T_1	30.0	K
4	Reactor level	L	2.0	m
5	Product A concentration	c_A	2.85	mol/m^3
6	Product B concentration	c_B	17.11	mol/m^3
7	Reactor temperature	T_2	80.0	K
8	Coolant flowrate	F_5	0.9	m^3/s
9	Product flowrate	F_4	0.25	m^3/s
10	Coolant inlet temperature	T_3	20.0	K
11	Coolant inlet pressure	PCW	56250.0	Pa
12	Level controller output	CNT$_1$	74.7	-
13	Coolant controller output	CNT$_2$	0.9	-
14	Coolant setpoint	CNT$_3$	59.3	-
15	Inventory	r_1	0.0	-
16	Mol balance	r_2	0.0	-
17	Cooling water pressure drop	r_3	0.0	-
18	Effluent pressure drop	r_4	0.0	-

Table II
PROCESS FAULTS

#	Fault name	Affected parameter
1	No fault	-
2	Blockage at tank outlet	R_1
3	Blockage in jacket	R_9
4	Jacket leak to environment	R_8
5	Jacket leak to tank	R_7
6	Leak from pump	R_2
7	Loss of pump pressure	PP
8	Jacket exchange surface fouling	UA
9	External heat source (sink)	Q_{ext}
10	Primary reaction activation energy	β_1
11	Secondary reaction activation energy	β_2
12	Abnormal feed flowrate	F_1
13	Abnormal feed temperature	T_1
14	Abnormal feed concentration	c_{A0}
15	Abnormal cooling water temperature	T_3
16	Abnormal cooling water pressure	PCW
17	Abnormal jacket effluent pressure	JEP
18	Abnormal reactor effluent pressure	REP
19	Abnormal level controller setpoint	SP$_1$
20	Abnormal temperature controller setpoint	SP$_2$
21	Control valve 1 stuck	V_1
22	Control valve 2 stuck	V_2
23	Sensor fault(s) (sensed variables)	'MEAS'

to an abrupt change of the process variables and should make classification easier.

APPENDIX A. CSTR SIMULATION SYSTEM

This section describes the variables and static and dynamic equations of the CSTR simulator.

A. Controllers

The system uses three PI controllers, one for the reactor level and a cascade controller for the reactor temperature and coolant feed valve. The discrete controller outputs are calculated as

$$\mathrm{CNT}(t_k) = \mathrm{CNT}(t_{k-1}) + K_p\left[e(t_k) - e(t_{k-1})\right] + \frac{K_i}{2}\Delta t\left[e(t_k) + e(t_{k-1})\right],$$

Table A.1
CSTR SIMULATOR SYSTEM VARIABLES, UNITS AND NOMINAL VALUES IN SQUARE BRACKETS

α_B, α_C	Primary and secondary Arrhenius rate constant pre-exponential factor [1/min]
β_B, β_C	Primary and secondary activation energy [kJ/kmol]
$\Delta H_B, \Delta H_C$	Primary and secondary heat of reaction [kJ/kmol] [30000.0] [-10000.0]
$\Delta t = t_{k+1} - t_k$	Sample interval of the simulator [0.02 min]
ρ	Density of coolant [1000 kg/m^3]
A	Floor area of reactor [1.5 m^2]
A_H	Heat exchange area between jacket and reactor [m^2]
c_{A0},c_A,c_B,c_C	Concentrations [mol/m^3]: Feed [20.0], Reactant A [2.85], Product B [17.11], Product C [0.0226]
CNT$_1$,CNT$_2$,CNT$_3$	Controller output signals [74.7], [0.9], [59.3]
C_p	Specific heat capacity of coolant [4.2 kJ/(kg °C)]
F_1, F_2, F_3, F_4	Flows [m^3/min]: reactant feed [0.25], reactor exit [0.25], effluent leak [0.0], effluent [0.25]
F_5, F_6, F_7, F_8	coolant feed [0.9], jacket to reactor leak [0.0], jacket to environment leak [0.0], jacket effluent [0.9]
K_p, K_i	Controller gains of the three controllers [35.0,-0.04,-25.0], [5.0,-0.02,-75.0]
$L = V/A$	Liquid level of reactor [2.0 m]
PP	Pump differential pressure [48000 kg/m^2]
PB=$\rho g L$	Pressure at reactor outlet [2000 kg/m^2]
Q	Heat transfer from reactor to jacket [38020 kJ/min = W]
Q_{ext}	External heat source (sink) [0 W]
r_A, r_B, r_C	Reaction rates [1/min]
R_1, R_2, R_3, R_4	Flow resistances [min kg$^{\frac{1}{2}}$/m^4]: reactor exit pipe [100.0], pump leak [10^6], level control valve [19.85], effluent pipe [500.0]
R_5, R_6, R_7, R_8	coolant feed pipe [72.0], coolant feed valve [45.95], jacket to tank leak [10^6], jacket to exterior leak [10^6],
R_9, R_{10}	blockage in jacket [10^6], coolant effluent pipe [65.0]
SP$_1$, SP$_2$, SP$_3$	Set points of the three controllers: reactor level, reactor temperature, coolant flow rate [2.0,80.0,0.9]
T_1, T_2, T_3, T_4	Temperatures [°C] of reactant feed [30], reactor [80], coolant feed [20], coolant in jacket [40]
UA_H	heat transfer coefficient U, multiplied by A_H [1901 kJ/(min °C)]
V	Reactor volume [3.0 m^3]

where $e(t_k) = \text{SP}(t_k) - \text{MEAS}(t_k)$ is the measures error at time instance t_k. Moreover, the controller outputs are cropped to the interval $[0, 100]$ if they exceed these limits. The valve positions are determined as the complement of the control signal, hence

$$V_1 = 100.0 - \text{CNT}_1, \qquad V_2 = 100.0 - \text{CNT}_3,$$

and are also limited to $[0, 100]$. Finally the resistances of the level control and coolant flow valves are mapped exponentially as

$$R_3 = 5.0 \exp(0.0545 V_1), \qquad R_6 = 5.0 \exp(0.0545 V_2).$$

B. Jacket

Based on the electrical circuit analogy (2), the global resistance of the cooling circuit becomes

$$R_{\text{coolant}} = R_5 + R_6 + \left[\frac{1}{R_7} + \frac{1}{R_8} + \frac{1}{R_9 + R_{10}}\right]^{-1}. \quad \text{(A.1)}$$

The pressure difference caused by the coolant pipe and flow regulating valve, using (1) is

$$\Delta P_{5,6} = [F_5(R_5 + R_6)]^2,$$

and the global relevant pressure balance of the jacket is then

$$\Delta P_c = \text{PCW} - \text{JEP} - \Delta P_{5,6},$$

where PCW is the pressure of the coolant feed and JEP a faulty pressure drop of the jacket. Using (1), the coolant flow and the two leak flows are

$$F_5 = \frac{\sqrt{\text{PCW} - \text{JEP}}}{R_{\text{coolant}}}, \qquad F_6 = \frac{\sqrt{\Delta P_c}}{R_7}, \qquad F_7 = \frac{\sqrt{\Delta P_c}}{R_8},$$

and finally, the flow out of the jacket is the inflow, subtracted by the leak to the environment and the leak into the reactor, hence

$$F_8 = F_5 - F_6 - F_7.$$

The heat transfer Q_{jacket} between the reactor and the jacket is equivalent to the heat transfer caused by the outflow of the warmed coolant, so

$$Q_{\text{jacket}} = UA_H(T_2 - T_4) = \rho C_p F_8 (T_4 - T_3). \quad \text{(A.2)}$$

Since the heat transfer is slow, the updated jacket temperature can be calculated from (A.2) by solving for T_4.

C. Reactor

Analogously to (A.1) the global resistance of the product effluent resistance is

$$R_{\text{effluent}} = R_1 + \left[\frac{1}{R_2} + \frac{1}{R_3 + R_4}\right]^{-1}. \quad \text{(A.3)}$$

The global relevant pressure balance of the reactor is

$$\Delta P = \text{PB+PP-REP},$$

and hence the reactor exist flow, leak flow and effluent flow by virtue of (1) become

$$F_2 = \frac{\sqrt{\Delta P}}{R_{\text{effluent}}}, \quad F_3 = \frac{\sqrt{\Delta P - (F_2 R_1)^2}}{R_2}, \quad F_4 = F_2 - F_3.$$

In a normal operational state, the volume V of the reactor remains invariant, since the feed flow F_1 equals the reactor exit flow F_2. Faults in the form of leaks or blockages can change the volume dynamically, so

$$\frac{dV}{dt} = F_1 + F_6 - F_2. \quad \text{(A.4)}$$

This is a first order ordinary differential equation and solved in the simulator by a simple Euler method to update the reactor volume (and level $L = V/A$) as

$$V(t_{k+1}) = V(t_k) + \Delta t \left[F_1 + F_6 - F_2\right].$$

The remaining model equations of the reactor are necessary to obtain the updated reactor temperature T_2. The reaction rates for the two first-order reactions $A \to B, A \to C$, reactions with $-r_A = r_B + r_C$, using the Arrhenius Rate Equation are

$$r_B = c_A \alpha_B \exp(-\beta_B/(R\tilde{T}_2))$$
$$r_C = c_A \alpha_C \exp(-\beta_C/(R\tilde{T}_2))$$

where $R = 8.31446 \text{ J}/(\text{mol} \cdot K)$ is the gas constant and $\tilde{T}_2 = T_2 + 273.15$ is the reactor temperature in Kelvin. The material balance of the reactant and product moles, supposing dynamic concentrations and/or volume (especially when a fault occurs yield

$$\dot{c_A} = -r_B - r_C + \frac{1}{V}\left[(c_{A0} - c_A)F_1 - c_A F_6\right]$$
$$\dot{c_B} = r_B - \frac{c_B}{V}(F_1 + F_6)$$
$$\dot{c_C} = r_C - \frac{c_C}{V}(F_1 + F_6),$$

which again are solved by the Euler method.

The energy balance of the reactor is

$$\frac{dQ}{dt} = \rho C_p F_1 T_1 - \rho C_p F_2 T_2 + \rho C_p F_6 T_4 + (\Delta H_B r_B + \Delta H_C r_C)V - Q_{\text{jacket}} + Q_{\text{ext}}. \quad (A.5)$$

The first and second term on the right hand side are the energy change to to the inflow and outflow of the liquid, the third term the energy change caused by the leak from the jacket into the tank, the fourth term is the energy created by the exothermic reaction, the tank to jacket heat exchange is defined in (A.2). The energy stored by the liquid in the tank is

$$Q = \rho C_p V T_2, \quad (A.6)$$

and since the temperature *and* volume can change in case of a fault, its derivative is

$$\frac{dQ}{dt} = \rho C_p \frac{d(VT_2)}{dt} = \rho C_p \left[V\frac{dT_2}{dt} + T_2\frac{dV}{dt}\right]. \quad (A.7)$$

Solving for $\frac{dT_2}{dt}$ in (A.7), under consideration of (A.4), (A.5) and (A.6), the updated reactor temperature T_2 can be found by the Euler method.

D. Constraints and Security System

The simulator possesses a security mechanism that in the case of a real operation would shut down the system. In the simulation, a shutdown flag is set and a message is issued, the simulation however continues until its timeout. The security system if triggered if the nominal tank level of 2 m falls outside the interval $[1.2, 2.75]$ or the nominal reactor temperature of 80°C is higher than 130°C.

Moreover, additional features in the form of constraints are available that can aid the fault diagnosis. These four parameters are incorporated into the 14 sensed variables vector of table I to form the final 18-dimensional feature vector $\mathbf{x}$.

Table A.2
SECURITY CONSTRAINTS OF THE CSTR SIMULATOR. SUPERSCRIPT 'N' MEANS NOMINAL VALUE IN NORMAL OPERATION, C.F. TABLE A.1. DIFFERENTIAL EXPRESSIONS $d(.)/dt$ ARE APPROXIMATED BY EULER METHOD.

Constraint name	Definition
Inventory	$r_1 = V - V^N - d(F_1 - F_4)/dt$
Mol balance	$r_2 = (c_A + c_B + c_C^N)V - 60.0 - d[c_{A0}F_1 - (c_A + c_B + c_C^N)F_4]/dt$
Cooling water pressure drop	$r_3 = F_5 - \sqrt{\text{PCW}}/(R_6 + R_5^N + R_9^N + R_{10}^N)$
Effluent pressure drop	$r_4 = F_4 - \sqrt{\text{PB} + \text{PP}}/(R_3 + R_1^N + R_4^N)$

E. Simulation algorithm

The main simulation loop, after having initialized the system can be resumed as the following calculations

1) Output of the controllers (level, reactor temperature coolant flow)
2) Valve positions and valve resistances
3) Using the Kirchhoff analogy, the global resistances of the effluent and cooling circuit
4) Flow rates
5) Heat flux from reactor to jacket
6) Jacket temperature
7) Reactor volume
8) Reaction rate, using Arrhenius equation
9) Concentration of reactant A and products B and C
10) Reactor temperature

One of the reasons why e.g. the Tennessee Eastman simulator is popular and the MIT-CSTR practically unknown is that the first published the software online and the second is a pre-internet work where the original Fortran code is only available as a bitmap on the scanned Ph.D thesis of [1]. The code was transcribed from there and missing parts were recovered (for instance the Fortran random number routines `GGUBS`, `GGNML`, `MDNRIS`, `MERFI` were originally not included). The missing variable plotting routine `SIMPLOT` was substituted by a `gnuplot` interface that allows to visualize the temporal evolution of the sensed variables and constraints of table I. The software [2] consists of a single file that can be easily compiled by a standard Fortran compiler,

[2]Code and additional material at `sites.google.com/site/trauber/mit-cstr`

e.g. `gfortran` in Unix systems. A simple configuration file that emulates the manual input of the system parameters is sufficient to run the simulator in a single command.

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