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Lecture No-10 Heuristics in Process Synthesis and Design

Welcome to lecture 10 of plant design and economics. In this lecture we will talk about a set of heuristics or rules of thumb that will be very useful for process synthesis and design. These heuristics are based on experience and very easy to apply.

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So today's topic will be heuristics in process synthesis and design.

(Refer Slide Time: 00:48)



Heuristic rules are rules of thumb expedite the selection and positioning of processing operation and equipment when generating process alternatives. Heuristics are very easy to apply. Thus, several promising flow sheets or base-case design can be generated quickly with relatively little effort. These rules are based on experience and these rules hold in general, but this rule should be tested to ensure that they apply in the specific application.

For example for the particular problem you are solving you should test the validity of this heuristic rules may be by simulation.

(Refer Slide Time: 01:38)

This set of heuristics are taken from the reference given from the book Product and Process Design Principles by Seider, Seader, Lewin and Widagdo. So there are several heuristics rules of thumb in this book. We will play we will present not all the rules, but a set of rules which we think are more important at this point of time and we are using the same number those rules are numbered 1, 2, 3 etcetera and we are using the same number as given in this book.

Let us start to heuristic 1, select raw materials and chemical reactions to avoid, or reduce, the handling and storage of hazardous and toxic chemicals. Now storing hazardous and toxic chemicals can lead to dangerous situations. There was a very unfortunate accident at Union Carbide Pesticide plant in Bhopal India in 1984. Water was accidentally mixed with a highly reactive intermediate methyl isocyanate, which is used for pesticide.

This methyl isocyanate the plant stored in huge quantity and water was accidentally mixed. Now when water mixes with methyl isocyanate it leads to evolution of tremendous amount of heat it is an extreme exothermic reaction. Then what happened is the methyl isocyanate was it was no more possible for the storage tank to hold the methyl isocyanate and the vapours came out. This led to death of several thousands and affected several lakhs of people in Bhopal.

Consider the manufacture of ethylene glycol. Usually, it is manufactured in a two step process as shown first the partial oxidation of ethylene and then hydrolysis of the product to make ethylene glycol.

(Refer Slide Time: 04:27)



It is common in processes with two reaction states to store the intermediate so as to permit continuous operation. But storing hazardous and toxic chemical as we have just discussed is extremely dangerous. In fact, after the Bhopal incident the chemical process industries have started thinking to design processes where you actually do not have to store such dangerous intermediate highly reactive compounds in huge quantity.

Now coming back to the manufacture of ethylene glycol, which is generally done in a two step process, both the reactions are highly exothermic. A water spill into the ethylene oxide storage tank can lead to a dangerous accident. So, an efficient process will try to eliminate the storage of large quantities of reactive intermediates such as ethylene oxide. So, what are the alternatives? First alternative may be you use a single step, instead of two step reactions use a single step.

Ethylene may be reacted with sodium hydroxide and chlorine to produce Ethylene glycol. Note this alternative requires more expensive raw material. Certainly, Sodium hydroxide or caustic and chlorine are more expensive compared to oxygen that you get from here. Remember the previous two step reactions used partial oxidation of ethylene to form ethylene oxide. Now this single reaction step of producing ethylene glycol using chlorine and caustic completely eliminates the intermediate, of course it is more expensive process.

(Refer Slide Time: 07:11)



As the second alternative as the ethylene oxide is formed you react it with carbon dioxide to form ethylene carbonate. Now ethylene carbonate is a much less active intermediate. So this can be safely stored and later on you can produce ethylene glycol from this. So ethylene carbonate is a much less reactive intermediate and can be stored safely and later on hydrolyzed to form the ethylene glycol product.

(Refer Slide Time: 07:53)



Let us come to heuristic number 2, use an excess of one chemical reactant in a reaction operation to consume completely a valuable toxic or hazardous chemical reactant. So use an excess of one chemical reactant in a reaction operation to consume completely a valuable toxic or hazardous chemical reactant. The degree of excess of course is an important consideration. So, what should be the amount which we call excess amount?

Because the degree of excess will govern the cost of separation, recirculation, and of course thus influence process economics. Excess of one chemical will also be useful to absorb the heat of reaction and thereby maintain moderate temperatures. So maintaining moderate temperature can be done by absorbing heat of reaction when you take excess amount of one chemical. Excess of one chemical will also be useful to increase conversion of the limiting reactant and also to minimize side reactions.

(Refer Slide Time: 09:27)



Distribution of Chemicals: Inert Species, often impure feed streams contain species that are inert during chemical reaction operation. If nearly pure products are required then you have to remove this impurity. Now question is when should you remove the impurity? Should you remove the impurity before chemical reaction or should you remove the impurity after chemical reaction? So the heuristic related to this will tell you the answer.

Of course you have to assess the ease and cost of separation by examining the physical properties, on which the separations are based, size of separator etcetera. You can use simulation for this purpose. For example, if you are thinking of distillation as separation process then check the relative volatility. So, if the relative volatility differs widely the distillation will be easy to perform. Similarly if you are thinking of crystallization as a separation process, check the differences in freezing point.

Similarly if you are thinking of membrane separation processes, look at the permeability of the species. So by these you have to assess the ease and cost of separation by examining the physical properties on which the separations are based. You also have to take care of size of separators and these things can be done by performing simulations. So the heuristic related to inert species says, when relatively pure products are required eliminate inert species before the reaction operations when the separations are easily accomplished and when the catalyst is adversely affected by the inert.

So if separation can be done very easily and if catalysts adversely affected by the inert, then we should eliminate the inert species before the reaction operation. But this should not be followed when a large exothermic heat of reaction must be removed. Remember that if you have just in the previous heuristic we have talked about that excess of one chemical absorbs heat of reaction so inert species will absorb some amount of heat.

So when a large amount of exothermic heat of reaction must be removed, this should not be this particular this heuristic rule should not be followed.

(Refer Slide Time: 12:44)

Distribution of Chem	icals: Purge Streams
In continuous operations, inert accum Separation/reaction at low concentra synthesis – argon is purged.	nulate – needs to be removed. Ition is expensive – use purge. Consider NH ₃
Heuristic - 4	
Introduce liquid or vapor purge strea	ms to provide exits for species that
> enter the process as impurities in	the feed
> produced by irreversible side-read	ctions
when these species are in trace quan from the other chemicals.	tities and/or are difficult to separat
Lighter species leave in vapour purge in liquid purge streams.	streams, and heavier species exit
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Next purge systems, purge streams. In continuous operations inert will accumulate and must be removed from the system. If these are not removed from the system then it may be necessary to shut down the operation. Now the inert will be present in small quantity in the beginning. So separation or reactions at low concentrations is expensive. So if you are thinking of separation or reaction to remove the inert it will be expensive because the inert will be present at low concentrations.

So use purge, we have already seen in previous lectures how argon is purged in ammonia synthesis. Now heuristic 4 says: introduce liquid or vapour purge streams to provide exits for species that enter the process as impurities in the feed, produced by irreversible side reactions

when these species are in trace quantities and or are difficult to separate from the other chemicals.

Lighter species live in vapour purge streams and heavier species exit in liquid purge streams.

(Refer Slide Time: 14:35)



Heuristic – 5; do not purge valuable species or species that are toxic and hazardous even in small concentrations. For example, waste stream containing trace amount of rare metals. It will happen if your catalyst is impregnated on ceramic support. So under such cases, you should not use purge. Sometimes environmental regulation will also not allow you to use purge. Add separators to recover valuable species.

Add reactors to eliminate the possible toxic and hazardous species. So when you have toxic or hazardous species or valuable species do not use purge. Catalytic conversion of hydrocarbons and carbon monoxide in the exhaust gases from internal combustion engine. Instead of purging the exhaust gases from combustion engine catalytic converters are used to convert carbon monoxide and nitrogen oxides to carbon dioxide and nitrogen respectively.

So you do not use purge instead we use catalytic converters to convert carbon monoxide and nitrogen oxides, instead of releasing carbon monoxide and nitrogen oxides to environment. (Refer Slide Time: 16:15)



Heuristics 6 is about recycle byproducts that are produced in small quantities in reversible reactions are usually not recovered in separators or purged. Instead, they are usually recycled to extinction. So byproducts that are produced in small quantities in reversible reactions are usually not recovered in separators or purged instead, they are usually recycled to extinction. When the reaction proceeds irreversibly small quantities of byproducts must be separated.

Otherwise it will build up in the process and the process has to be shut down. When the reaction process reversibly it becomes possible to achieve an equilibrium conversion at steady state by recycling products species without removing them from the process. So, that is why in reversible processes, you can recycle up till extension, but when the reaction process irreversibly you have to separate it away otherwise it will build up in the process and you have to shut down the process.

(Refer Slide Time: 17:43)



Heuristic 7 is about selectivity. For series and parallel competing reactions adjust the temperature, pressure and catalyst to obtain high yield of the desired product. In the initial distribution of chemicals assume that these conditions can be satisfied before developing a base-case design obtain kinetic data and check that this assumption holds.

(Refer Slide Time: 18:12)



Heuristic 8 is about reactive separations. So you ask the question, can you perform both reactions and separations in the same process unit? Heuristic 8 says consider conducting reversible reactions in a separation device capable of removing the products and hence driving the reactions to the right. Such reaction separation operations lead to very different distributions of chemicals. Usually, separations follow reaction operations, we first perform reactions and then the effluent teams go to separating devices for separation.

The reactive separation allows task integration, that means the combinations of operations is possible in the same process units. Merging reactions and separations is possible in the reactive distillation towers, reactive absorption towers, reactive membranes etcetera.

(Refer Slide Time: 19:06)



Now let us consider reactive distillation of methanol and acetic acid to produce methyl acetate. Now this is the carried out in a reactive distillation tower where this part indicates the reaction zone. Methanol is more volatile compared to acetic acid and it is fed to the bottom of the reaction zone. When methanol is fed to the bottom of the reaction zone it concentrates in the vapour phase and contacts acetic acid, which is spread at the top of the reaction zone and concentrates in the liquid phase.

As methyl acetate is formed it concentrates in the vapour phase and leaves the tower from the top of the distillation column in the nearly pure form. The water leaves as bottom stream. Now what is the advantage here? The product chemicals are withdrawn from the reaction section, in the liquid form and the vapour form driving the reaction forward without excess reactant or changes in the pressure.

(Refer Slide Time: 20:41)



Separations involving liquid-liquid and vapour mixtures. Heuristic 9, separate liquid mixtures using distillation, stripping, enhanced distillations, such as extractive distillation, isotropic distillation, reactive distillation, liquid-liquid extraction, crystallization, and or adsorption. So we should separate liquid mixtures using distillation, stripping, enhanced distillation, liquid-liquid extraction, crystallization, crystallization, liquid-liquid extraction, crystallization, crystallization, liquid-liquid extraction, crystallization, crystalliza

Heuristic 10, attempt to condense all partially condensed vapour mixtures with cooling water or a refrigerant. Then use above heuristic 9, means you attempt to condense or partially condense vapour mixtures with cooling water or a refrigerant and then separate liquid mixture using distillation, stripping, enhanced distillation etcetera. Heuristic 11; separate vapour mixtures using partial condensation, cryogenic distillation absorption, adsorption, membrane separation and or desublimation.

(Refer Slide Time: 22:02)



Heuristic 12 is about separations involving solid particles. Crystallize inorganic chemicals from a concentrated aqueous solution by chilling when solubility decreases significantly with decreasing temperature. Use crystallization by evaporation when solubility does not significantly change with change in temperature. So you can crystallize inorganic chemicals from a concentrated aqueous solution by cooling it down when the solubility is a strong function of temperature.

So solubility should decrease rapidly with decrease in temperature. Then you can efficiently use crystallization. Use crystallization by evaporation when solubility does not change significantly with temperature. For example say sodium chloride, sodium chloride solution inverter. If you consider the solubility of the sodium chloride does not change much with change in temperature, the solubility is already very high.

But for crystallization to take place you have to decrease the solubility, so you can you evaporate the water. When decrease in the temperature does not decrease the solubility you can do evaporation we call that as evaporative crystallization. You can also use another solvent known as anti-solvent in which the solute will have low solubility, but these anti solvent will be soluble with the other solvent that is present.

So in this case anti solvent can be added let us say to aqua solution of sodium chloride. We can use alcohol as anti-solvent. So alcohol I mixed with water, but sodium chloride has very low solubility in alcohol. So this will work so the resulting solubility in the mix solvent will decrease and the crystallization can take place. But in this case, of course evaporative crystallization will be a very cost effective method.

Heuristic 13, Crystal growth rates and sizes are controlled by controlling super saturation usually in the range of 1.02 to 1.05. So, super saturation means that in the solution excess amount of salute is dissolved than permitted by the solubility at that temperature. So how much salute can be dissolved in a solvent at a given temperature can be obtained from the solubility data. So beyond that if it is dissolved we call the solution is supersaturated.

And super saturation is the practical driving force for crystallization. Of course the thermodynamic driving force will be the differences in chemical potential of the species in the solid phase and the solution phase but a practical driving force per crystallization to takes place is the super saturation. So the crystal growth rates and sizes are typically control in the range of 1.02 to 1.05 or super saturation.

Growth rates are influenced greatly by the presence of impurities and certain additives, so there are growth modifiers. So impurities in very small quantity have a very strong effect on the growth rate and if you can influence the growth rate of various phases of a crystal you can influence the shape of the crystals as well. However, the same set of impurity will not modify the growth rates of all crystals, so these are case specific.

Heuristic 14; separate organic chemicals by melt crystallization with cooling, followed by removal of crystals by settling, filtration, or centrifugation.

(Refer Slide Time: 26:51)



Heuristic 21; note that we are not talking about all the heuristics listed in the reference book that you mentioned. So heuristic 21 is about heat removal from exothermic reactors to remove a highly exothermic heat of reaction consider the use of excess reactant and inert diluents, or cold shots. These affect the distribution of chemicals and should be inserted early in process synthesis.

Heuristic 22; for less exothermic heat of reaction circulate reactor fluid to an external cooler or use a jacketed vessel or cooling coils. Also consider the use of intercoolers between adiabatic reaction stages. So to remove highly exothermic heat of reaction you consider use of excess reactant, we have discussed this earlier also and in a dilute or cold shots. But when the exothermic heats are not too much, so for less exothermic heat of reaction you can circulate reactor fluid to an external cooler or use a jacketed vessel or cooling coils.

(Refer Slide Time: 28:17)



Heat addition to endothermic reactors, we talked about heat removal from exothermic reactors. Now, let us talk about heat addition to endothermic reactors. To control temperature for a highly endothermic heat of reaction consider the use of excess reactant and inert diluent or hot shots. These affect the distribution of chemicals and should be inserted early in the process synthesis. Heuristic 24, for less endothermic heats of reaction circulate reactor fluid to an external heater or use a jacketed vessel or heating coils.

Also consider the use of inter heaters between adiabatic reaction stages. So the management of heat removal from exothermic reactor and heat addition to endothermic reactors are very much similar. So there we use cold shots we can use hot shorts here. There we are using cooling coil here we can use heating coils.

(Refer Slide Time: 29:27)



Now, some heuristics about heat exchangers and furnaces. Heuristic 26, near-optimal minimum temperature approaches depend on the temperature level as: 10 degree Fahrenheit or less for temperatures below ambient, 20 degree Fahrenheit for temperatures above ambient up to 300 degree Fahrenheit, 50 degree Fahrenheit for high temperatures 250 to 350 degree Fahrenheit in a furnace.

Heuristic 27, when using cooling water to cool or condense a process stream, assume a water inlet temperature of 90 degree Fahrenheit water is coming from cooling water cooling tower and a maximum outer outlet temperature of 120 degree Fahrenheit.

(Refer Slide Time: 30:18)



Heuristic 28, boil a pure liquid or close boiling liquid mixtures in a separate heat exchanger, using a maximum overall temperature driving force of 45 degree Fahrenheit to ensure nucleate boiling and avoid undesirable film boiling to ensure that nucleate boiling takes place and you need to avoid undesirable film boiling. Heuristic 31, estimate the heat exchanger pressure drops as follows.

1.5 psi for boiling and condensing 3 psi for a gas 5 psi for a low viscosity liquid 7 to 9 psi for a high viscosity liquid 20 psi for a process fluid passing through a furnace.

(Refer Slide Time: 31:09)

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Heuris	ic - 37	
For hea use a c	ds up to 3200 ft and flow rates in the ra entrifugal pump.	ange of 10 - 5000 gpm,
For hig recipro	h heads up to 20,000 ft and flow rates u cating pump.	p to 500 gpm, use a
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Heuristic 34, use a fan to raise the gas pressure from atmospheric pressure to as high as 1.47 psig. Use a blower or compressor to raise the gas pressure to as high as 30 psig. Use a compressor or a staged compressor system to raise pressure greater than 30 psig. Heuristic 37, for heads up to 3200 feet and flow rates in the range of 10 to 5000 gallons per minute use a centrifugal pump.

For high heads up to 20000 feet and flow rates up to 500 gallon per minute use a reciprocating pump.

(Refer Slide Time: 31:55)



There are few more heuristics about pumps and compressors. To increase the pressure of a stream pump a liquid rather than compress a gas unless refrigeration is needed. For a three-stage steam-jet ejector system used to achieve a vacuum of 2 torr, 100 pounds of 100 psig steam per pound of gas are required.

So these are some of the heuristics that you discussed which are useful for process synthesis and design there are several other heuristics and rules of thumb which engineers have accumulated over a long period of time through their experience. Some of those heuristics and rule of thumb we will discuss as you progress in the course with this we stop our discussion on heuristics in process synthesis and design. Thank you for watching.