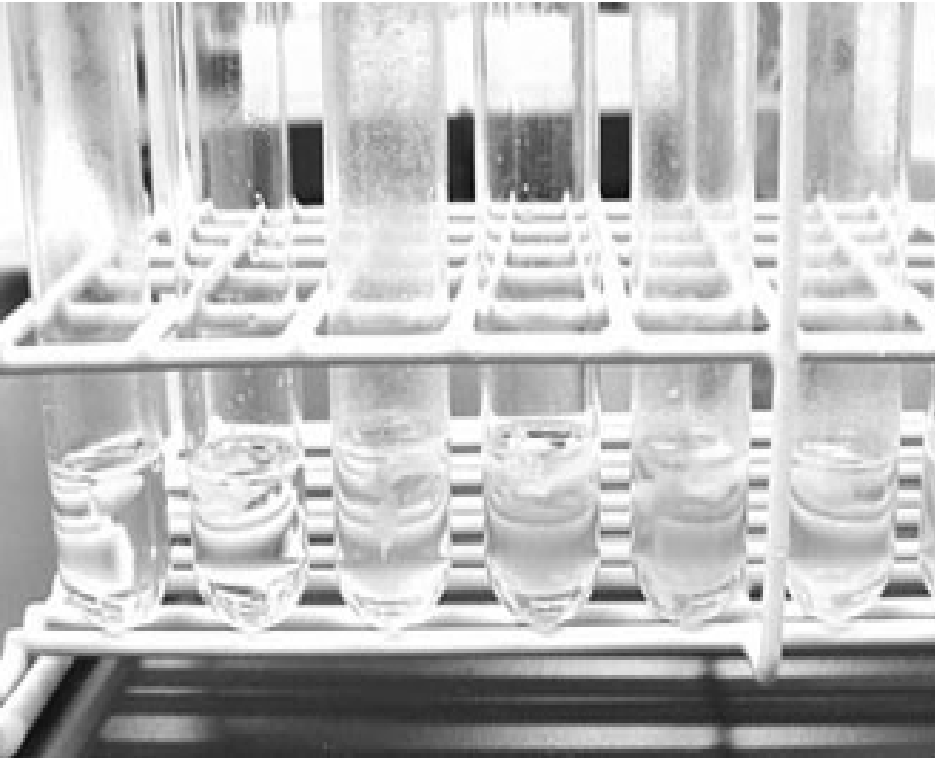


KIChE Fall Meeting

Industrial Practice for Process Operation and R&D – Present and Future

# Conceptual Design and Its Role in Process Design



October 2006

Dr. Yoshio Kumagae, preFEED Corporation

## Agenda

Freshman and Experienced Engineer

Challenges

Rigorous Simulation vs. Common Sense

1. Distillation, or not ?
2. Install Steam Turbine, or not ?
3. Which can capture the image ?

Recommendations

# Freshman vs. Experienced Engineer

# Size of a pipe for 100 m<sup>3</sup>/hr water ?



- If the velocity is 10 m/s, then the size is 59 mmD.
- If 100 m/s, then 19mmD.



- The diameter should be 130 – 190 mm,
- because the velocity must be 1-2 m/s for liquids.

# Experienced Engineer



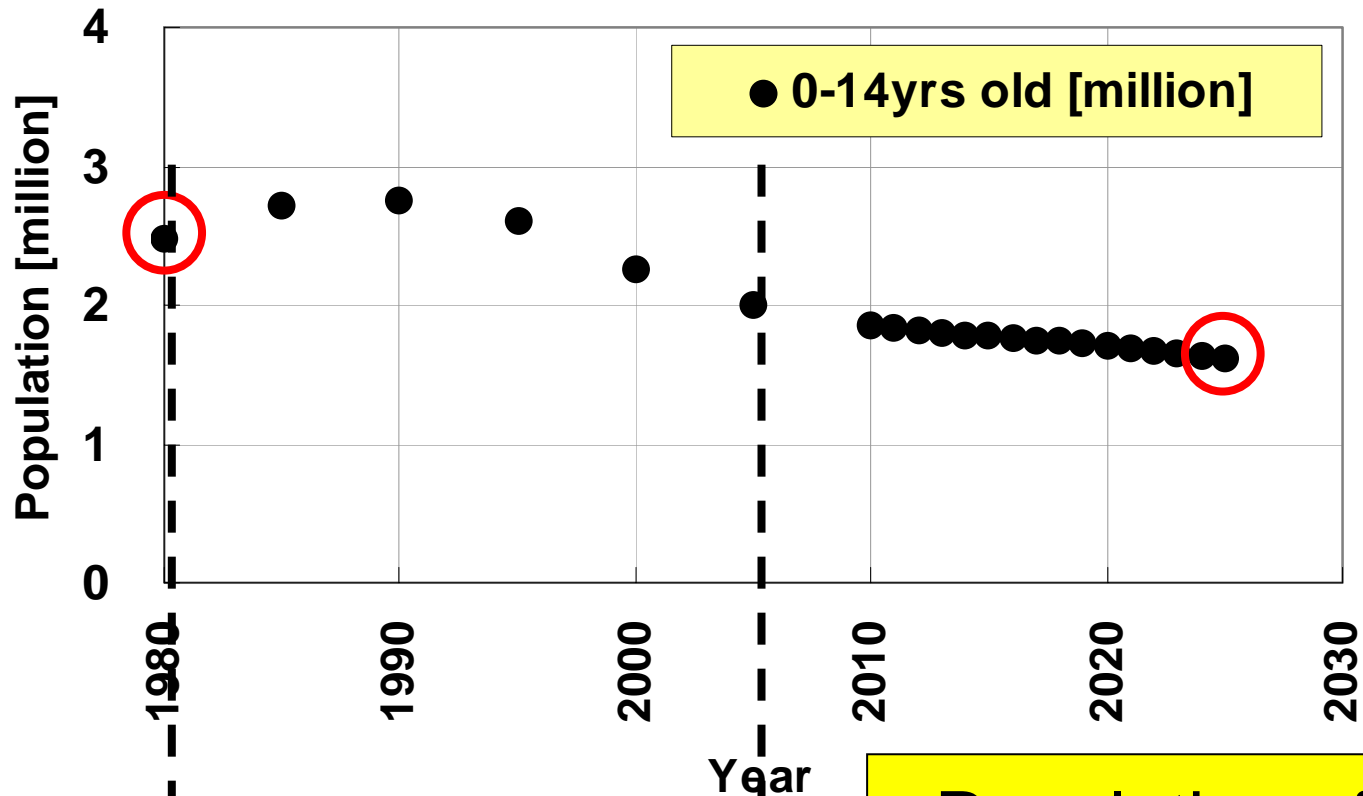
Experienced Engineer can

- estimate the approximate size of equipment without computer.
- check the detailed calculation without computer.

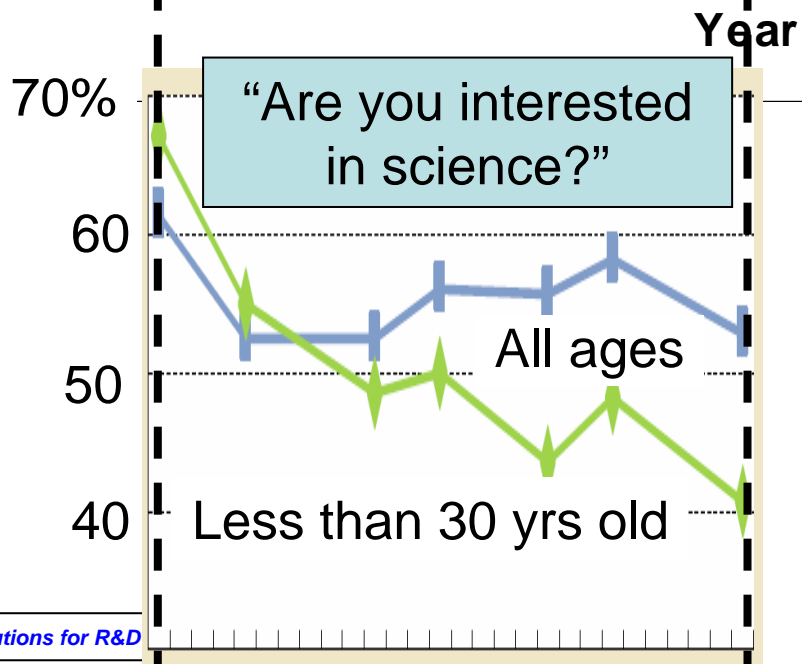
Experienced engineer has the knowledge of standard values, first question to ask, quick calculation, meaning of parameter value.

**He has common sense of process design !**

# Challenges



Future



- Population of 0-14 yrs old, source of future engineers, will decrease to 1/2 (2025/1980).
- The human resources will be reduced further.

How many years will your boss be patient for you to accumulate experience ?

Typical Answer by Managers:  
"5 years" after joining the company

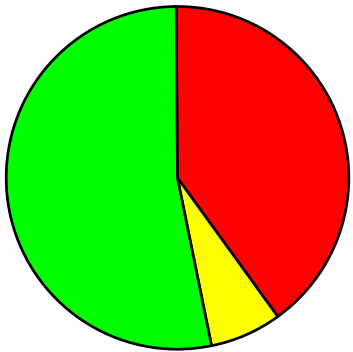


# How About **Today's** Engineers ?

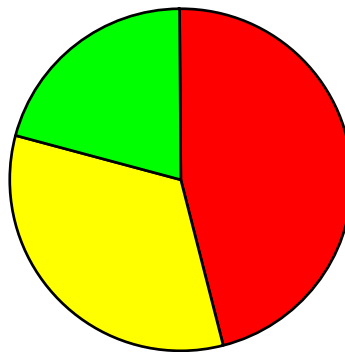
## Results of 100 Common Sense Questions

Know well   Not sure   Never heard of

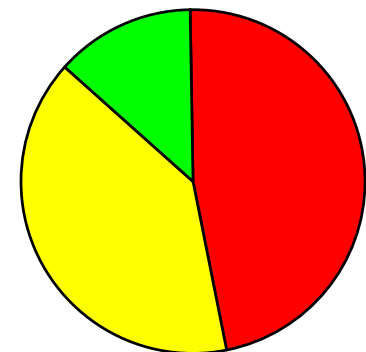
How to use triangle diagram ?



Meaning of parameter "B" of Antoine equation ?



If relative volatility is 2, is it a difficult separation ?



Concern over today and future

- Gap between expectation and reality
- Concern over future human resources

Reasons why we need to train our engineers

Train engineers so that (1) they can make the best use of process simulator if applicable and (2) they can design processes without simulator if not applicable.

# Rigorous Simulation vs. Common Sense

Many design options are theoretically feasible, but only a small number of designs have survived. They have technical and/or economical reasons.

The knowledge related to them are accumulated in each experienced engineers after a long trial and error efforts.

They are called “**rule-of-thumb**”, “**heuristics**”, “**back-of-the-envelope calculation**”, “**common sense** (of process design”, which are related to **conceptual process design**.

# Rigorous Simulation vs. Common Sense

## 1. Distillation, or not ?

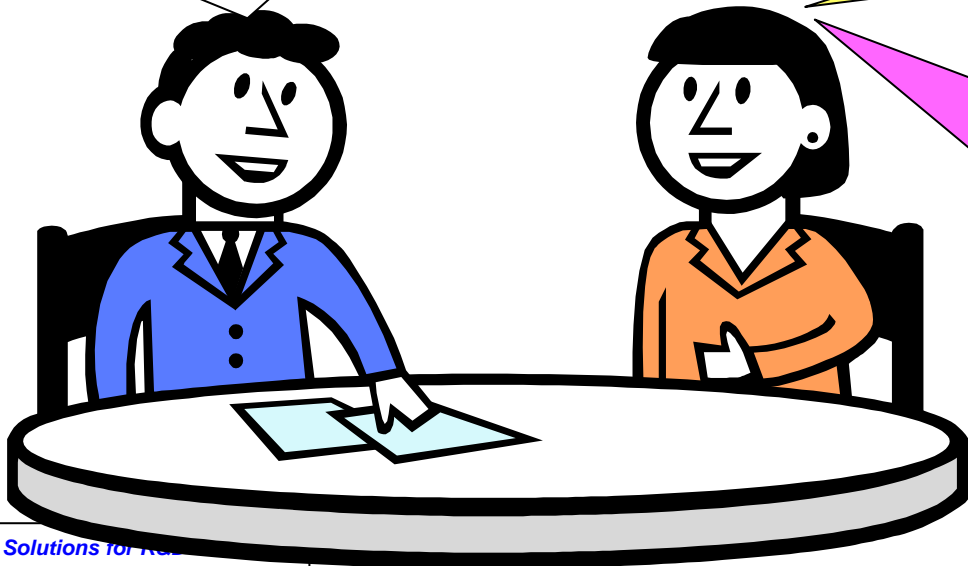
# Separation of o-/p- dichlorobenzene (bp=180/174 C)

I used AspenPlus to calculate the distillation column. It looks the separation is not easy. Should I continue the case studies? Or do you have some suggestions?

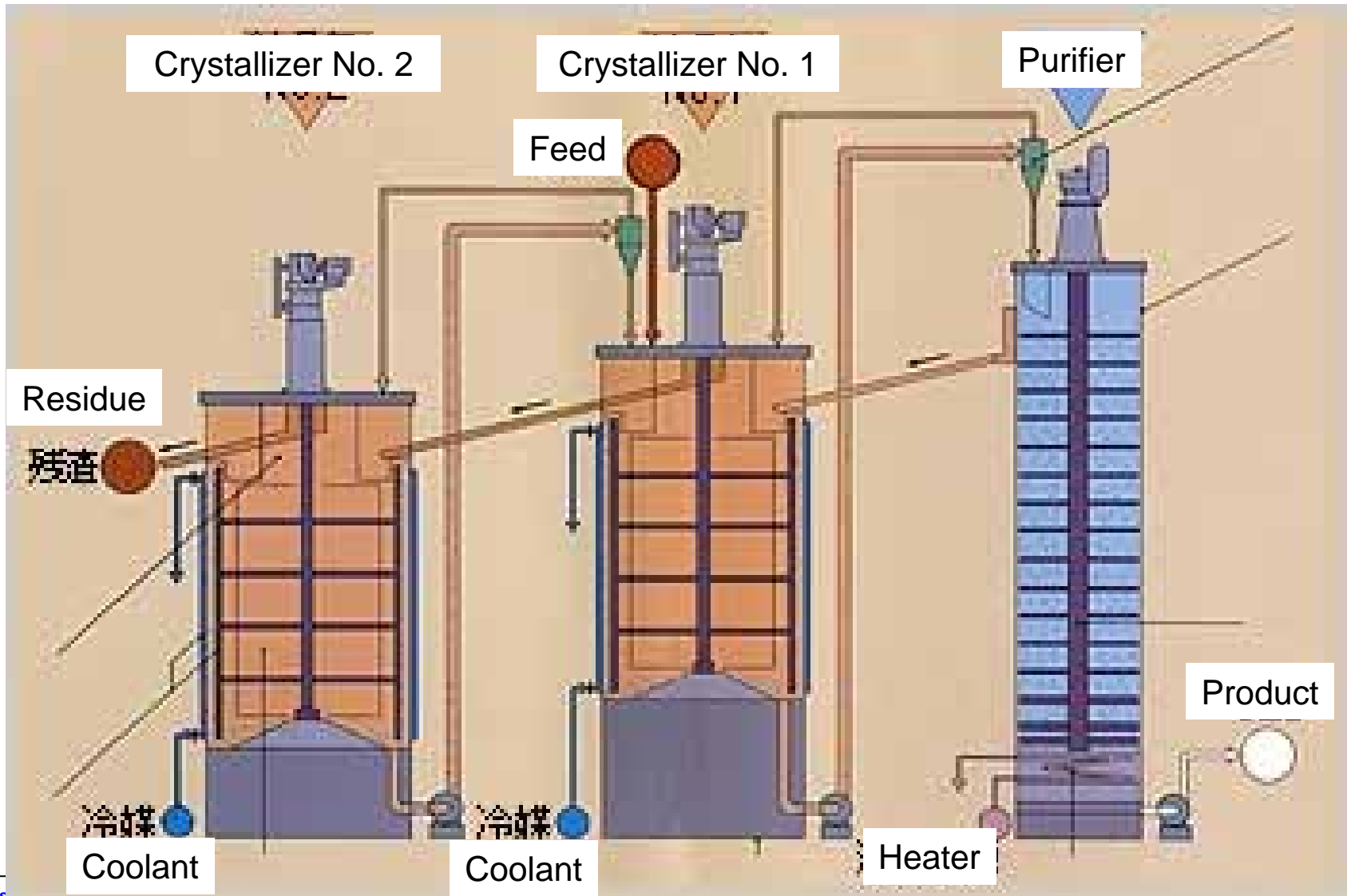
A: Let me check your calculation first. Can you send me the simulation file?

B: Run more case studies. Nth= 50, 100, 150 and RR= 10, 50, 100.

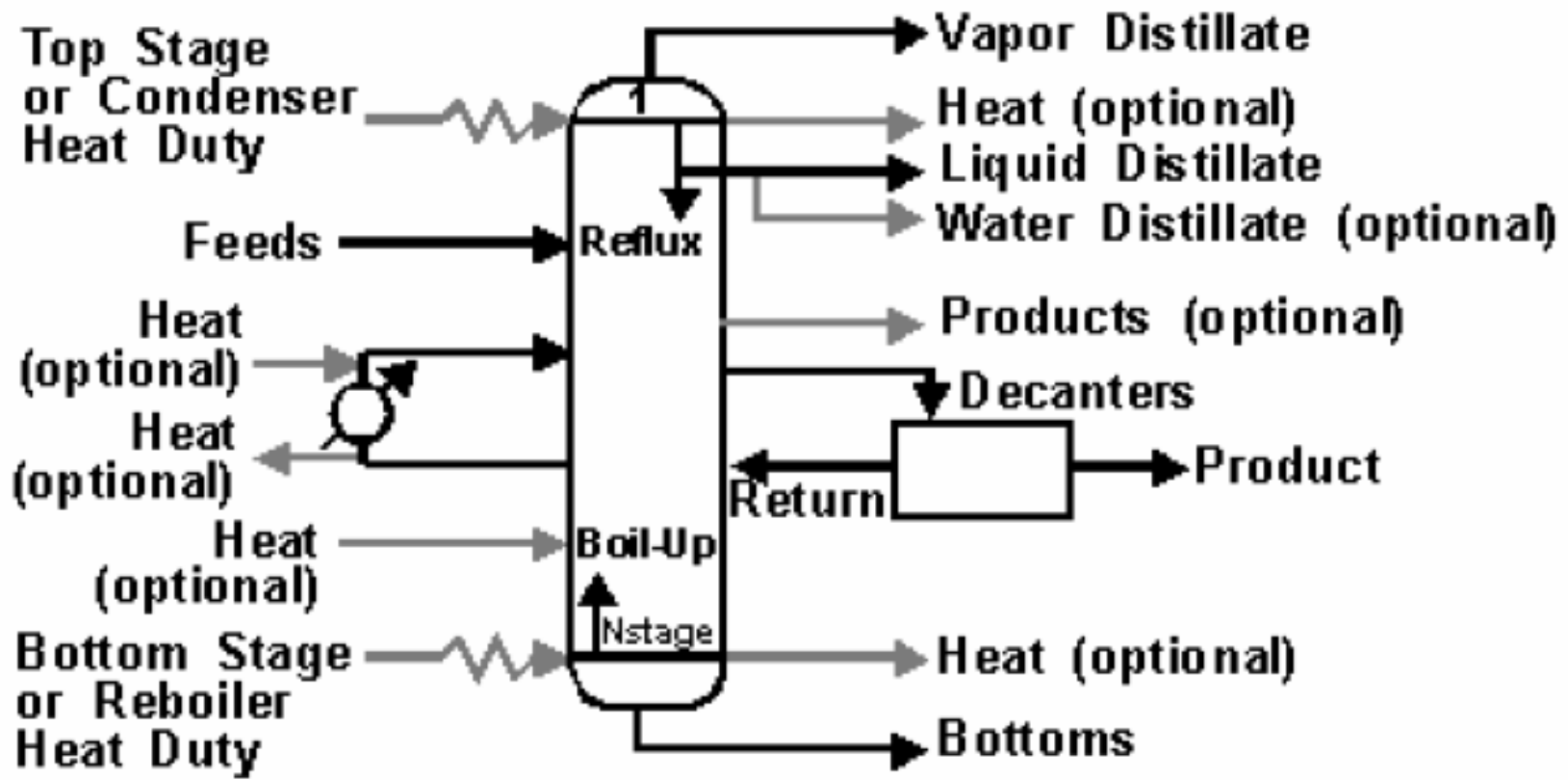
C: As the boiling points difference is only 6C, distillation is not practical. Make research on other separations.



# Crystallization for p-dichlorobenzene production



# Why 6C Difficult for Distillation ?



We may realize this fact after many case studies.

Better way ?



# Why 6C Difficult for Distillation ?

$$N_{\text{act}} = 1350 / \Delta T$$

Rigorously speaking, we need components, VLE, target purity to calculate the number of stages.

However, existing columns have common features.

“Molecular Chemical Engineering for Process Design”  
(Kawai, Mitsubishi Kasei, November 1987)

Common Sense As

“Quick calculation method from experience”

# Rigorous Simulation vs. Common Sense

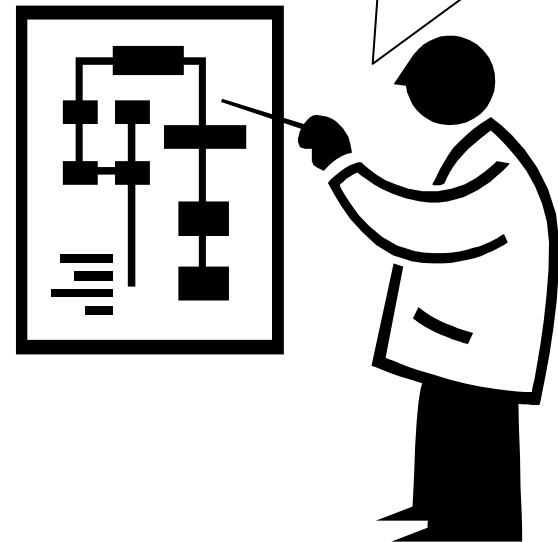
## 2. Install Steam Turbine, or not ?

# What Is Best for Energy Saving ?

Do you think it a good idea to install steam turbine to save energy of my plant site?

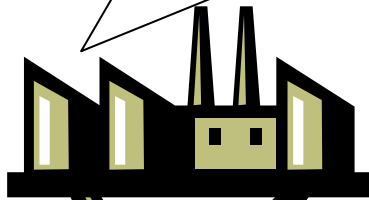


Maybe. Do you know the steam demand and electricity demand on your site?

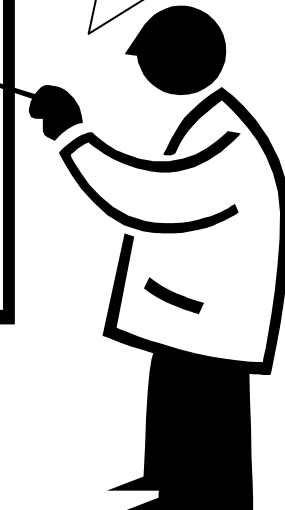
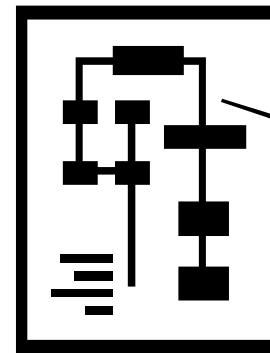


# Energy Saving Planning

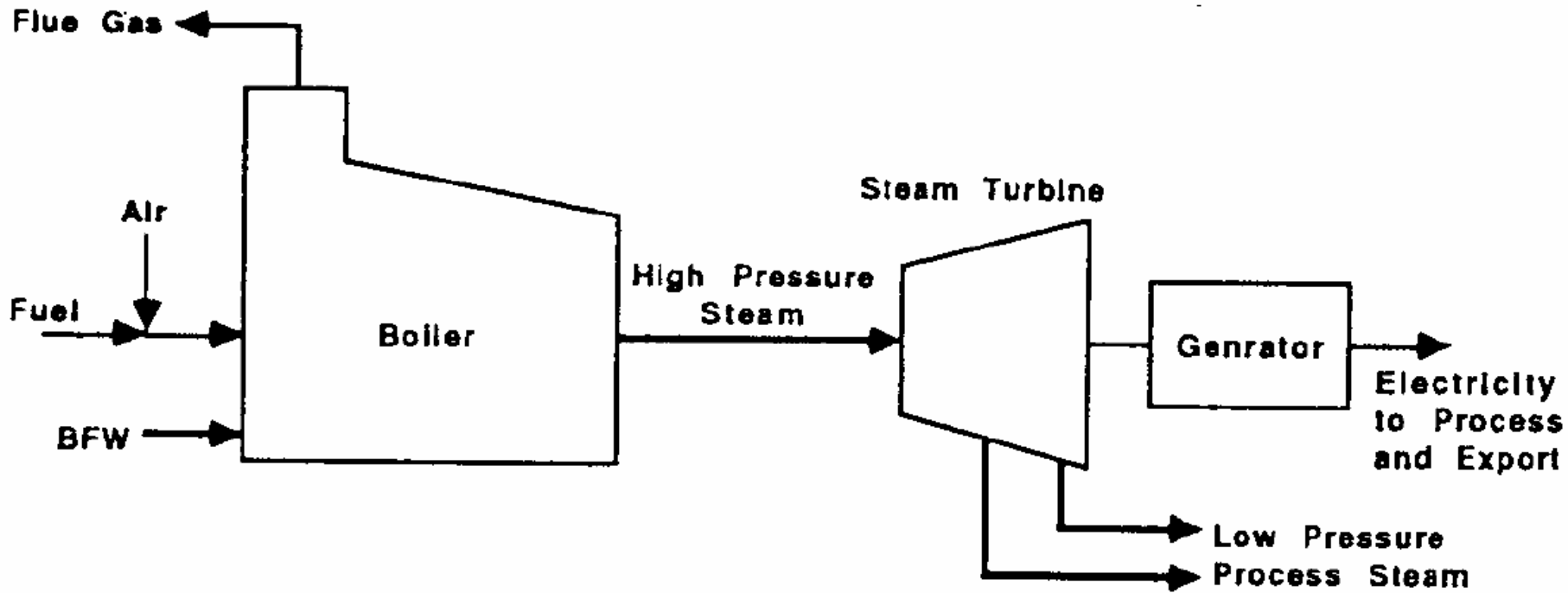
Total steam consumption is 300 t/hr and electricity consumption is 100 MW.



My suggestion is that you consider Gas Turbine first. You can also study steam turbine to combine with gas turbine.

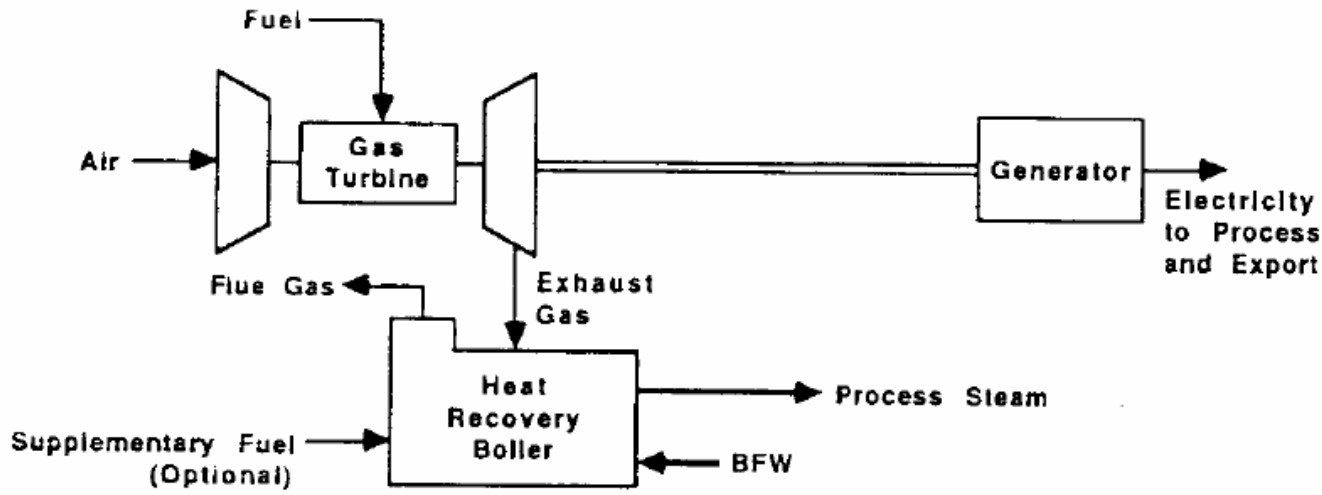


## A. STEAM TURBINE TOPPING CYCLE



Steam turbine system produces steam [t/h] and electricity [MW] with the ratio of 6-17.

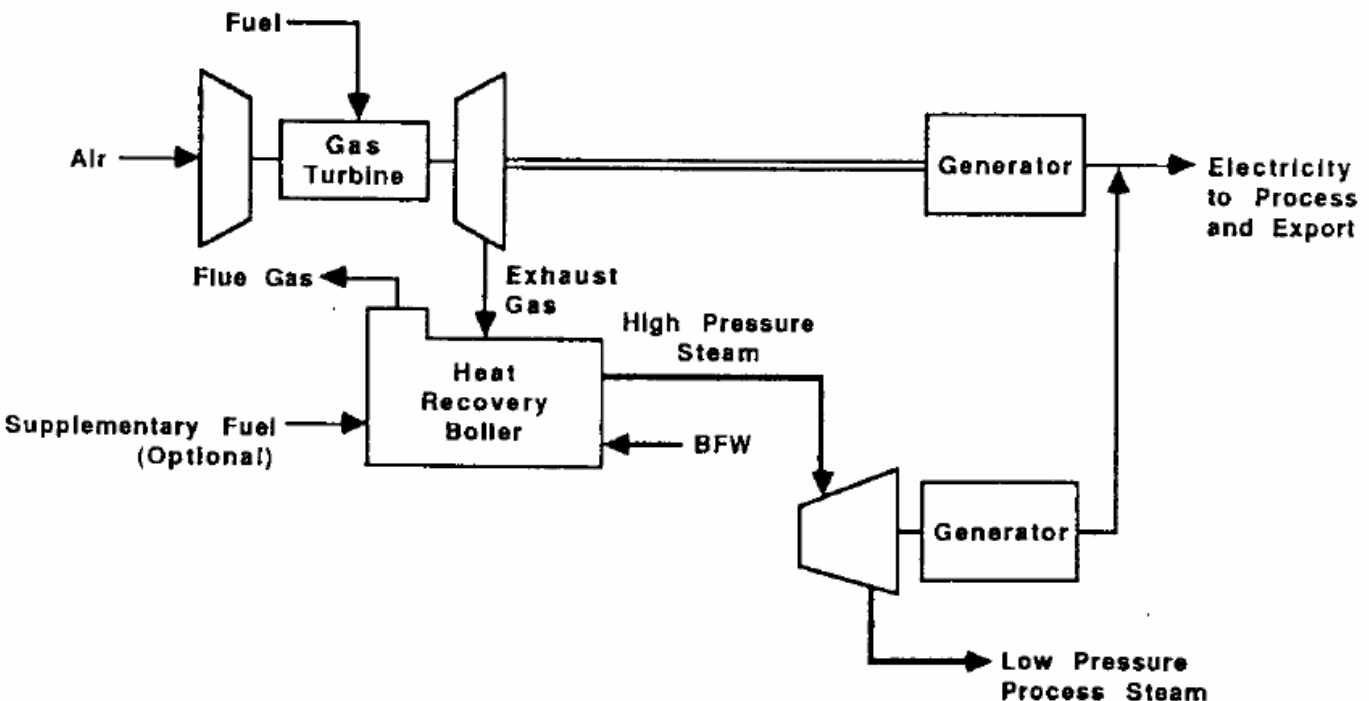
**B. GAS TURBINE TOPPING CYCLE**



$$\frac{\text{steam}[t / hr]}{\text{electricity}[MW]}$$

**= 2 - 4**

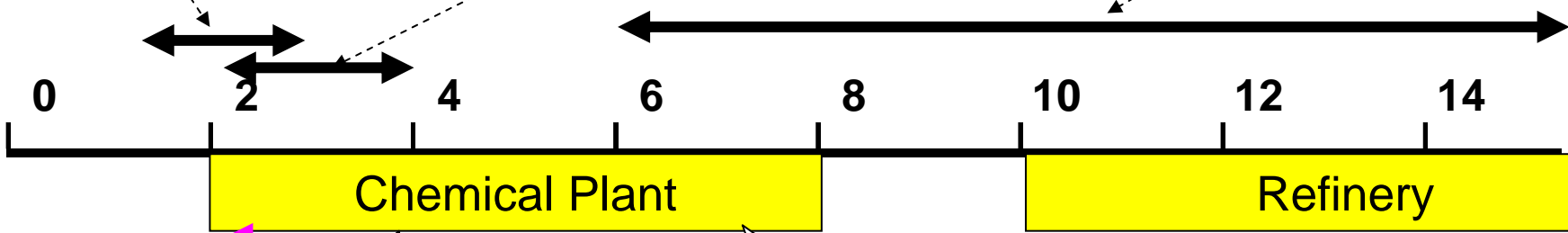
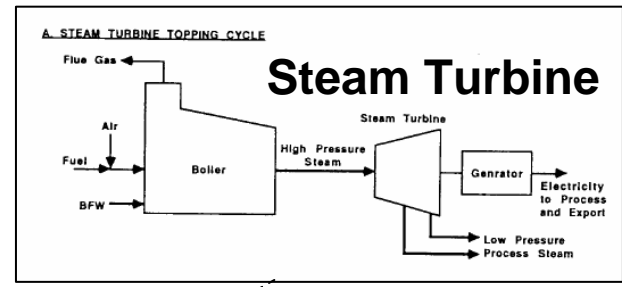
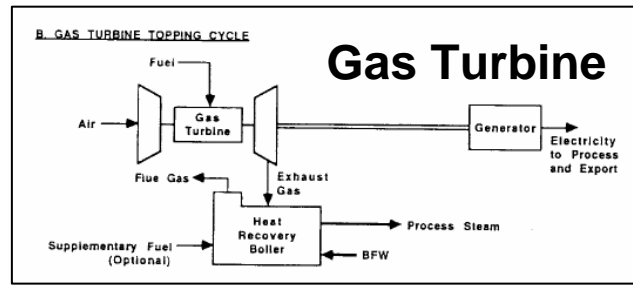
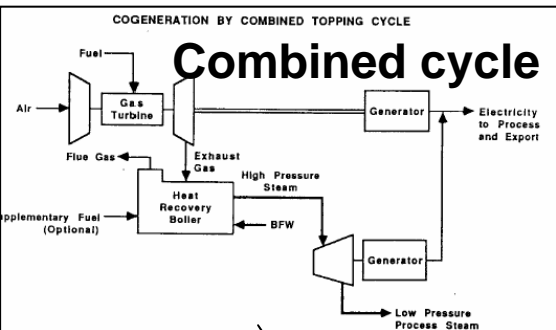
**COGENERATION BY COMBINED TOPPING CYCLE**



**= 1.5 - 3**



# Common Sense As "Procedure and figures from experience"



Further energy saving is difficult.

Install Gas Turbine and Combined Cycle to reduce electricity further.

Introduce site steam turbine system to reduce electricity cost.

Start the energy saving here. Steam is easier to reduce than electricity

# Rigorous Simulation vs. Common Sense

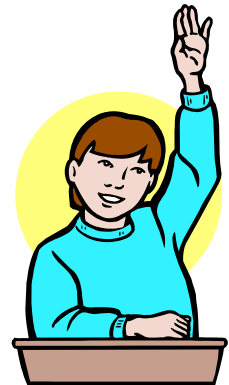
3. Which can capture the image ?





“We conducted experimental study, ran simulator and found (A) this reaction is in 1<sup>st</sup> order and (B) the rate constant is 10 [1/min].”

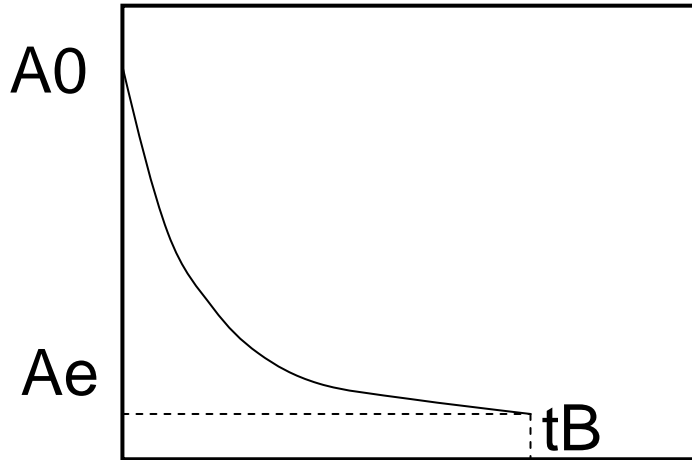
“Is it a fast reaction ?”



# Answer #1

- Look at unit of  $k=10$  [1/min].
- [1/min] is not familiar to us, but [min] is a familiar unit.
- Take the inverse of [1/min], then we obtain 0.1 [min].
- This must be some time constant related to this reaction. 0.1min is 6 sec.
- This sounds like a fast reaction, but I should compare it with other time constants such as residence time of reactor.

# Answer #2, more theoretically



$$\frac{dA}{dt} = -kA$$

$$\frac{A_e}{A_0} = e^{-kt_B}$$

1. half-time =  $\ln(2)/k = 0.693/10 = 0.0693 \text{ min} = 4.2 \text{ sec}$

1'. "time to  $1/e$  ( $\approx 40\%$ ) =  $1/k = 0.1 \text{ min} = 6 \text{ sec}$

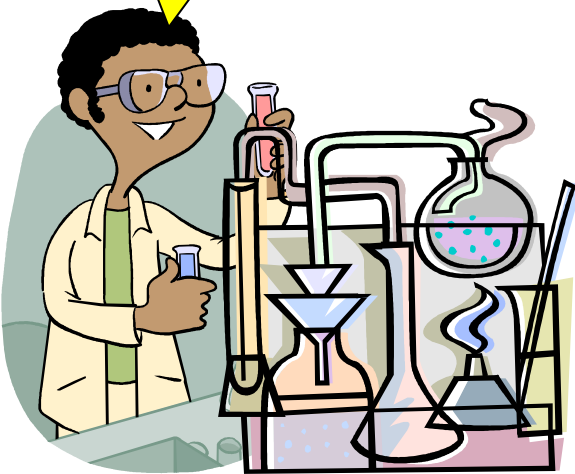
2. We need other time constants for comparison.

Common Sense From  
Theory (Physical Chemistry)

# Recommendation

- Common sense, rule-of-thumb, heuristics, back-of-the-envelope calculation are critical for correct judgment to complicated calculations.
- Their sources are not only experience but also physical chemistry.
- They are essential compliment to process simulation for conceptual process design.

Check the results with Rule-Of-Thumb



Experimental Work

A new finding

Prediction from initial model

Additional data

Refined model



Check the results with Rule-Of-Thumb



Modeling & Simulation



**Thank you for your attention !**

**PreFEED Corporation provide**

- (1) Advanced Chemical Engineering Training (Data Analysis; Phase Equilibrium; Batch vs. Continuous; Modeling; Rule-Of-Thumb)**
- (2) Modeling Consultancy**
- (3) Support to Equation Solver**