

Chapter 6. SYSTEM SIMULATION

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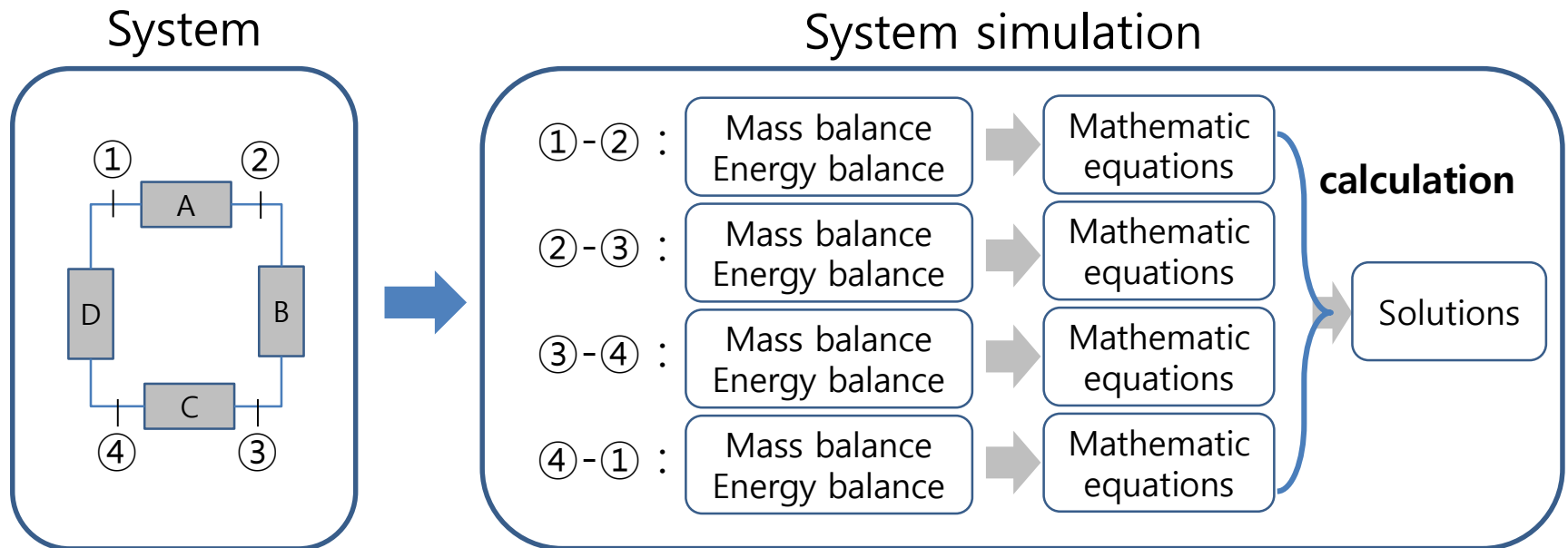


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Chapter 6. SYSTEM SIMULATION

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.



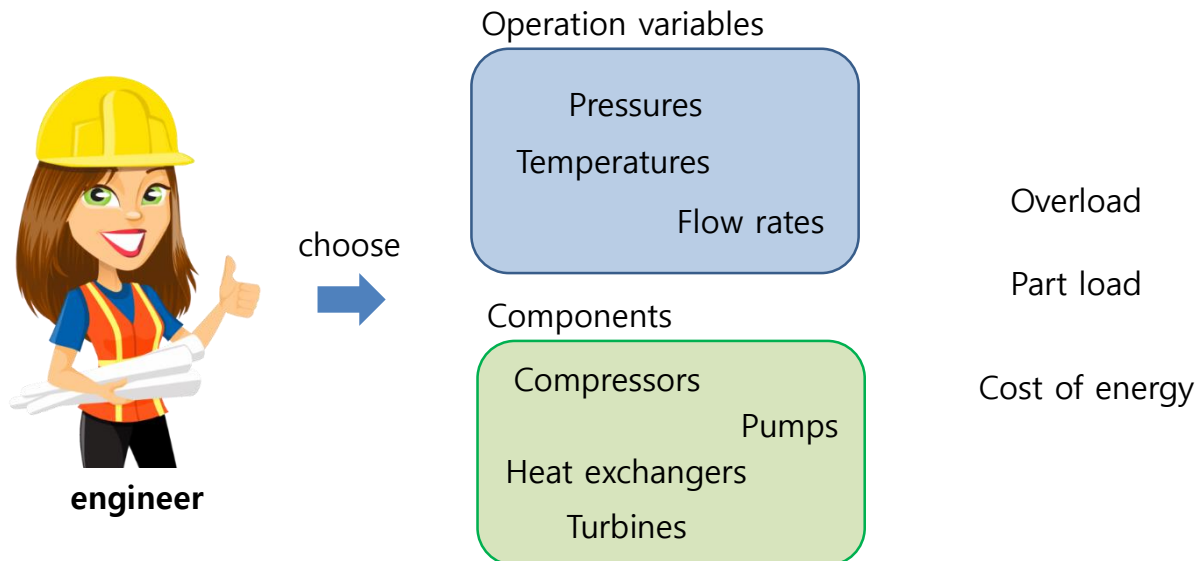
- characteristics of all components
- thermodynamic properties

- a set of simultaneous equations

Chapter 6. SYSTEM SIMULATION

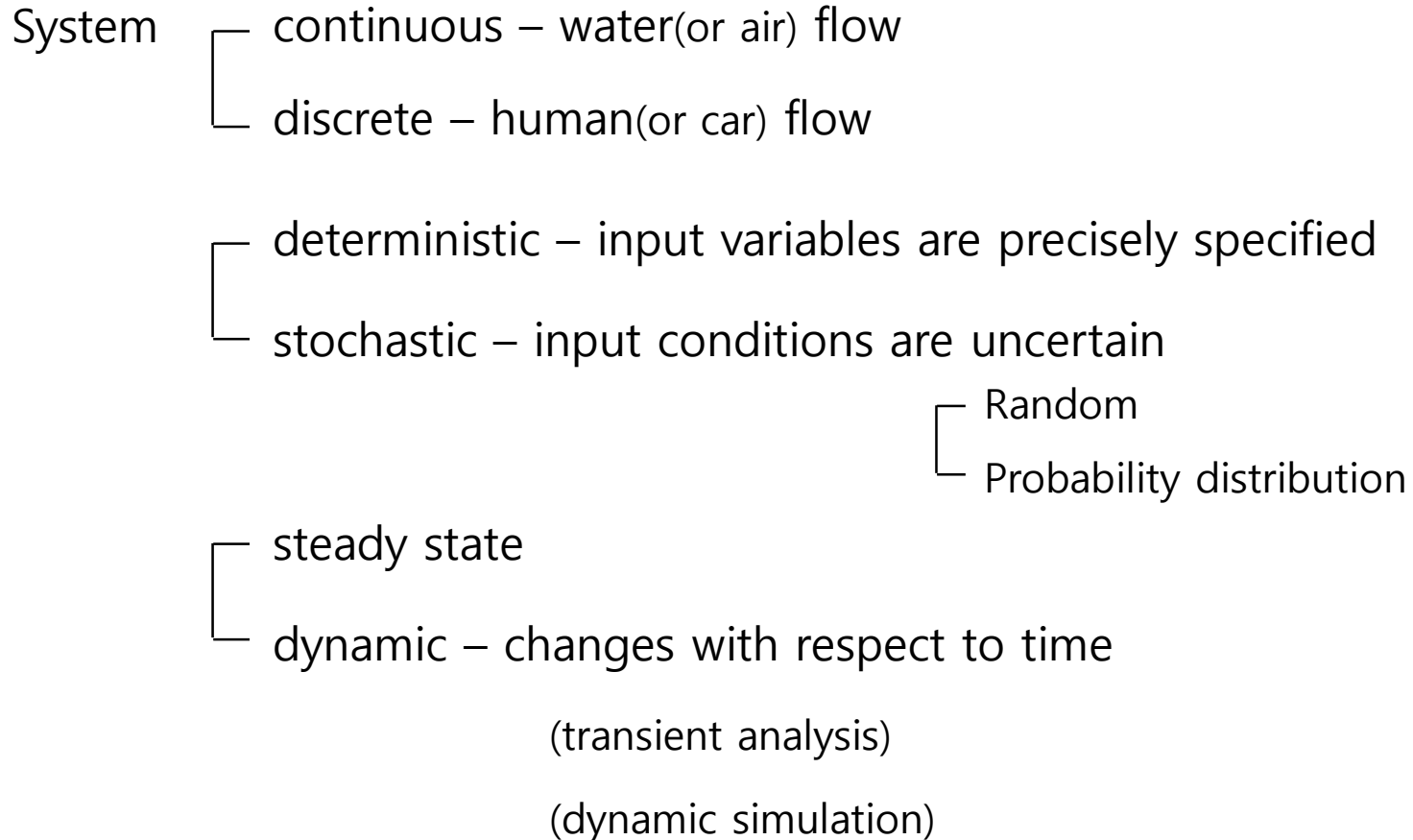
6.2 Some uses of simulation

- Design stage – to achieve **improved design**
- Existing system – to explore prospective **modifications**
- Design condition
 - Off design condition (part load / over load) ← normal operation



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6.3 Classes of simulation



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6.4 Information-flow diagrams

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

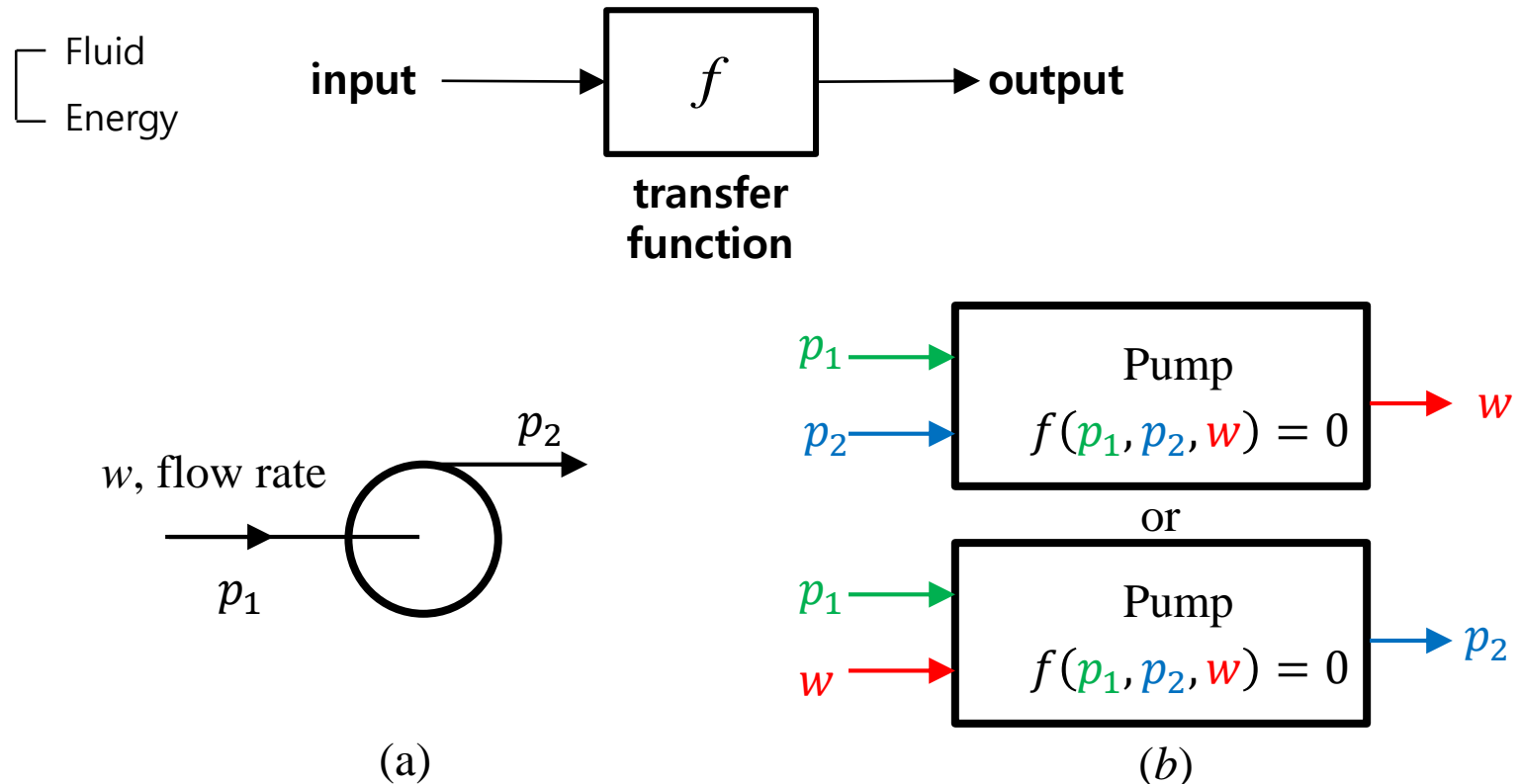


Fig. (a) Centrifugal pump in fluid-flow diagram (b) possible information-flow blocks representing pumps.

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6.4 Information-flow diagrams

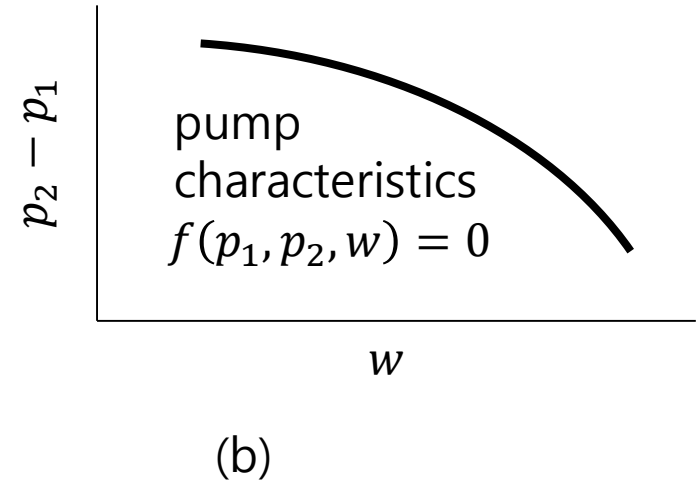
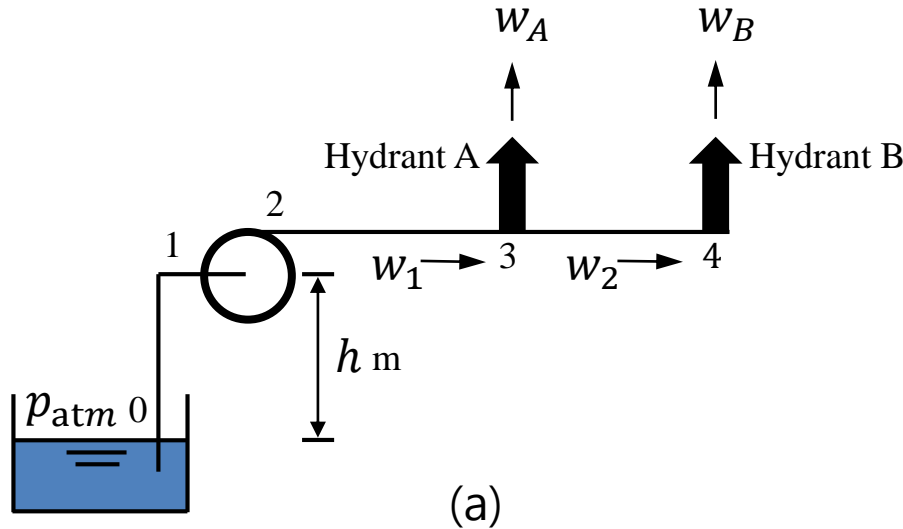


Fig. (a) Fire-water system (b) pump characteristics.

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

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

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

$$\text{Section 1-2 : } p_2 - p_3 = C_2 w_1^2$$

$$\text{Section 2-3 : } p_3 - p_4 = C_3 w_2^2$$



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

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

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

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

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

Chapter 6. SYSTEM SIMULATION

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 $w_2 = w_B$

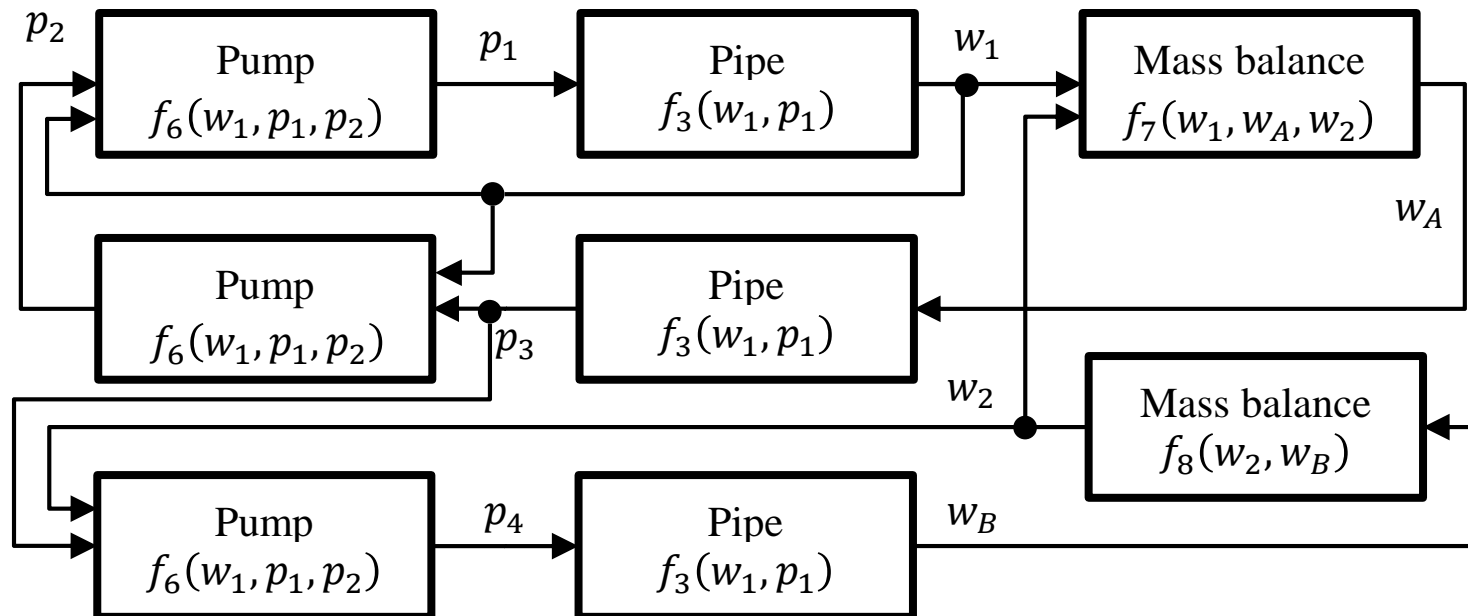
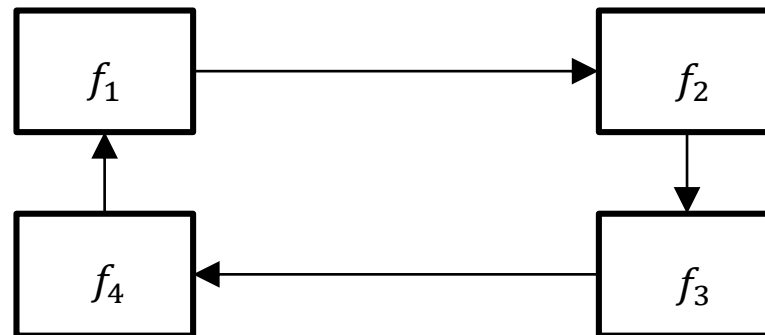


Fig. Information-flow diagram for fire-water system.

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 Δp , w_1 , w_2 and w by using successive substitution.

<Given>

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

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

$$\text{The friction in the pipe} = 7.2w^2$$

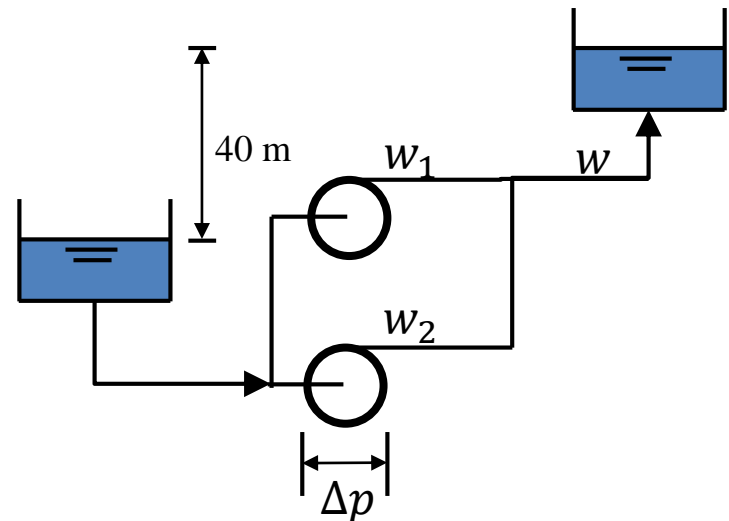


Fig. Water-pumping system

Chapter 6. SYSTEM SIMULATION

6.7 Successive substitution

<Solution>

- ✓ Pressure difference due to elevation and friction :

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

- ✓ Pump 1 : $\Delta p = 810 - 25w_1 - 3.75w_1^2$
- ✓ Pump 2 : $\Delta p = 900 - 65w_2 - 30w_2^2$
- ✓ Mass balance : $w = w_1 + w_2$

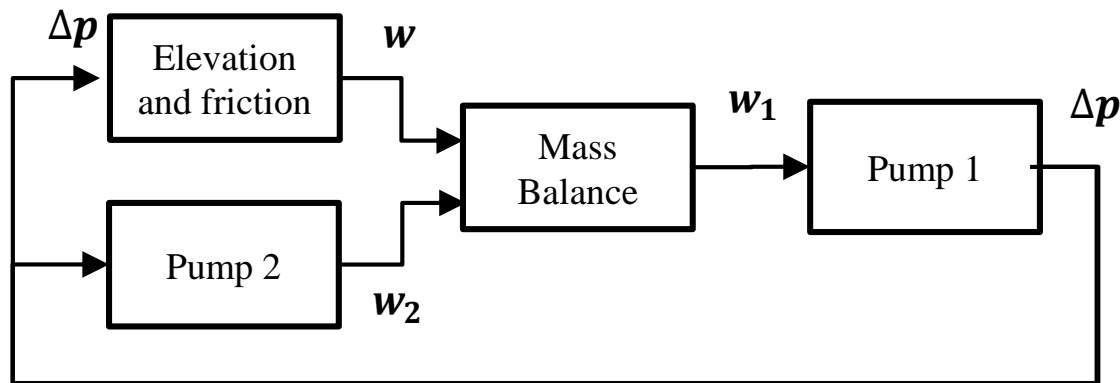


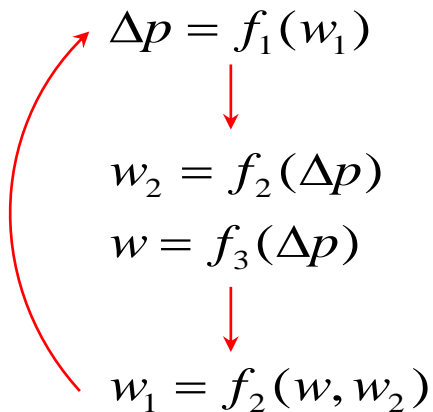
Fig. Information-flow diagram

Chapter 6. SYSTEM SIMULATION

6.7 Successive substitution

<Solution>

✓ Iteration with initial assumption : $w_1 = 4.2$



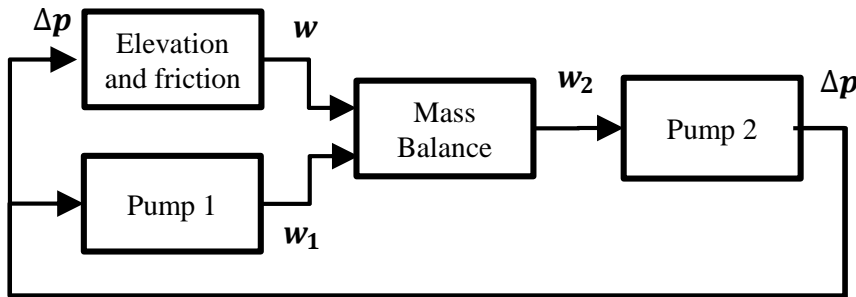
Iteration	Δp	w_2	w	w_1
1	638.85	2.060	5.852	3.792
2	661.26	1.939	6.112	4.174
3	640.34	2.052	5.870	3.818
4	659.90	1.946	6.097	4.151
⋮	⋮	⋮	⋮	⋮
47	649.98	2.000	5.983	3.983
48	650.96	1.995	5.994	3.999
49	650.04	2.000	5.983	3.984
50	650.90	1.995	5.993	3.998

Chapter 6. SYSTEM SIMULATION

6.7 Pitfalls in successive substitution

Diagram 2

✓ initial assumption : $w_2 = 2.0$

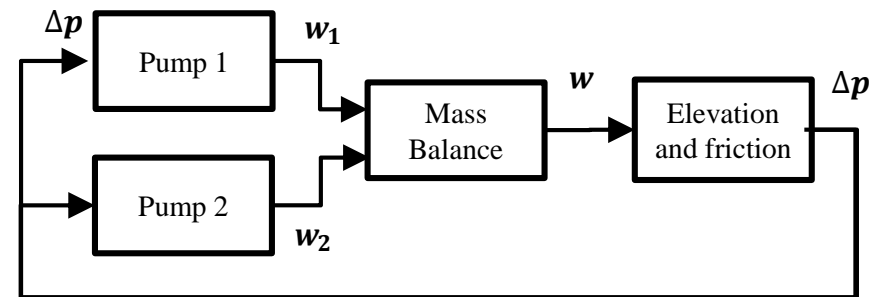


Iteration	w_1 [kg/s]	w_2 [kg/s]	w [kg/s]	Δp [kPa]
1	4.000	<u>2.000</u>	5.983	650.00
2	3.942	1.983	6.019	653.16
3	4.258	2.077	5.812	635.53
4	2.443	1.554	6.814	726.54
5	11.353	4.371	divergence	42.87

✓ 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	<u>6.000</u>	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)

Chapter 6. SYSTEM SIMULATION

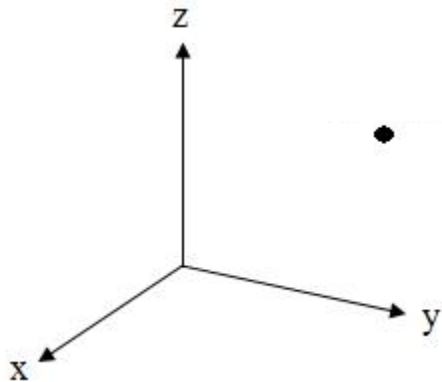
6.9 Taylor-series expansion

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

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

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

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



$$c_0 = z(a, b)$$

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

$$c_1 = \frac{\partial z(a, b)}{\partial x}$$

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

$$c_2 = \frac{\partial z(a, b)}{\partial y}$$

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

Chapter 6. SYSTEM SIMULATION

6.9 Taylor-series expansion

$$y = y(x)$$

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

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

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

$$\begin{aligned} y &= y(a_1, a_2, \dots, a_n) + \sum_{j=1}^n \frac{\partial y(a_1, a_2, \dots, a_n)}{\partial x_j} (x_j - a_j) \\ &\quad + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \frac{\partial^2 y(a_1, a_2, \dots, a_n)}{\partial x_i \partial x_j} (x_j - a_i)(x_j - a_j) \\ &\quad + \dots \end{aligned}$$

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>

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

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

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

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

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

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

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

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

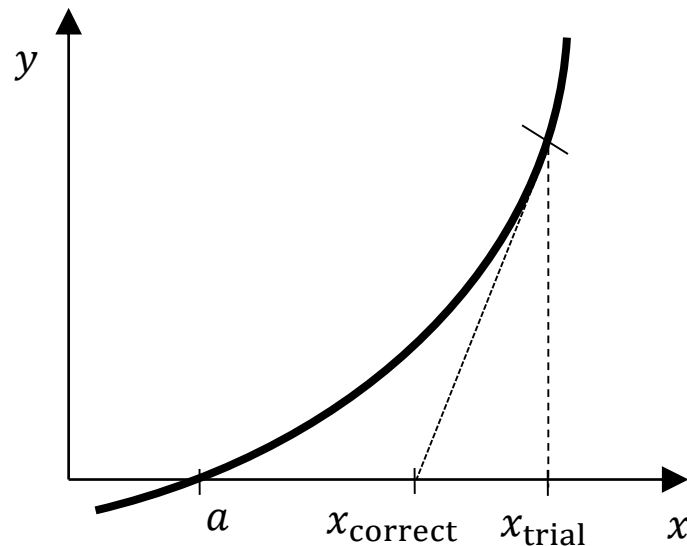
Chapter 6. SYSTEM SIMULATION

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.

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

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



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

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

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

Chapter 6. SYSTEM SIMULATION

6.10 Newton-Raphson with one equation and one unknown

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

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

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

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	

Chapter 6. SYSTEM SIMULATION

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}

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

Chapter 6. SYSTEM SIMULATION

6.11 Newton-Raphson with multiple equations and unknowns

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

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

Chapter 6. SYSTEM SIMULATION

6.11 Newton-Raphson with multiple equations and unknowns

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

<Solution>

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

$$f_2 = \Delta p - 810 + 25w_1 + 3.75w_1^2 = 0$$

$$f_3 = \Delta p - 900 + 65w_2 + 30w_2^2 = 0$$

$$f_4 = w - w_1 + w_2 = 0$$

✓ 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

Chapter 6. SYSTEM SIMULATION

6.11 Newton-Raphson with multiple equations and unknowns

<Solution>

$$\checkmark \begin{bmatrix} 1.0 & 0.0 & 0.0 & -72.0 \\ 1.0 & 47.5 & 0.0 & 0.0 \\ 1.0 & 0.0 & 155.0 & 0.0 \\ 0.0 & -1.0 & -1.0 & 1.0 \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \Delta x_3 \\ \Delta x_4 \end{bmatrix} = \begin{bmatrix} 177.7 \\ 48.75 \\ 15.0 \\ 0.50 \end{bmatrix} \quad \Delta x_i = x_{i,t} - x_{i,c}$$

$$\checkmark \Delta x_1 = 98.84, \Delta x_2 = -1.055, \Delta x_3 = -0.541, \Delta x_4 = -1.096$$

$$\checkmark \text{corrected variable : } \Delta p = 750 - 98.84 = 651.16 \quad w_1 = 4.055, \quad w_2 = 2.041, \quad w = 6.096$$

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

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

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