Chemical Process Intensification.
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Model 5: Optimisation from Process Intensification.
Lecture 1: Introduction on Stochastic Optimisation.

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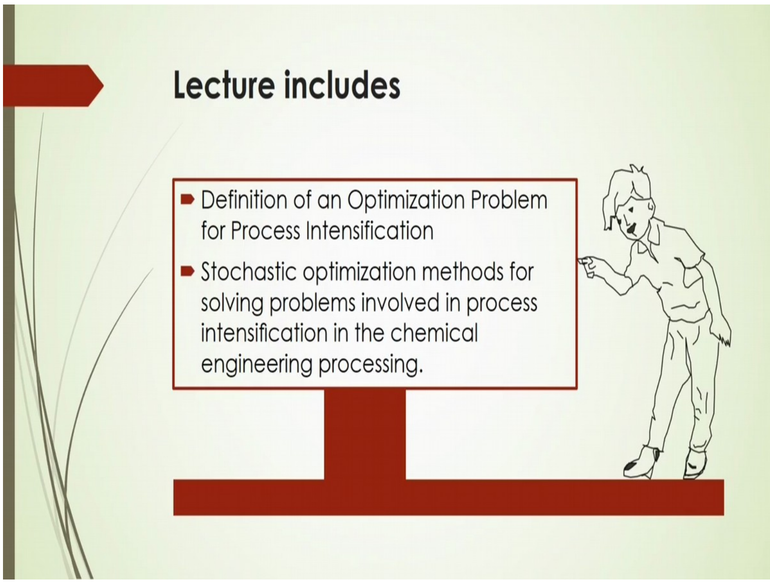

Welcome to massive open online course on chemical process intensification. In this module as optimisation for process intensification, we will discuss something about optimisation and chemical process intensification and also some algorithms and how to actually get the solution for that, we will be discussing in this module 5. And under this module 5, in the 1st lecture we will discuss something about the stochastic optimisation, basic things. So, in this lecture we will be including the definition of an optimisation problem for process intensification.

And types of optimisation problem for the process intensification also special attention to be given to the stochastic optimisation methods for solving problems involved in process intensification in the chemical engineering process. In the previous module we have discussed regarding the different scale and stages of that sustainable design and also what are the different methodology and for that what are the computer-aided tools are being used for the sustainable design.

So, based on that whenever you are going to design that certain process, that design should be also based on the optimisation techniques, optimisation aspects. So, here that is why we should learn something about that basic of that optimisation problem for the process intensification.

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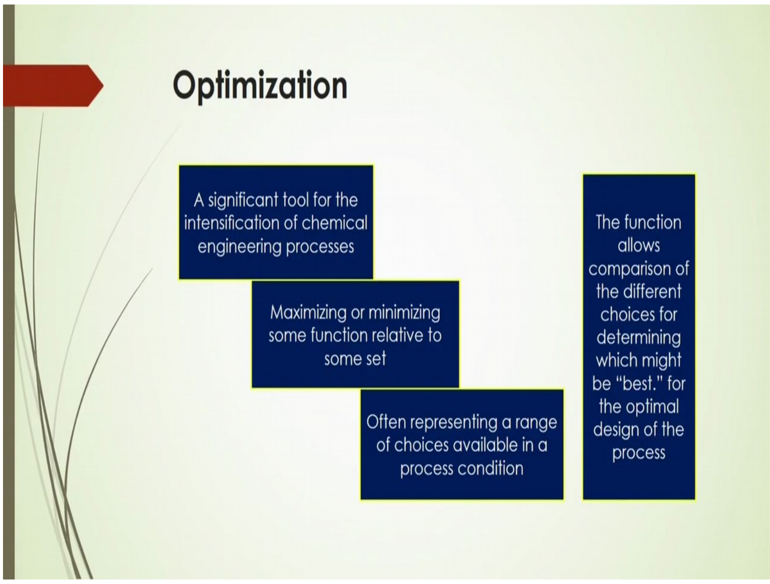

Now what is that optimisation, you know this optimisation is a tool for the intensification of chemical engineering process, especially if you consider that maybe this optimisation will be for other type of processes. And based on this optimisation tool, your objective is to maximising or minimising some function that will be related to some set based on that process condition.

And also this optimisation will often represent a range of choices available in a process condition. So, what are the variables to be taken for the analysis of that process and based on which that design should be further considered. And whatever functions will be considered based on that operating conditions that function will allow the comparison of the different choices for.

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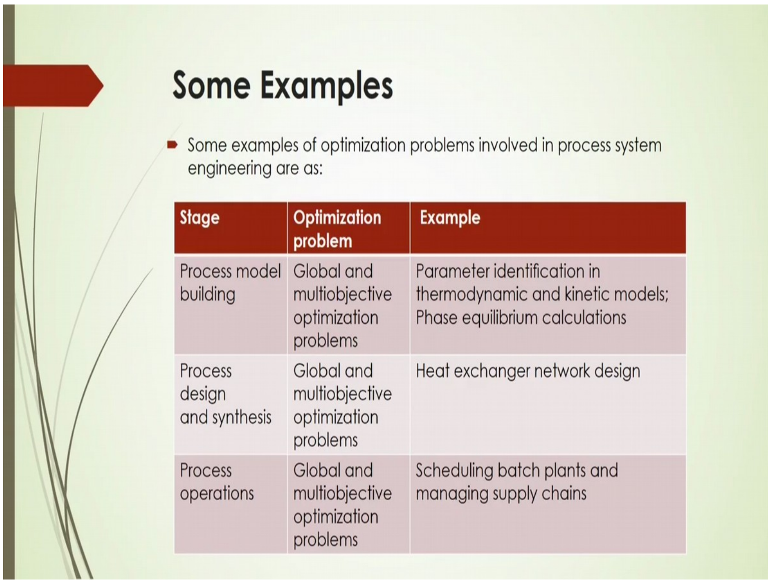

Here are some examples are given for the optimisation problems which is involved in process system engineering, such as, if I consider that there are several stages of that operation. So, in that case process model building stage that we have discussed in the earlier lectures also, different stages and different levels of solving that for the design of that sustainable processes. So, in that case the stage or process model building, process design and synthesis, process operations, those are stages, in that case what are the optimisation problems are actually coming that also to be considered.

So, in the stage of process model building you will see the optimisation problems will be global and multi-objective optimisation problems. Such as parameter identification in thermodynamic and kinetic analysis of the process and also what are the phase equilibrium conditions that also to be actually calculated based on this optimisation process.

And the process design and synthesis in that case again that optimisation problem is global and multi-objective and in that case you can have an example like heat exchanger network design, in that case you have to choose that optimisation problem as a global and multi-objective optimisation. And process operation, that is also global and multi-objective optimisation problem. In this case scheduling waste plants and managing the supply chains are the examples for this stage of process operation for optimisation problem.

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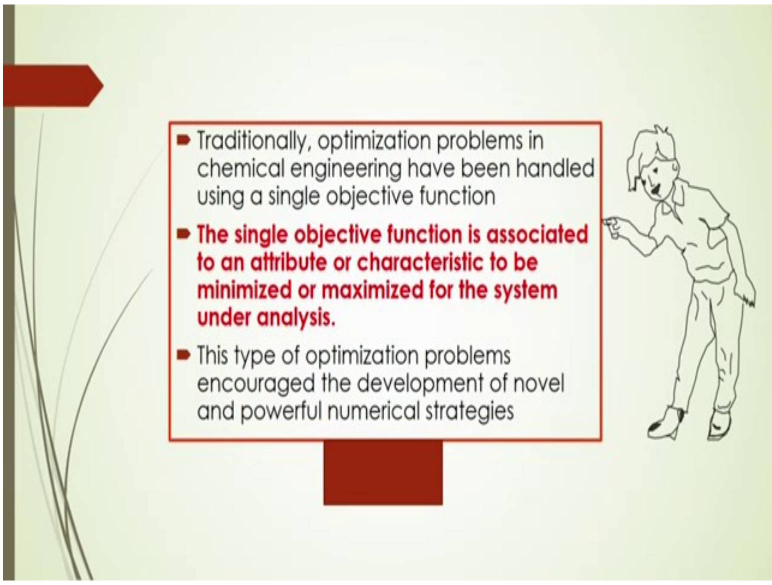

So, in this case we have to say that traditionally the optimisation problems in chemical engineering actually have been handled using a single objective function. In that case the single objective function is generally related to an attribute or you can say the characteristic to be minimised or maximise for the system under analysis. So, these types of optimisation problems encouraged the development of noble and powerful numerical strategies.

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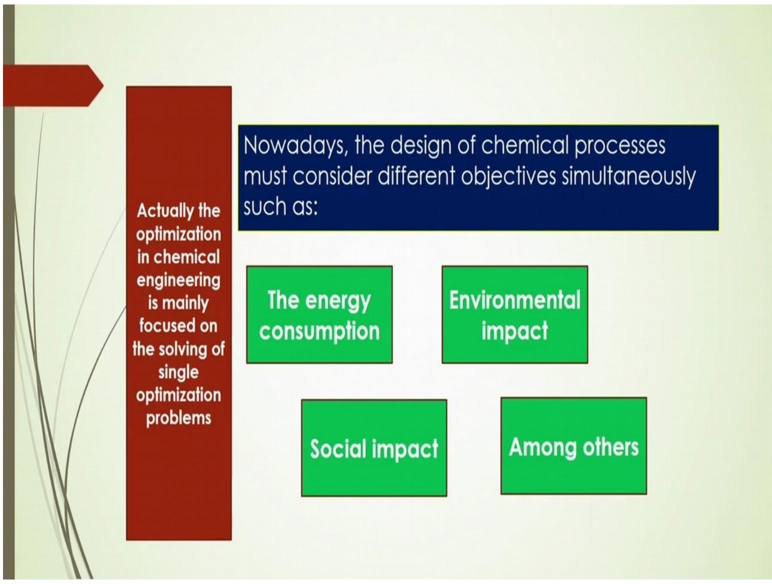

So, that is why the traditional optimisation problems may not be useful nowadays because whenever we are going to design any chemical process based on the process intensification, there are several different objective is simultaneously will come for this, in that case you have to consider all those that different objective for the design. So, that is why whatever optimisation actually techniques earlier was used, that was mainly focused on the solving of the single optimisation problem.

But for process intensification and nowadays the design of chemical engineering processes must consider that different objective simultaneously. What are those different objective to be considered, like what are the energy consumptions, what are the environmental impact and also what are the social impact, also among others there are various objective should be considered for this design of chemical engineering process. And in that case you have to compare this multi-objective optimisation process with the single objective, then you will realise that how process intensification actually will act a role based on this optimisation problem.

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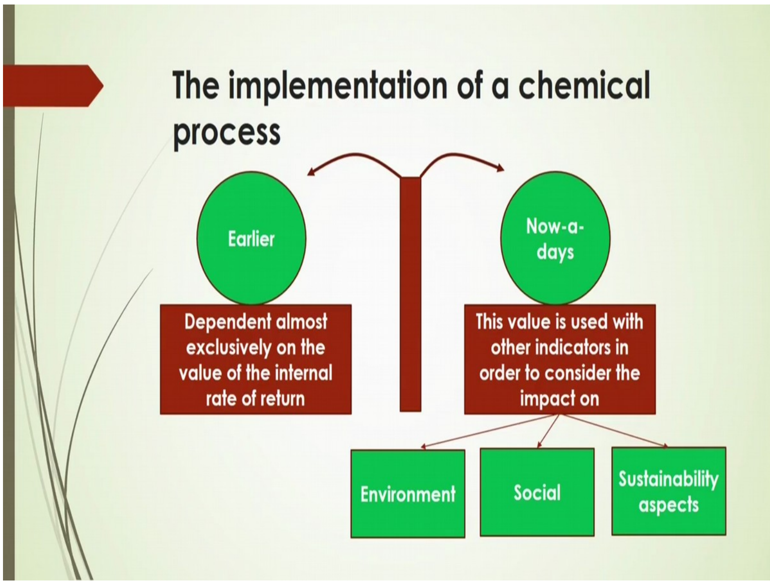

And then after that you have to, you know that implement that chemical engineering process based on that by comparing that earlier and also nowadays you know that problems solutions in the design aspect. So, in earlier stages you will see that, it will depend almost exclusively on the value of the internal rate of return whereas nowadays this value is used with other indicators in the order to consider the impact on like environmental, social and sustainability aspects.

So, that is why whenever you are going to implement that chemical process, that you know internal rate of return value of course should be based on that environmental, social and sustainability aspects. So, that earlier stage, you know that only single objective, single conditions actually being used for that analysis of that design or optimisation process.

Whereas nowadays it is being used based on that environmental, social and sustainability criteria.

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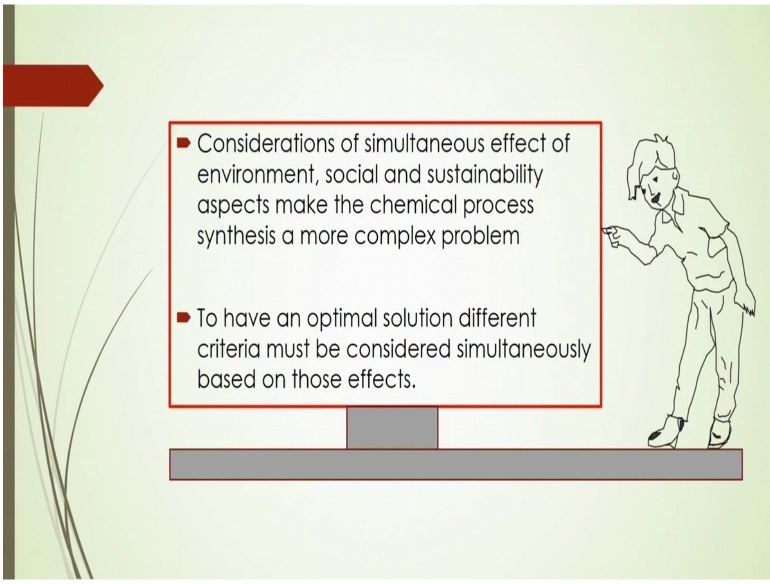

Now considerations of simultaneous effects of environment, social and sustainability aspects make the chemical process synthesis a more relatively complex problem. And in that case to have an optimal solution, different criteria should be considered simultaneously based on those effects. So, by considering these 3 effects of environment, social and sustainability, whenever you are getting that complex phenomena, you may not get that single optimal solution there, maybe different you know that multi-optimal solutions you can expect for that.

But to get an optimal solution, that a different criteria should be considered based on those effects that means there are several you know that variables that are effects on the objective functions. So, those objective functions to be considered based on that effects.

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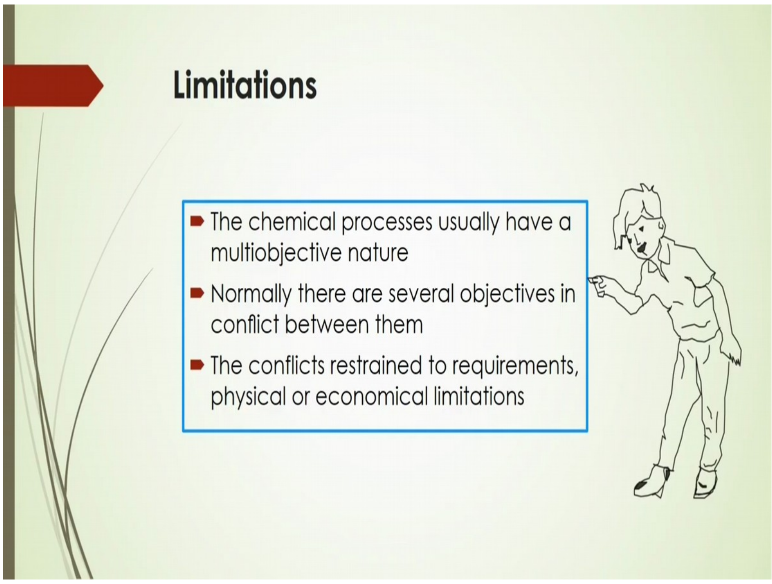

Now, what are the limitations of that optimisation problems, in that case the chemical processes generally use a multi-objective nature. And also that normally there are several objectives in conflict between them. So, that complex restraint to requirements, physical or economical limitations.

So, that is why there are some limitations that you have to consider during your optimisation problems, how to actually segregate those conflicts of several variables between them, so that you can you know that several objectives in the conflict between them can be you know that you can wisely consider by just neglecting that conflict of that multi-objective nature of that variable.

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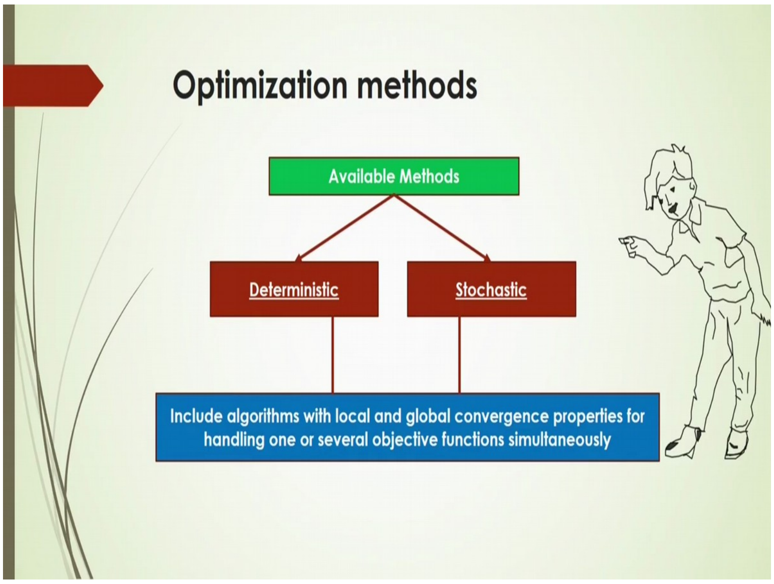

Optimisation methods are generally in this case, if we talk to that, what are the different methods are available to get this optimisation of this chemical engineering process. So, in that case available methods are deterministic and stochastic, in that case both the methods include algorithms with local and global conversion properties for handling once or several objective functions simultaneously.

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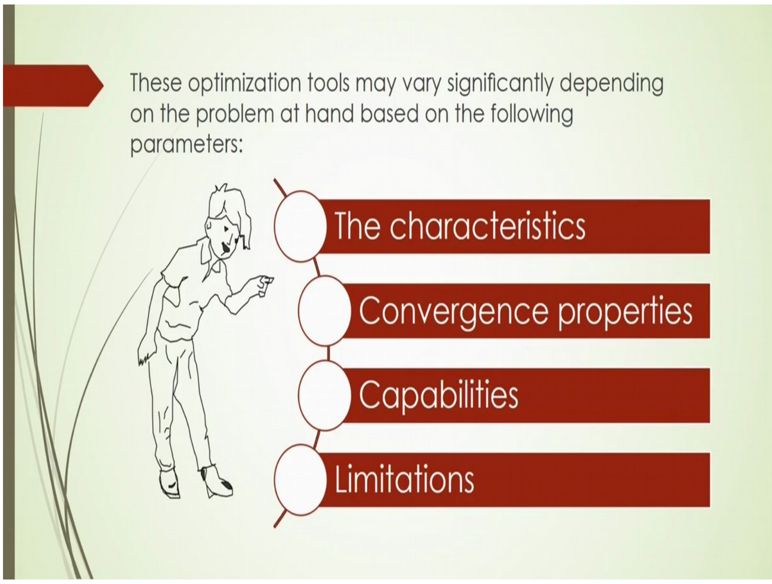

So, first of all let us consider that how these optimisation tools may vary significantly depending on the problem at hand based on the parameters. Now what are the parameters actually that effect on that optimisation tools, like you know that characteristic features and the convergence properties, capabilities and limitations. These are the 4 parameters that affects on the optimisation tools significantly.

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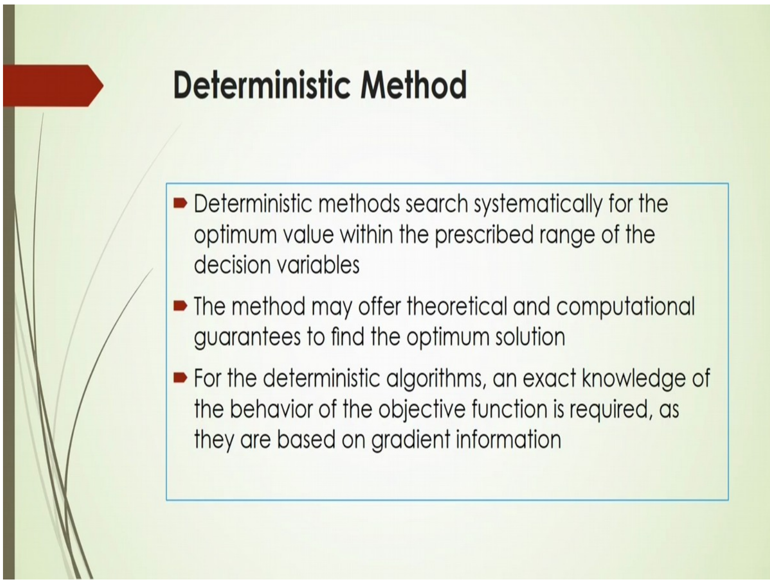

Also, if we consider that deterministic method, in that case the method actually search systematically for the optimum value within the prescribed range of the decision variables. So, these deterministic methods will give you the theoretical and computational guarantees to find the optimum solution.

And for the deterministic algorithms, an exact knowledge of the behaviour of the objective function is required, otherwise actually there will be some, you know that information to be missed for that. So, that is why based on that gradient information, exact knowledge of the behaviour of the objective function should be you know that considered. So, that is why these deterministic methods are useful for critical and computational methods which will guarantee to find out the optimal solution.

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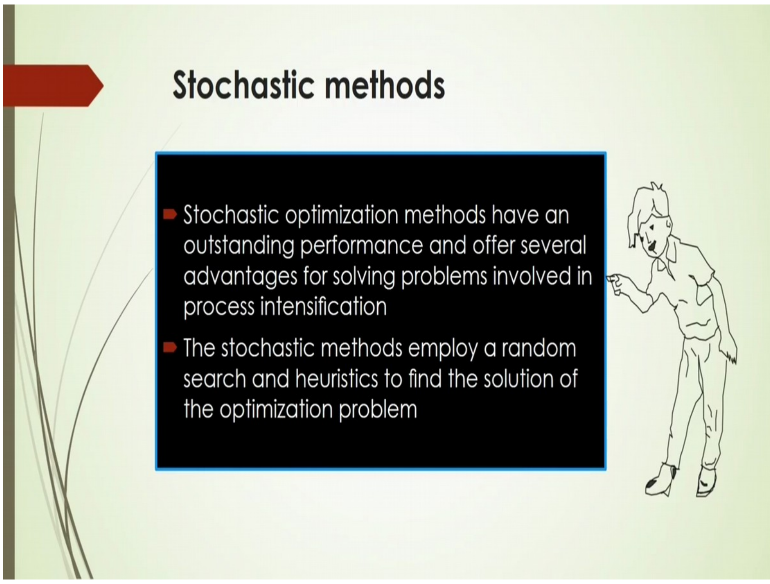

Whereas stochastic methods have an outstanding performance and offers several advantages for solving problems involved in process intensification. In this case you know that methods employ a random search and heuristics to find the solution of the optimisation problem. So, in this case we will see there are several advantages and disadvantages also you will find here. That because you know that in stochastic methods, sometimes you have to search the random variables and also you know the some heuristics you have to consider to find the solution of that optimisation problem.

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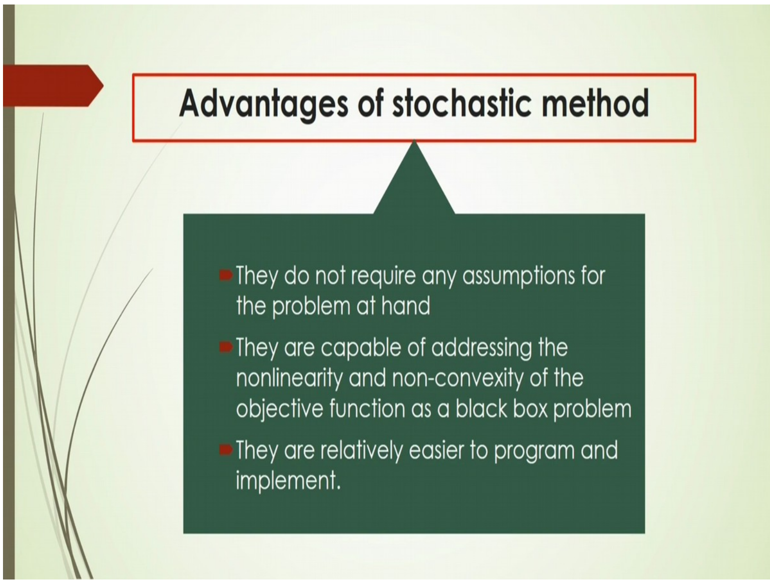

What are those advantages of that stochastic method? In this case, these methods, you know to not require any other options for the problem at hand here. So, these are the advantages. And they are capable of addressing the nonlinearity and non-convexity of the objective function as a black box problem. And they are relative easier to program and implement.

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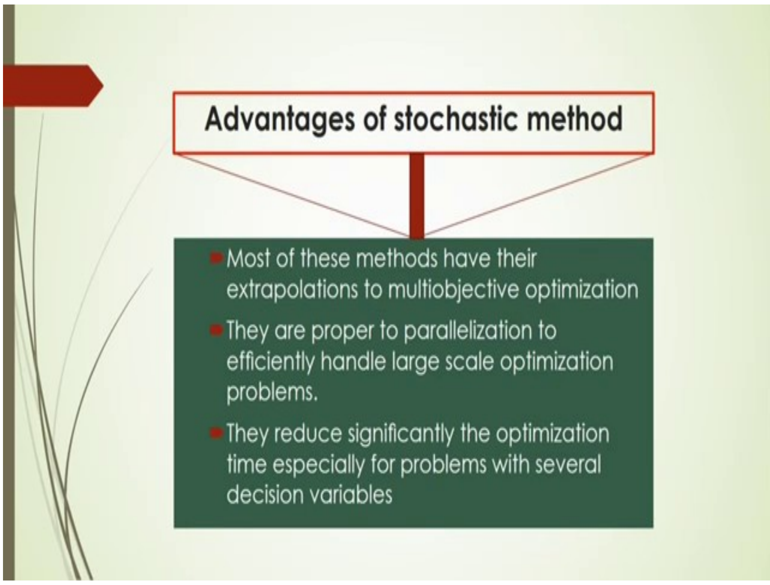

And also most of the methods have their extrapolations to multi-objective optimisations and also they are proper to you know that parallelisation too, efficiency or efficiently handle larger scale optimisation problems. So, they reduce significantly the optimisation time, especially for the problems with different decision variables.

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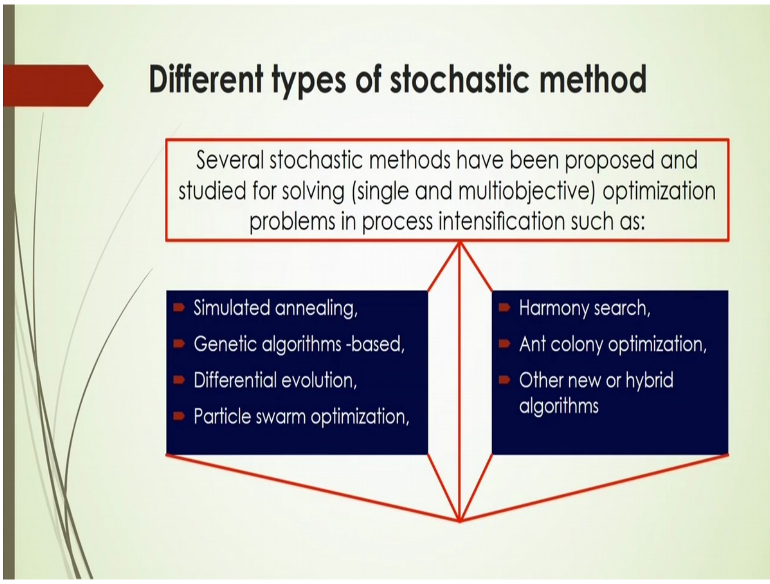

So, what are the different types of stochastic methods that you have to know. Several methods actually based on the stochastic considerations are you know proposed, so in that case these methods actually solve the single and multi-objective optimisation problems in process intensification.

So, what are those different types of stochastic methods like you know simulated, annealing, genetic algorithm based, differential evaluation or evolution and particle swarm optimisation, harmony search, Ant colony optimisation other new or hybrid algorithms are there. So, these are the several stochastic methods which are being used for solving the single and multi-objective optimisation problems in process intensification.

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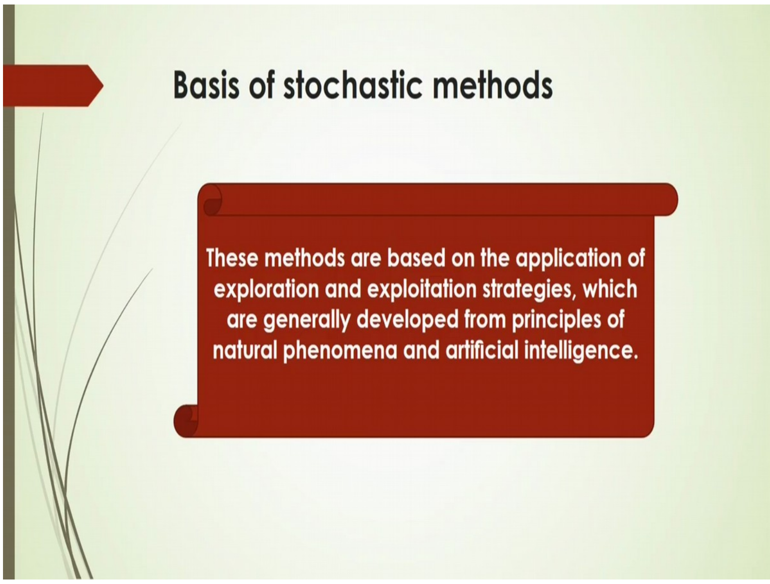

What are the basis of stochastic methods? Actually these methods are based on the application of exploration and exploitation strategies, which are generally developed from principles of natural phenomena and artificial intelligence. So, this was the basis for that stochastic methods.

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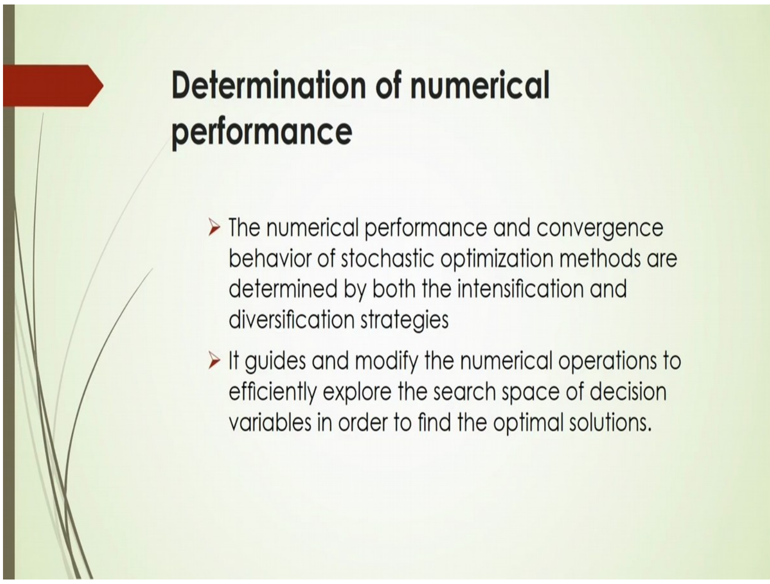

Now, to get the numerical performance, you have to converse the behaviour of the stochastic optimisation methods and which are to be determined by both the intensification and diversification strategies. And it guides and modifies the numerical operations to sufficiently explore the search space of decision variables in order to find the optimal solutions.

So, here very interesting that whenever you are going to find out that numerical performance, you have to consider both the intensification criteria, why this process intensification is done, on what basis this intensification is done, that that several criteria, several aspects, several you know that change of geometry, either change by geometry or not.

Either change by concentration variations or either you are changing that process intensification based on that you know that surface properties or some other to know that like the reduction of equipment or you can say that reduction or you know that suitable using solvent, even suitable material, even what are the suitability of the environmentally packed positive or negative.

All those actually factors to be you know considered for the performance of that optimisation problem. So, in that case you have to sometimes modify that numerical operations based on those factors and also you have to search that decision variables among of them to find out that optimal solutions based on those decision variables.

So, the decision variables to be found, based on that, you may search that the decision variables, based on that building block phenomena that we have discussed in the previous class also, there are different phenomena based building blocks like mixing characteristic, reaction phenomena, even the separation, even you know that Two-phase mixing, multiphase mixing, single phase mixing, even the geometry, some dividing rule. So, all those phenomena based building blocks to be considered.

Among those building blocks that you have to search some suitable phenomena based building blocks and based on which you have to make a set of simultaneous phenomena based building blocks. And those simultaneous phenomena based building blocks you can identify the decision variables to find out the optimal solution also. So, to determine the numerical performance and the convergence behaviour of the stochastic optimisation methods, what is that you have to determine both the intensification and diversity case in strategies based on that phenomena of the operating variables.

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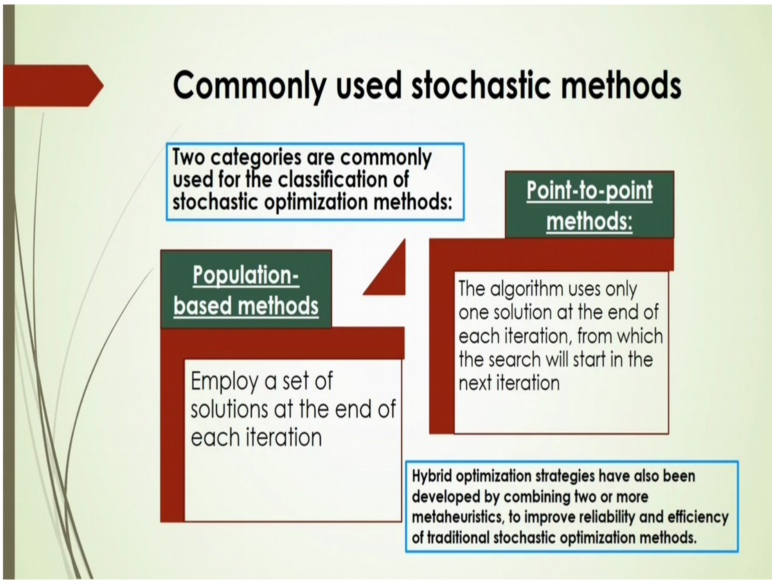

Commonly used stochastic methods are generally of two categories, like population-based methods and point-to-point methods. In this case these two categories are commonly used for the classification of these stochastic optimisation methods. The first classification is called population-based method, in this case generally employs a set of solutions at the end of each iteration. So, you can get the set of solutions at the end of each iteration.

Whereas the point-to-point methods provide solution based on the algorithms which are being used on the one solution at the end of the each iteration from which the search will start in the next iteration. So, that is why point-to-point methods, for that you have to use some algorithm where your search of that solution will be based on that iteration of the previous part. And hybrid optimisation strategies may also been developed by combining two or more meta heuristics to improve reliability and efficiency of traditional stochastic optimisation methods.

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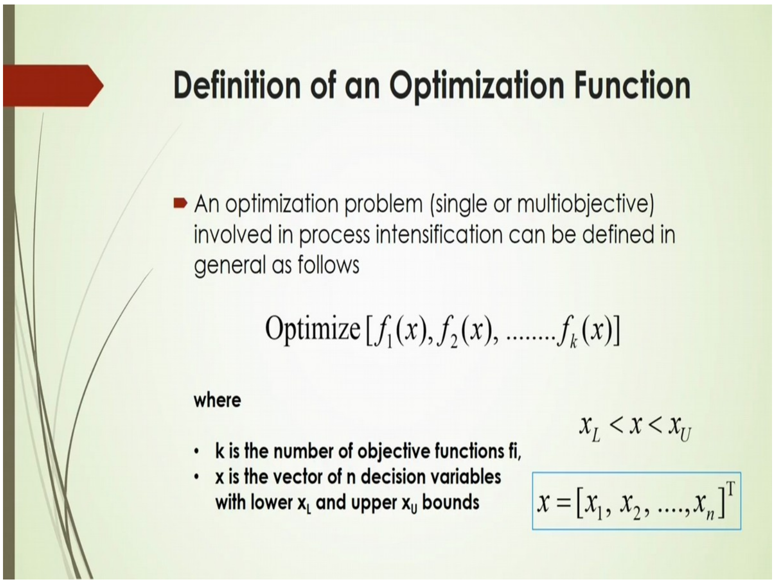

What are the definition of optimisation function, how to define the optimisation function? And optimisation problem, single or multi-objective, whatever it is, that involves in process intensification, which can be defined based on that different operating variables. You have to use this optimisation problems as optimise of that, what is that

$$\text{Optimize}\,[f_1(x), f_2(x), \ldots\ldots.. f_k(x)].$$

$$x_L < x < x_U$$

$$x = [x_1, x_2, \ldots., x_n]^T$$

Now x, what is that? x is the vector of n number of decision variables with lower bound an upper bound.

And these functions, you know that f here is an optimisation function, based on that decision variables. And k is the number of objective functions, how many objective functions you are making and also what are the limits of that decision variables should be lower bound to the upper abound. And this x should be a set of like this $x_1, x_2, x_3 \ldots x_n$. So, this is a way how to actually that optimisation function can be defined.

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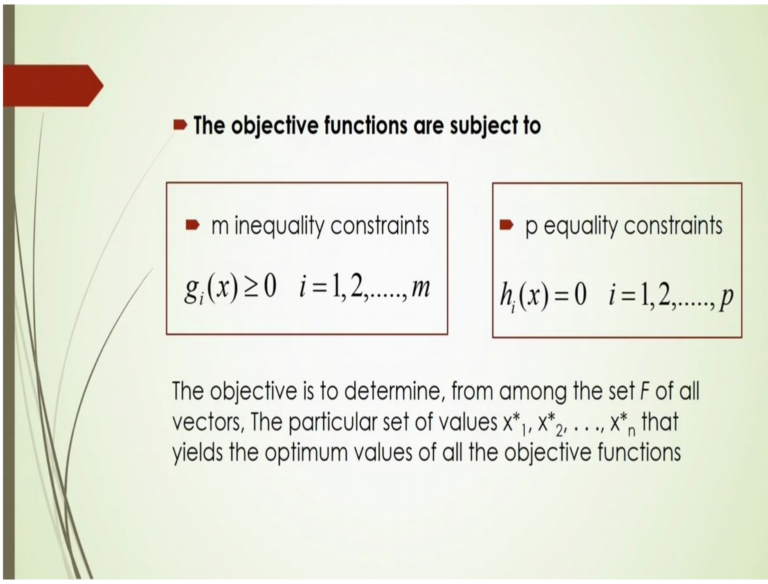

The objective functions are subject to certain constraints, so what are those constraints. Maybe, different types of constraints will be there. Sometimes m number of inequality constraints will be there, where

$$g_i(x) \quad 0 \quad i = 1, 2, ..., m$$

to be represented and which should be greater than equal to 0, where i here is 1, 2… m like this m number of inequality constraints. And P is the equality constraints there, some equality constraints should be considered as a constraint there. In that case it should be represented by

$$h_i(x) = 0 \quad i = 1, 2, ..., p$$

that should be equal to 0.

And in this case p number of equality constraints to be there. So, the objective to determine from among the set of all vectors and in this case like this $g_i(x)$ and $h_i(x)$ for the function of those vectors, variables and particular set of values, here in this case x_1 star, x_2 star,… x_N star, that will yield the optimum values of all the objective functions. So, the solutions will be like this x_1 star, x_2 star,… x_N star for this objective function for the maximisation or minimisation based on this constraints of M number of inequality constraints and P number of equality constraints.

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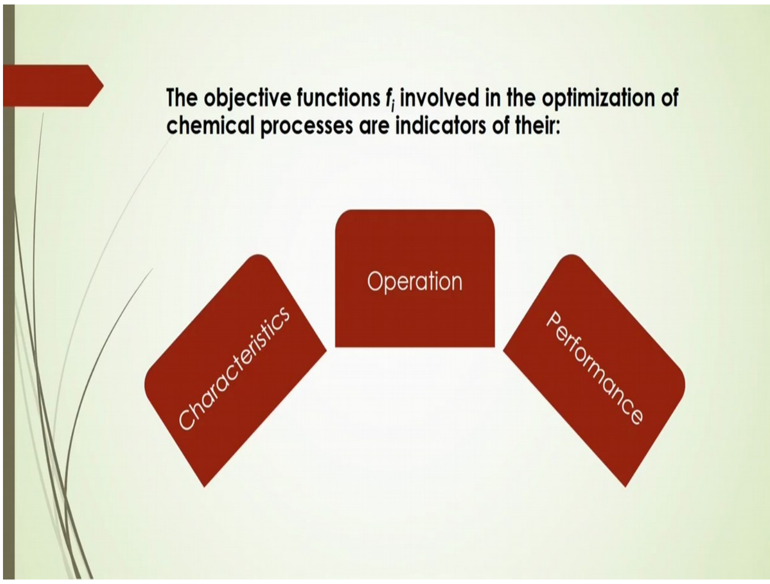

And the objective functions FI involved in the optimisation of chemical process are indicators of the characteristics, operation and performance. These 3 important indicators are very important to consider during your definition of that objective function.

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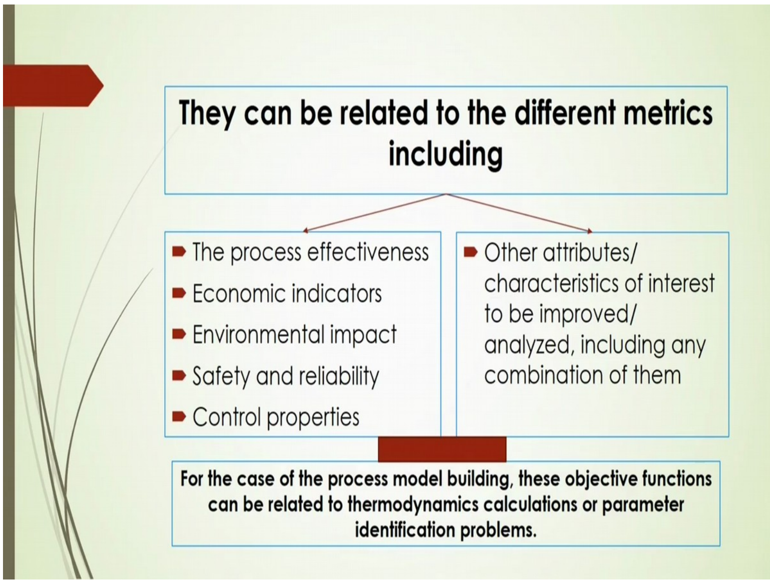

And they can be related to the different metrics, like the process effectiveness, economic indicators, environmental impact, even environmental assessment, life cycle assessment, safety and reliability, control properties and other attributes, characteristic of interest that is to be improved and also the analysis and also including any combination of them also to be considered for the optimisation.

And for the case of process model building, these objective functions can be related to different, again factors like thermodynamic factors, thermodynamic calculations or parameters that identify the problem. So, that is why for the case of the process model building, these objective functions can be related to the thermodynamic calculations or parameter indication problems.

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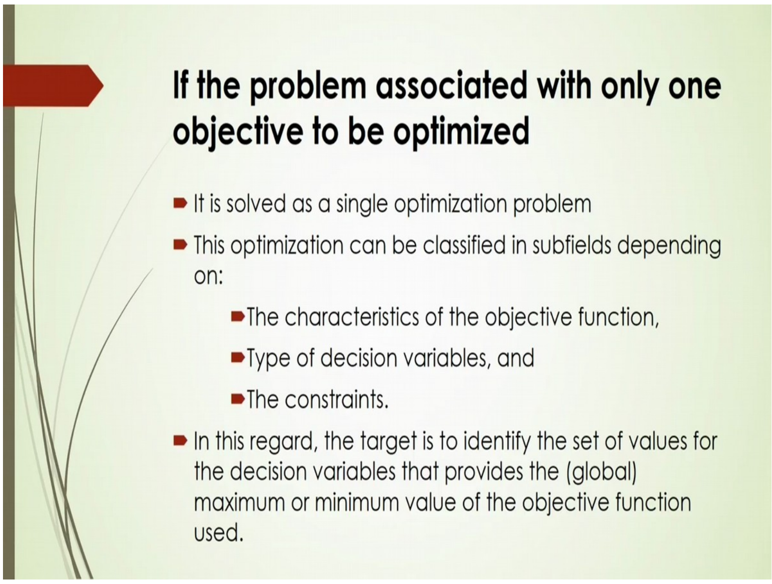

If the problem associated with only one objective to be optimised, in that case it can be solved as a single optimisation problem. And this optimisation can be classified in subfield depending on the characteristics of the objective function, types of decision variables and the constraints. Now, types of decision variables may be based on that suitability of that phenomena based decision variables can be taken there.

And also that type of the constraints, for type of the constraints that you have considered, that also to be considered for that optimisation. In this regards the target is to identify the set of values for the decision variables that provides the maximum or minimum value as a global of the objective function that are being used.

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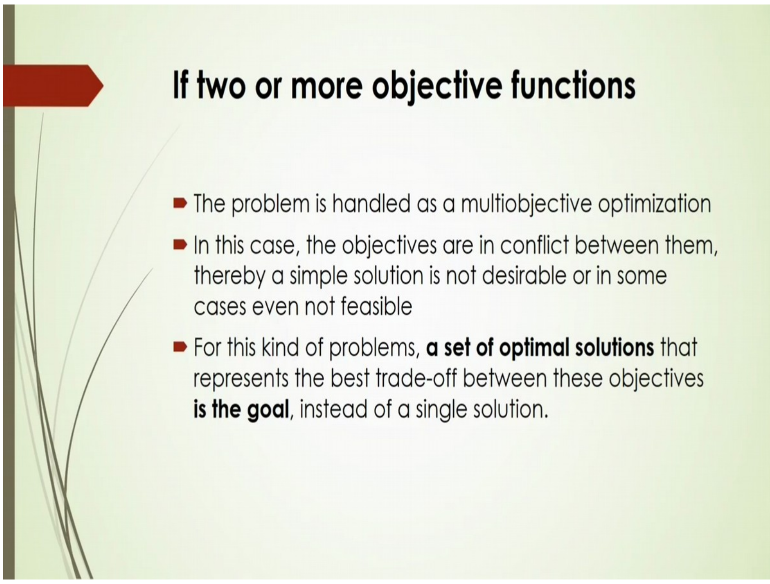

If 2 or more objective functions are to be considered, in that case the problem will be handled as a multi-objective optimisation problem. In this case the operatives are in conflict between them. Whereby a simple solution is not, that is desirable or in some cases it is not feasible. For these kind of problems, set of optimal solutions that are present the best trade-off between these objectives in the goal.

And in that case it is not actually considered that single solution to be obtained here. So, instead of single solution, set of optimal solutions to be obtained, based on that kind of problems. So, whether it is multi-objective optimisation or not, that should be of course there. So, multi-objective optimisation, in that case you will have a set of optimal solutions instead of a single solution.

So, whereas in the single objective functions, that maybe you know that only single solution you can expect. So, in the case of multi-objective functions, the objectives are in conflict between them, thereby a simple solution is not desirable or in some cases even not feasible also because in this case you are considering several decision variables based on that you know the environment, social and also other considerations.

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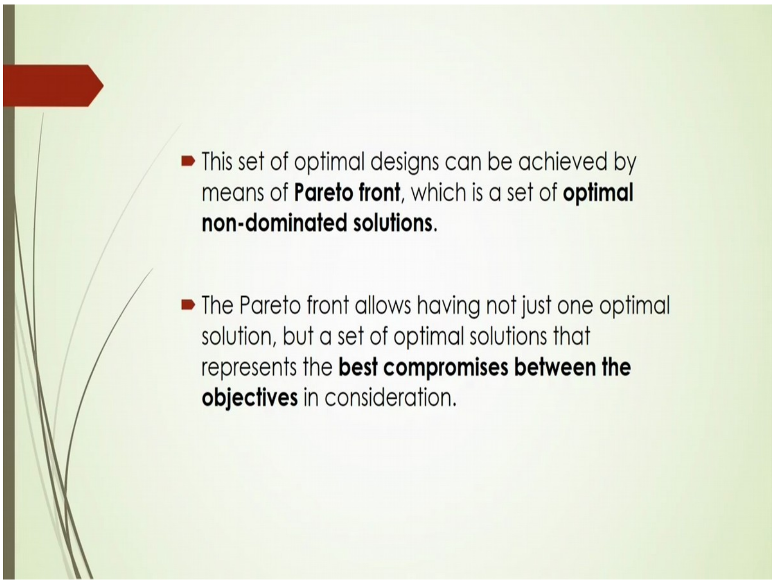

So, the set of optimal designs can be achieved by you know Pareto front. What is that Pareto front, this is generally a set of optimal non-dominated solutions. And the Pareto front allows having not just one optimal solution but a set of optimal solutions that represents the best compromises between the objectives is in consideration.

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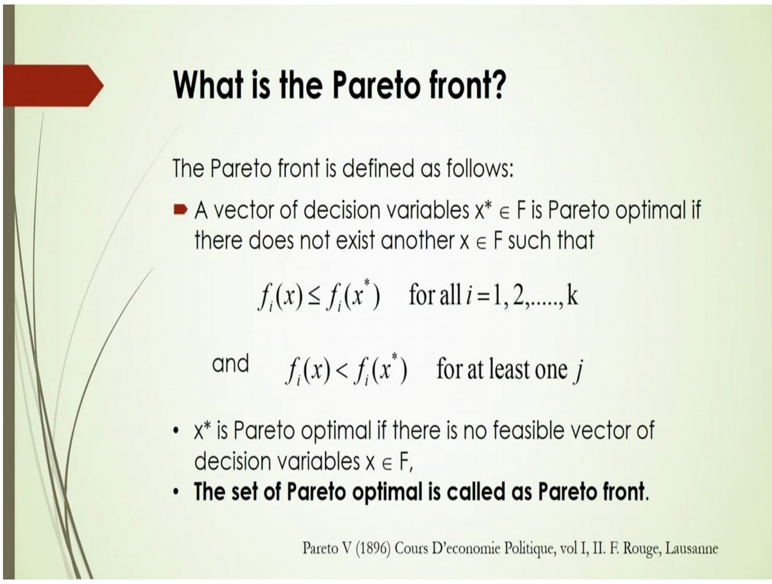

So, Pareto front should be considered here. What is that Pareto front? A Pareto front is defined as a vector of decision variables x star which belongs to that objective function. So, it is called a Pareto optimal, if that does not exist another x which belongs to optical function. Such as

$f_i(x) \le f_i(x^*)$ for all $i = 1, 2, \ldots, k$

$f_i(x) < f_i(x^*)$ for at least one j

Here as shown in the slide that here in this case that Pareto function, that is, this region variables of x star for that function should be greater than or equal to $f_i(x)$ that is function of x which is exist or not exist another x function. So, for all i equal to 1, 2 and k and also $f_i(x)$ should be less than or equal to fix star for at least one change. And this x star is Pareto optimal if there is no feasible vector of the decision variables, x belongs to F functions. A set of Pareto optimal is called as Pareto front. So, Pareto front is nothing but the set of Pareto optimal solutions.

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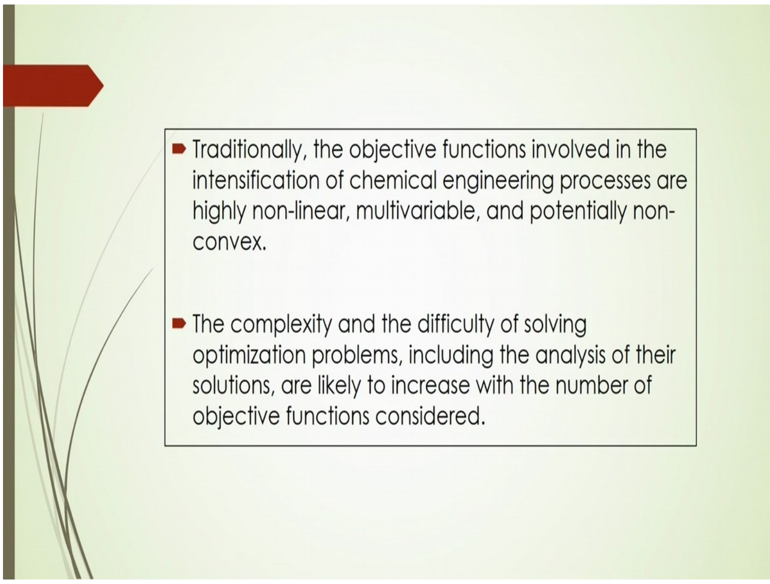

Traditionally, the objective functions involved in the intensification of chemical engineering processes are highly nonlinear multivariable and potentially non-convex. So, this is to be considered, in this case that in this case of course whatever solutions you will get, maybe you know based on that nonlinear functions multivariable or potentially non-convex function. And the complexity and the difficulty of this, solving of this optimisation problem will be there.

In this case it will include the analysis of the solutions are likely to increase with the number of objective functions that are being considered. So, in this case you have to wisely select the decision variables to get that you know optimal solutions. They are especially for that multivariable objective function.

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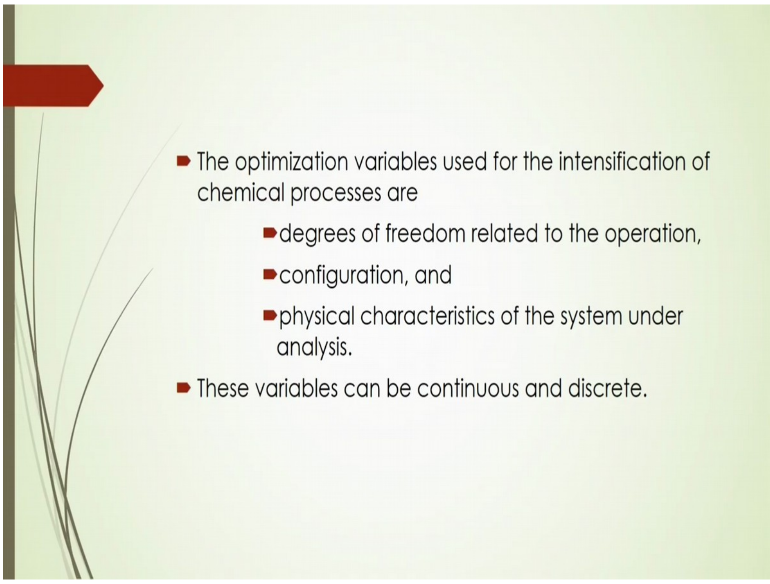

And the optimisation variables which are being used for the intensification of the chemical processes generally are degrees of freedom related to the operation and of configuration and physical characteristics of the system under analysis. And these variables can be you know that continuous or discrete also. So, these are the different optimisation techniques that we have discussed in this lecture.

And we are getting different types of optimisation and deterministic and also you can say that stochastic optimisation techniques. There are several advantages of the stochastic optimisation techniques relative to do deterministic techniques. Generally these stochastic techniques are being used for that optimisation of these chemical processes that are being you know that in process intensification of this chemical engineering process.

So, in that case you know sometimes you will consider that the stochastic methods have some decision variables to be considered and also different aspects of social, economical and also other different conditions to be considered for your process optimisation. So, you have to define that objective functions there, whether these objective functions are multi-objectives or single objective case you may get the single solution but it will be easier. But whereas multi-objective functions, in that case the solution will be very complex and also in that case the constraints of that multi-objective variable will be more.

So, in that case wisely you have to select that decision variables based on that other criteria of the processes. Now, whenever you are going to intensify the process, based on that intensification, what are the different variables that you are actually optimising? And because process intensification phenomena will actually be based on the different criteria, it may be based on the surface properties, maybe based on the mixing characteristics, it may be based on the geometry of the system, maybe the number of the equipment, it may be the flow patterns. So, all those hydrodynamic characteristics, even reaction kinetics also to be considered for the constraints.

So, not only these technical parts you have to consider, even some other, you know that impact of the, environmental impact should be also considered in that case. So, there you know that configurations, analysis of the degrees of freedom, physical characteristics of the system and its analysis of course to be done beforehand and also to get that optimisation problems based on this characteristics of the different variables, you may get that multiple solutions, multiple optimal solutions, so that is why optimal Pareto form will be obtained, that is a set of different nonlinear solutions or you can say that different optimal solutions, set of different optimal solutions to be obtained there.

So, those optimal solutions maybe obtained based on the variables which are maybe sometimes continues, sometimes discrete. So, here we have actually gone through some basics of that optimisation techniques. And for these optimisation techniques you need some algorithms, computer-based algorithms also, some tools also sometimes are being used, that already we have discussed in the previous lecture that what are the different types of computer-aided tools are being used for the process design.

And that process design based on this optimisation problem. So, there are several tools also available and algorithms also are available there, so we will discuss in the late next lecture what the different types of algorithms there are for these optimisation techniques.

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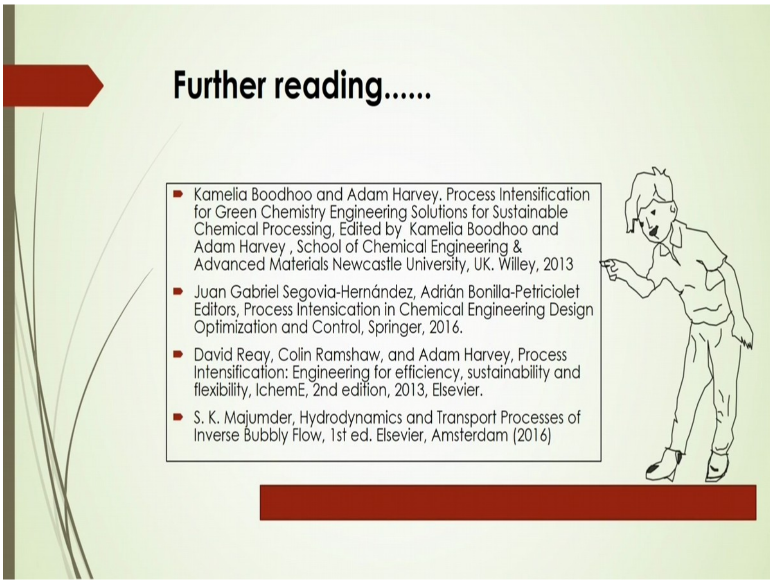

So, I would suggest to read further about these optimisation techniques. This textbook as well as some other reference also you can follow for this. So, I think we have discussed something about that optimisation, how it can be used and what are the objective functions? So, next lecture we will discuss about the algorithm of these optimisation techniques. So, thank you for this lecture.