

# Exam

## Pan American Advanced Studies Institute Program on Process Systems Engineering

Name: \_\_\_\_\_

### Module: Optimization

Nonlinear programming (30 pts) \_\_\_\_\_

Mixed-integer programming (30 pts) \_\_\_\_\_

Global Optimization (30 pts) \_\_\_\_\_

### Module: Process and Product Design

Metabolic networks (30 pts) \_\_\_\_\_

Mass exchange networks (30 pts) \_\_\_\_\_

Heat integration (30 pts) \_\_\_\_\_

### Module: Scheduling and Supply Chain

Scheduling (30 pts) \_\_\_\_\_

Supply chain (30 pts) \_\_\_\_\_

New product development (30 pts) \_\_\_\_\_

### Module: Process Control

Process Dynamics/Control (30 pts) \_\_\_\_\_

Model Predictive Control (30 pts) \_\_\_\_\_

Process Control Design (30 pts) \_\_\_\_\_

TOTAL (360 pts) \_\_\_\_\_

**Pan American Advanced Studies Institute**  
**Program on Process Systems Engineering**  
**Part 1. Nonlinear Programming and Dynamic Optimization**  
**Exam Questions**

1. Consider the NLP:

$$\begin{aligned} \text{Min } & (x_2)^2 \\ \text{s.t. } & x_1 - x_2 + 1 \leq 0 \\ & -x_1 - x_2 + 1 \leq 0 \end{aligned}$$

- a) Convert this problem to bound constrained and write the KKT conditions for this problem.
- b) Identify the basic and nonbasic variables. How many superbasic variables are there? Are the sufficient second order KKT conditions satisfied?
- c) Solve this problem with a barrier method. Quantitatively describe the trajectory of  $x(\mu)$  and  $f(x(\mu))$  as  $\mu \rightarrow 0$ .

2. Using the coordinate basis, apply range and null space decomposition and solve for the linear system:

$$\begin{bmatrix} W & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} d \\ \lambda \end{bmatrix} = - \begin{bmatrix} \nabla f \\ c \end{bmatrix} \quad \text{with } W = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad A = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \quad \nabla f = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad c = [2]$$

3. Consider the reactor optimal control problem below. Assume that temperature is a function of time.

$$\begin{aligned} \text{Max } & c_2(1.0) \\ \text{s.t. } & dc_1/dt = -k_1(T) c_1^2, c_1(0) = 1 \\ & dc_2/dt = k_1(T) c_1^2 - k_2(T) c_2, c_2(0) = 1 \end{aligned}$$

where  $k_1 = 4000 \exp(-2500/T)$ ,  $k_2 = 62000 \exp(-5000/T)$  and  $298 \leq T(t) \leq 398$ .

- a) Write the optimality conditions for this optimal control problem.
- b) Formulate this problem as an NLP using orthogonal collocation on finite elements. Choose two collocation points and 10 elements. Do not solve.

## Part 1. Exam. Mixed-Integer Optimization

1. The logic condition  $y_1 \Rightarrow y_2, \neg y_1 \vee \neg y_2$  can be represented with the constraints  $y_1 = 0, y_2 = \delta, \delta = 0, 1, 0 \leq y_1, y_2 \leq 1$ . Is this a better, equal or worse model than using the following linear inequalities that are derived from CNF form,  $y_1 \leq y_2, y_1 + y_2 \leq 1, y_1, y_2 = 0, 1$ ?
2. Formulate mixed-integer linear constraints for the following disjunction, using both big-M and convex-hull formulations:  
Either  $0 \leq x \leq 10$  or  $20 \leq x \leq 30$
3. Consider the mixed-integer linear programming problem

$$\begin{aligned} \min Z &= a^T x + b^T y \\ \text{s.t.} \quad & Ax + B y \leq d \\ & x \geq 0, y \in \{0, 1\} \end{aligned}$$

Assume it is desired to solve this problem by Benders decomposition where the 0-1 variables are treated as "complicating" variables for the master problem. If the LP subproblems for fixed  $y^k, k=1, 2, \dots, K$  are feasible with an optimal solution  $x^k$  and multipliers  $\lambda_k$ , show that the master problem can be formulated as follows:

$$\begin{aligned} Z_L^K &= \min \alpha \\ \text{st } \alpha &\geq b^T y + \lambda_k^T [B y - d] \quad k = 1, 2, \dots, K \\ \alpha &\in R^1, y \in \{0, 1\} \end{aligned}$$

## Part 1. Global optimization. Exam questions

**Question 1.** Find the generating sets for the convex and concave envelopes of the function  $f = (x_1x_2 + x_3x_2)/y$  over  $\{0 < x_i^L \leq x_i \leq x_i^U \text{ for } i = 1, \dots, 3, 0 < y^L \leq y \leq y^U\}$ .

**Question 2.** Find the generating sets for the convex and concave envelopes of the function  $g = x/y + 3x + 4xy + 2xy^2$  over  $\{0 < x^L \leq x \leq x^U, 0 < y^L \leq y \leq y^U\}$ .

**Question 3.** Consider the following pooling problem (Haverly, 1978):

$$\begin{aligned} \min \quad & -9x_5 - 15x_9 + 6x_1 + 16x_2 + 10x_6 \\ \text{s.t.} \quad & x_1 + x_2 = x_3 + x_4 \\ & x_3 + x_7 = x_5 \\ & x_4 + x_8 = x_9 \\ & x_7 + x_8 = x_6 \\ & x_{10}x_3 + 2x_7 \leq 2.5x_5 \\ & x_{10}x_4 + 2x_8 \leq 1.5x_9 \\ & 3x_1 + x_2 = x_{10}(x_3 + x_4) \\ & (0,0,0,0,0,0,0,0,1) \leq \mathbf{x} \\ & \mathbf{x} \leq (300,300,100,200,100,300,100,200,200,3) \end{aligned}$$

(a) Solve this pooling problem by branch-and-bound manually:

- Disaggregate products and use the convex and concave envelopes of the bilinear terms to construct a relaxation.
- You may use GAMS/MINOS or GAMS/CPLEX or any other LP code to solve the relaxed problems.
- Use the best-bound node selection rule to select nodes.
- Use bisection of longest edge for branching but branch on the incumbent when possible.
- You may use GAMS/MINOS or your favorite local search every three branch-and-bound iterations using the corresponding relaxation point as the starting point.
- Terminate the search as soon as your lower and upper bounds are within 0.001.

(b) Solve the same model (after product disaggregation) with GAMS/BARON in two different ways:

- 1 Using default BARON settings.
- 2 Using BARON settings to apply the above algorithm (best-bound node selection, bisection of longest edge, branching on incumbent, local search every three branch-and-bound iterations, termination within an absolute gap of 0.001).  
*Hint:* If BARON outperforms your algorithm, it is because you need to change some of its default options.

## Problem Set

**Problem 1:** Consider the small-scale *Escherichia coli* metabolic network comprised of 92 reactions and 58 metabolites. The GAMS file “mininetwork.inc” provides the stoichiometry of the reactions in a GAMS-compatible format and the spreadsheet “smallnetwork.xls” shows the reaction network and metabolites. These 92 reactions include both internal and transport reactions. Similarly, there are both intracellular and extracellular metabolites in the model. An example of extracellular metabolite is SUCCxt (i.e. extracellular succinate). The suffix (xt) designates the extracellular metabolites. Some reactions lead to a drain of metabolites such as formate (reaction 88) and glycerol (reaction 91). The biomass formation in the network is treated as a drain of precursors in the appropriate ratios (reaction 79).

Assume that the organism can only uptake glucose (rxn 1) at a fixed rate of (10 mmol/gDW.hr) and unlimited amounts of phosphate (reaction 12) and oxygen (reaction 8). This means that the flux through all other transport reactions (i.e., 2, 4, 6, 9, 10 and 13) should be set to zero in this study.

- (i) Identify the maximum biomass formation in the network given a glucose uptake of 10 mmol/gDW.hr
- (ii) Pinpoint which single reaction deletions and thus corresponding gene knock-outs, in the network are lethal (i.e. they lead to zero biomass formation).
- (iii) Identify one or more reactions whose deletion lead to the formation of the maximum amount of ethanol (reaction 7) when biomass is maximized.

**Problem 2:** Use OptKnock (optknock.gms) to identify a single, double and triple knock-out strategy that maximizes ethanol production. Any alternate optima ?

**Problem 3:** Given that the network uptakes a fixed amount of glucose (10 mmol/gDW.hr) to form biomass, determine

- (i) If there exist any “blocked” reactions in the network.
- (ii) Which reaction pairs out of the following set of reactions *pfkA*, *pgk*, *gnd*, *acnA* and *adhE* are fully, partially or directionally coupled?

## Practice Exercises for Mass Integration and Pollution Prevention

1. Consider the VAM process described in the lecture. A new reaction pathway has been developed and will to be used for the production of VAM. This new reaction does not involve acetic acid. The rest of the process remains virtually unchanged and the AA losses with the product are 100 kh/hr. What are the targets for minimum fresh usage and discharge/losses of AA?
2. Consider the food processing plant shown in the simplified flowsheet of Fig. 1. The primary feedstocks are first pre-washed then processed throughout the facility. The gaseous waste of the process is cleaned in a water scrubber prior to discharge. Therefore, the process has two sinks that consume fresh water: the washer and the scrubber. Table 1 provides the data for these two sinks. The process results in two aqueous streams that are sent to biotreatment but may be considered for recycle: condensate I from the evaporator and condensate II from the stripper. The data for the two process sources are given in Table 2.

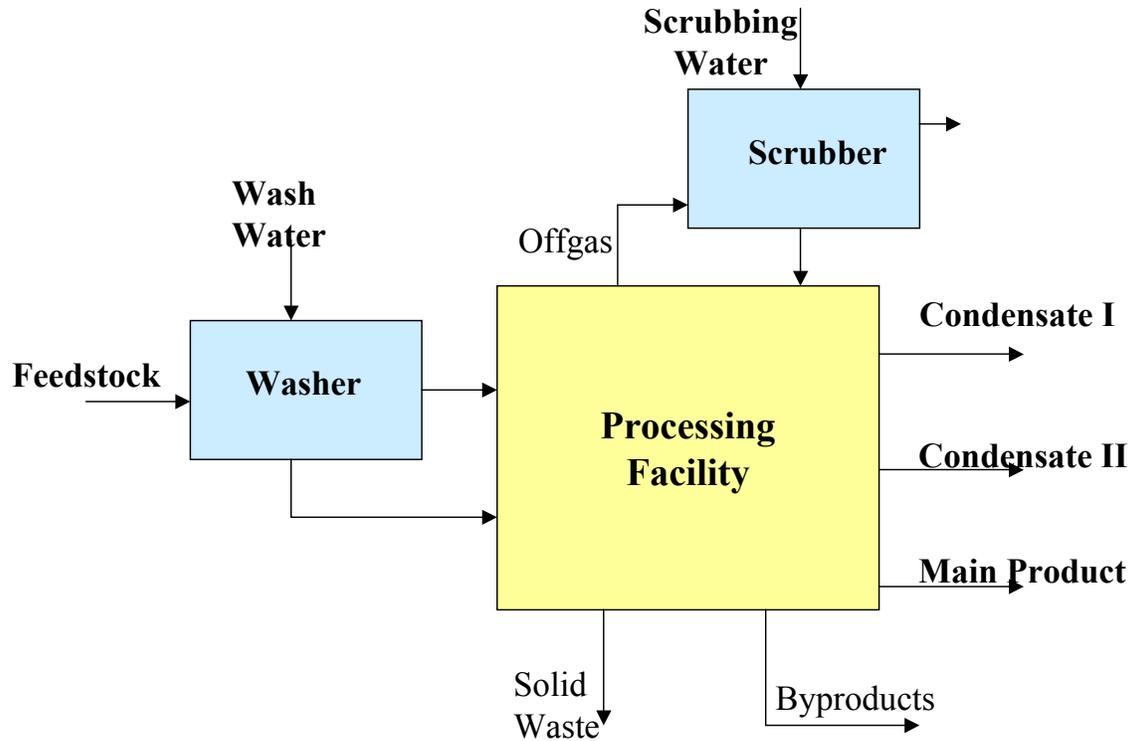


Fig. 1. A Simplified Flowsheet of the Food Processing Plant

Table 1. Sink Data for the Food Processing Example

Sink	Flowrate kg/hr	Maximum Inlet Mass Fraction	Maximum Inlet Load, kg/hr
Washer	8,000	0.03	240
Scrubber	10,000	0.05	500

Table 2. Source Data for the Food Processing Example

Source	Flowrate kg/hr	Maximum Inlet Mass Fraction	Maximum Inlet Load, kg/hr
Condensate I	10,000	0.02	200
Condensate II	9,000	0.09	810

At present, the plant uses fresh water for the washer and the scrubber. In order to reduce the usage of fresh water and discharge of wastewater (condensate), the plant has decided to adopt direct-recycle strategies. An engineer has proposed that Condensate I be recycled to the scrubber (Fig. 2). The result of this project is to eliminate the need for fresh water in the scrubber, reduce overall fresh water consumption to 8,000 kg/hr, and reduce wastewater discharge (Condensate II) to 9,000 kg/hr. Critique this proposed project (compare it with the minimum water-using solution, describe the differences, discuss why an integrated approach yields insights unseen by localized approaches, etc.).

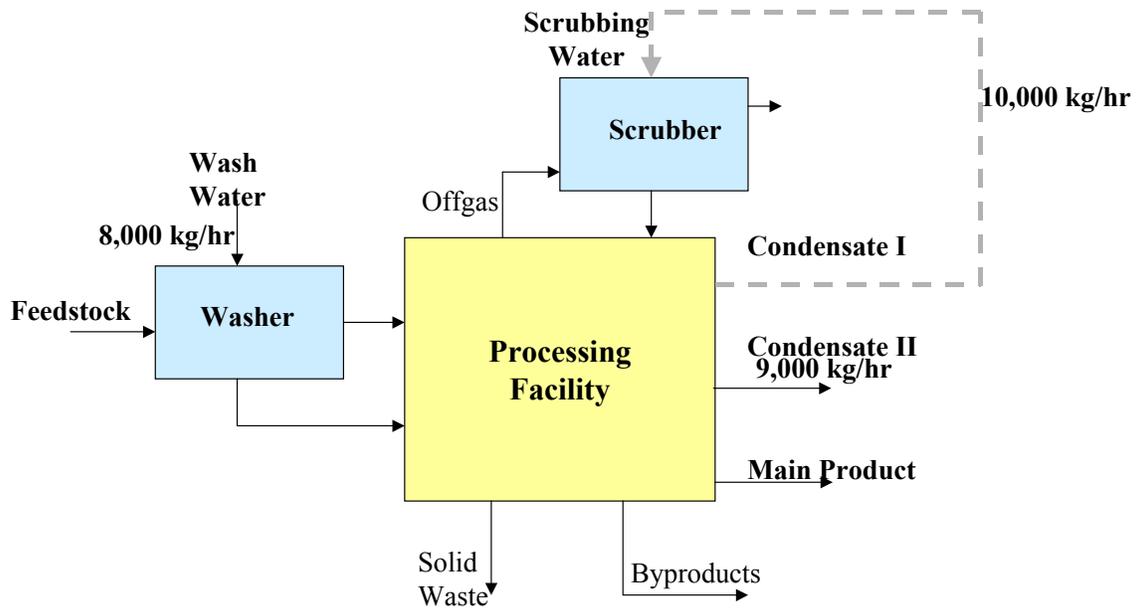
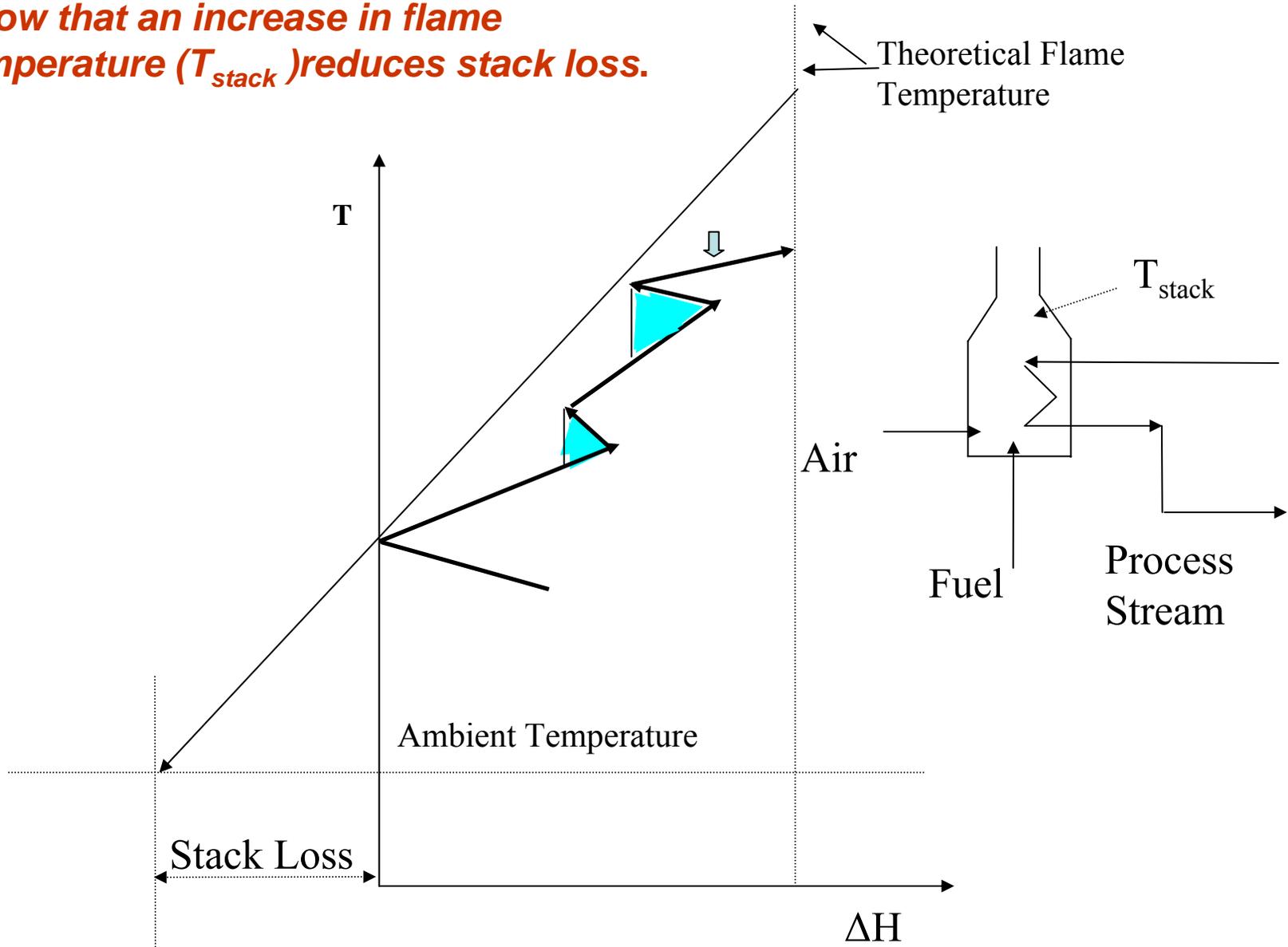


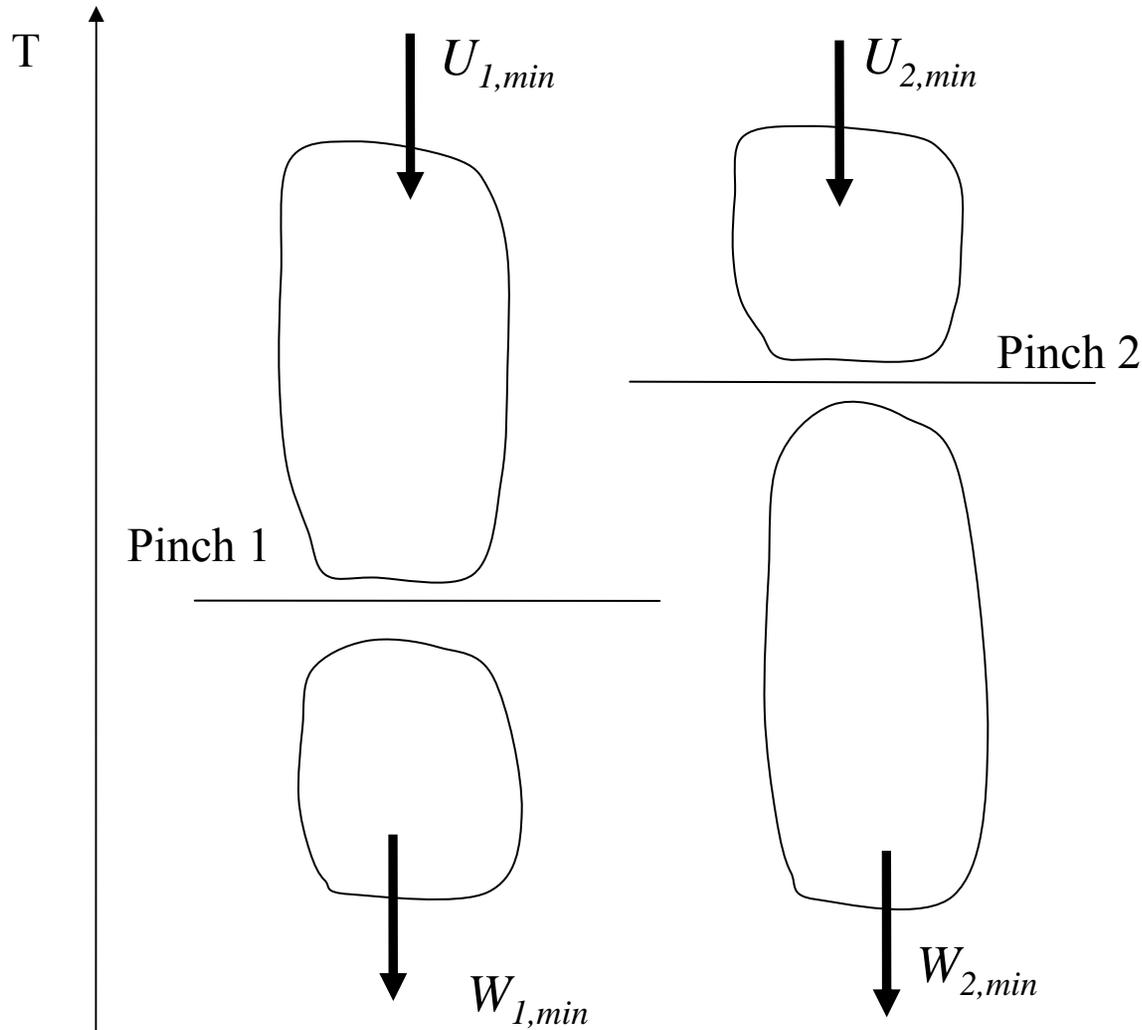
Fig. 2. Proposed Recycle Project

# Question 1

*Show that an increase in flame temperature ( $T_{stack}$ ) reduces stack loss.*



# Question 2



Consider two plants with the following Minimum utility and pinch points.

Assume  $Q_T$  is to be transferred between pinches. State under what conditions one would also want to transfer heat between plants at temperatures above Pinch 2.

# Question 3

Consider the following data

STREAM	FCp (kW/°C)	Tin (°C)	Tout (°C)
S1	0.15	300	80
S2	0.225	200	40
S3	0.2	40	180
S4	0.3	140	280

Use  $\Delta T_{\min} = 10$  °C.

- a) Design the maximum energy recovery network.**
- b) Use Loops and Paths to Relax the network.**

## Pan American Advanced Institute Program on Process Systems Engineering

### BATCH SCHEDULING

#### EXERCISES

1. A chemical plant producing a pair of final products P1 and P2 is to be scheduled in order to maximize the profit over a time horizon of 24 h. The process involves the production of three intermediates (I1, I2, I3) from feedstocks A and B, which are subsequently transformed into the end products P1 and P2 (see Table 1). Intermediate I3 is synthesized from a (60:40)-mix of intermediates I1 and I2 through Task-3. The quantity of I3 yielded by Task-3 is then applied to the synthesis of the final products P1 and P2 in equal amounts (50:50). Five processing tasks are to be performed in three equipment units (E1, E2, E3), with each one being devoted to a subset of the tasks as shown in Table 2. Capacities of the processing units in Kg are also given in Table 2. Data related to intermediate and final products are included in Table 3.

Task	States Consumed	States Produced
Task-1	Feed-A	I1
Task-2	Feed-B	I2
Task-3	I1, I2 (60% : 40%)	I3
Task-4	I3 (50%)	P1
Task-5	I3 (50%)	P2

Table 1. States consumed and produced by each task

Task	E1	E2	E3
Task-1	3	4	
Task-2	5	5	
Task-3	6	5	
Task-4			3
Task-5			7
Capacity (Kg)	100	200	400

Table 2. Constant task processing times (in h)

State	Initial Inventory (Kg)	Dedicated Tank Capacity (Kg)	Minimum Demand (Kg)	Unit Price (\$/Kg)
Feed-A	2000	Unlimited		1
Feed-B	2000	Unlimited		2
I1	--	200	--	-
I2	--	200	--	-
I3	80	500	--	-
P1	50	Unlimited	250	8
P2	50	Unlimited	200	12

Table 3. State Data

- a) Find the production schedule that maximizes the profit using:
- a discrete-time scheduling model
  - a continuous-time scheduling formulation
- b) Let now assume that Task-1 and Task-2 both require heat provided by steam. The coefficient values for the fixed and variable steam consumption terms are:

Task	$\mu_{ir}$	$v_{ir}$
Task-1	5	0.20
Task-2	4	0.25

Table 4. Steam consumption coefficients for tasks 1 & 2

Find the new best production schedule maximizing the profit.

2. Let us consider a make-to-stock sequential batch facility involving three processing stages (S1, S2, S3) where a single batch of five different products (P1, P2, P3, P4, P5) all following the same routing (S1 → S2 → S3) are to be produced. In each stage, several identical units are running in parallel (Table 1). Table 2 includes the batch processing time for every product at each stage. Setup times are negligible.

Stage	Set of Equipment Units
S1	E1, E2
S2	E4, E5
S3	E6, E7

Table 1. Set of parallel units in each stage

Product	S1	S2	S3
P1	18	12	9
P2	16	13	11
P3	15	15	12
P4	10	12	15
P5	12	14	10

Table 2. Processing times (in h)

- a) Find the production schedule that minimizes the time required to complete all the batches by using:
- the slot-based continuous time model
  - the global general precedence continuous formulation
- b) Let us consider the following sequence-dependent setup times:

	P1	P2	P3	P4	P5
P1		1.5	1.0	1.2	3.0
P2	1.3		0.9	1.2	1.4
P3	0.8	0.9		0.5	1.0
P4	1.1	2.5	0.7		1.6
P5	1.0	1.4	0.5	.6	

Table 3. Sequence-dependent setup times

Find the new best production schedule minimizing the makespan.

### Part 3. Exam. Supply chain optimization

#### 1. Capacitated Plant Location Model (Chopra and Meindl, 2004)

SC consulting, a supply chain consulting firm, has to decide on the location of its home offices. Their clients are primarily located in the 16 states in Table 1 below. There are four potential sites for home offices: Los Angeles, Tulsa, Denver, and Seattle. The annual fixed cost of locating an office in Los Angeles is \$165,428, Tulsa is \$131,230, Denver is \$140,000 and Seattle is \$145,000. The expected numbers of trips to each state and the travel costs from each potential site are also shown in Table 1.

Table 1. Travel costs and number of trips

State	Travel costs (\$)				Number of trips
	Los Angeles	Tulsa	Denver	Seattle	
Washington	150	250	200	25	40
Oregon	150	250	200	75	35
California	75	200	150	125	100
Idaho	150	200	125	125	25
Nevada	100	200	125	150	40
Montana	175	175	125	125	25
Wyoming	150	175	100	150	50
Utah	150	150	100	200	30
Arizona	75	200	100	250	50
Colorado	150	125	25	250	65
New Mexico	125	125	75	300	40
North Dakota	300	200	150	200	30
South Dakota	300	175	125	200	20
Nebraska	250	100	125	250	30
Kansas	250	75	75	300	40
Oklahoma	250	25	125	300	55

Each consultant is expected to take at most 25 trips each year.

- If there are no restrictions on the number of consultants at a site and the goal is to minimize costs, where should the home offices be located and how many consultants should be assigned to each office? What is the annual cost in terms of the facility and travel?
- If at most 10 consultants are to be assigned to a home office, where should the offices be set up? How many consultants should be assigned to each office? What is the annual cost of this network?
- What do you think of a rule where all consulting projects out of a given state should be assigned to one home office? How much is this policy likely to add to cost compared to allowing multiple offices to handle a single state?

2.

Sunchem, a manufacturer of printing inks, has five manufacturing plants worldwide. Their locations and capacities are shown in Table 2 along with the cost of producing one ton of ink at each facility. The production costs are in the local currency of the country where the plant is located. The major markets are North America, South America, Europe, Japan, and the Rest of Asia. Demand at each market is shown in Table 2. Transportation costs from each plant to each market in US dollars are shown in Table 2. Management has to come up with a plan for 2006.

- (a) If exchange rates are expected as in Table 3, and no plant can run below 50% capacity, how much should each plant produce and which markets should each plant supply?
- (b) If there are no limits on the amount produced in each plant, how much should each plant produce?
- (c) Can adding 10 tons of capacity in any plants reduce costs?
- (d) How should Sunchem account for the fact that exchange rates fluctuate over time?

Table 2.

	North America	South America	Europe	Japan	Asia	Capacity (tons/year)	Production cost/ ton
USA	600	1,200	1,300	2,000	1,700	185	\$10,000
Germany	1,300	1,400	600	1,400	1,300	475	6,400 Euros
Japan	2,000	2,100	1,400	300	900	50	1,800,000 Yen
Brazil	1,200	800	1,400	2,100	2,100	200	14,000 Real
India	2,200	2,300	1,300	1,000	800	80	400,000 rupees
Demand (tons/year)	270	190	200	120	100		

Table 3. Exchange rates

	US\$	Euro	Yen	Real	Rupee
US \$	1.000	0.840	111.6	2.366	43.53
Euro	1.190	1	132.9	2.815	51.82
Yen	0.00896	0.00750	1	0.0212	0.390
Real	0.42267	0.35510	47.1747	1	18.40
Rupee	0.02297	0.01930	2.56368	0.0543	1

### 3. Managing Growth at SportStuff.com

In December 2000, Sanjay Gupta and his management team were busy evaluating the performance at SportStuff.com over the last year. Demand had grown by 80 percent over the year. This growth, however, was a mixed blessing. The venture capitalists supporting the company were very pleased with the growth in sales and the resulting increase in revenue. Sanjay and his team, however, could clearly see that costs would grow faster than revenues if demand continued to grow and the supply chain network was not redesigned. They decided to analyze the performance of the current network to see how it could be redesigned to best cope with the rapid growth anticipated over the next three years.

#### **SPORTSTUFF.COM**

Sanjay Gupta founded SportStuff.com in 1996 with a mission of supplying parents with more affordable sports equipment for their children. Parents complained about having to discard expensive skates, skis, jackets, and shoes because children outgrew them rapidly. Sanjay's initial plan was for the company to purchase used equipment and jackets from families and any surplus equipment from manufacturers and retailers and sell

these over the Internet. The idea was very well received in the marketplace, demand grew rapidly, and by the end of 1996 the company had sales of \$0.8 million. By this time a variety of new and used products were sold and the company received significant venture capital support.

In June 1996, Sanjay leased part of a warehouse in the outskirts of St. Louis to manage the large amount of product being sold. Suppliers sent their product to the warehouse. Customer orders were packed and shipped by UPS from there. As demand grew, SportStuff.com leased more space within the warehouse. By 1999, Sportstuff.com leased the entire warehouse and shipped to customers all over the United States. Management divided the United States into 6 customer zones for planning purposes. Demand for each customer zone in 1999 was as shown in Table 4. Sanjay estimated that the next three years would see a growth rate of about 80 percent per year, after which demand would level off.

### THE NETWORK OPTIONS

Sanjay and his management team could see that they needed more warehouse space to cope with the anticipated growth. One option was to lease more warehouse space in St. Louis itself. Other options included leasing warehouses all over the country. Leasing a warehouse involved fixed costs based on the size of the warehouse and variable costs that varied with the quantity shipped through the warehouse. Four potential locations for warehouses were identified in Denver, Seattle, Atlanta, and Philadelphia. Warehouses leased could be either small (about 100,000 sq. ft.) or large (200,000 sq. ft.). Small warehouses could handle a flow of up to 2 million units per year whereas large warehouses could handle a flow of up to 4 million units per year. The current warehouse in St. Louis was small. The fixed and variable costs of small and large warehouses in different locations are shown in Table 5.

Sanjay estimated that the inventory holding costs at a warehouse (excluding warehouse expense) was about  $\$600 \sqrt{F}$  where  $F$  is the number of units flowing through the warehouse per year. Thus, a warehouse handling 1,000,000 units per year incurred an inventory holding cost of \$600,000 in the course of the year. Use the following inventory costs:

Range of F	Inventory Cost
0-2 million	$\$250,000 + 0.310F$
2-4 million	$\$530,000 + 0.170F$
4-6 million	$\$678,000 + 0.133F$
Over 6 million	$\$798,000 + 0.113F$

SportStuff.com charged a flat fee of \$3 per shipment sent to a customer. An average customer order contained four units. SportStuff.com in turn contracted with UPS to handle all its outbound shipments. UPS charges were based on both the origin and the destination of the shipment and are shown in Table 6. Management estimated that unbound transportation costs for shipments from suppliers were likely to remain unchanged, no matter what the warehouse configuration selected.

### QUESTIONS

1. What is the cost SportStuff.com incurs if all warehouses leased are in St. Louis?
2. What supply chain network configuration do you recommend for SportStuff.com?

Table 4.

Zone	Demand in 1999	Zone	Demand in 1999
Northwest	320,000	Lower Midwest	220,000
Southwest	200,000	Northeast	350,000
Upper Midwest	260,000	Southeast	175,000

Table 5.

Location	Small Warehouse		Large Warehouse	
	Fixed cost (\$/year)	Variable cost (\$/unit flow)	Fixed cost (\$/year)	Variable cost (\$/unit flow)
Seattle	300,000	0.20	500,000	0.20
Denver	250,000	0.20	420,000	0.20
St. Louis	220,000	0.20	375,000	0.20
Atlanta	220,000	0.20	375,000	0.20
Philly	240,000	0.20	400,000	0.20

Table 6.

	Northwest	Southwest	Upper Midwest	Lower Midwest	Northeast	Southeast
Seattle	\$2.00	\$2.50	\$3.50	\$4.00	\$5.00	\$5.50
Denver	\$2.50	\$2.50	\$2.50	\$3.00	\$4.00	\$4.50
St. Louis	\$3.50	\$3.50	\$2.50	\$2.50	\$3.00	\$3.50
Atlanta	\$4.00	\$4.00	\$3.00	\$2.50	\$3.00	\$2.50
Philly	\$4.50	\$5.00	\$3.00	\$3.50	\$2.50	\$4.00

4.

Moon Micro is a small manufacturer of servers that currently builds all of its product in Santa Clara, California. As the market for servers has grown dramatically, the Santa Clara plant has reached capacity of 10,000 servers per year. Moon is considering two options to increase its capacity. The first option is to add 10,000 units of capacity to the Santa Clara plant at an annualized fixed cost of \$10,000,000 plus \$500 labor per server. The second option is to have Molelectron, an independent assembler, manufacture servers for Moon at a cost of \$2,000 for each server (excluding raw materials cost). Moon sells each server for \$15,000 and raw materials cost \$8,000 per server.

Moon must make this decision for a two-year time horizon. During each year, demand for Moon servers has an 80 percent chance of increasing 50 percent from the year before and a 20 percent chance of remaining the same as the year before. Molelectron's prices may change as well. They are fixed for the first year but have a 50 percent chance of increasing 20 percent in the second year and a 50 percent chance of remaining where they are.

Use a decision tree to determine whether Moon should add capacity to its Santa Clara plant or if it should outsource to Molelectron. What are some other factors that would affect this decision that we have not discussed?

5.

Steel Appliances (SA) manufactures high-quality refrigerators and cooking ranges. SA has one assembly factory located near Denver from which it has supplied the entire US. Demand has grown rapidly and the CEO of SA has decided to set up another factory to serve eastern markets. The supply chain manager is asked to find a suitable location for the new factory, which will serve markets in Atlanta, Boston, Jacksonville, Philadelphia and New York. The coordinate location, the demand in each market, the required supply from each parts plant, and the shipping cost for each supply source is shown in Table 7.

Table 7.

Sources/Markets	Transportation cost \$/(ton.mile)	Quantity in tons	Coordinates	
			x	y
<b>Supply sources</b>				
Buffalo	0.90	500	700	1200
Memphis	0.95	300	250	600
St. Louis	0.85	700	225	825
<b>Markets</b>				
Atlanta	1.50	225	600	500
Boston	1.50	150	1050	1200
Jacksonville	1.50	250	800	300
Philadelphia	1.50	175	925	975
New York	1.50	300	1000	1090

Determine the optimal location of the new site.

## Purpose

- Present the 2 building blocks used in the SimOpt framework
- Illustrate the advantages and limitations of the two methodologies in dealing with stochastic systems

## General features of new product development pipelines

- A number of new product candidates is available for development
- There are dependencies between the candidates
- There are resources with limited capacity
- The development of each project requires multiple activities with specific predecessor-successor relationships

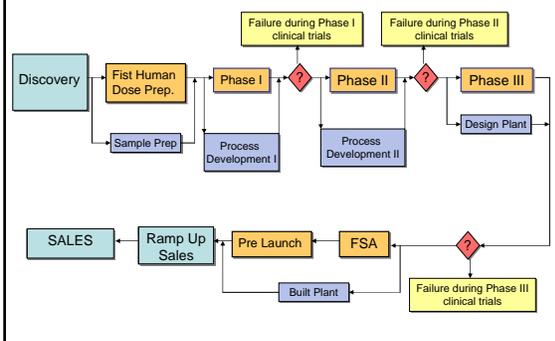
## General features of new product development pipelines

- Limited time horizon (first mover advantage, expiration of patents, etc)
- Variable rewards and costs
- Variable resource requirements and activities duration
- There are tasks with success/failure probability

## Case study characteristics

- All the characteristics of the problem will be kept but:
  - Variable costs
  - Dependencies
  - Variable resource requirements and activities duration
- All projects will have the same resource requirements and activity durations
- The negative cash flows incurred at each stage are the same

## Development



## Problem data

Activity	Mean duration (days)	Mean resource usage (\$MM)	Resource capacity (\$MM)
FHD Prep	400	80	275
Phase I	300	80	175
Phase II	500	80	200
Phase III	775	200	300
FSA	375	20	100
Pre-Launch	100	50	75
Ramp Up 1	365	12	25
Ramp Up 2	365	22	50
Ramp Up 3	365	40	70
Mature Sales	365	150	1000
Sample Prep	400	2	10
Process Development I	730	10	16
Process Development II	730	10	16
Design Plant	730	10	13
Build Plant	730	60	120

## Problem data

Project	Phase I Succ. prob	Phase II Succ. prob	Phase III Succ. prob	Cumulative prob.	Mean Rewards*	Expected Rewards
0	90	30	90	0.243	900	218.70
1	85	20	85	0.1445	500	72.25
2	90	15	95	0.12825	2000	256.50
3	87	22	88	0.168432	1000	168.43
4	100	45	99	0.4455	200	89.10
5	90	20	86	0.1548	650	100.62
6	88	15	88	0.11616	2000	232.32
7	93	30	97	0.27063	1500	405.95
8	90	40	92	0.3312	1200	397.44

\* The rewards are normally distributed (N-(u, (0.2u)<sup>2</sup>))

## Mathematical program nomenclature

- Indices:
  - j = a project
  - k = an activity
  - r = a resource
  - t = time
- Parameters
  - $w_{jk}$  = The reward weight for activity k of project j (mature sales reward \* cumulative probability of unresolved uncertainties)
  - $a_{jk}$  = The duration of activity k of project j
  - $k_{rk}$  = The amount of resource r required by activity k of project j
  - $K_r$  = The capacity of resource r
- Sets
  - $P_{jk}$  = The set of activities that precedes activity k of project j
- Decision Variables
  - $X_{jkt}$  = 1 if activity k of project j is started at time t

## Mathematical program

$$\max \sum_{j=\text{project}} \sum_{k=\text{task}} \sum_{t=\text{period}} w_{jk} e^{-r(t+a_{jk})} x_{jkt}$$

Resource constraints

$$\sum_j \sum_k k_{rjk} \sum_{q=-a_{jk}+1}^t x_{jqk} \leq K_r \quad \forall r,$$

Allocation constraints

$$\sum_r x_{jkr} \leq 1 \quad \forall j, k,$$

Precedence constraints

$$-\sum_r t \cdot x_{jkr} + \sum_t (t + a_{jh}) x_{jht} \leq T(1 - \sum_r x_{jkr})$$

$$\sum_t x_{jht} - \sum_t x_{jkt} \leq 1 - \sum_t x_{jkt} \quad \forall j, k, h \in P_{jk}$$

## Mathematical program results

	Time horizon		
	6 years	10 years	14 years
last activity scheduled	x[0][4][13]	x[0][4][13]	x[0][6][45]
	x[1][2][5]	x[1][4][21]	x[1][4][21]
	x[2][4][9]	x[2][11][34]	x[2][13][42]
	x[3][4][14]	x[3][4][14]	x[3][4][14]
	x[4][4][18]	x[4][4][18]	x[4][4][18]
	x[5][4][17]	x[5][4][17]	x[5][4][17]
	x[6][4][10]	x[6][4][10]	x[6][12][47]
	x[7][4][5]	x[7][8][30]	x[7][11][52]
	x[8][6][13]	x[8][6][29]	x[8][7][45]
sln time	5	17	676
sequence	872603541	278603541	267803541

## Discrete-event simulator Results

sequence	sequence criteria	ENPV (\$MM)	P(NPV<0)
012345678	ENPV can be negative	-15	0.622
782345610	Prioritize 2 main projects	1760	0.4
782603541	expected rewards	1855	0.381
786203541	switch 2 projects	1843	0.379
782603514	switch 2 projects	1959	0.361
872603541	math program 6 years	1820	0.383
278603541	math program 10 years	1636	0.372
267803541	math program 14 years	1313	0.513
267830514	rewards	1308	0.508
782603	less projects in the pipeline	2521	0.355

## Summary

- Mathematical programs
  - Strength: Generate optimal policies
  - Weakness: Unable to capture the complete stochastic nature of practical systems
- Discrete-event simulations
  - Strength: Captures the behavior of highly complex stochastic systems
  - Weakness: Limited scope for optimization
- Main limitation of the ENPV objective fun
  - Unable to capture the flexibilities in the system (delay or abandonment options) and control risk level
- Challenges:
  - Develop a framework that integrates information from the math program and the discrete-event simulation
  - Develop math programming approaches capable of incorporating decision making flexibilities and risk minimization

## How to run the Mathematical Program

- Access the server catalyst.ecn.purdue.edu using a secure shell\*
  - Username:
  - Password: PASI2005
- Open directory Matprogram/bin (cd Matprogram/bin)
- Type OP [discretization factor] [time horizon in years] [number of projects] [resource availability factor in percentage]
- Type more solution.txt to see the results
- If you want to access the source code the header file is in the directory include and the files are in the directory src

\*A secure shell can be downloaded from <http://ftp.ssh.com/pub/ssh/SSHSecureShellClient-3.2.9.exe>

## How to use the PPD Discrete event simulator

- FTP the server catalyst.ecn.purdue.edu
  - username:
  - password: PASI2005
- Download the file in the directory PPD and open it with a browser
  - Allow blocked content if you have a pop up blocker
- Scroll down and input the sequence of projects (0-8) prioritized from top to bottom
  - Change select to 0 if you don't want a specific project to be part of the simulation
- Click on sequence and scroll up to see the behavior of the pipeline in real time
  - Each sequence is run 5000 times
- If you want to slow down the simulation click on delay. If you want to speed it up again click on speed
- If you want to change the resource availability input the new value in the resources table and click on capacity

# Advanced Process Dynamics and Control

## Exam Questions

1. What is the algebraic multiplicity  $a$  and the geometric multiplicity  $g$  of the eigenvalue  $\lambda = -1$  of the matrix

$$\mathbf{A} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

2. Design a state feedback control law  $\mathbf{u}(t) = -\mathbf{K} \mathbf{x}(t)$  that places the closed-loop eigenvalues as indicated by the set  $\{-1, -1\}$  for an LTI system characterized by the matrices

$$\mathbf{A} = \begin{bmatrix} -1 & 0 \\ 1 & 2 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

3. Design a state feedback control law  $\mathbf{u}(t) = -\mathbf{K} \mathbf{x}(t) - \mathbf{K}_r \mathbf{r}(t)$  that places the closed-loop eigenvalues at  $\{-1, -1\}$  for the LTI system given in question 2, and that ensures zero-offset behavior with respect to all set-point signals  $\mathbf{r}(t)$  that have a constant final value.

## Exam Problems for Model Predictive Control

Prepared by Jay H. Lee

Pan American Advanced Studies Institute Program on Process Systems Engineering

1. Suppose the process has three inputs  $u_1, \dots, u_3$  and three outputs  $y_1, \dots, y_3$ .  $y_1$  and  $y_2$  has the setpoints of 0.2 and 0.8 respectively. In addition, these two outputs must be kept below 0.25 and 0.85 and above 0.15 and 0.75, respectively, at all times (soft constraints). If these two outputs can be controlled at their setpoints, it is then desirable to drive  $y_3$  to its maximum value of 2 (a secondary requirement). All three inputs must operate in the range of  $\pm 0.5$ . Write down a reasonable *quadratic* objective to use for MPC. Use the prediction horizon of  $p$  and the control horizon of  $m$ .

2. Consider the following SISO system.

$$\begin{aligned} \begin{bmatrix} x_1(k+1) \\ x_2(k+1) \end{bmatrix} &= \begin{bmatrix} 0.4 & 0.1 \\ 0 & 0.2 \end{bmatrix} \begin{bmatrix} x_1(k) \\ x_2(k) \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} u(k) \\ y(k) &= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} x_1(k) \\ x_2(k) \end{bmatrix} \end{aligned} \quad (1)$$

- (a) Calculate the impulse response and step response coefficients. What is the reasonable truncation point for this system?
  - (b) Write down the step response model that corresponds to the above state space system.
  - (c) Write down the prediction equation for the above system with  $p = 2$  and  $m = 2$ .
  - (d) Derive the unconstrained control law for the above system with  $\Lambda^y = 2$  and  $\lambda^u = 0.5$ .
  - (e) How would you derive the unconstrained MPC law for  $p = \infty$  and  $m = 2$ .
  - (f) How would the prediction equation change if the state space model is used directly?
3. Consider the following FIR system model:

$$y(k) = h_1 u(k-1) + h_2 u(k-2) + h_3 u(k-3) + \frac{1}{1-q^{-1}} \varepsilon(k) \quad (2)$$

- (a) Derive the expression for the one-step-ahead predictor and the prediction error.
- (b) Suppose you are given experimentally obtained time series data  $y(1), \dots, y(12)$  and  $u(1), \dots, u(12)$ . Derive the formula for obtaining the parameters  $h_1, h_2, h_3$  that minimize the prediction error for the given data.

# Process Control Design. Tom Marlin

## Questions

1. The snow-ball effect was discussed during the class.
  - a. Describe the snow-ball effect in a recycle system.
  - b. An alternative design is proposed for the CSTR with recycle. It is given in the Figure 1. Discuss the behavior of this control system to the same disturbance considered in the class workshop, i.e., a feed impurity that reduces the reaction rate constant by 10%.

Specifically, does the snow-ball effect occur in this design for the specified disturbance? In your response, describe the qualitative dynamic behavior of key variables, including whether the final values are greater, less, or equal to their initial values.

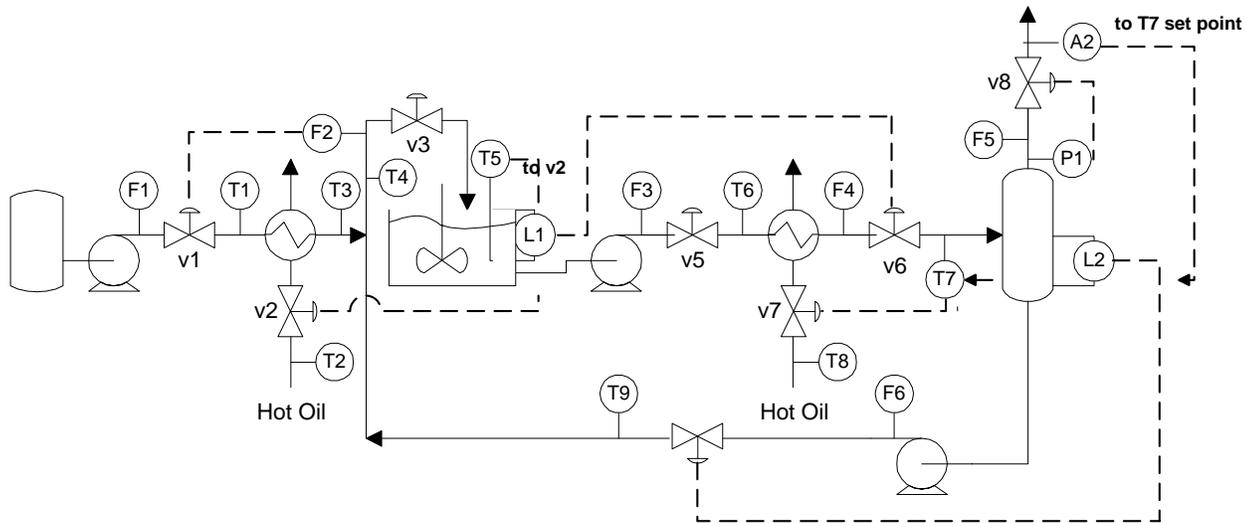


Figure 1

Notes:

1. The heat of reaction is 0.0.
2. The reaction is  $A \rightarrow B$  with first order kinetics.
3. You may not add or modify controllers, sensors, valves or other process equipment.

2. You would like to design analyzer controls for the distillation tower in Figure 2. You decide to retain the pressure and level control; thus, you have a 2x2 control system to design. The transfer function model for the system is given in the following for the feedback process and a feed flow rate disturbance.

$$\begin{bmatrix} XD(s) \\ XB(s) \end{bmatrix} = \begin{bmatrix} \frac{12.8e^{-s}}{16.7s+1} & \frac{-18.9e^{-3s}}{21s+1} \\ \frac{6.6e^{-7s}}{10.9s+1} & \frac{-19.4e^{-3s}}{14.4s+1} \end{bmatrix} \begin{bmatrix} F_R(s) \\ F_V(s) \end{bmatrix} + \begin{bmatrix} \frac{3.8e^{-8.1s}}{14.9s+1} \\ \frac{4.9e^{-3.4s}}{13.2s+1} \end{bmatrix} F(s)$$

- a. Evaluate whether the product purities are controllable in the steady-state.
- b. Evaluate the integrity of all possible 2x2 multiloop control systems. Comment on the implications for the final design.
- c. For all control systems with acceptable integrity, determine if the interaction is favorable for
  - i. A set point change to the distillate controller.
  - ii. The feed flow rate disturbance for which the model is given.
- d. Would you recommend decoupling to improve the closed-loop feed-flow disturbance response?

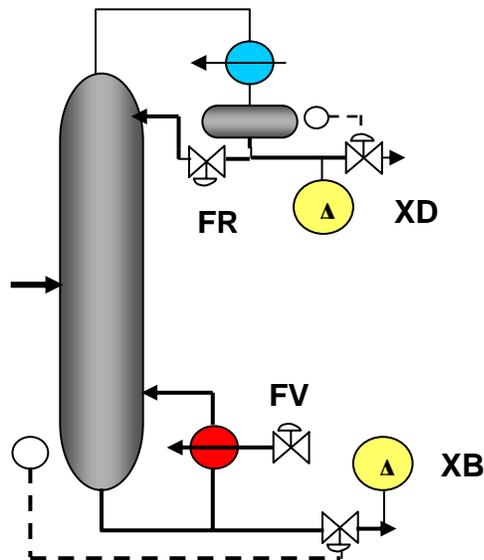
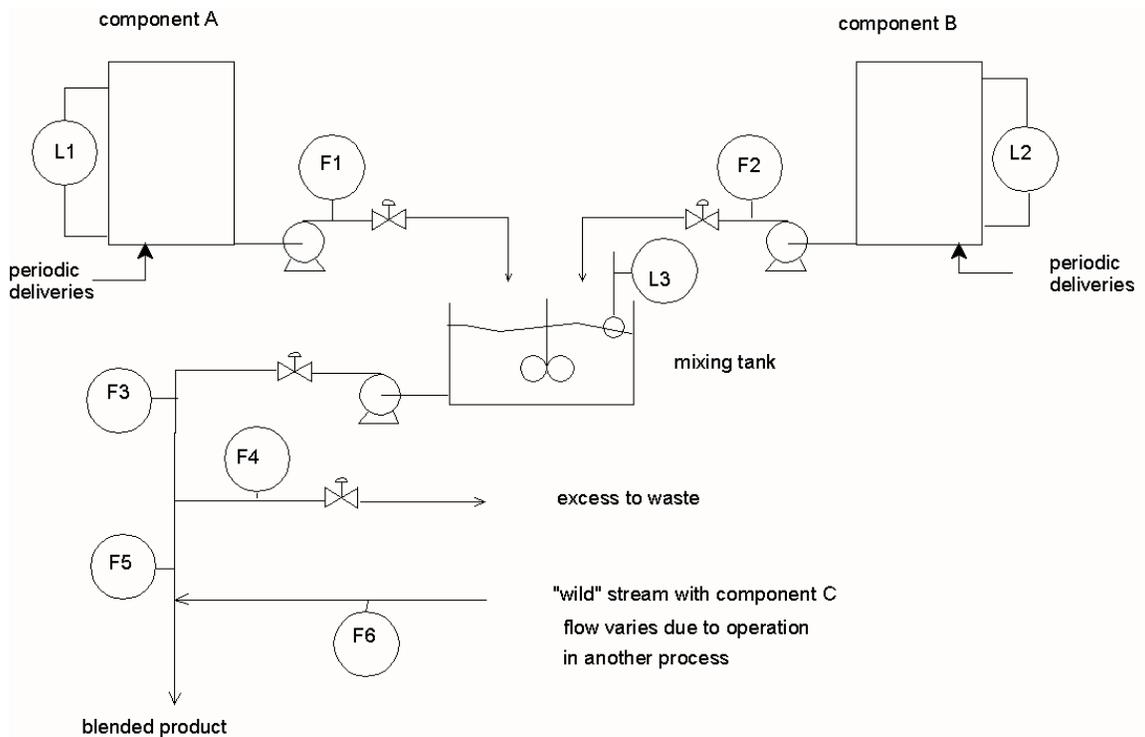


Figure 2.

3. The mixing process in Figure 3 involves a tank to mix components A and B. The effluent from the mixing tank is blended with a stream of component C. The flow of F6 stream is "wild", i.e. it changes to accommodate operations in another process and cannot be adjusted by this control strategy. Note that the flow to waste is to be minimized.
- Using only the equipment shown in the figure, design a control system to tightly control the percentages of A, B, and C in the blended product. Can you achieve this and also control the total flow of blended product?
  - Improve your result in (a) by adding an on-stream analyzer that can measure all of the components in one stream. Decide the proper location and use it in the control system. Discuss why the analyzer would improve the performance.



**Figure 3.**