Chemical Process Intensification
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Lecture 11
Methods and Tools of Achieving Sustainable Design

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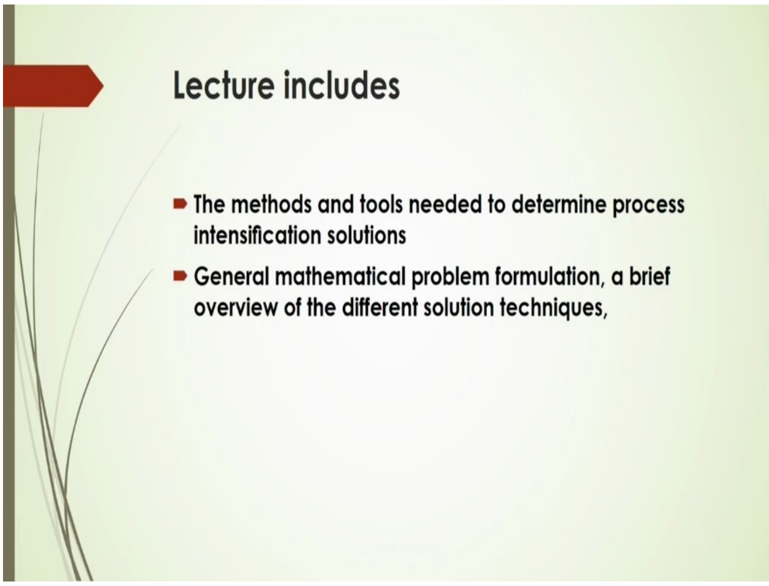

Welcome to Massive Open Online Course on Chemical Process Intensification. In this module we will discuss methods and tools for achieving sustainable design. In the previous notes we have discussed the scale and stages of design for the sustainable design and processes and in this lecture, we will cover this, under this method and tools, how to determine the process intensification solution and also what should be the mathematical problem formulation, brief overview of the solution techniques will be considered here.

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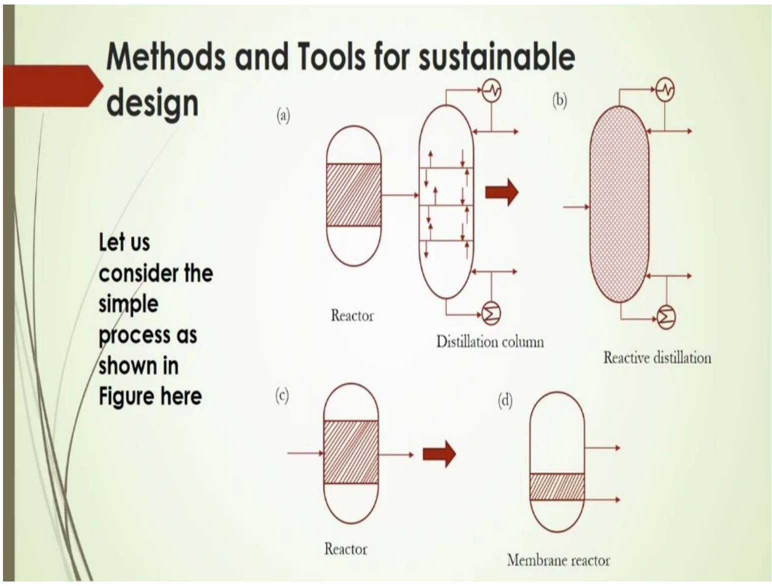

Now, if we consider the methods and tools for the sustainable design, in that case we have to, you know consider that, you know that scale and also unit operations. And if we consider that the simple process like as shown here in the figure, like a reactor distillation column, reactive distillation, even reacted to the membrane reactor, you will see there will be a conversion of this, you know the flow of this unit operation, scale to the unit operation, then task and then that final stages of that unit process.

So, here, now if we consider that for the sustainable design, and if we do the separate process of reactor, reaction engineering in the reactor and distillation in the distillation column, we have seen that there are, you know that more energy losses, even sometime will be less yield and also other different difficulties in the operation of the you know that processes.

So, conjugating these you know two operations like reactor and the distillation, where this, conjugation of these two processes of reaction and separation process, we can say that we can design of the reactive distillation, just by considering the economic and also some other operational factors to get the sustainable design.

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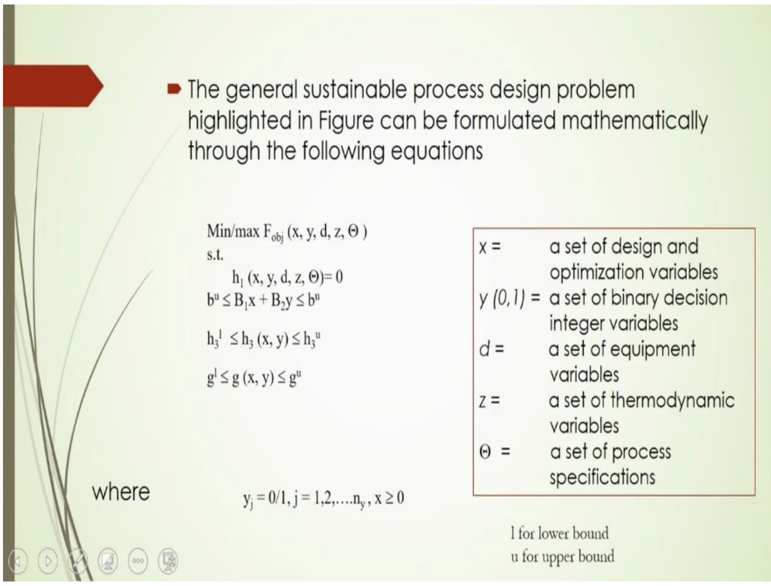

And some other examples like reactor, to you know that membrane for the separation, then reactive, or membrane reactor we can say there. So, in this way if we consider that certain, you know that process and, in that case, to design the general sustainable process, in that case you have to, you know that formulate these things by a mathematics and for that mathematical expression, you have to you know consider that different the different you know parameters.

And in that case if we express this by mathematical expression, like you have to minimise or maximise the objective of several you know operating variables where this sustainable design to be obtained. Based on this or subject to this some other, you know some other parameters here. In this case this equation we are given that 1, 2, I think 5, that if objective as a function of that is XY dz and you know that theta and subject to s1 into X, Y, D, Z and theta, that should be equal to 0.

$$Min \vee Max\, F_{obj}(x, y, d, z, \Theta)$$

s.t

$$h_1(x, y, d, z, \Theta) = 0$$

$$b^l \leq B_1 x + B_2 y \leq b^u$$

$$h_3^l \leq h_3(x, y) \leq h_3^u$$

$g^l \leq g(x, y) \leq g^u$

where

$y_j = 0/1, j = 1, 2, \ldots, n_y, x \geq 0$

And under this limit of you know up are bound in lower bound, it will be as that B lower bound should be less than equal to what is that B1 X plus B2 Y, these things should be less than equals to B, the upper bound. So, in this case and also some other parameters like h3, another parameter is a function of X and Y within a upper bound of this h3l to h3U. And also that GL to GU, and G is a function again based on that operating variables. Now, X is the set of design and optimisation variables, Y is a set of binary decision and these are variables.

And D is equal to a set of equipment variables and also Z that given here in the equation a set of thermodynamic variables and theta is a set of process specifications. And Y is a set of binary decision integer variables should be 0 or 1 and, in that case, also that objective functions should be a set of binary decision integer variables. That variables should be you know 1 to Z and which should be greater than or equal to 0.

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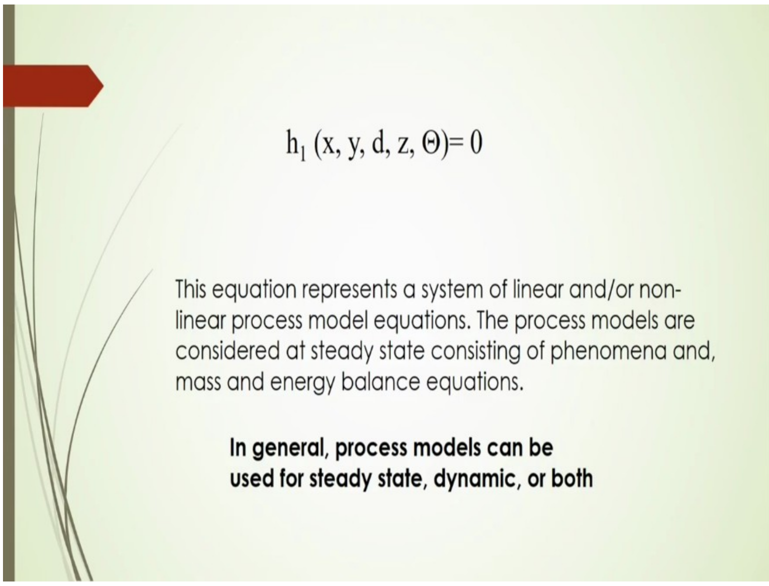

And in this case, this h1 is a function of X, Y, D, Z and Theta will be equals to 0,

$h_1(x, y, d, z, \Theta) = 0$

this equation represents a system of linear and nonlinear process model equations. In the process models are considered at steady-state that will consist of phenomena and mass and energy balance equations.

So, in general the process models can be used for steady-state, dynamic and or both modes. So this equation is very important whether you are representing the model equation as a linear system or non-linear system. So, the process models should be considered generally for the steady-state, which will consist of phenomena mass and energy balance equations.

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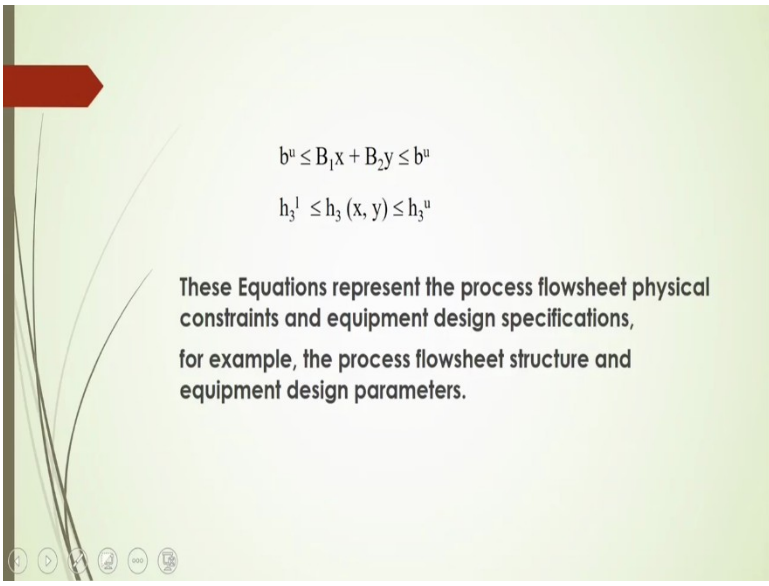

Whereas these equations B, that is B1X plus B2 Y and X3 is a function of X and Y,

$$b^l \le B_1 x + B_2 y \le b^u$$

$$h_3^l \le h_3(x, y) \le h_3^u$$

this you know, these equations represent the process flow sheet physical constraints and equipment design specifications. For example, the process flow sheet structure and equipment design parameters. So, by these equations, you can represent this process flow sheet physical constraints.

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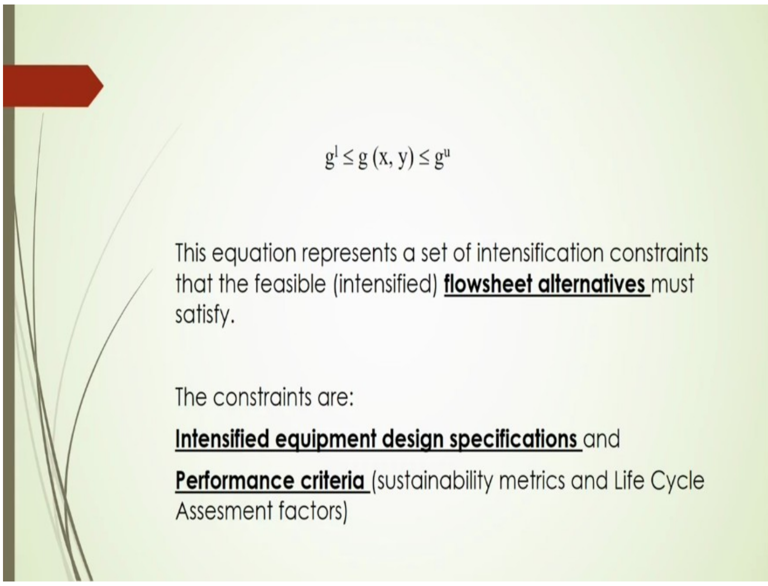

And also this equation, like G less than equal to G x, y, is a function of X and Y,

$$g^l \le g(x, y) \le g^u$$

was there a limit of lower to upward, this equation represents a set of Intersection constants at the feasible intensifies flow sheet alternative must be satisfied based on this equation. The constraints are intensified equipment design specifications and perform its criteria, which will be sustainability metrics and life cycle assessment factors. So, these constraints to be considered for your, you know that optimisation process for your sustainable design.

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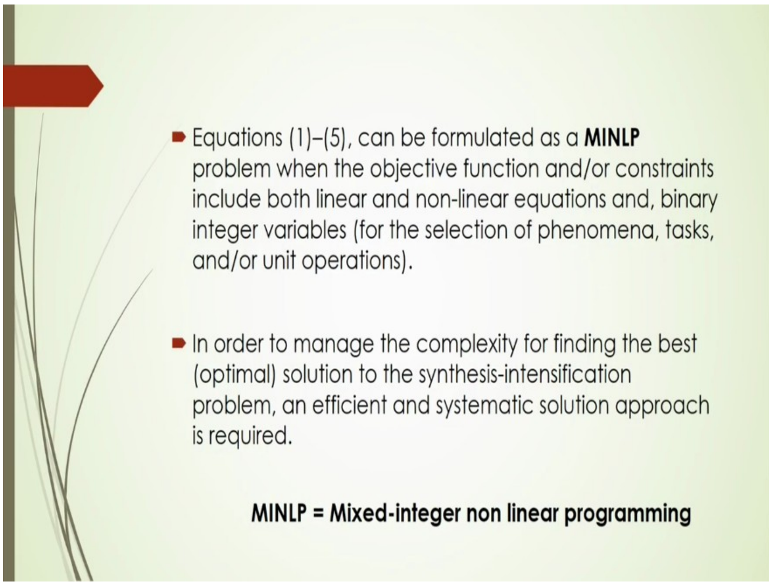

Now, equation 1 to 5, that I do not that in the beginning, that what are the equations can be formulated as a, you know that MINLP problem, when the objective function and/or constraints include both linear and nonlinear equations. And binary integers are variables for the selection of phenomena, tasks and unit operations.

In order to manage the complexity of you know finding the best or optimal solution to the synthesis intensification problem, an efficient and systematic solution approach is required. So, this MINLP, you know that problem should be considered when objective function or constraints, both will include linear and nonlinear equations. And also, binary integer variables for the selection of phenomena and tasks or unit operations to be considered. So, MINLP is mixed integer nonlinear programming.

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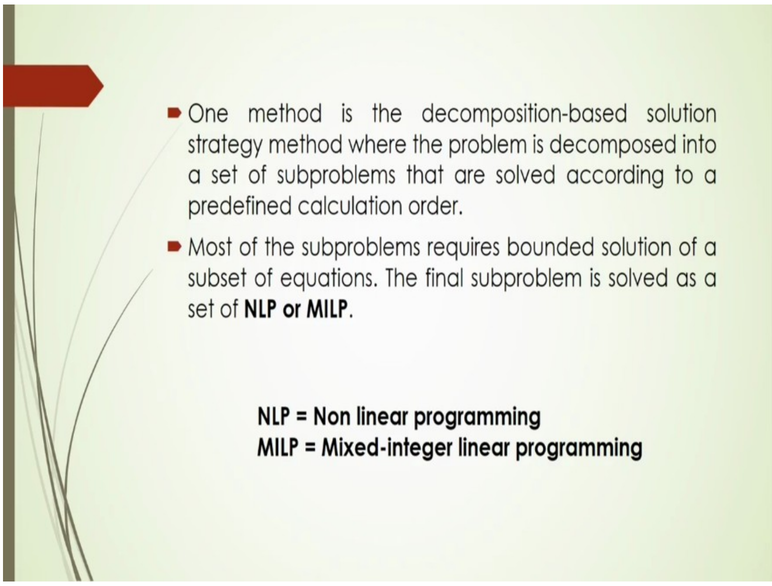

And also, one method is the decomposition-based solution strategy for this, you know where the problem is decomposed into a set of some problems that are solved according to the predefined calculation order. Most of the sub problems require a bounded solution of a subset of equations. The final sub problem is solved as a set of NLP or MILP. What is NLP? NLP is called Nonlinear Programming, whereas M ILP is called Mixed Integer Linear Programming.

So, one method to solve this problem it is called decomposition-based solution. And in that case the problem will be decomposed into a set of sub problems and that have solved according to a predefined calculation order. Most of the sub problems require bounded solutions, in that case and the final sub problem is solved as a set of, that is mixed integer linear programming or non-linear programming.

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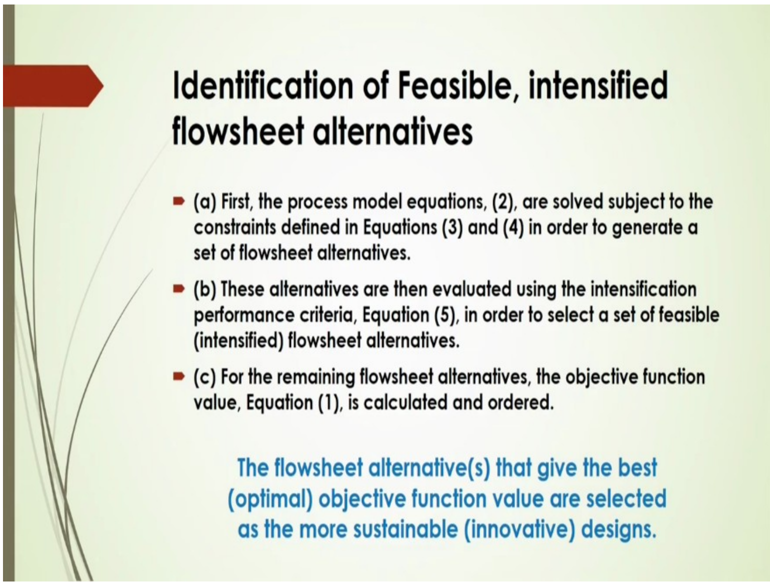

Now, what are the, you know that alternatives for the feasible, intensified flow sheet. 1st of all you have to consider the process model equations and which will be actually solved subject to the constraints that is defined in equation number 3 and 4 that earlier I have given in order to generate a set of flow sheet alternatives. These alternatives are then evaluated using the intensification performance criteria.

Equation 5 days in order to select a set of feasible flow sheet alternative. So, here you remember that equation that I have given, that will be sequentially 1, 2, 3, 4, though I have, it is not mentioned here but it will be considered as 1, 2, 3, 4, 5. Now for the remaining flow sheet alternatives, the objective function value equation 1 is calculated and ordered.

So, in that case you have to remember that the flow sheet alternatives that give the best optimal objective function value, that are selected as the more sustainable design. So, to identify the feasible and intensified flow sheet alternatives, you have to consider those model equations. That is given in equation number 2 and that should be solved subject to the constants even in equation number 3 and 4.

So, these alternatives, after that you have to evaluate using the intensification performance criteria and then finally equation 5, in order to select a set of feasible flow sheet alternatives. And for the remaining flow sheet alternatives, the objective function values that is equation is to be calculated and it should be ordered.

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Performance criteria	Improvement					
	Raw material utilisation	Separation efficiency	Energy efficiency	Waste minimization	Process economics	Environment outlook
Effective use of resources	*			*	*	*
New processing policies	*	*	*	*	*	*
Equipment capital investment		*	*		*	*
Utility consumption	*	*	*	*	*	
Sustainablity metrics			*	*	*	
LCA factors			*	*	*	
Integration of unit operations (sustainable technologies)	*	*	*	*	*	*
Integration of tasks	*	*	*	*	*	*
Integration of phenomena	*	*	*	*	*	*

Now, as per performance criteria, improvement in performance criteria for performing the process intensification, we can say that different performance criterion is there. So, there will be effective use of resources, that will be new processing policies, equipment capital investment, utility consumption, sustainability metrics, life cycle analysis factors and integration of unit operations or sustainable technologies like integration of tasks, integration of phenomena, all should be considered as a performance criterion.

So, improvement will be, you know that based on that raw material utilisation, separation efficiency, energy efficiency, waste minimisation, even process economics, even environmental outlook there. So, in this case here in the table, star will indicate the performance criteria that are used as a measure of improvements. So, in this case multiple performance criteria can also be used.

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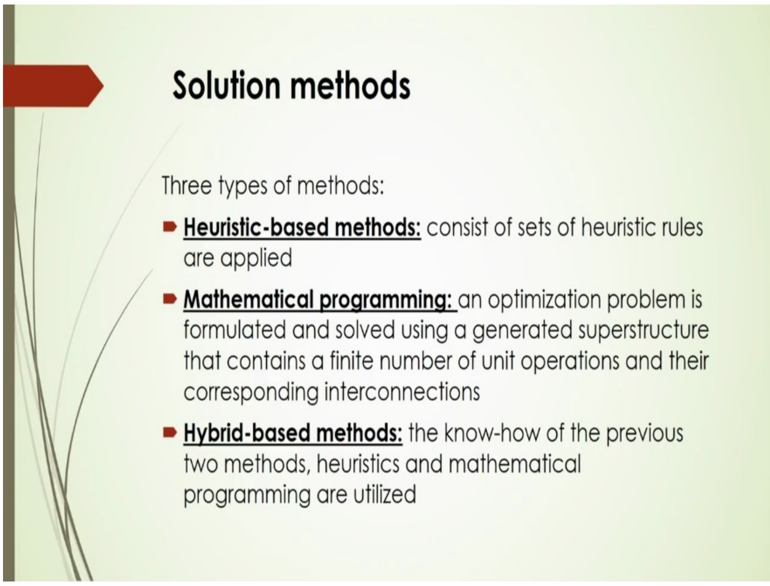

Now, what are the different solution methods to get that optimised, you know that process design. There are generally 3 types of methods, one is called heuristic based methods, it generally consists of sets of heuristic rules and also mathematical programming are one of the important you know that solution methods among the 3 methods of this given in the slides.

So, mathematical programming is an optimisation problem, which is formulated and solved using a generated you know superstructure that contains a finite number of unit operations and their corresponding interactions and who also interconnections.

Now, hybrid-based method is also another important, this is basically the know-how of the previous 2 methods, like heuristic and mathematical programming. And in that case, you know that based on the knowledge of this heuristic and mathematical programming, the hybrid method can be procured or developed to get that optimised solution.

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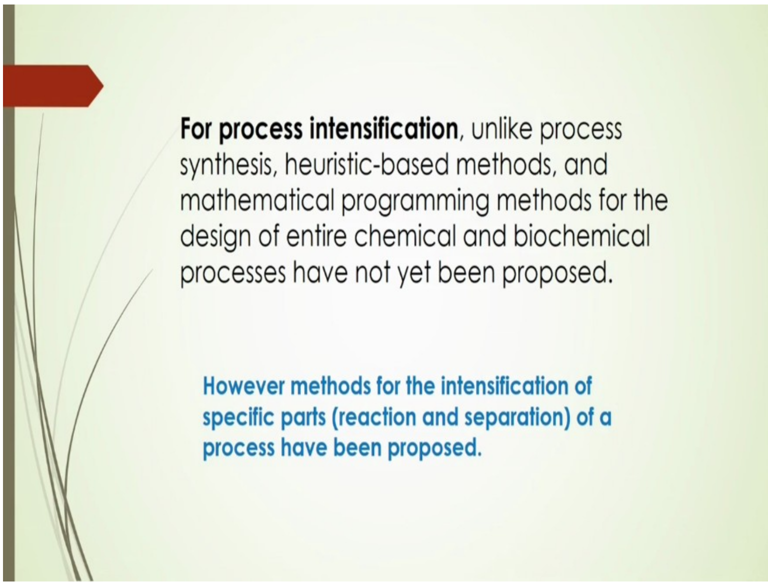

Now, for process intensification, unlike the process synthesis, heuristic based methods and mathematical programming methods, these 2 methods for the design of entire chemical and biochemical process have not yet been actually proposed as per literature. However, the methods for the intensification of the specific parts, that is reaction and separation of a process have been processed, have been actually proposed in the later research.

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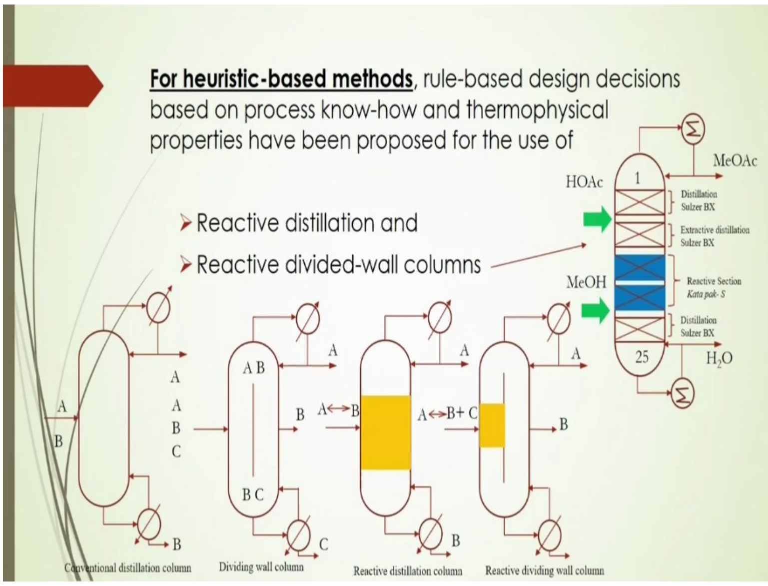

So, for heuristic based methods, it is generally rule-based, you know or design, decision based on process know-how and Thermo physical properties that have been proposed for the use of reactive distillation and reactive divided wall columns as shown in the figure in the slide. Here you can see the conventional distillation column from the left of this figure, A and B will be you know that reactants to be sent to that and to be separated that A and B and also that dividing wall column, there is another option to get that process intensification, here A, B, C will be supplied to that dividing wall column, where you can separate it with AB and BC at the bottom and the top of this column.

And after that this B should be separated from that ABC mixture and then, you know that A will be separated from the top of the column and C will be separated from the bottom of that column. Whereas, if you are using that reactive distillation column, that A and B will be used for reaction as well as the separation of this products of A and B and unreacted A and B and also product.

So, that product should be you know that taken care after separating of A and B from its top and bottom parts of the reactive distillation column. And you know that reactive dividing wall column also there, 1st of all this A and B will be giving the products as C and after that A will give you the product B and C and you have to separate that ABC by this wall separated, that is this column, dividing wall column. So, here you will see that B will be separated from this A and C from the top and bottom parts of the column.

Another important examples here, suppose you are going to actually produce that methyl acetate from the methanol and acetic acid mixture, first of all you have to allow it and the reaction of this, this methanol and acetic acid and whatever products will be coming. And that product should be, you know that separated by that distillation process or extraction process.

First of all, extraction, and then distillation, then you know that distillation. Now, finally that after reaction to the reactive extraction and distillation you can get from the top that methyl acetate as a product, whereas from bottom you can have this water solution water from the bottom. So, in this way you can date in that you know sustainable design of this certain process based on this heuristic method.

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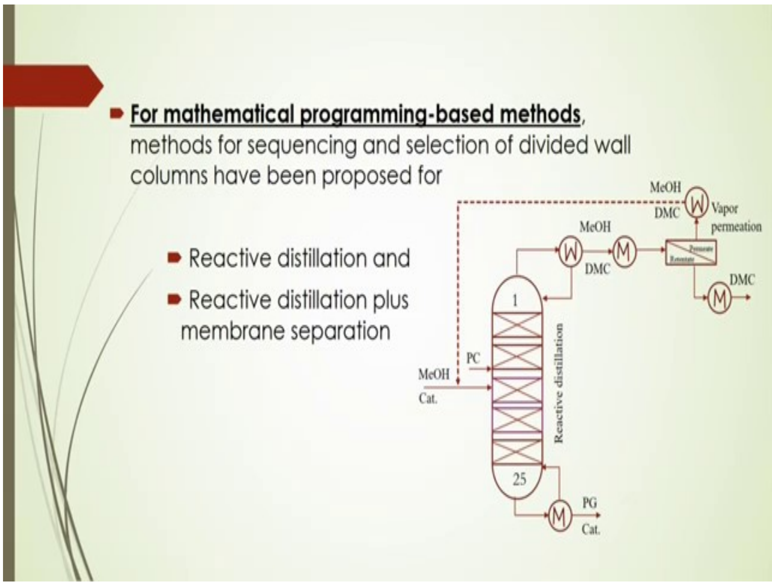

For mathematical programming-based methods, in that case these methods are actually generally for sequencing and selection of divided wall columns and in this case reactive distillation as well as reactive distillation plus membrane separation can be considered here. So, if suppose there is the methanol with catalyst should be, you know that used for that reactive distillation here like PC and PG are to be used, then that PC and after that you know after reactive distillation it will be separated as that methanol and DMC and as a bottom product PG and catalyst.

And also, after that it will be you know that separated by the membrane, to get that methanol and DMC and by vapour permeation that you can actually separate that DMC from that methanol. Of course, that DMC will be, some extent will be there with a mixture of methanol, it will be sent back to the distillation column. So, in this way that combination or you can say that integration of this process can be used and mathematically expressing this, you know this process, phenomena, then you can, of course, solve based on the operating variables, what are considered in this case.

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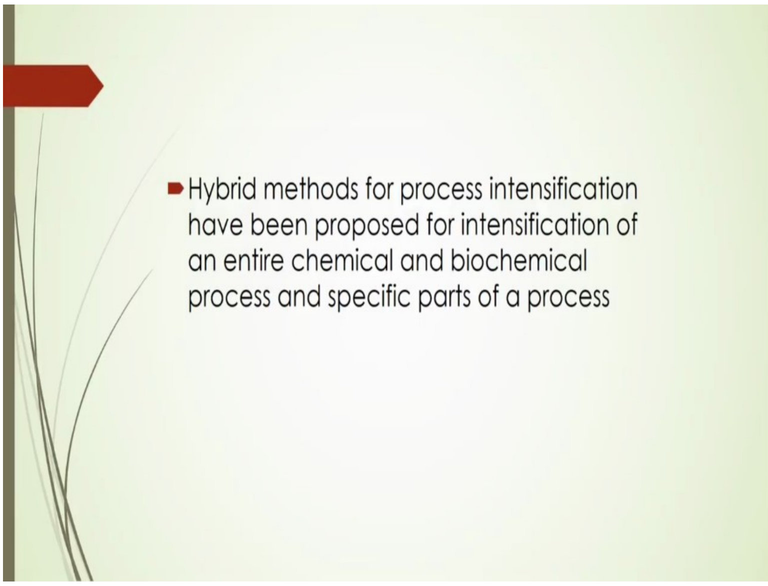

And hybrid methods for process intensification have been proposed for intensification of an entire chemical and biochemical process and specific parts of the process that we have to note down here.

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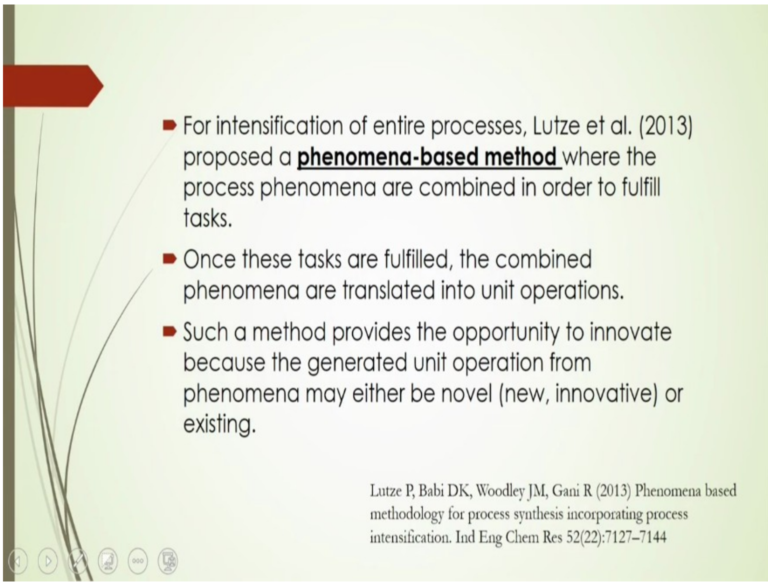

And for intensification of entire process Lutze et al. In 2013, they have proposed a phenomena-based method, where the process phenomena are combined in order to fulfil tasks. Like once these tasks are fulfilled, the combined phenomena are translated into unit operations. Such a method that will provide the opportunity to innovate because the generated unit operations from the phenomena may either be novel or maybe new, innovative or existing there. So, there it is why phenomena-based methods can be used to fulfil the task. And in that case, you have to that combine the phenomena, that should be translated into unit operations.

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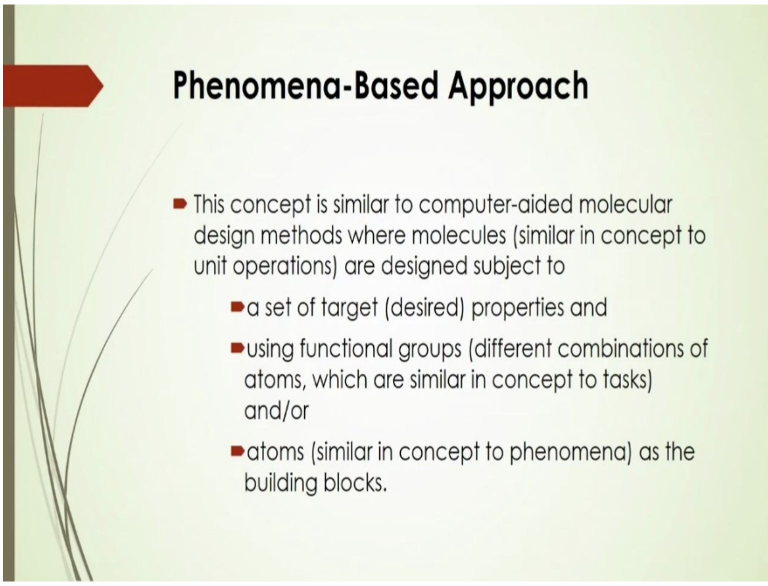

And based on that concept it is actually similar to the computer aided molecular design methods where molecules, that is similar in concept to unit operations are designed. That is subject to a set of you know target properties and using functional groups that is different combinations of the items which are similar in concept to task or you can say that atoms, that is similar in concept to phenomena as the building blocks.

So, you know you have to make a building block for this phenomena based approach where the set of target or desired properties to be identified and using that functional groups of different combinations of atoms, which are actually similar in concept to tasks that should be also it you know taken care and also atoms that is similar in concept to phenomena that also to be you know identified to get the you know that solution based on this phenomena based approach.

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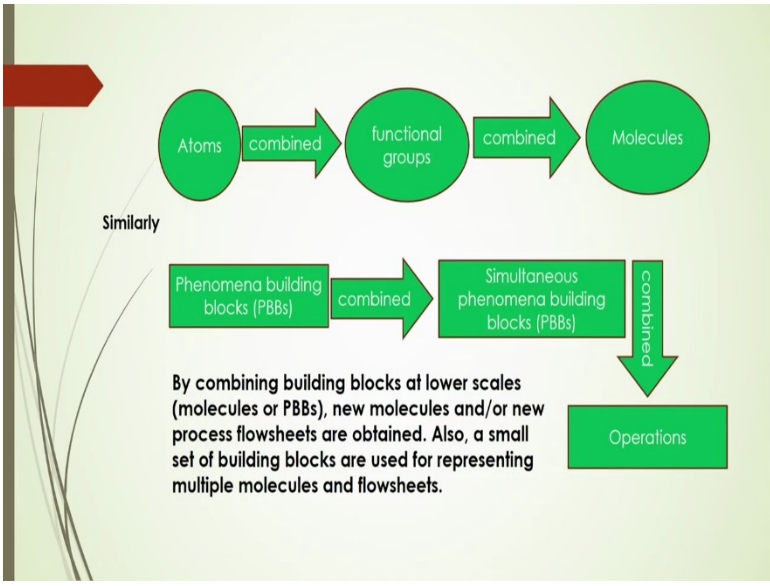

Now, for these atoms are to be combined, that will give you the functional groups and then it will be combined to molecules and after that what will happen that phenomena building blocks to be made based on this atoms or combined phenomena, that is phenomena-based building blocks and it will be combined to give you the simultaneous phenomena building blocks as compared to the atoms to molecules. And you know that then if you combine the simultaneous phenomena building blocks, it is called the SPB, that instead of PBB, that is the set of PBB, that is called SPB, it is called simultaneous phenomena building blocks and it will be combined to give you the final operations there.

So, based on the concept of atoms to the molecules where the atoms combined to functional groups and to molecules, similarly you can make that block wise, that is block concept of the phenomena-based blocks, you can develop or you can make to give you the final operations there. Like phenomena building blocks, it will be combined to that simultaneous building blocks and then finally it will get, it will give you the operations based on that combination of this phenomena-based building blocks.

So, by combining building blocks at lower scales, that is molecular's or PBBs, a new molecule or a new process flowsheet you can say are to be actually developed to get that design. Also, a small set of building blocks are used for representing the multiple molecules and the flowsheets there.

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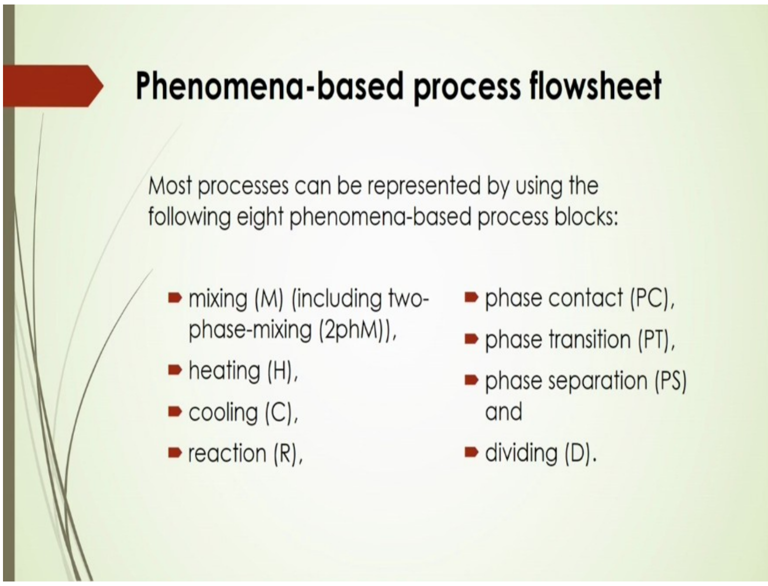

And most of the process can be represented by using the following, you know that eight phenomena-based process blocks like mixing, including two phase mixing and heating, you can say that cooling, reactor, phase contact, phase transition, phase separation and dividing. So, these are the different phenomena-based process blocks, so if you are combining these different phenomena-based blocks to form that PBB and after that combining more PB, it will give you the simultaneous building blocks and finally you can get the, you know that final operational flowsheets there.

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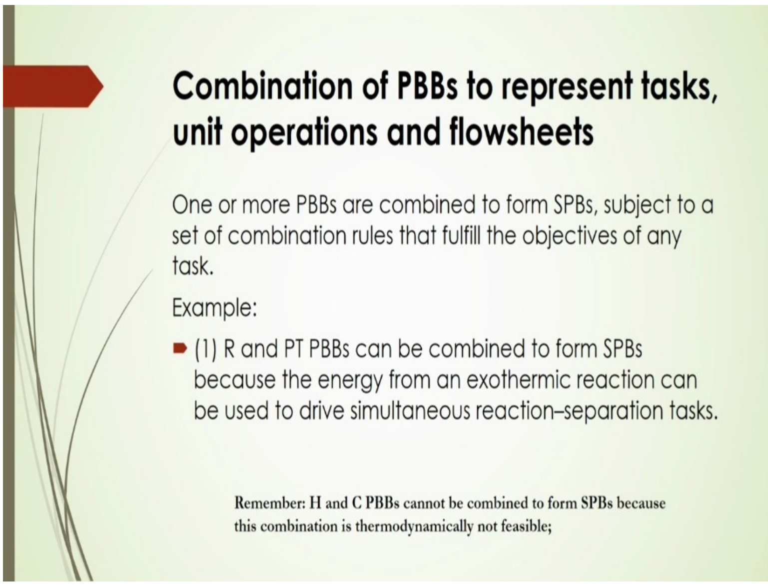

So, one or more PBBs are combined to form that SPBS, it is called Simultaneous phenomena-based building blocks, subject to asset of combination rules, that fulfil the objectives of any tasks there. Example, suppose if you are considering that reaction and also the phase transition, so this reaction and phase transition phenomena-based building blocks can be combined to form this simultaneous phenomena-based building blocks.

Because the energy that is from an exothermic reaction can be used to drive the simultaneous reaction separation tasks. So, that is why you have to combine SPBBs to form that simultaneous PBS, where the energy and neck Superbike reactions to be utilised to drive the simultaneous reaction separation operation tasks.

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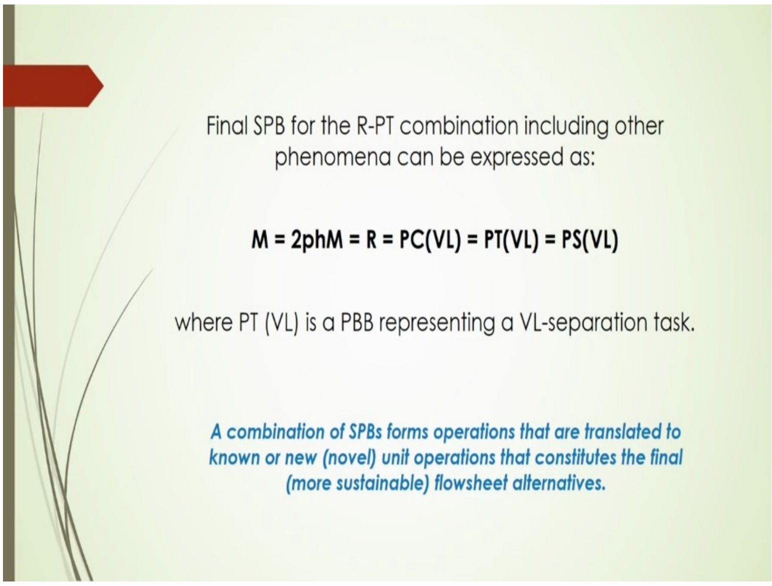

Final, that SPB for the RPT, that is you know the reaction and phase transition combination, that including other phenomena also can be expressed as this, by mathematics like, you know that M will be equal to 2phM, that is 2 phase mixing, that is equal to reaction that PC (VL) and PT(VL) and PS(VL), VL means vapour liquid, PC means phase contact between these vapour and liquid.

Phase transition vapour and liquid and phase separation vapour and liquid. For that PT (VL) is a PPV representing a vapour liquid separation task. So, a combination of this SPVS forms operations, that are translated to know or new novel unit operations, that constitute the final, you can say more sustainable flow sheet alternatives. So, that is why final SPVS for this combination of PBB can be formed based on that building blocks of that phenomena-based variables. In combination of those, this SPVS will give you the final flow sheet alternatives.

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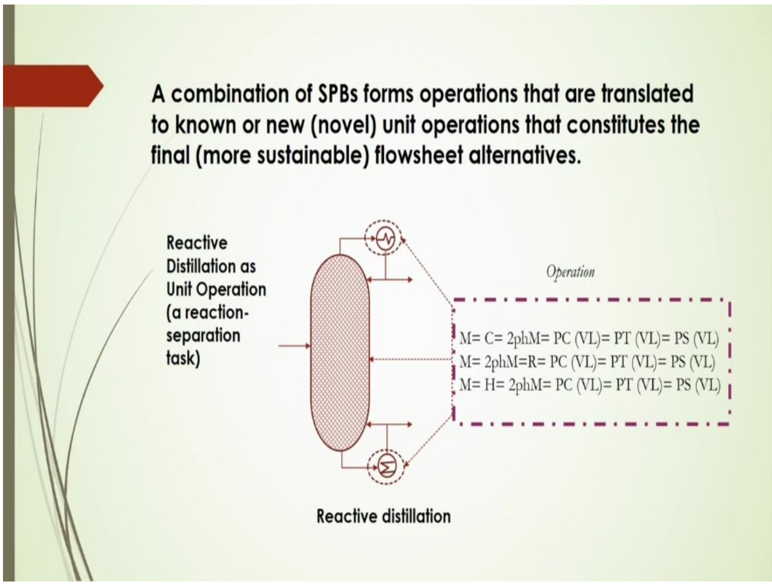

Now a combination of this SPBs form operations that are translated to know or new unit operations that constitutes the final flow sheet alternatives. So, based on we can here have this reactive distillation where reactive distillation will be considered as a unit operation, that is a reaction separation task.

So, in this case you will see there, where condensation and the heat exchanger to be used there, so in that case that operation will be, based on that mixing, you know that contact, even you know 2 phase mixing, even PC, that is vapour liquid, phase contact and also phase transition will be there between that vapour and liquid. Also phase separation will be there. So, in this way that M to PSM, that will be equal to R in equal to PC of VL and PT of VL and PS of VL and in this way you can form this operational flowsheet for this reactive distillation.

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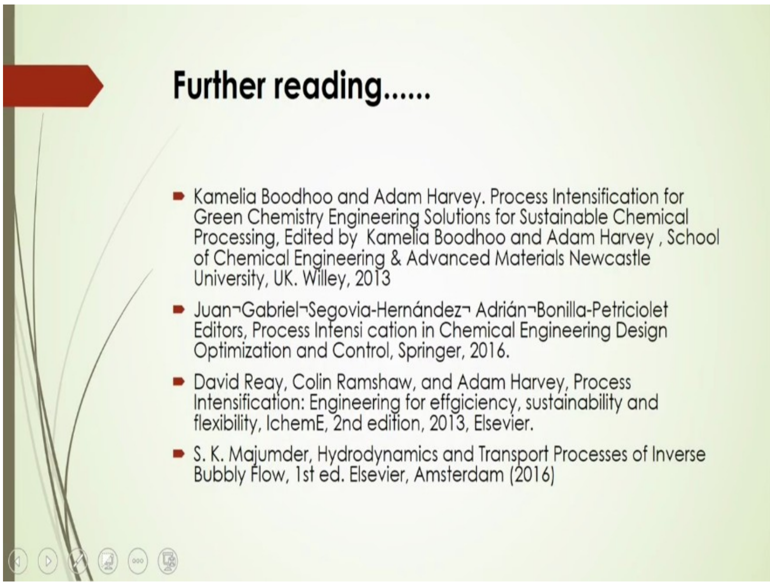

Now, I will suggest to read further about this, that operational methods or solution methods to get that final solution of this optimisation or representing the process intensification design, based on the different constraints and different phenomena based variables, based on which you can form the building blocks and which is based on the concept of you know that atoms to the molecules and how then these PBBs, that is phenomena based building blocks can be formed based on the phenomena of the variables and also from that PPB.

How it can be formed to that simultaneous phenomena-based building blocks which will give you the final alternatives of the process flowsheet. And that is why we can use that concept of the atoms to molecules for the design of the sustainable process based on this building block concept. So, I will suggest you to go further this textbook to know about the solution of the techniques of sustainable design for this process intensification. So, thank you for this lecture today.