EngrD 2190 – Lecture 7

Concept: Process Analysis – Mathematical Modeling

Context: Mass Balances – a Freezer Desalinator with Two Products

Defining Question: What are the requirements for a solvable mathematical model?

Read Chapter 3 pp. 99-106 (mass balances)

Lecture 8 will cover the same concepts,
but in a different context.

Professional Practice, Part 1: Résumés

- Résumés due today at 5 p.m.

  email as attachment to Professor Bauer (btb42)
  with subject line: EngrD 2190, Your Name, Resume
  and attached file named: Lastname_Resume.doc

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A Strategy for Design

Define the *Real* Problem.

Generate Ideas.

iterate

Evaluate.

Create many designs,
choose the best.

How to choose the best?

Build each design? No - Impractical.

Evaluate each design.

1. Build a convenient model.

$$\boxed{\text{small model}} \xrightarrow{\text{dynamic scaling}} \boxed{\text{micro system}}$$

Chapter 5.

2. Create a mathematical model. Chapter 3.

   Translate the physical & chemical description into equations.

3. Create a graphical model. Chapter 4.

   Translate the physical & chemical description into a geometric construction.

Mathematical Models

A mathematical description of a process or a unit operation.

A mathematical model predicts the performance of a process or unit given operating conditions – concentrations, flow rates, temperatures, and equipment costs, for example.

Mathematical modeling is a hallmark of chemical engineering.

Key Requirement:
Every equation must have an explicit source.

A Method of Mathematical Modeling

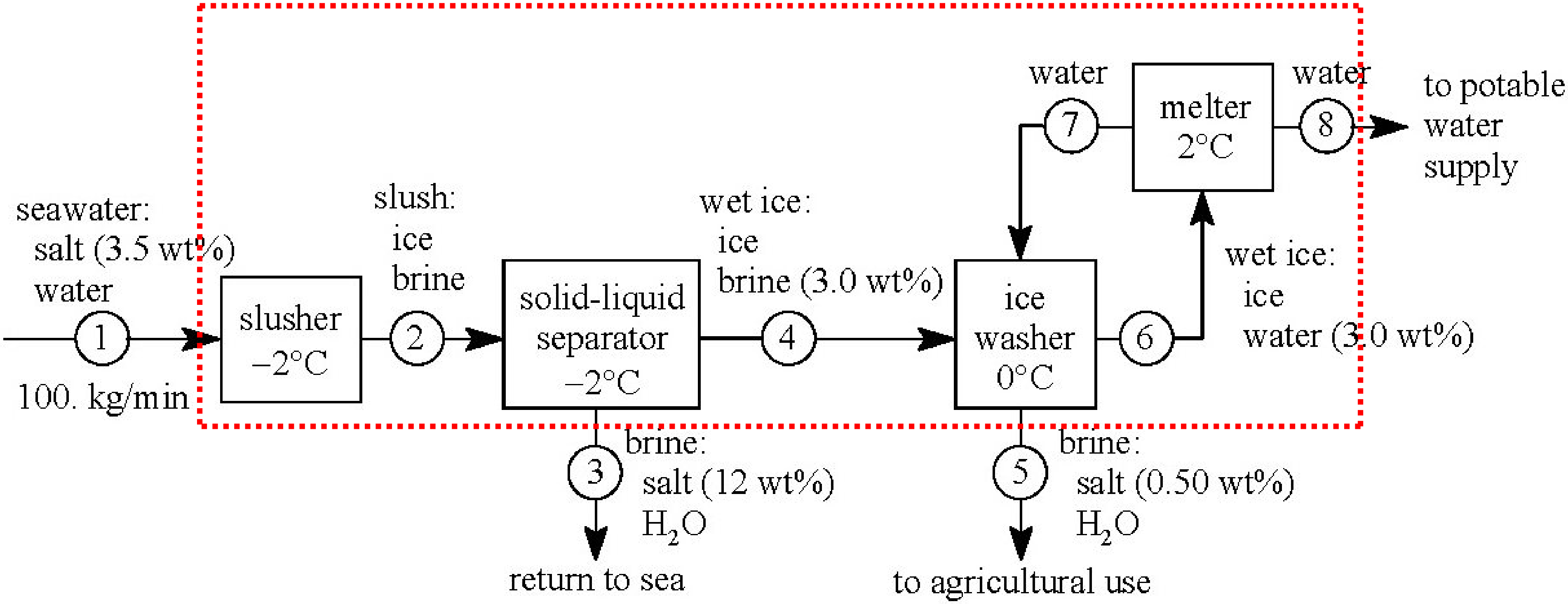
1. Define a system. Draw system borders on the process flowsheet.

1. Define a system – draw system borders

external streams internal stream (recycle)

Model 1:
Fig 3.8, p. 96

Calculate $\boxed{F_{T,3}, F_{T,5}, F_{T,8},}$ and $\boxed{F_{T,7}.}$



Model 1: (4 streams) × (2 parameters/stream) = 8 parameters

A Method for Mathematical Modeling

1. Define a system. Draw system borders on the process flowsheet.

2. State conditions & assumptions.

The process is at steady state. No chemical reactions.

3. Choose a set of n–1 parameters. 3 parameters: total = H_2O + salt

Choose 3 – 1 = 2 parameters.

options: total + H_2O

$\boxed{\text{total + salt}}$ Because stream compositions are in wt% salt

salt + H_2O

4. Define nomenclature.

$F_{i,\,n} \equiv$ mass flow rate of substance i in stream n, in kg/min.

$W \equiv H_2O$ existing as any phase; water, ice, or steam.

$S \equiv$ salt

A Method for Mathematical Modeling, cont'd

5. Translate into equations.

template equation shorthand for steps 1 and 2.

Mass Balances: rate in = rate out

total: $F_{T,1} = F_{T,3} + F_{T,5} + F_{T,8}$ (1)

salt: $F_{S,1} = F_{S,3} + F_{S,5} + F_{S,8}$ (2)

Process Specifications: $F_{T,1} = 100.\ \text{kg/min}$ (3)

"salt = 3.5% × stream 1" $F_{S,1} = 0.035F_{T,1} = 3.5\ \text{kg/min}$ (4)

"salt is 12% of stream 3" $F_{S,3} = 0.12F_{T,3}$ (5)

$F_{S,5} = 0.005F_{T,5}$ (6)

$F_{S,8} = 0$ (7)

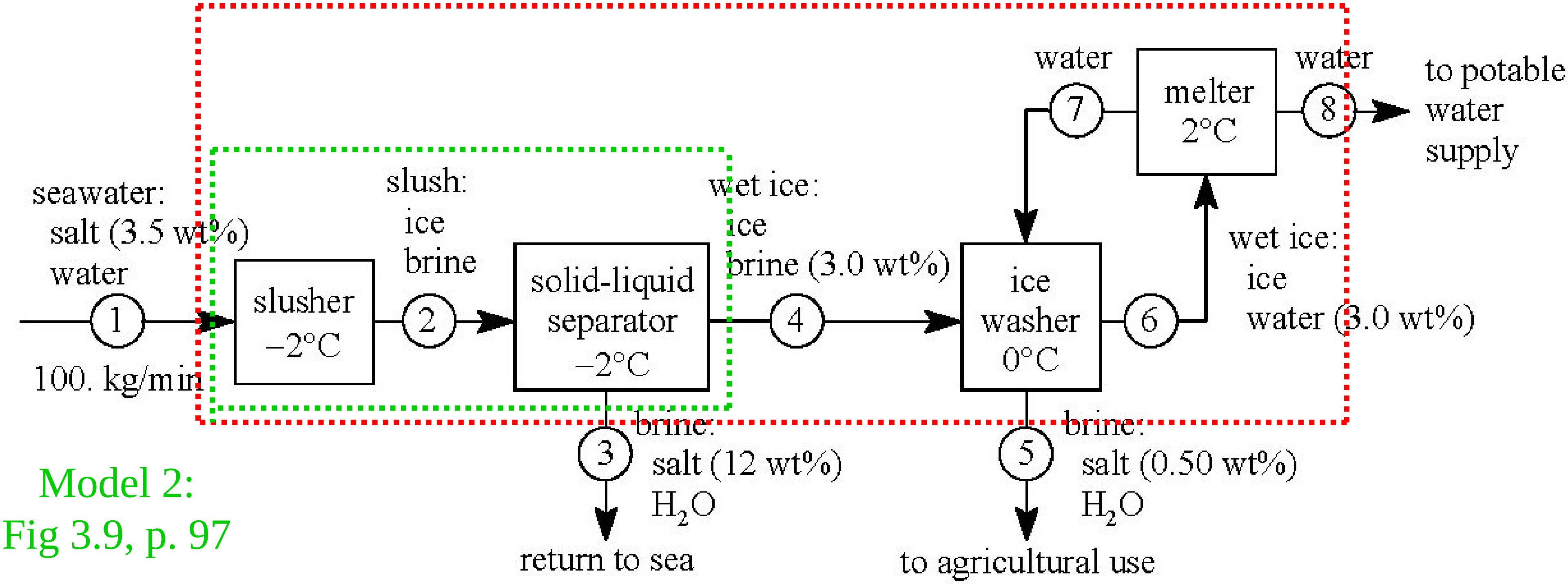
We have 8 parameters and 7 equations. We need one more equation.

Define a new system to obtain the 8th equation.

external streams internal stream (recycle)

Model 1:
Fig 3.8, p. 96

Calculate $\boxed{F_{T,3}, F_{T,5}, F_{T,8},}$ and $\boxed{F_{T,7}.}$



Model 2:
Fig 3.9, p. 97

Model 1: (4 streams) × (2 parameters/stream) = 8 parameters

Model 2: (3 streams) × (2 parameters/stream) = 6 parameters

Model 2 – slusher + solid-liquid separator

Mass Balances: rate in = rate out

total: $F_{T,1} = F_{T,3} + F_{T,4}$ (2.1)

salt: $F_{S,1} = F_{S,3} + F_{S,4}$ (2.2)

implies green borders and steady state

If you omit this template equation, you must describe borders and state assumptions.

Process Specifications:

"salt is 12 wt% of brine; brine is 3 wt% of stream 4"

$$F_{S,4} = 0.12 \times (\text{brine})$$

$$F_{S,4} = 0.12 \times (0.03 F_{T,4})$$

$$F_{S,4} = 0.0036 F_{T,4} \qquad (2.3)$$

$$F_{T,1} = 100.\ \text{kg/min} \qquad (2.4)$$

$$F_{S,1} = 3.5\ \text{kg/min} \qquad (2.5)$$

$$F_{S,3} = 0.12 F_{T,3} \qquad (2.6)$$

Six equations,
Six parameters.
Solvable!

Model 2 – solving the equations

$$F_{T,1} = F_{T,3} + F_{T,4} \quad (2.1)$$

$$F_{S,1} = F_{S,3} + F_{S,4} \quad (2.2)$$

$$F_{S,4} = 0.0036F_{T,4} \quad (2.3)$$

$$F_{T,1} = 100.\ \text{kg/min} \quad (2.4)$$

$$F_{S,1} = 3.5\ \text{kg/min} \quad (2.5)$$

$$F_{S,3} = 0.12F_{T,3} \quad (2.6)$$

Substitute equations (2.5), (2.6), (2.3) into equation (2.2).

$$F_{S,1} = F_{S,3} + F_{S,4} \quad (2.2)$$

$$3.5 = 0.12F_{T,3} + 0.0036F_{T,4} \quad (2.7)$$

Substitute equation (2.4) into equation (2.1).

$$F_{T,1} = F_{T,3} + F_{T,4} \quad (2.1)$$

$$100 = F_{T,3} + F_{T,4}$$

$$F_{T,4} = 100 - F_{T,3} \quad (2.8)$$

Substitute equation (2.8) into equation (2.7).

$$3.5 = 0.12F_{T,3} + 0.0036(100 - F_{T,3})$$

8th equation for Model 1

$$\boxed{F_{T,3} = 26.98\ \text{kg/min}}$$

$$F_{T,4} = 73.02\ \text{kg/min}$$

$$F_{S,3} = 3.24\ \text{kg/min}$$

$$F_{S,4} = 0.26\ \text{kg/min}$$

Model 1 – solving the equations

$$F_{T,1} = F_{T,3} + F_{T,5} + F_{T,8} \quad (1)$$

$$F_{S,1} = F_{S,3} + F_{S,5} + F_{S,8} \quad (2)$$

$$F_{T,1} = 100.\text{ kg/min} \quad (3)$$

$$F_{S,1} = 3.5\text{ kg/min} \quad (4)$$

$$F_{S,3} = 0.12F_{T,3} \quad (5)$$

$$F_{S,5} = 0.005F_{T,5} \quad (6)$$

$$F_{S,8} = 0 \quad (7)$$

$$F_{T,3} = 26.98\text{ kg/min} \quad (8)$$

Substitute equation (8) into equation (5).

$$F_{S,3} = 0.12F_{T,3} = 0.12(26.98) = 3.24\text{ kg/min} \quad (9)$$

Substitute equations (4), (9), (6), and (7) into equation (2).

$$F_{S,1} = F_{S,3} + F_{S,5} + F_{S,8} \quad (2)$$

$$3.5 = 3.24 + 0.005F_{T,5} + 0 \quad \Rightarrow \quad F_{T,5} = 52.58\text{ kg/min} \quad (10)$$

Substitute equations (3), (8), and (10) into equation (1).

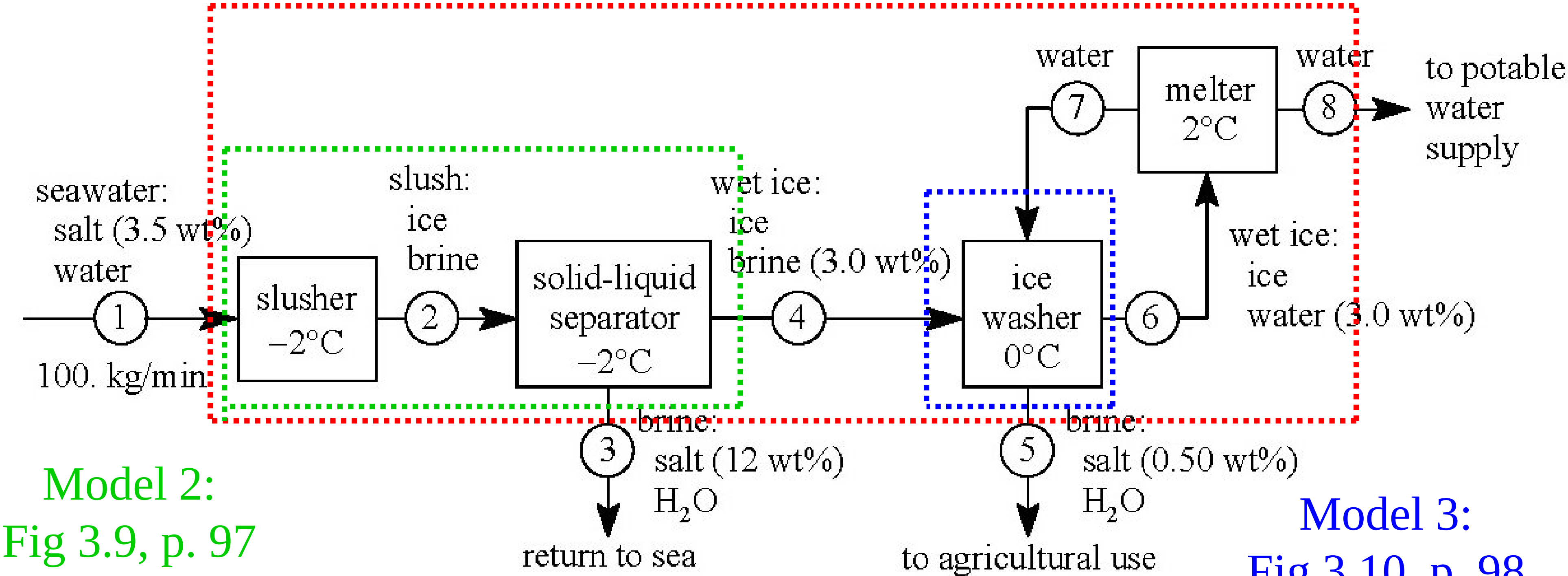
$$F_{T,1} = F_{T,3} + F_{T,5} + F_{T,8} \quad (1)$$

$$100 = 26.98 + 52.58 + F_{T,8} \quad \Rightarrow \quad F_{T,8} = 20.44\text{ kg/min} \quad (11)$$

external streams internal stream (recycle)

Calculate $\boxed{F_{T,3}, F_{T,5}, F_{T,8},}$ and $\boxed{F_{T,7}.}$

Model 1:
Fig 3.8, p. 96



Model 2:
Fig 3.9, p. 97

Model 3:
Fig 3.10, p. 98

Model 1: (4 streams) × (2 parameters/stream) = 8 parameters

Model 2: (3 streams) × (2 parameters/stream) = 6 parameters

Model 3: (4 streams) × (2 parameters/stream) = 8 parameters

Model 3 – ice washer

Mass Balances: rate in = rate out

implies blue borders and steady state

total: $F_{T,4} + F_{T,7} = F_{T,5} + F_{T,6}$ (3.1)

salt: $F_{S,4} + F_{S,7} = F_{S,5} + F_{S,6}$ (3.2)

If you omit this template equation, you must describe borders and state assumptions.

Process Specifications: "5% of ice in stream 4 melts."

$\Rightarrow$ (ice in stream 6) = 0.95(ice in stream 4)

"ice is wet with 3% water" $\Rightarrow$ (ice in stream 6) = $0.97F_{T,6}$

$$0.97F_{T,6} = 0.95(0.97F_{T,4})$$

$$F_{T,6} = 0.95F_{T,4} \quad (3.3)$$

"salt is 0.5 wt% of stream 5" $F_{S,5} = 0.005F_{T,5}$ (3.4)

"stream 6 is pure water" $F_{S,6} = 0$ (3.5)

Model 3 – ice washer

From Model 2:

$$F_{T,4} = 73.02 \text{ kg/min} \quad (3.6)$$

$$F_{T,5} = 52.58 \text{ kg/min} \quad (3.7)$$

$$F_{S,4} = 0.263 \text{ kg/min} \quad (3.8)$$

8 equations and
8 parameters –
Solvable!

Substitute equation (3.6) into equation (3.3).

$$F_{T,6} = 0.95 F_{T,4} \quad (3.3)$$

$$F_{T,6} = 0.95(73.02) = 69.37 \text{ kg/min} \quad (3.9)$$

Substitute equations (3.6), (3.7), and (3.9) into equation (3.1).

$$F_{T,4} + F_{T,7} = F_{T,5} + F_{T,6} \quad (3.1)$$

$$73.02 + F_{T,7} = 52.58 + 69.37$$

$$F_{T,7} = 48.93$$

For Homework, you must summarize your results.

Waste brine - Stream 3:	27. kg/min
Agricultural brine - Stream 5	53. kg/min
Potable water - Stream 8:	20. kg/min
Recycled water - Stream 7:	49. kg/min

Must include units!

Must box the answer!

Must use correct significant figures!

Done? No! Check your answers!

total in = total out? $100 = 27 + 53 + 20?$

$100 = 100$ ✓

salt in = salt out? $3.5 = 0.12 \times 27 + 0.005 \times 53 + 0 \times 20?$

$3.5 = 3.5$ ✓

A Method for Mathematical Modeling

1. Define a system.
2. State conditions & assumptions.
3. Choose a set of n–1 parameters.
4. Define nomenclature.
5. Translate into equations.
6. Solve.

Key Requirement:
Every equation must have an explicit source.

Your mathematical model must have no ambiguities, no uncertanties.