Chemical Process Intensification.
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Lecture 4.3: Multilevel Computer-aided tools.

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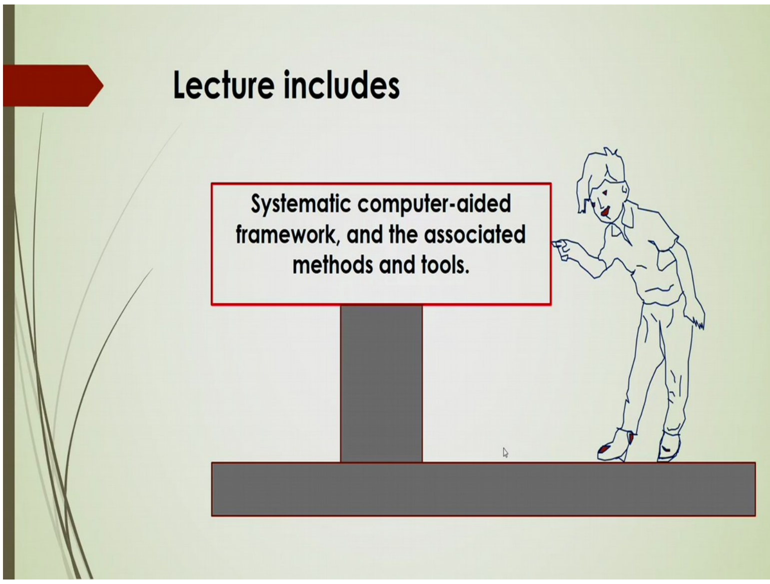

Welcome to Massive Open Online Course on chemical process intensification. Here we are discussing in the model for regarding the design techniques of process intensification. Earlier we have discussed about the stages and the scale of processes for the sustainable design and in the previous lecture we have discussed about the methodology of the process intensification and how it can be designed for the sustainable design. And also we have discussed that different, you know that stages by which you can get the sustainable design.

In this lecture we will try to discuss about the multilevel computer-aided tools, where it will be applicable for the design process intensification techniques. So, here we will discuss that topic in systematic way, that how that computer-aided framework can be made and also how it is actually associated with the methods and tools.

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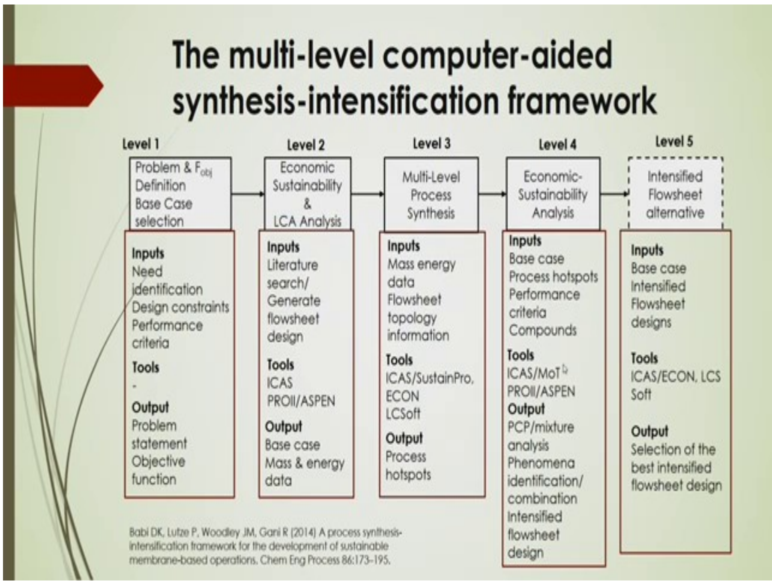

Now, if we consider about that multilevel computer-aided for the synthesis process, for the process intensification and for that some framework should be required. Before going to that, you know that, applying the tools to solve that different techniques of process design. So, there are several levels of course here are to be considered, like level 1 to level 5, here we have given as per by Babi et al.,

They have given this actually, level by the actually framework for the process intensification. They have discussed that there should be at least 5 level to get that in sustainable design for the process intensification. And they have discussed that some membrane-based operations which will be sustainable and how it can be developed for that process intensification in chemical engineering process. And also, they have given that some framework for that particular membrane-based operation for the sustainable process.

So, in that case as a level 1, they have considered that some problems and the objectives of the actually design and how it can be functionalised, so objective functions should be defined and it should be based on the base case selection and in that case some inputs to be considered like you know that it requires some you know that identification, you know the some identification of phenomena, even some design constraints and also you know that what should be the performance criteria that also to be actually considered.

So, as a level 1, as an input, here you have to actually keep that inputs for the basic needs and also you know that identification of the constraints and the process performance criteria. And as a level one, there should not be any actually there is no tools actually being used in this level and but without using tools you can have some output, that output should be represented as what should be the problem identification, what should be the statement for that and also you know that what should be the objective function that you have to define. So, this is the output as the level I.

After that love to go to level II, in that case you have to analyse the economic and also that life cycle assessment there. So, for the sustainability that economic consideration is required and, in that case, along with that life cycle analysis also required. So, in the level II that economic sustainability and LC analysis to be done and as an input here, in that case literature search, generate, flowsheet, design, these are the things to be required.

So you have to assess the you know different, you know the possibility how to solve, how to analyse, all those things and how actually the researchers, they have analysed and they have made the objective function and on what basis they have made that objective function, what are the different constants that may come and how it will be acting on, you know that how it will be affecting on that optimisation problem.

And also, if is there any you know flowsheet type design, that also you have to find out. So, in this level, that literary survey should be done, even some flowsheet, you know and also how to design that flowsheet, that should be considered. And in this case for designing that flowsheet and also generation of that flowsheet, you have to use some tools, like ICAS or Aspen, you can use these types of tools for designing that flowsheet there.

And in that case as a output you can say that some base case mass and energy data to be actually segregated or you can say to be considered there for analysis of this sustainable and economic and also life-cycle assessment. So, after completion of this level 2, you have to go to the level III where multilevel process synthesis is being done.

So, based on that multilevel process synthesis, you have to consider some inputs for that synthesis, like what should be the mass energy data that you have to consider and what should be the flowsheet topology information, that also to be you know that considered in this case. And for that the tools to be used as ICAS or Sustain Pro, software or ECON or LCS or LC Soft is called to be used for you know that analysis of that multi-process synthesis.

And as an output you can get here some process, you know that yield and also some you know that localised hotspot region there, where that heat, how it will be distributed or energy or some other form of you know that mass concentration, how it will be, you know that distributed that you can also get based on the mass and energy data. And in the level 4, in that case again that economic sustainability analysis is to be done, where inputs to be given as you know that what are the base case process hotspots and also what should be the process criteria that should be also considered.

And also, what are the compounds for that, given that process criteria, that also to be considered here. Here also the tools like ICAS or MOT Pro 2 or Aspen, you have to use. And as an output that you can get that you know some Mixer analysis and also phenomena identification combination or intensified flowsheet design, those things you can get at this level.

And at the final level, in that case they intensified flowsheet alternatives to be also developed there, so for that you have to use some inputs like what are the base case flowsheets to be designed, based on that you have to intensify those actually designed flowsheets and how to intensify for that you have to actually use some tools.

In that case again you can use that LC Soft and ICAS or ECON software that you can use to get the intensified way of that flowsheet design for the alternatives. And as output you can get the selection of the best intensified flowsheet design at this level. So, these are the different levels that you have to consider for the intensification framework based on which you can get the sustainable design for that particular process.

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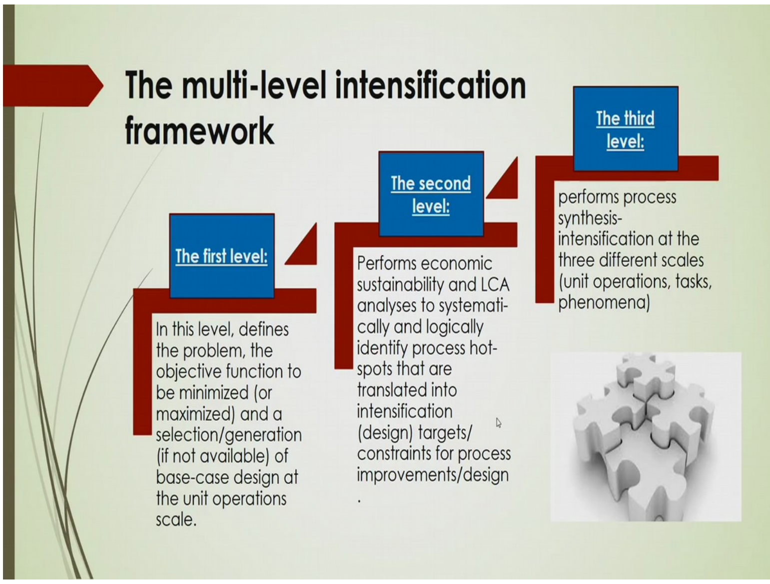

Now, you know that there are several levels that I told that is, but in that case the first level, 2nd level and 3rd levels are the main important, where some optimisation phenomena based on the economic sustainability and life cycle analysis to be done. And in that case, the process synthesis which are being performed at a different scale, like unit operation, task of phenomena level, that what we have discussed in the previous lecture. Based on this framework we can analyse this performance of the process by this different scales and also economic analysis.

So, as a first level, we can say in this level defines the problem, the objective function to be minimised or maximised and you can say that selection or generation of the base case design for the unit operation. And after that economic sustainability to be performed and also parallelly you have to consider the life cycle assessment do you know that systematically and logically to identify the process hotspots that are actually translated into intensification design. Or you can say that what is your targets that should be obtained.

After that, of course, you have to improve the process design based on this economic analysis and life cycle analysis by considering some constraints there what is coming whenever you are operating any unit operations. So, for that to design, you have to consider the constraints what is coming, what are the different operating variables, how that operating variables are interacting to each other, even you know that is there any hydrodynamic parameters are taking part for that and what are the different physical properties of phenomena that should be also considered as a constraint there.

And after getting all those optimisation functions, subject to the constraints for that you know process improvement or design, after that you have to analyse the performance of the process synthesis by identification of those three different scales, like unit operation, task and phenomena. So, these are the multilevel intensification framework which is to be considered for the sustainable design.

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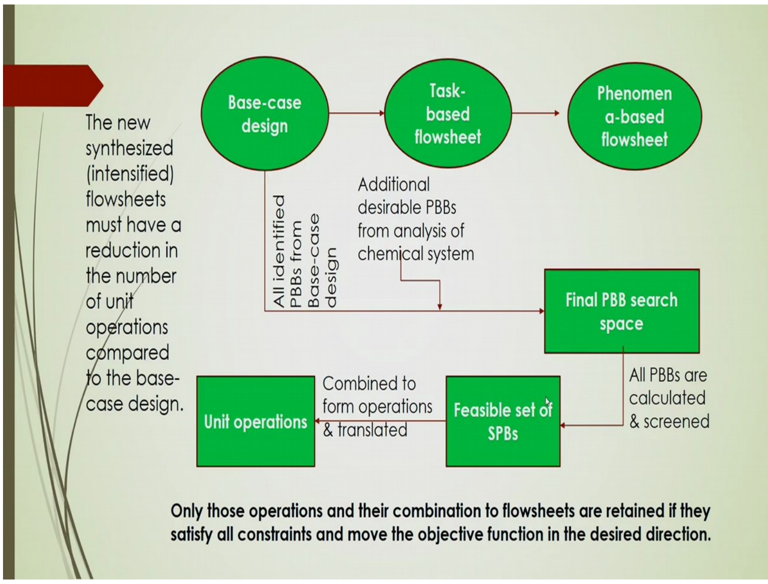

Now, to get the new synthesised, intensify flowsheets, you have to, you know that reduce the number of unit operations that should be compared to the base case design. So, it is a must whenever you are getting any process flowsheet alternatives by intensification, you have to compare it with the, you know the base case design. So, how or what extent of that intensification is being done based on your process intensification from the base case design to be analysed there.

So, in that case you have to consider first you know base case design after that task-based flowsheet to be formed and then you know the phenomena-based flowsheet to be considered. Now, from the base case design, all identified that phenomena-based building blocks that we have discussed in the previous lectures, that all phenomena-based building blocks are to be formed based on these base case design. And from that base case the then, you have to go to the final phenomena-based building blocks/space. And sometimes to conjugate those PB, you will get that SPB, that means here simultaneous phenomena-based building blocks.

And in this case additional desirable phenomena-based building blocks from the analysis of chemical system to be considered, whenever you are going to search that final PBB space there. So, after that searching of final PBB, all PBs are to be calculated, that is all phenomena-based building blocks to be calculated and also screened down, so that you can get the most possible and useful phenomena-based building blocks to be used for final feasible design.

For that you have to segregate that phenomena-based building blocks out of all PBBs and you have to make a set of some, you know that specialised or you can say sometimes called simultaneous phenomena-based building blocks after calculating and screening up of those PBBs. PBB's means phenomena-based building blocks. Now, if you combine all these SPBs, it will give you the formation of operations and it will be translated to the unit operations. So, finally we are getting this unit operations based on the setting of a feasible SPB from the domain of PBBs, all PBBs.

So, you have to first calculate all phenomena or you can say that constraints of that PBBs and based on that you have to segregate which actually PBB will be useful for the sustainable design. And after getting all, you know that possible and useful PBBs, you have to make SPBS. And again, after combining all SPBS, you can design that unit operations finally. Now, only those operations and their combinations to flowsheets are retained, if they satisfy all constraints and movie objective function in the desired direction.

So, this is to be remembered that you cannot use all those PBS to get to the combination of flowsheets. So, you have to screen down some PBBs and based on which, which PBBs will satisfy the constraints that should be considered. And move that objective function in the desired direction based on that satisfied constraints.

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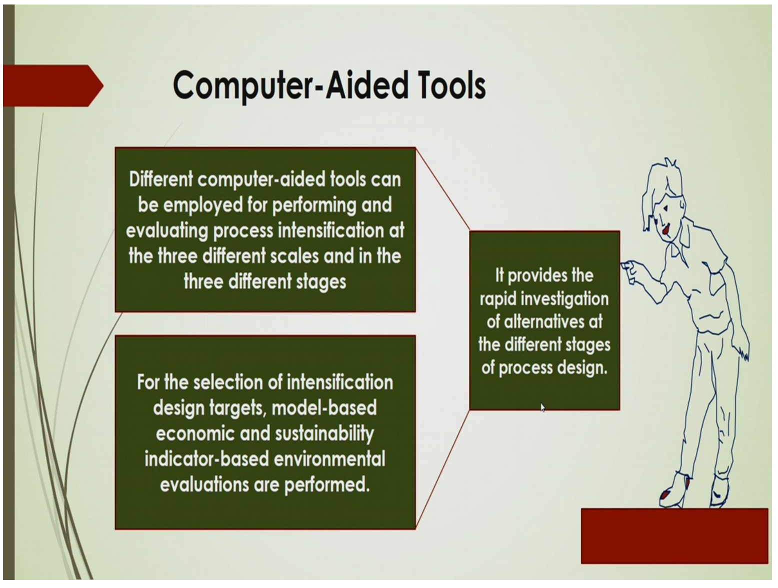

Now, Computer-aided tools, in that case different computer-aided tools actually can be used for performing and evaluating that process intensification at the 3 different scales and in the different stages that we have discussed in the previous lectures regarding that scales and stages. And for the selection of that intensification, design targets, you have to evaluate and perform the mortal based economic and sustainability indicator-based environmental aspects.

So, there because you are not actually getting that intensify design targets, based on that economic and sustainability indicator, you will not be proceed for that further for the process intensification. Because it provides the rapid investigation of the alternatives at the different stages of process design, otherwise you will see there will be a mixed up of that phenomena paste building blocks, where some interactions of the unnecessary and also un-useful or you can say that is not feasible at all, that should be directing to the design.

So, diverted to segregate all those non-feasible PBBs, based on that selection of that design targets and also for that you have to, of course, use the different tools for segregating PBBs and making that set of SPB based on that computer-aided tools. Now, that is why you will see that computer-aided tools will give you the rapid investigation of the alternatives at the different stages of process design.

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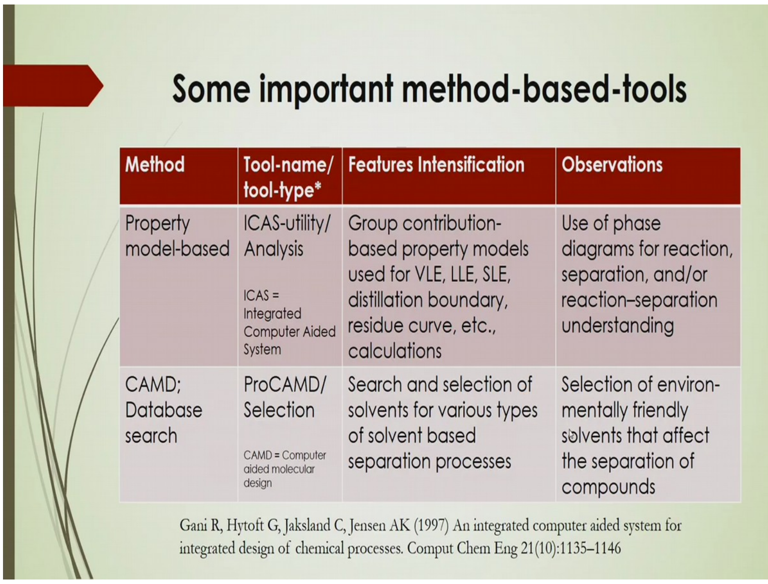

Method	Tool-name/ tool-type*	Features Intensification	Observations
Property model-based	ICAS-utility/ Analysis ICAS = Integrated Computer Aided System	Group contribution-based property models used for VLE, LLE, SLE, distillation boundary, residue curve, etc., calculations	Use of phase diagrams for reaction, separation, and/or reaction–separation understanding
CAMD; Database search	ProCAMD/ Selection CAMD = Computer aided molecular design	Search and selection of solvents for various types of solvent based separation processes	Selection of environ-mentally friendly solvents that affect the separation of compounds

Now, in this case some important method-based tools, here we can see in this table, it is given, in this case we thank to Gani et al. They have actually you know compiled all those tools based on their observations. So, we can see here some, you know methods and also what are the tools, what type of tools are being used and what are the features, intensifications are there and also what are their observations and, in this case, we can see from this table.

Now, if we consider that property model-based, so in that case some tools like ICA S utility or analysis tools should be used. ICAS means integrated computer aided system and in this case, what are the intensification features are being used there, group contributions-based property models used for vapour liquid equilibrium, liquid-liquid equilibrium, solid liquid equilibrium, even distillation boundary, residue curve, etc. and also calculations based on this you know tools.

So, property model-based method we can use this type of ICAS utility and analysis also, for the VLE, LLE, SLE and also other process parameters like residue curve, distillation boundary, etc. And in this case use of phase diagrams for the reactions separation or reactions separation understanding are very important because without these phase diagram for the reaction, or separation, you will not be able to use these tools. Next, CAMD, database search, like your tool S pro, CAMD or selection, in that case you can search by this tool regarding the solvents and also how the solvents can be used for various types of you know separation processes.

So, you can use this CAMD method or database search method by this you know pro CAMD tool for the search and selection of solvents for various types of solvent-based separation processes. And in this case selection of environmentally friendly solvents that will affect the separation of compounds in a better way because here you are going to search or select the solvents which will not be you know that hazardous or that is before going to solve that, you know that optimisation problem based on that optimisation function, you are selecting that solvent, which should be more appropriate for that separation processes.

Because all those physical properties, all of all these solvents to be actually segregated beforehand to go through this solution. So, that is why selection of environmentally friendly solvents that affect the separation of compounds based on this database search very well. Now, CAMD, computer-aided molecular design and another method is called driving force-based method.

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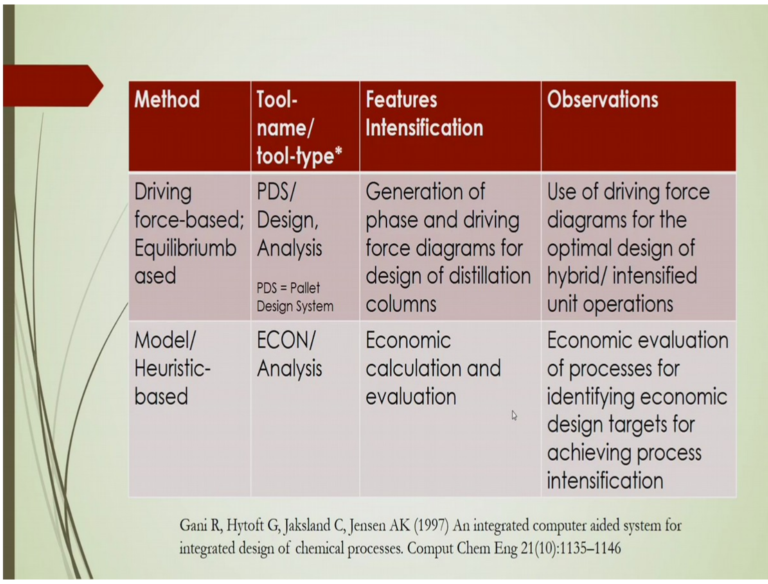

Method	Tool-name/ tool-type*	Features Intensification	Observations
Driving force-based; Equilibriumb ased	PDS/ Design, Analysis PDS = Pallet Design System	Generation of phase and driving force diagrams for design of distillation columns	Use of driving force diagrams for the optimal design of hybrid/ intensified unit operations
Model/ Heuristic-based	ECON/ Analysis	Economic calculation and evaluation	Economic evaluation of processes for identifying economic design targets for achieving process intensification

Gani R, Hytoft G, Jaksland C, Jensen AK (1997) An integrated computer aided system for integrated design of chemical processes. Comput Chem Eng 21(10):1135–1146

In this case you know that equilibrium based, it is called the method, in this case some PDS or design analysis tool should be used. PDS means here palate design system. In this case is very interesting that you have to know first the driving force of that concentration or energy or that is call temperature differences, all those things, based on the diagrams, that is called driving force diagram.

So, you have to generate that phase and driving force diagrams for the design of specially distillation columns. Because distillation column is generally vapour liquid operation where the phase, you know that equilibrium diagram is very important for that separation process in distillation column.

Now, in this case you have to use the driving force diagram for the optimal design of hybrid or intensified unit operations like this separation of crude selection or crude oil distillation, even you know that extractive selection, even you know that adsorb distillation, even reactive distillation, all those intensified are hybrid units can be analysed by this driving force-based method by the tool of this PDS or design analysis tool.

So, another important method, it is called model or heuristic-based model or method, in this case econ or analysis tool to be used for the analysis of economic feasibility of the process and also that calculation of that investment criteria for that process design and also what should be the economic targets that can also be identified by this model or heuristic-based method.

In this case you will see that the targets of the process intensification, economic evaluation is very important because without you know that economic evaluation or calculation, you will not be able to analyse the cost-effective factor based on which how you are going to intensify the process. So, for analysis of that, economic feasibility, you have to use this heuristic-based method by this ECON software.

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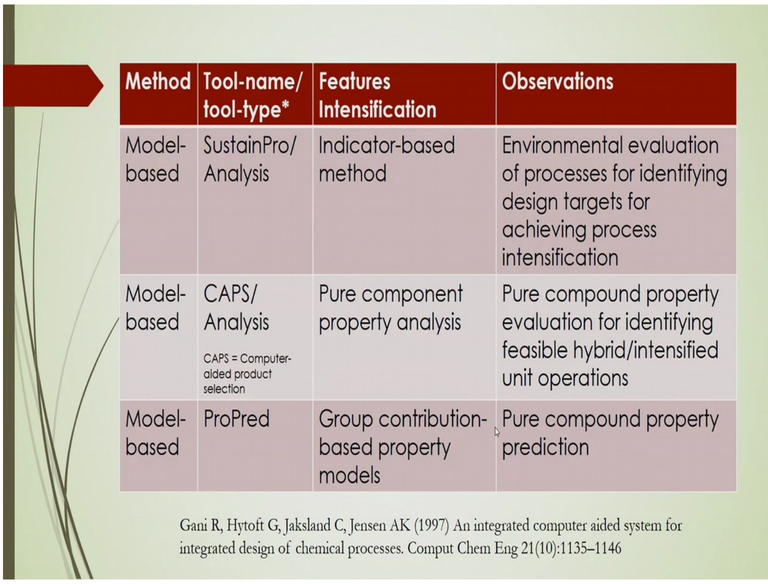

Method	Tool-name/ tool-type*	Features Intensification	Observations
Model-based	SustainPro/ Analysis	Indicator-based method	Environmental evaluation of processes for identifying design targets for achieving process intensification
Model-based	CAPS/ Analysis CAPS = Computer-aided product selection	Pure component property analysis	Pure compound property evaluation for identifying feasible hybrid/intensified unit operations
Model-based	ProPred	Group contribution-based property models	Pure compound property prediction

Gani R, Hytoft G, Jaksland C, Jensen AK (1997) An integrated computer aided system for integrated design of chemical processes. Comput Chem Eng 21(10):1135–1146

Another model-based method where this Sustain Pro or analysis tool can be used, in this case it is called the indicator-based method for you know that analysis of feature of intensification. And in this case environmental evaluation of process for identifying design targets for achieving process intensification. So, this can be done by this Sustain Pro software.

Again, another software, it is called CAPS software, it is called computer-aided product selection. In that case what other features, actually for that intensification, generally pure component property is being analysed by this CAPS software. It is very important to evaluate the pure compound property for the identification of the feasible or hybrid you know that feasible hybrid intensified unit operations. ProPred is also another important tool where you know that sometimes multiphase phenomena where the group-based contribution of the property is to be analysed there.

There are several fluids which are being used or taking part in the particular process. So, in that case what will become mixed properties of that phenomena, that is being actually analysed by this ProPred. In that case he or compound property prediction can be done based on that ProPred analysis software.

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Method	Tool-name/ tool-type*	Features Intensification	Observations
Equation oriented problem solution	MoT, Aspen Custom Modeller/ Analysis	Indicator-based methodProcess and property models can be generated and solved for evaluation.	Model-based evaluation and design of intensi-fied/hybrid unit operations
Model-based calculati ons	Aspen Plus, PROII/ Analysis	Models for well-known and hybrid/intensified unit operations	Model-based simulation and analysis of multiple intensified Process alternatives

Gani R, Hytoft G, Jaksland C, Jensen AK (1997) An integrated computer aided system for integrated design of chemical processes. Comput Chem Eng 21(10):1135–1146

Another method, it is called equation-oriented problem solution where MOT Aspen, custom, modular or analysis tools can be used. In this case indicator-based method, process and property models can be generated and solved for the evaluation. So, for the intensified or hybrid unit operations for those designs this model-based evaluation is important and you have to of course use this equation-oriented problem, solution method for the analysis of the design of intensified or hybrid unit operations.

Another important computer tool, it is called Aspen plus or pro 2 analysis tool pack for the model-based calculation methods. In that case what are the models to be used, that can be selected properly by this Aspen plus or pro 2 software for the analysis of hybrid or intensified unit operations. And that model can be done or intensified for that or model can be refined based on this model-based calculation for the hybrid or intensified unit operations. And in this case model-based simulation and analysis of multiple intensified process alternatives also can be you know that identified or procured based on this tool like Aspen plus or pro 2 analysis tool pack.

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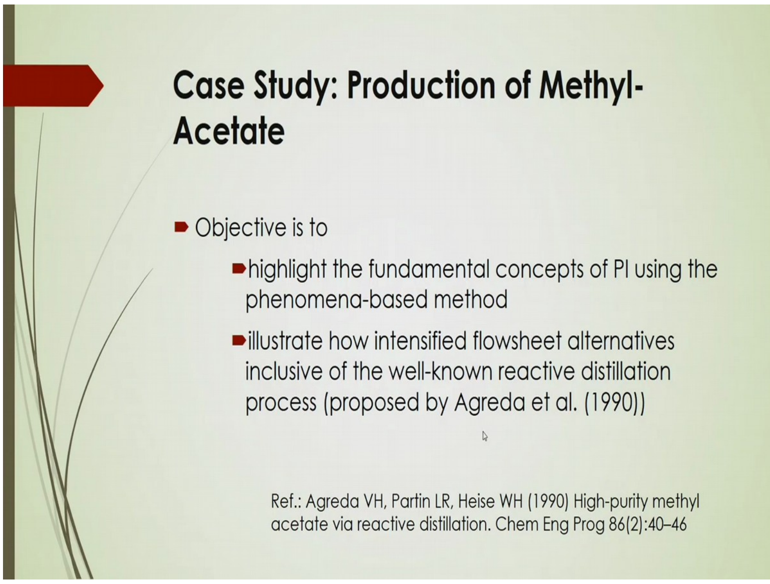

Now let us consider one case study for the production of methyl acetate. In this case again that Agreda et al, 1990, they have given this case study for the production of methyl acetate. And they have analysed this process intensification based on that fundamental concepts of process intensification based on the phenomena-based method. And their objective was to highlight the fundamental concepts of process intensification using phenomena-based method. And also, they have illustrated how intensified flowsheet alternatives, inclusive of the well-known reactive distillation process that they have actually discussed in this case study.

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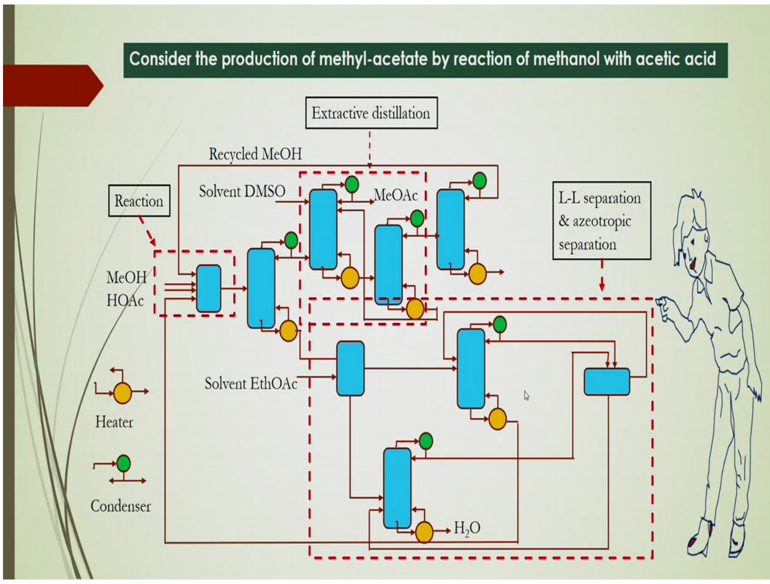

So, in that case they have considered the production of myth elicited by the reaction of methanol with acetic acid. So, here in this slide, I see the process pro diagram here, there are stages of reaction, extractive distillation and then what is that, separation process. So, all these 3 processes are integrated and then they have analysed based on that this phenomena-based method. Now, in this case the reaction stage methanol and acetic acid is being reacted in a reactor and then that with the solvent like DMSO, that is being separated and is being distilled for the extraction of methyl acetate. And then after that it is being separated to get the water and some other products as per this flowsheet.

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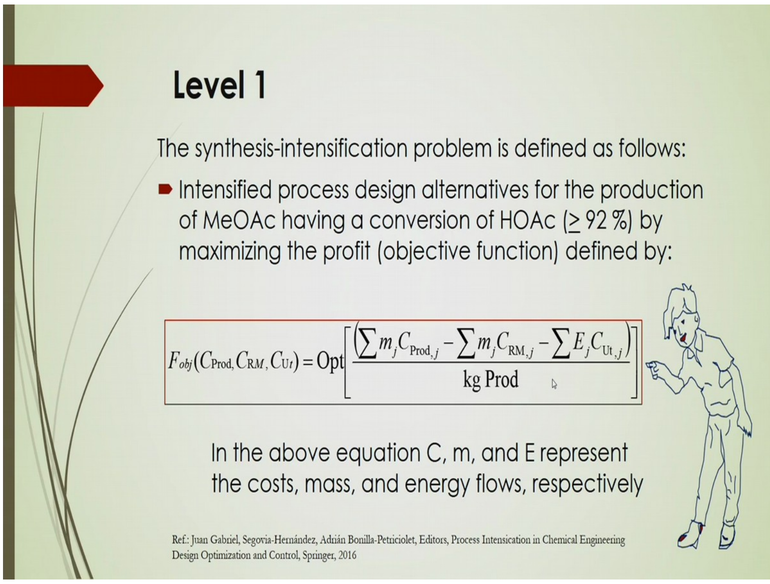

Now, if we consider this flow diagram and the process flowsheet, we can discuss the level wise what are the different problem analysis for this particular process. Now, as the level I, this is the synthesis intensification problem is defined as follows. In this case intensified process design alternatives for the production of methyl acetate having a conversation of an acetic acid more than 92 percent by maximising the profit.

That is why they have made that objective function

$$F_{obj}(C_{\text{Prod}}, C_{\text{RM}}, C_{\text{Ut}}) = \text{Opt}\left[\frac{\left(\sum m_j C_{\text{Prod},j} - \sum m_j C_{\text{RM},j} - \sum E_j C_{\text{Ut},j}\right)}{\text{kg Prod}}\right]$$

which is defined by an objective, that is C production, C RM, C UT and which is to be optimised based on this optimisation function, here it is given in the slide, that is summation of MJ, C product at J, minus summation of MJ into C RM J minus summation of J CUTJ divided by amount of production in KG. So, in this case you will see some notations are F for functions, C actually represents the cost, M represents the mass and you see that energy is representing the E is representing the energy.

And also, some you know subscript of production RM, like reaction mixing, and also some utility with respect to time like this so these are the things to be considered and the objective function to be made like this.

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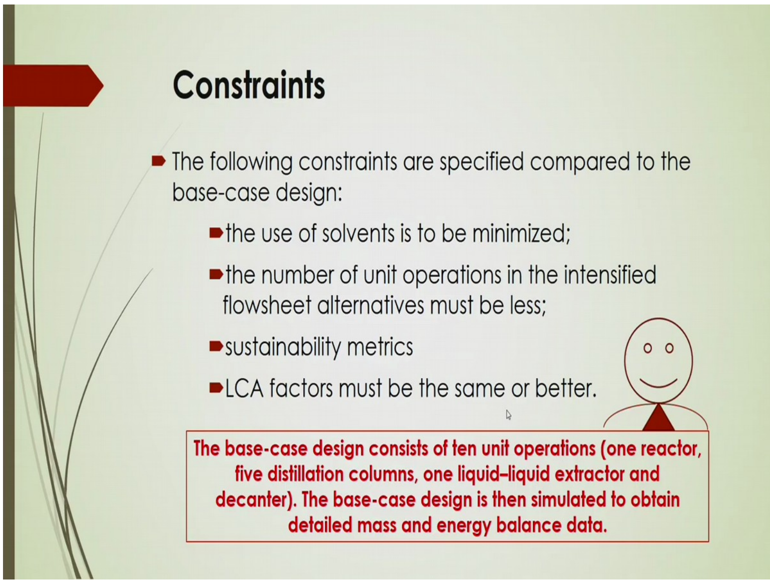

Now, what are the constants that become based on the production of methyl acetate. In this case the constraints which are to be actually specified compared to the base case design are: the use of solvents which is to be minimised. And the number of unit operations in the intensified flowsheet alternatives that should be of course less. And sustainability metrics to be considered there and also the LCA factor must be the same or better for your process design.

So, whenever you are going to make that constraints, you have to also think about the specific problems, that is constraints may not be the same for all processes, it is actually process-based constraint because different processes will have different types of constraints there. So, in this particular case, you have to think about the solvents and you cannot use that solvent in arbitrary amount, so that should be minimised and also you have to think about the number of unit operations to be used, which can be useful for the flowsheet for intensified way.

And also for that flowsheet alternatives to be developed and that should be very last in amount. And what are the sustainability metrics, all those factors, economic, environment and also the other policy optimisation should also be considered for that, capital cost should be also considered for that metrics.

And also, life-cycle analysis ofcourse are to be considered for that. So, base case design consists of in this particular case is 10 unit operations, that is one reactor, 5 distillation columns, as per the previous diagram here, you will see that one liquid-liquid extractor and a canter. The base case design is then simulated to obtain detailed mass and energy balance data.

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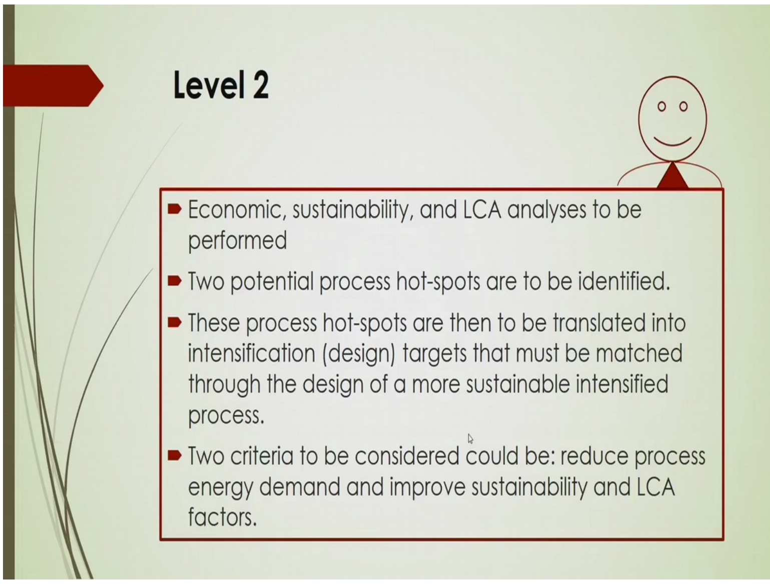

Now, after that you have to go to the level II, where economic sustainability and LC analysis to be performed. And in that case two potential process hotspots are to be identified and these process hotspots are then to be translated into intensification design targets, where you have to match them through the design of a more sustainable intensified process. And 2 criteria to be considered, like reduced process energy demand and improve sustainability and LCK factor, life cycle assessment factors to be considered as a criterion.

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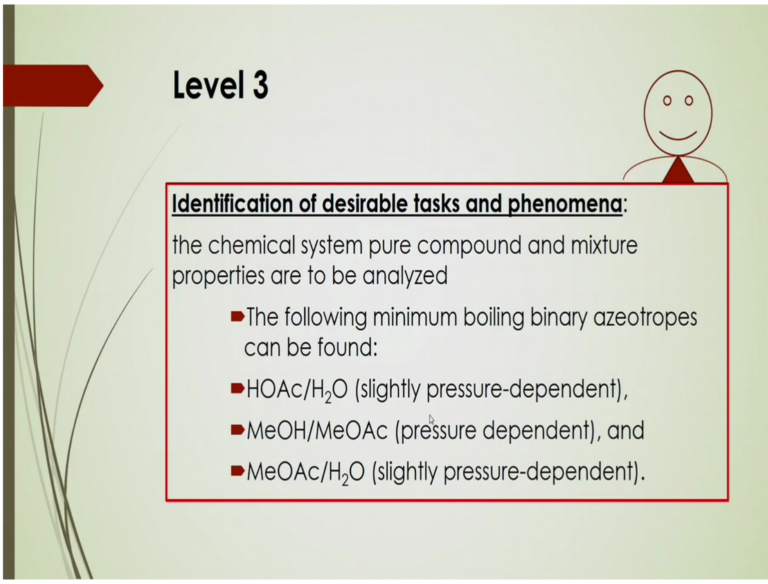

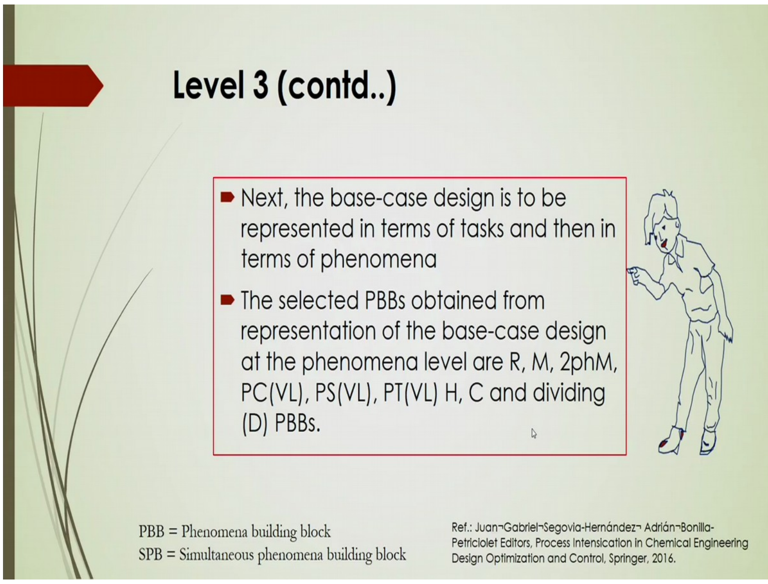

Next you have to go to the level III where identification of desirable tasks and phenomena to be done. In that case the chemical systems which are being used, that should be pure compound end mixture properties are to be analysed and also to be analysed if suppose more than more fluid should be used, then you have to consider the mixture properties there. Whether that mixture properties will be depending on the hold-up of that phases. Hold-up means volume fraction of the phases in that mixture.

So, the following minimum boiling binary azeotropes to be found, in that case for this phenomena-based analysis here, you know that an acetic acid and water mixture, where slightly it will be pressure dependent. And methanol and methyl acetate will be your pressure dependent and also methyl acetate and water mixture, that is also slightly pressure dependent.

So, whenever you are considering the separation that depends on the boiling temperature of those components.

So, you have to consider that boiling phenomena because sometimes if these mixtures will have almost same boiling points. That is the boiling point difference is very less, so in that case you may get the azeotropic phenomena there. That is at a certain mole fractions you will see there will be no separation. So, you have to consider that, mole fraction of those components in such a way that azeotropes should not be formed. So, that is why you have to consider that boiling phenomena to actually avoid that azeotrope.

And if you are considering that azeotropes, then you have to consider that pressure dependent phenomena, even some other factors where that equilibrium condition of paper and liquid there. So, at this level that you have to identify the desirable task and phenomena based on these criteria. Also, the last case design is to be represented in terms of tasks and then in terms of phenomena.

And after selection of that phenomena-based building blocks that are obtained from the representation of the base case design at the phenomena level, like you know that what are those phenomena-based building blocks, that should be reaction, that should be mixing, that should be to phase mixing, that should be phase contact, vapour liquid phase contact, maybe you know that phase separation. You can say that phase transition, you can say that heating, you can say that cooling and also other types like dividing rules there.

So, those are called PBB, like phenomena-based building blocks. So, here this R means here, it is given the short form here, R means reaction, M for Mixture or mixing, you can say that is called phenomena. And 2PI means 2 phase mixing, PC means phase contact between vapour and liquid, PS means phase separation between vapour and liquid, PT means phase transition whenever liquid is going to convert to vapour, that is at the transition, that is PT, it is called phase transition.

S for heating, C for cooling and dividing for D. So, these are the building blocks that should be actually formed at this level. Now, the additional or desirable you can say that some building blocks phenomena-based building blocks to be also added based on the thermodynamic insights, like you know that phase separation, phase transition and phase transition between vapour and vapour, phase transition between vapour and liquid, phase transition between vapour and vapour.

So, these are the additional, sometimes it will be desired or sometimes beneficial to analyse those optimisation problems in intensification. And considering all possible combinations of the identified, this phenomena-based building blocks, you have to make a set of simultaneous phenomena-based building blocks and out of which some should be you know that considered for the feasible design by using the combination of rules of that PBBs to SPPS.

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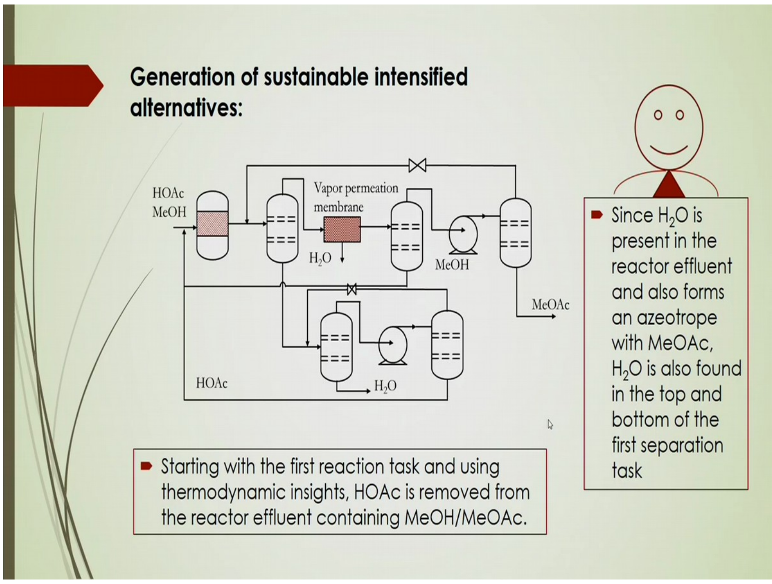

Now what are the generation of sustainable intensified alternatives? Now, how to actually procure that alternatives of that building blocks? So, like in this again that same process, in this case you have to start with the first reaction task and using thermodynamic insights like phase separation of vapour and phase contact between vapour and liquid and phase transition, so all those insights to be considered, where based on that consideration, that here in this particular cases, acetic acid can be removed from the reactor effluent that will contain that you know that methanol and methyl acetate effluent.

So, to remove that acetic acid from those mixtures, that you have to consider that alternative building blocks or intensified alternatives, you can say that based on this process specialised form. But it may not be the case for other processes. So, it is actually based on the process type. So, since in this case particular methyl acetate production, water is present in the reactor effluent and also acetic acid is also present there and that water in the mixture of methanol and methyl acetate will sometimes form that azeotropes.

So, that may be a very difficult case for separation at this azeotrope form. So, you have to you know that consider the operation at a certain condition so that the separation will be easier at this particular azeotropic condition also. So, there you know that concentration or you can say that mole fraction of those water or methanol or methyl acetate to be considered just by changing the pressure or equilibrium temperature or equilibrium pressure so then you can have the different concentration and different mole fractions, based on which you can get the separate ability criteria and you can get that separation.

So, you have to design that process, you have to make the building blocks in such a way that the azeotropic conditions to be considered and in that case in the top and bottom part of that separation call to be considered as a task for this particular special form of azeotropic condition.

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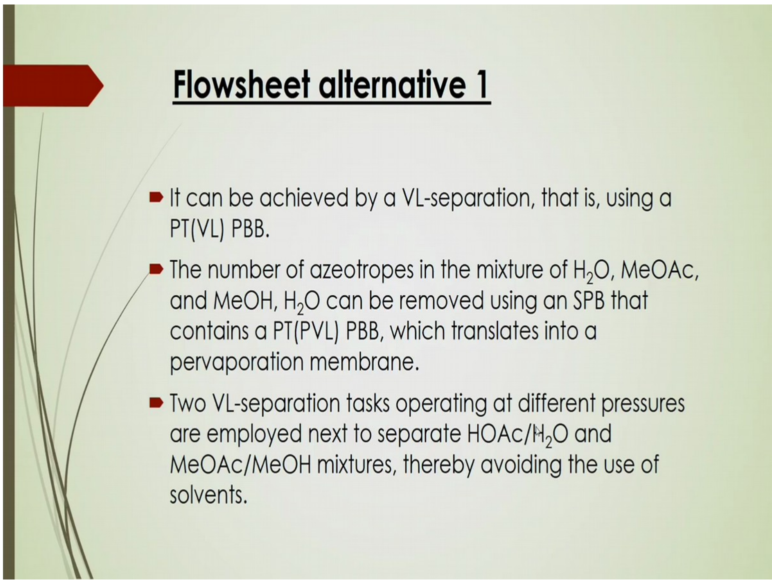

Now, flowsheet alternative 1 is that it can be achieved by a vapour liquid separation, that is using a phase transition criterion. And the number of azeotropic in the mixture of water or methyl acetate or methanol and water, that can be removed by using and simultaneous phenomena-based building blocks, that contains phase transition.

Even you can say that mixing characteristics, even other like you know the 2 phase mixing phenomena, even the separability criteria there, maybe that it can be what I can say that this is absorption criteria or you can say that it is called the extraction criteria or you can say that transportation of the molecules from one place to another, that is mass transfer phenomena. So, all those things to be considered in that phenomena-based building blocks for this azeotropic condition.

And how many actually azeotropes can be formed, that depends on that as products and by-products that are coming in the effluent. Now, here myth elicited and also methanol, both will become, so 2 azeotropes will be formed along with that water is coming in the effluent. Because water and ethanol, water and methyl acetate, these 2 you know the easier troops will form.

So, this number of azeotropes in the mixture of those water and methyl acetate or ethanol and water can be removed by considering the special, that is simultaneous phenomena-based building blocks that will contain phase transition phenomena-based building blocks in these particular cases, which will translate this into a membrane-based separation module there.

That may be for vaporisation, membrane module to be used for that for the separation of this azeotropic mixture. Now, 2 vapour liquid separation tasks that is operating at different pressures are employed next to separate that acetic acid and water and also methanol or methyl acetate mixtures. So, in that case you can avoid the use of that solvent for the separation of this azeotropes there.

So, without using that solvent you can separate this azeotropic mixture just by changing temperature on pressure than also that composition of that mixture. So, that is why you have to consider that flowsheet alternative of this separation task taste on this vapour liquid equilibrium condition.

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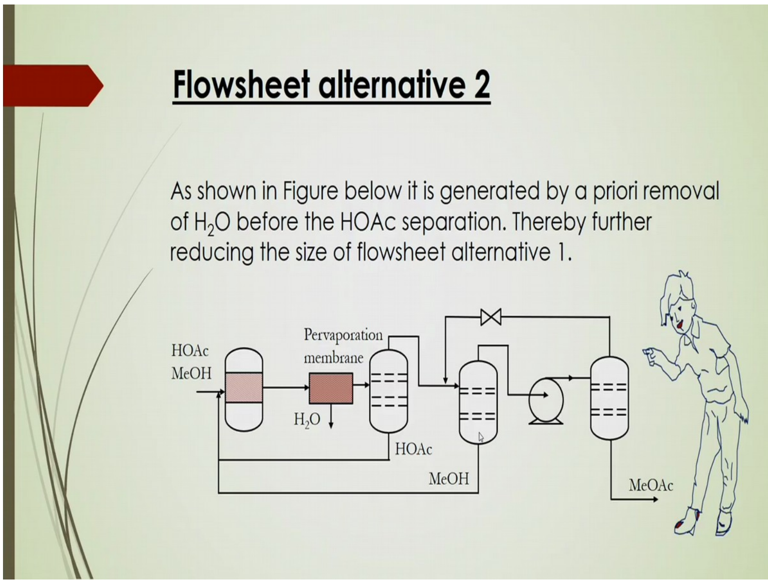

Now, as a flowsheet alternative 2, we can say that here it can be generated by a priori removal of water before the acetic acid separation. Thereby you have to reduce the size of flowsheet alternative 1, just by considering that, there will be a removal of water before the separation of acetic acid there.

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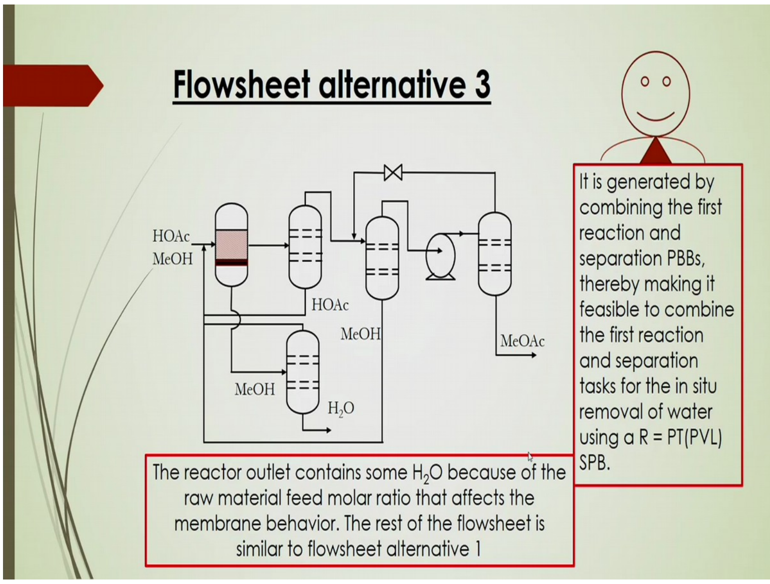

And flowsheet alternative 3, where you can also consider that when that reactor outlet contains some water, in that case that may affect the membrane behaviour. So, you have to select some other alternatives of that flowsheet to actually remove that water content in the reactor outlet, so that will not be coming, you know that to the effluent, to make your use number of azeotropic mixtures there. Because there are several other you know by-products will come along with that effluents, not only the methyl acetate, acetic acid, maybe some other components, so along with that water, that may be at certain temperature and pressure azeotropes will form.

So, it is better to remove that amount of water from the reactor outlet so that it will not come to that effluent after separation also. So, it is generated by combining the first reaction and separation of that separation based on that phenomena based building block, thereby making it feasible to combine the first reaction in separation task for in situ removal of water using the reaction that will be PT, PVL, SPV.

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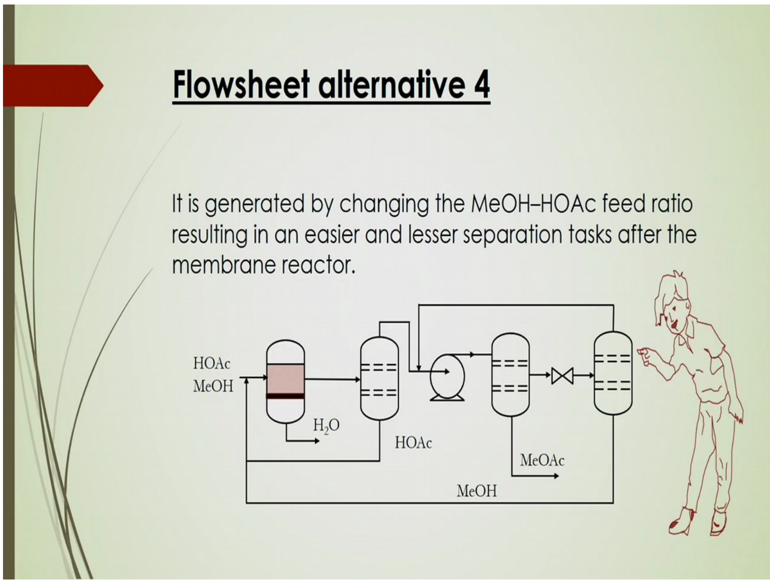

And as a flowsheet alternative 4, degenerated by changing the methanol acetic acid feed ratio, that results in anywhere and lesser separation task after the membrane reacted.

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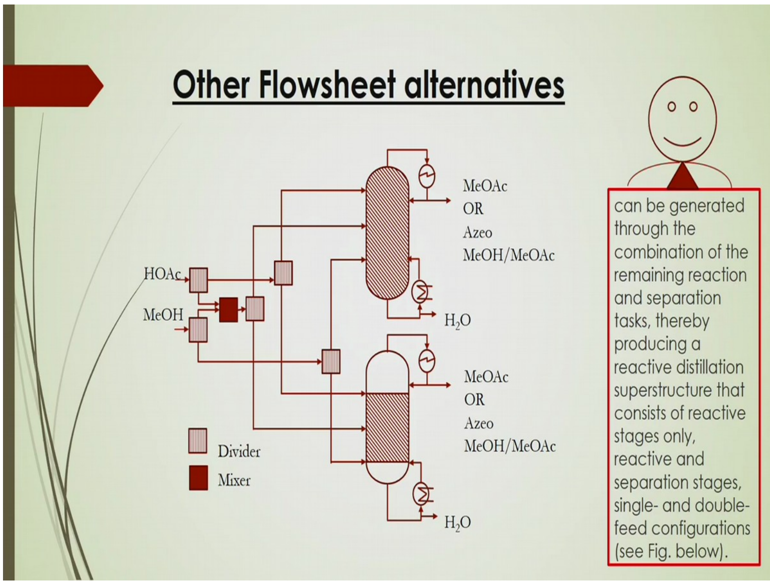

Other flowsheet alternative is also to be considered in this case by combination of the remaining reaction and separation tasks. And in that case, you can produce reactive distillation, superstructure or design a superstructure so that that reactive stages reactive or separation stages, single- and double-feet configurations also to be considered for that flowsheet alternatives.

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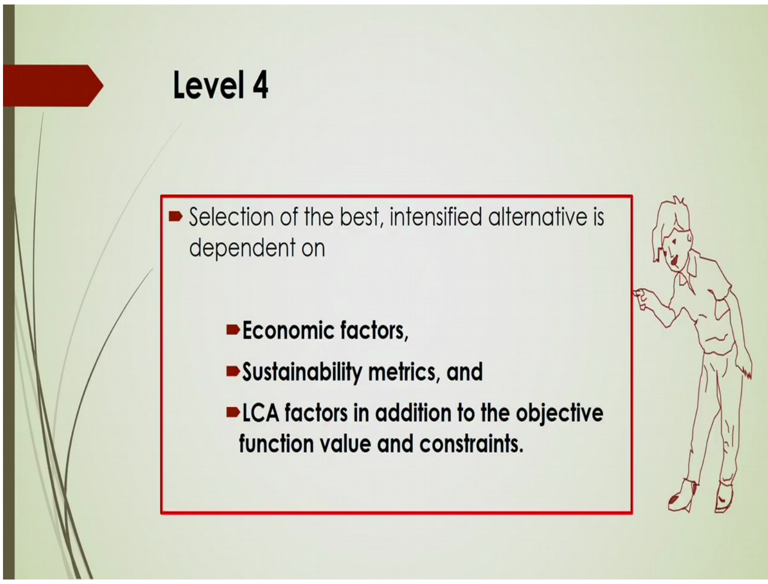

So, this and level 4 here, in that case you have to consider the economic factor sustainability metrics, LCA factors in addition to the objective function value and the constraints.

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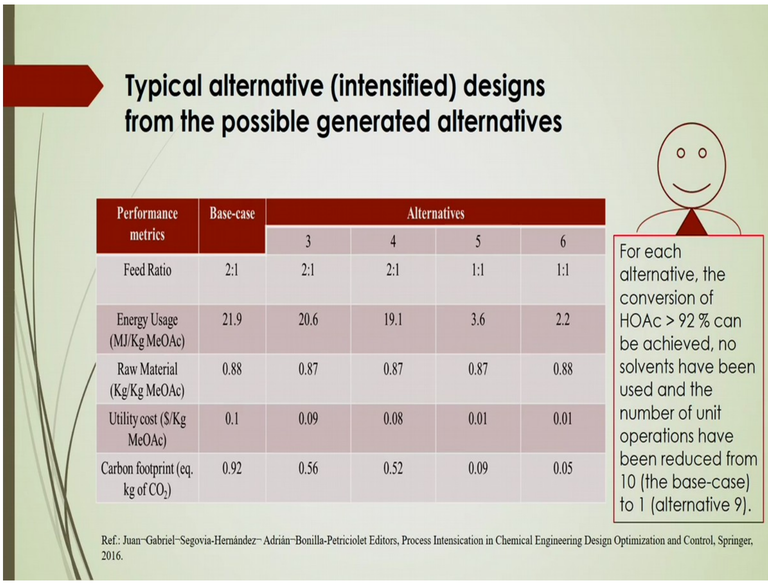

Here some typical alternative designs from the possible generated alternatives, here, 1, 2, 3, 4, 5, 6 alternatives are given here based on the feed ratio, energy uses, raw material, utility cost and carbon footprint. So, for each alternatives the conversion of acetic acid should be greater than 92 percent and it can be achieved where the no solvents have been used and the number of unit operations are actually reduced from 10 to 1 by alternative 9.

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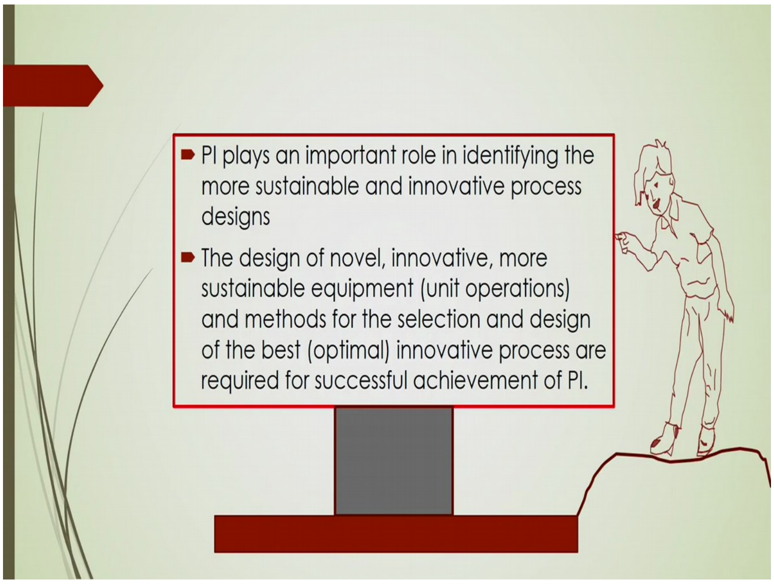

Now, in this case you have to remember that this process intensification plays an important role in identifying the more sustainable and innovative process designs based on this phenomena-based building blocks. And this you know that innovative sustainable equipments to be developed for that unit operations and along with that method for the selection and design of the best innovative process and it is of course required for the achievement of the process intensification.

And also, no design concepts for unit operations for multiple applications to be also thought about as a research and development and also accurate models, refinement of their existing models also to be needed to a better understanding of the complex behaviour of the reacting and separation and also you know that hybrid or based on the separation mixtures in unit operations.

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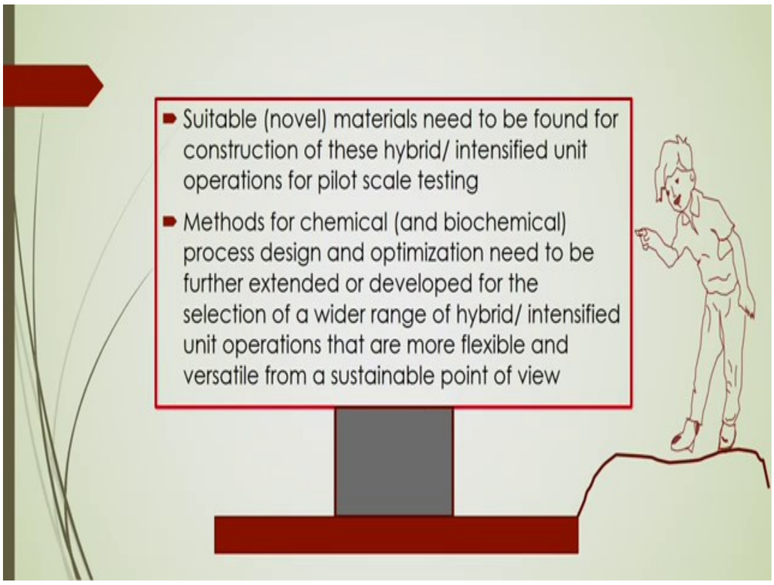

So, as, you know that research and development sections, they are actually trying to make a suitable material that is needed to found the construction of this hybrid or intensified unit operations or pilot scale testing. Also, method for chemical or biochemical process design or optimisation that also to be refined for further understanding and the instalment of those hybrid processes in industrial scale.

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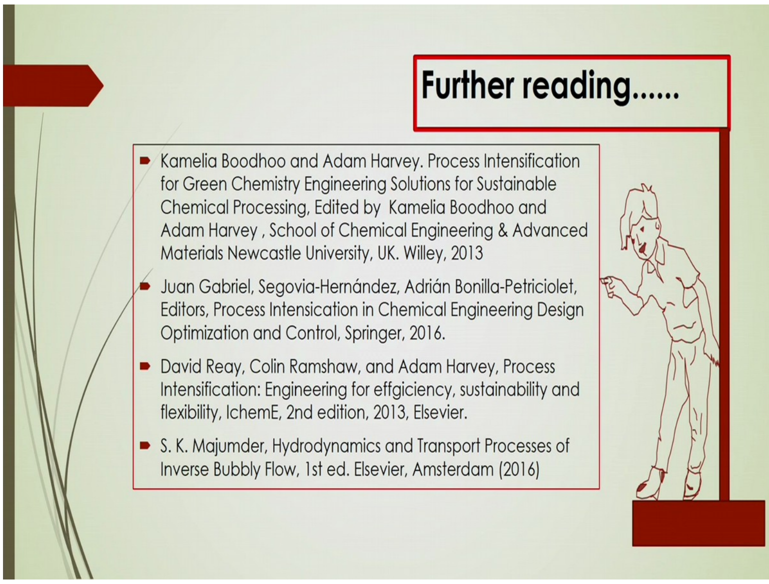

So, I would suggest to read further these books for further information regarding these computer-aided tools where it can be used for the particular process design by you know that hybrid or intensified way, how it can be developed based on the phenomena-based building blocks. So, thank you for this lecture today.