Optimal Design of Energy Systems (M2794.003400)

Chapter 6. SYSTEM SIMULATION

Min Soo KIM

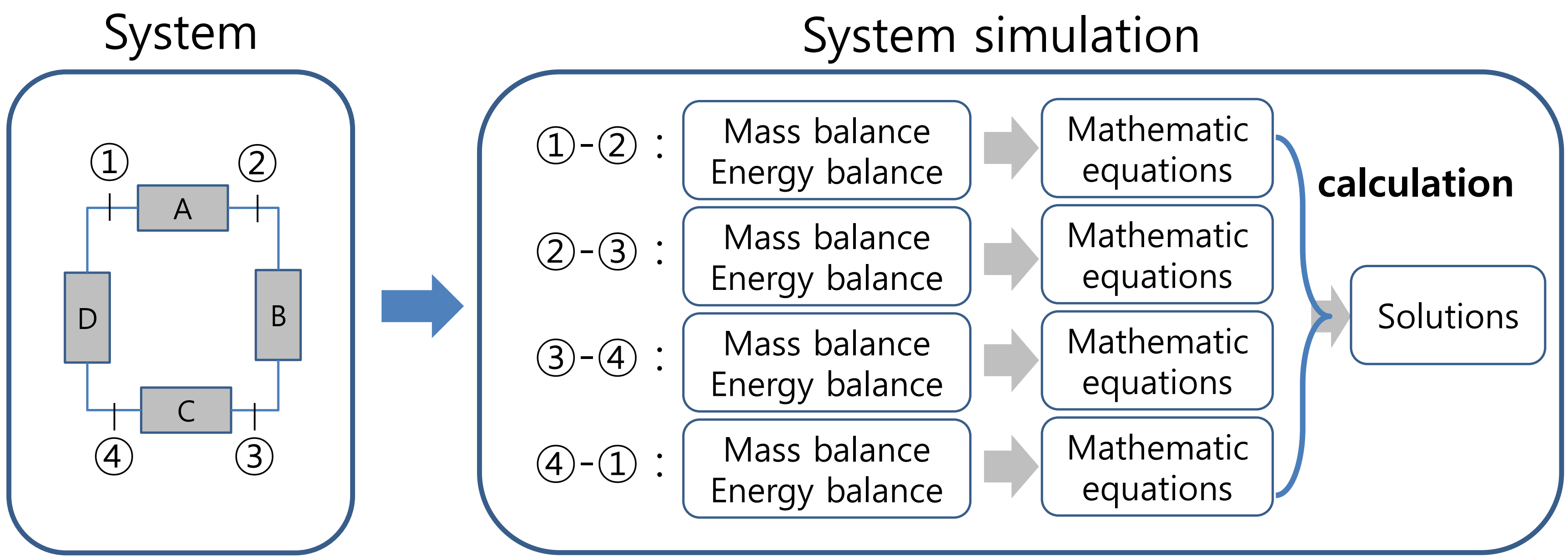
Department of Mechanical and Aerospace Engineering
Seoul National University

ENGINEERING
COLLEGE OF ENGINEERING
SEOUL NATIONAL UNIVERSITY

Chapter 6. SYSTEM SIMULATION

6.1 Description of system simulation

- **Calculation** of operating variables(pressure, temp., flow rate, etc…) in a thermal system operating in a steady state.
- **To presume performance** characteristics and equations for thermodynamic properties of the working substances.



- characteristics of all components
- thermodynamic properties
- a set of simultaneous equations

Chapter 6. SYSTEM SIMULATION

6.2 Some uses of simulation

- Design stage – to achieve **improved design**
- Existing system – to explore prospective **modifications**

- Design condition
- Off design condition (part load / over load) ← normal operation

engineer

choose

Operation variables

- Pressures
- Temperatures
- Flow rates

Components

- Compressors
- Pumps
- Heat exchangers
- Turbines

Overload

Part load

Cost of energy

Chapter 6. SYSTEM SIMULATION

6.3 Classes of simulation

System

- continuous – water(or air) flow
- discrete – human(or car) flow

- deterministic – input variables are precisely specified
- stochastic – input conditions are uncertain
  - Random
  - Probability distribution

- steady state
- dynamic – changes with respect to time

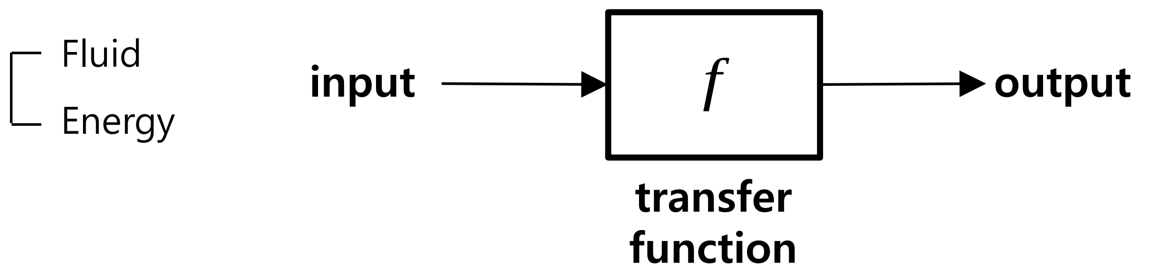
  (transient analysis)

  (dynamic simulation)

Chapter 6. SYSTEM SIMULATION

6.4 Information-flow diagrams

- A block signifies that an output can be calculated when the input is known



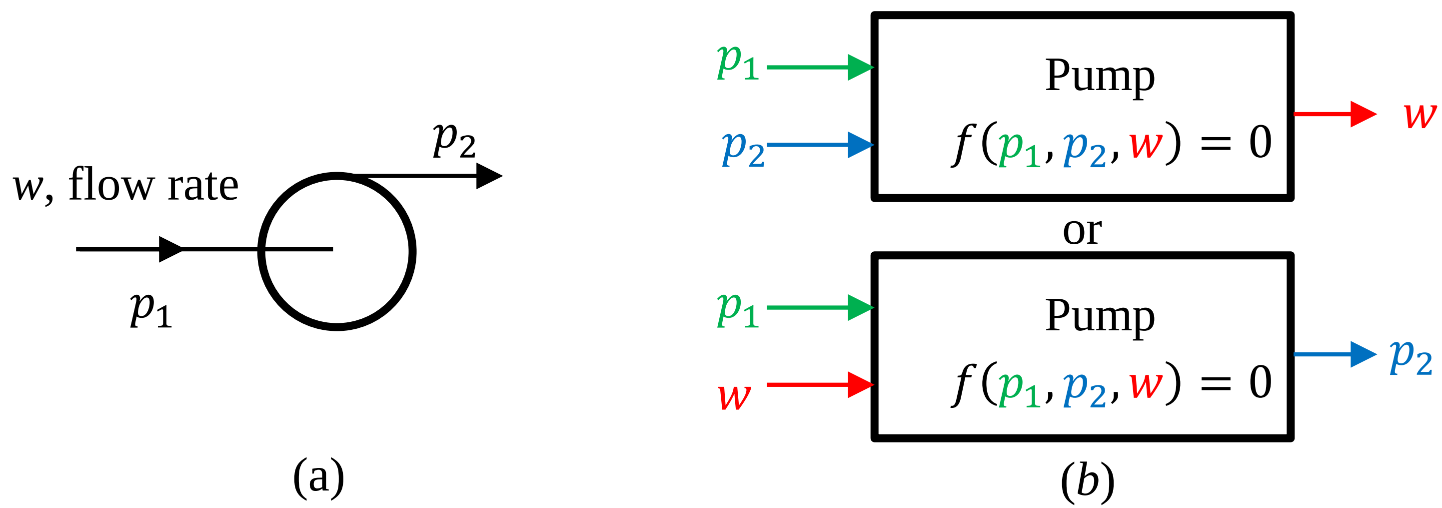
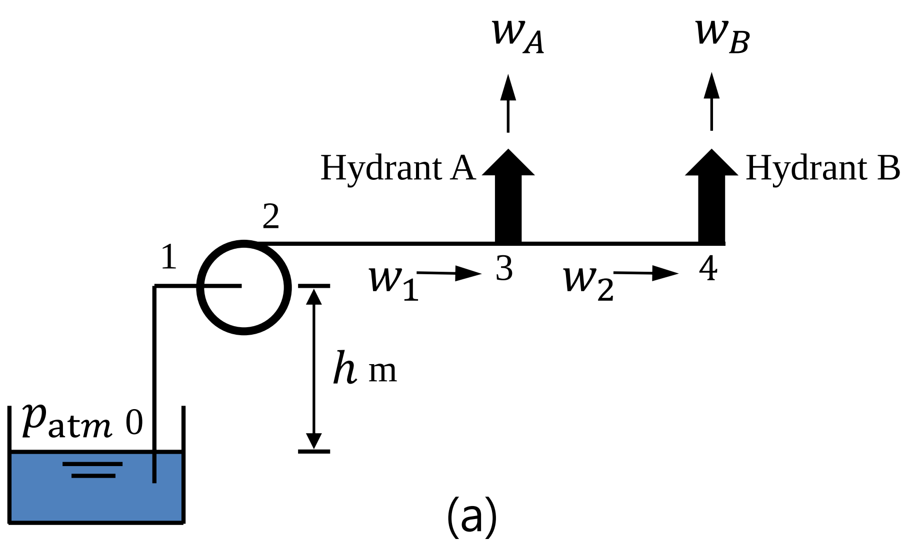


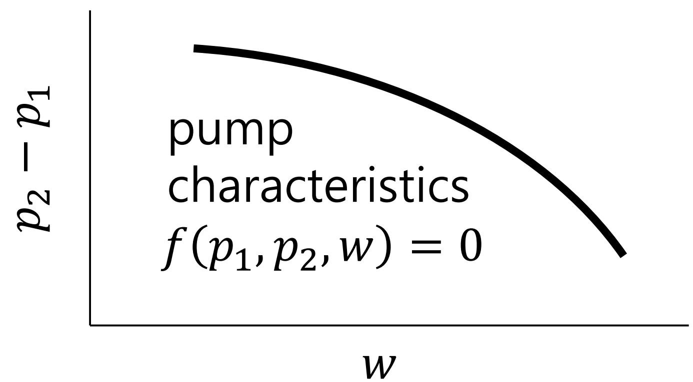
Fig. (a) Centrifugal pump in fluid-flow diagram (b) possible information-flow blocks representing pumps.

Chapter 6. SYSTEM SIMULATION

6.4 Information-flow diagrams



(a)



(b)

Fig. (a) Fire-water system (b) pump characteristics.

$$w_A = C_A\sqrt{p_3 - p_{\text{atm}}}$$

$$w_B = C_B\sqrt{p_4 - p_{\text{atm}}}$$

Section 0-1 : $p_{\text{atm}} - p_1 = C_1 w_1^2 + \rho g h$

Section 1-2 : $p_2 - p_3 = C_2 w_1^2$

Section 2-3 : $p_3 - p_4 = C_3 w_2^2$

$$f_1(w_A, p_3) = 0$$

$$f_2(w_B, p_4) = 0$$

$$f_3(w_1, p_1) = 0$$

$$f_4(w_1, p_2, p_3) = 0$$

$$f_5(w_2, p_3, p_4) = 0$$

6.4 Information-flow diagrams

Pump characteristics : $f_6(w_1, p_1, p_2) = 0$

Mass balance : $f_7(w_1, w_A, w_2) = 0$ or $w_1 = w_A + w_2$

$f_8(w_2, w_B) = 0$ or $w_2 = w_B$

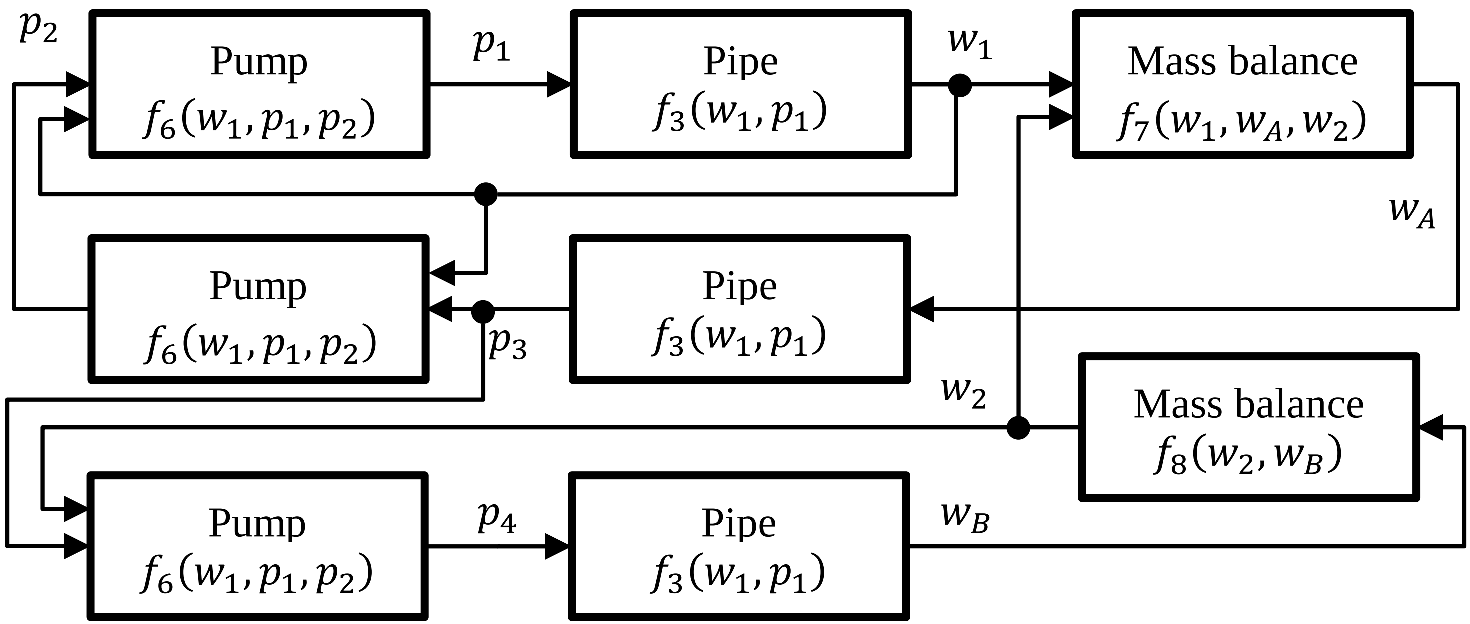
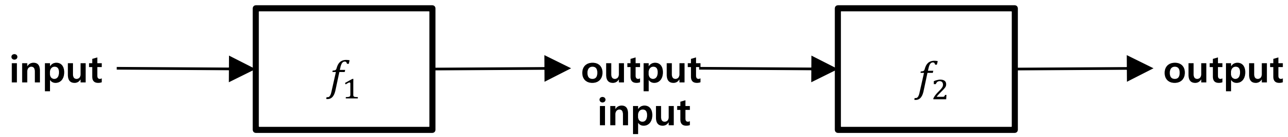


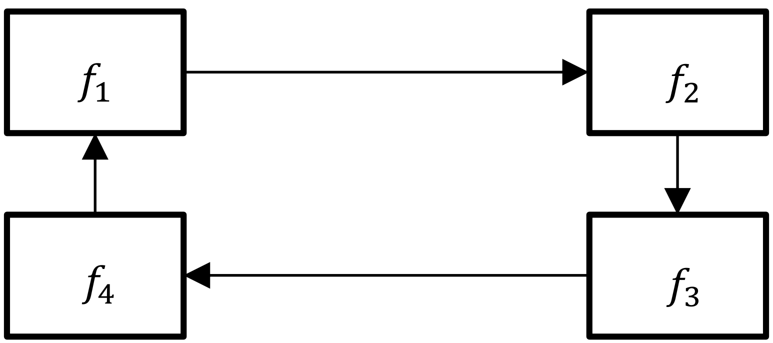
Fig. Information-flow diagram for fire-water system.

Chapter 6. SYSTEM SIMULATION

6.5 Sequential and simultaneous calculations

- Sequential calculation
- Simultaneous calculations





Chapter 6. SYSTEM SIMULATION

6.6 Two methods of simulation:

Successive substitution

Newton-Raphson

- To solve a set of simultaneous algebraic equations
- The **successive substitution** is a straight-forward technique and is closely associated with the information-flow diagram of the system.
- The **Newton-Raphson** method is based on a Taylor-series expansion.
- Each method has advantages and disadvantages

Chapter 6. SYSTEM SIMULATION

6.7 Successive substitution

- **Assume** a value of one or more variables and **begin** the calculation **until** the originally-assumed variables have been **recalculated**.
- The recalculated values are **substituted successively**, and **the calculation loop is repeated** until satisfactory convergence is achieved.

<Example 6.1>

Determine the values $\Delta p, w_1, w_2$ and w by using successive substitution.

<Given>

Pump 1: $\Delta p = 810 - 25w_1 - 3.75w_1^2$ [kPa]

Pump 2: $\Delta p = 900 - 65w_2 - 30w_2^2$ [kPa]

The friction in the pipe = $7.2w^2$

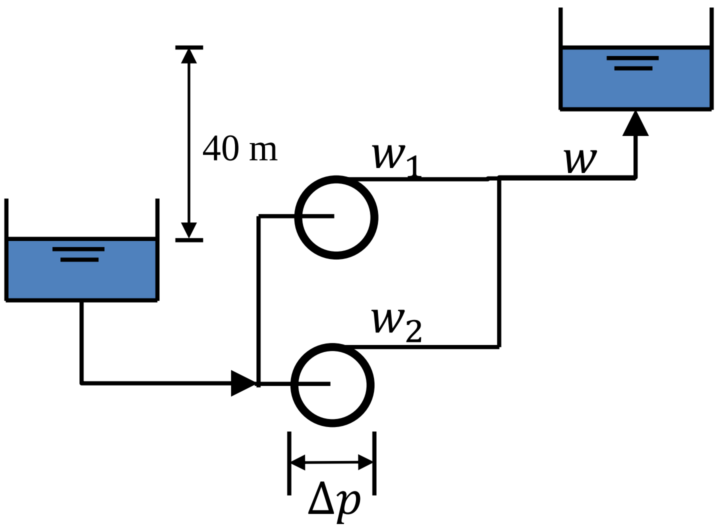


Fig. Water-pumping system

6.7 Successive substitution

<Solution>

✓ Pressure difference due to elevation and friction :

$$\Delta p = 7.2w^2 + \frac{(40\ \mathrm{m})(1000\ \mathrm{kg/m^3})(9.807\ \mathrm{m/s^2})}{1000\ \mathrm{Pa/kPa}}$$

✓ Pump 1 : $\Delta p = 810 - 25w_1 - 3.75w_1^2$

✓ Pump 2 : $\Delta p = 900 - 65w_2 - 30w_2^2$

✓ Mass balance : $w = w_1 + w_2$

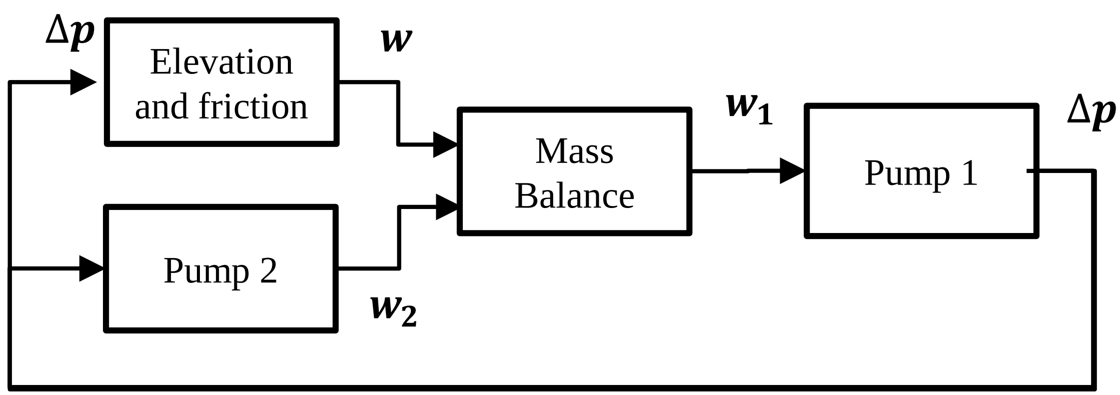


Fig. Information-flow diagram

Chapter 6. SYSTEM SIMULATION

6.7 Successive substitution

<Solution>

✓ Iteration with initial assumption : $w_1 = 4.2$

$$\Delta p = f_1(w_1)$$

$$w_2 = f_2(\Delta p)$$

$$w = f_3(\Delta p)$$

$$w_1 = f_2(w, w_2)$$

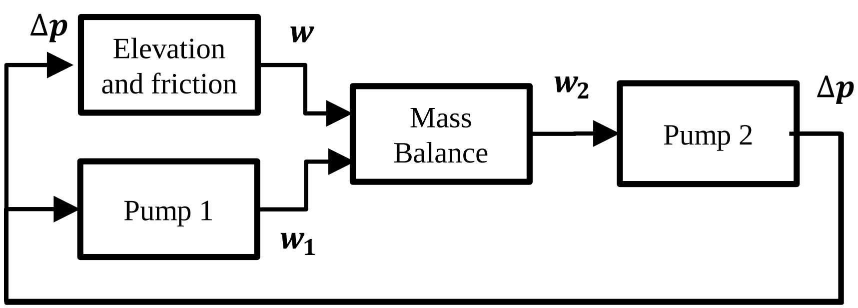
Iteration	Δp	w_2	w	w_1
1	638.85	2.060	5.852	3.792
2	661.26	1.939	6.112	4.174
3	640.34	2.052	5.870	3.818
4	659.90	1.946	6.097	4.151
⋮	⋮	⋮	⋮	⋮
47	649.98	2.000	5.983	3.983
48	650.96	1.995	5.994	3.999
49	650.04	2.000	5.983	3.984
50	650.90	1.995	5.993	3.998

Chapter 6. SYSTEM SIMULATION

6.7 Pitfalls in successive substitution

Diagram 2

✓ initial assumption : $w_2 = 2.0$

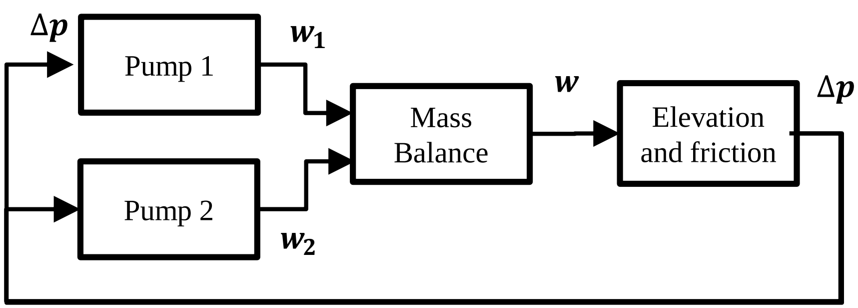


Iteration	w_1 [kg/s]	w_2 [kg/s]	w [kg/s]	Δp [kPa]
1	4.000	**2.000**	5.983	650.00
2	3.942	1.983	6.019	653.16
3	4.258	2.077	5.812	635.53
4	2.443	1.554	6.814	726.54
5	11.353	4.371	**divergence**	42.87

✓ Divergence occurs

Diagram 3

✓ initial assumption : $w = 6.0$



Iteration	w_1 [kg/s]	w_2 [kg/s]	w [kg/s]	Δp [kPa]
1	3.973	1.992	**6.000**	651.48
2	4.028	2.008	5.965	648.47
3	3.916	1.975	6.036	654.61
⋮	⋮	⋮	⋮	⋮
9	**divergence**		8.811	951.23

✓ Divergence occurs

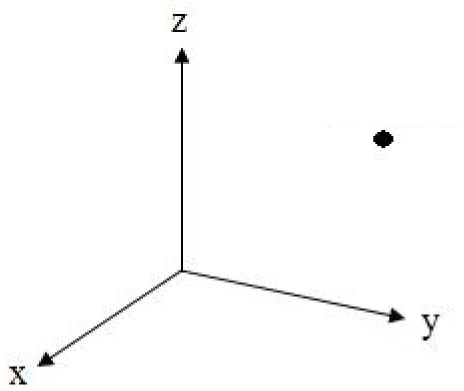
➡ Check the flow diagram in advance (Ch.14)

6.9 Taylor-series expansion

- The Newton-Raphson method is based on a Taylor-series expansion.

$$z = z(x, y)$$

Near the point $(a,\ b,\ z(a,b))$



$$z = c_0 + c_1(x-a) + c_2(y-b)$$
$$+c_3(x-a)^2 + c_4(x-a)(y-b) + c_5(x-a)^2 + \cdots$$

$$c_0 = z(a,b) \qquad c_3 = \frac{1}{2}\frac{\partial^2 z(a,b)}{\partial x^2}$$

$$c_1 = \frac{\partial z(a,b)}{\partial x} \qquad c_4 = \frac{\partial^2 z(a,b)}{\partial x \partial y}$$

$$c_2 = \frac{\partial z(a,b)}{\partial y} \qquad c_5 = \frac{1}{2}\frac{\partial^2 z(a,b)}{\partial y^2}$$

Chapter 6. SYSTEM SIMULATION

6.9 Taylor-series expansion

$$y = y(x)$$

$$y = d_0 + d_1(x-a) + d_2(x-a)^2 + \cdots$$

$$d_0 = y(a) \quad d_1 = \frac{dy(a)}{dx} \quad d_2 = \frac{1}{2}\frac{d^2y(a)}{dx^2}$$

$$y = y(x_1, x_2, \cdots, x_n)$$

$$y = y(a_1, a_2, \cdots, a_n) + \sum_{j=1}^{n} \frac{\partial y(a_1, a_2, \cdots, a_n)}{\partial x_j}(x_j - a_j)$$

$$+ \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial^2 y(a_1, a_2, \cdots, a_n)}{\partial x_i \partial x_j}(x_j - a_i)(x_j - a_j)$$

$$+ \cdots$$

Chapter 6. SYSTEM SIMULATION

6.9 Taylor-series expansion

<Example 6.2> Express $z = \ln(x^2 / y)$ as a Taylor-series expansion at (x=2,y=1)

<Solution>

$$z = \ln \frac{x^2}{y} = c_0 + c_1(x-2) + c_2(y-1) + c_3(x-2)^2 + c_4(x-2)(y-1) + c_5(y-1)^2 + \cdots$$

$$c_0 = \ln \frac{2^2}{1} = 1.39$$

$$c_1 = \frac{\partial z(2,1)}{\partial x} = \frac{2x / y}{x^2 / y} = 1$$

$$c_2 = \frac{\partial z(2,1)}{\partial y} = -\frac{x^2 / y^2}{x^2 / y} = -1$$

$$c_3 = \frac{1}{2} \frac{\partial^2 z(2,1)}{\partial x^2} = \frac{1}{2}\left(-\frac{2}{x^2}\right) = -\frac{1}{4}$$

$$c_4 = \frac{\partial^2 z(2,1)}{\partial x \partial y} = 0$$

$$c_5 = \frac{1}{2} \frac{\partial^2 z(2,1)}{\partial y^2} = \frac{1}{2} \frac{1}{y^2} = \frac{1}{2}$$

$$\therefore \quad z = 1.39 + (x-2) - (y-1) - \left(\frac{1}{4}\right)(x-2)^2 + \left(\frac{1}{2}\right)(y-1)^2 + \cdots$$

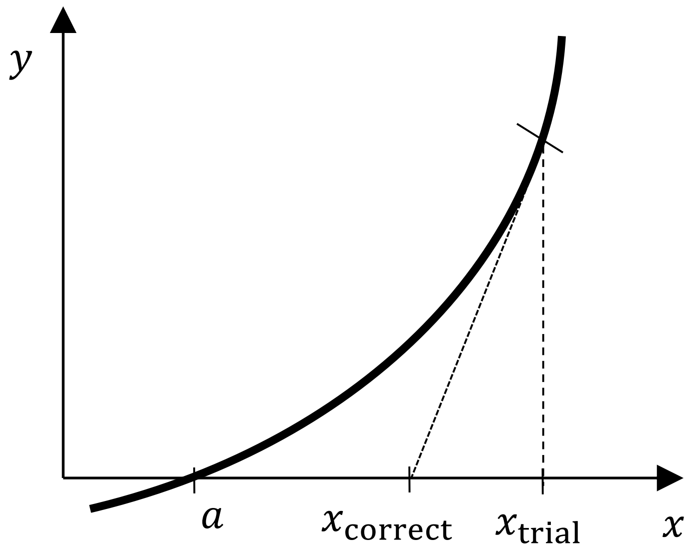
Chapter 6. SYSTEM SIMULATION

6.10 Newton-Raphson with one equation and one unknown

- In the Taylor-series expansion when x is close to a, the higher order terms become negligible.

$$y = y(a) + \frac{dy(a)}{dx}(x-a) + \left[\frac{1}{2}\frac{d^2y(a)}{dx^2}\right](x-a)^2 + \cdots$$

$$\rightarrow \quad y \approx y(a) + \frac{dy(a)}{dx}(x-a) = y(a) + y'(a)(x-a) \qquad (\because x \approx a)$$



$$y(x_t) = y(x_c) + \frac{y(x_t) - y(x_c)}{x_t - x_c}(x_t - x_c)$$

$$x_c = x_t - \frac{y(x_t)}{y'(x_t)}$$

$$x_{new} = x_{old} - (x_{trial} - x_{correct})$$

6.10 Newton-Raphson with one equation and one unknown

ex) $y(x) = x + 2 - e^x$ $\qquad y(x_c) = 0$

$x_t = 2 \longrightarrow y(x_t) = x_t + 2 - e^{x_t} = -3.39$

$$y \approx y(x_c) + y'(x_c)(x - x_c) \longrightarrow x_c = x_t - \frac{y(x_t)}{y'(x_t)} = 2 - \frac{-3.39}{1 - e^2} = 1.469 \longrightarrow x_{t,new}$$

Iteration	x_t	y(x)	y'(x)	x_c
1	2.000	-3.389	-6.389	1.470
2	1.470	-0.878	-3.347	1.207
3	1.207	-0.137	-2.345	1.149
4	1.149	-0.006	-2.154	1.146
5	**1.146**	0.000	-2.146	

6.11 Newton-Raphson with multiple equations and unknowns

$$f_1(x_1, x_2, x_3) = 0$$
$$f_2(x_1, x_2, x_3) = 0$$
$$f_3(x_1, x_2, x_3) = 0$$

trial value : x_{1t}, x_{2t}, x_{3t}

$$f_1(x_{1t}, x_{2t}, x_{3t}) = f_1(x_{1c}, x_{2c}, x_{3c}) + \frac{\partial f_1(x_{1t}, x_{2t}, x_{3t})}{\partial x_1}(x_{1t} - x_{1c})$$

$$+ \frac{\partial f_1(x_{1t}, x_{2t}, x_{3t})}{\partial x_2}(x_{2t} - x_{2c})$$

$$f_2 = \cdots$$

$$+ \frac{\partial f_1(x_{1t}, x_{2t}, x_{3t})}{\partial x_3}(x_{3t} - x_{3c})$$

$$f_3 = \cdots$$

$$+ \cdots$$

Chapter 6. SYSTEM SIMULATION

6.11 Newton-Raphson with multiple equations and unknowns

$$\begin{bmatrix} \dfrac{\partial f_1}{\partial x_1} & \dfrac{\partial f_1}{\partial x_2} & \dfrac{\partial f_1}{\partial x_3} \\ \dfrac{\partial f_2}{\partial x_1} & \dfrac{\partial f_2}{\partial x_2} & \dfrac{\partial f_2}{\partial x_3} \\ \dfrac{\partial f_3}{\partial x_1} & \dfrac{\partial f_3}{\partial x_2} & \dfrac{\partial f_3}{\partial x_3} \end{bmatrix} \begin{bmatrix} x_{1t} - x_{1c} \\ x_{2t} - x_{2c} \\ x_{3t} - x_{3c} \end{bmatrix} = \begin{bmatrix} f_1(x_{1t}, x_{2t}, x_{3t}) \\ f_2(x_{1t}, x_{2t}, x_{3t}) \\ f_3(x_{1t}, x_{2t}, x_{3t}) \end{bmatrix}$$

$$\rightarrow \quad x_{i,new} = x_{i,old} - (x_{i,t} - x_{i,c})$$

6.11 Newton-Raphson with multiple equations and unknowns

<Example 6.3> Solve Example 6.1 by Newton-Raphson method

<Solution>

- ✓ requirement : $f_1 = \Delta p - 7.2w^2 - 392.28 = 0$

$$f_2 = \Delta p - 810 + 25w_1 + 3.75{w_1}^2 = 0$$
$$f_3 = \Delta p - 900 + 65w_2 + 30{w_2}^2 = 0$$
$$f_4 = w - w_1 + w_2 = 0$$

- ✓ trial value : $\Delta p = 750,\ \ w_1 = 3,\ \ w_2 = 1.5,\ \ w = 5$

$$\rightarrow\ \ f_1 = 177.7,\ \ f_2 = 48.75,\ \ f_3 = 15.0,\ \ f_4 = 0.50$$

	$\partial/\partial\Delta p$	$\partial/\partial w_1$	$\partial/\partial w_2$	$\partial/\partial w$
$\partial f_1/\partial$	1	0	0	$-14.4w$
$\partial f_2/\partial$	1	$25+7.5w_1$	0	0
$\partial f_3/\partial$	1	0	$65+60w_2$	0
$\partial f_4/\partial$	0	-1	-1	1

6.11 Newton-Raphson with multiple equations and unknowns

<Solution>

- ✓ $$\begin{bmatrix} 1.0 & 0.0 & 0.0 & -72.0 \\ 1.0 & 47.5 & 0.0 & 0.0 \\ 1.0 & 0.0 & 155.0 & 0.0 \\ 0.0 & -1.0 & -1.0 & 1.0 \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \Delta x_3 \\ \Delta x_4 \end{bmatrix} = \begin{bmatrix} 177.7 \\ 48.75 \\ 15.0 \\ 0.50 \end{bmatrix} \qquad \Delta x_i = x_{i,t} - x_{i,c}$$
- ✓ $\Delta x_1 = 98.84,\ \Delta x_2 = -1.055,\ \Delta x_3 = -0.541\ \Delta x_4 = -1.096$
- ✓ corrected variable : $\Delta p = 750 - 98.84 = 651.16\ \ w_1 = 4.055,\ \ w_2 = 2.041,\ \ w = 6.096$

Iteration	w_1 [kg/s]	w_2 [kg/s]	w [kg/s]	Δp [kPa]	f_1	f_2	f_3	f_4
1	3.000	1.500	5.000	750.00	177.720	48.750	15.000	0.500
2	4.055	2.041	6.096	651.16	-8.641	4.171	8.778	0.000
3	3.992	1.998	5.989	650.48	-0.081	0.015	0.056	0.000
4	<u>3.991</u>	<u>1.997</u>	<u>5.988</u>	<u>650.49</u>	0.000	0.000	0.000	0.000

$$\therefore\ \Delta p = 650.49,\ \ w_1 = 3.991,\ \ w_2 = 1.997,\ \ w = 5.988$$

Chapter 6. SYSTEM SIMULATION

6.13 Overview of system simulation

- The system simulation operate to achieve **improved design** or to explore prospective **modifications**
- Choosing the combinations of dependent equation is important. But in large system is may not be simple to choose it.
- Successive substitution is a straight-forward technique and is usually easy to program. Its disadvantages are that sometimes the sequence may either converge very slowly or diverge.
- The Newton-Raphson technique is based on a Taylor-series expansion. It is powerful, but it is able to diverge on specific equations