**Chemical Process Intensification**
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**Lecture 14**
**Optimization Algorithms**

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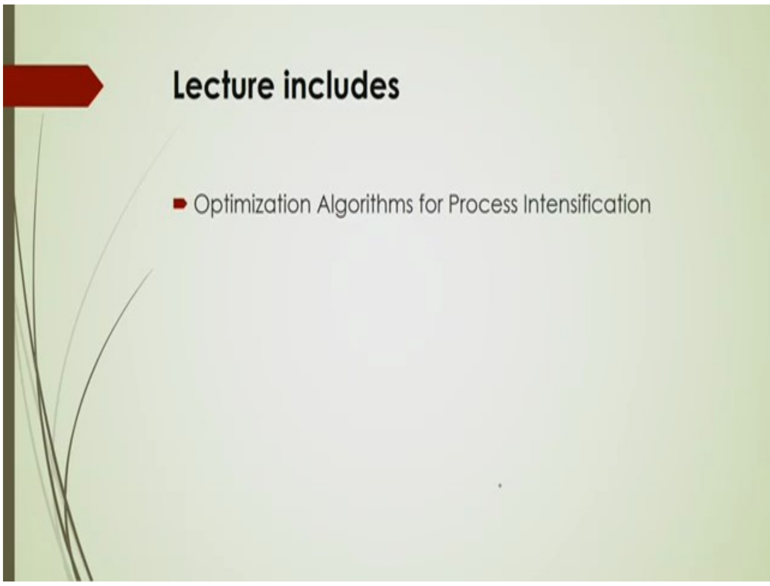


Welcome to massive open online course on Chemical Process Intensification. This is module optimisation for process intensification, this is module 5 and the lecture is 2 under this module. And in this module the optimisation algorithms are to be discussed. So, this lecture includes the optimisation algorithms for process intensification. In the previous lecture, under this optimisation techniques, we have discussed some introduction regarding that different types of optimisation and how that optimisations can be implemented.

And here in this lecture we will try to discuss something about that, what are the different algorithms that are being used for that optimisation techniques for the process intensification.

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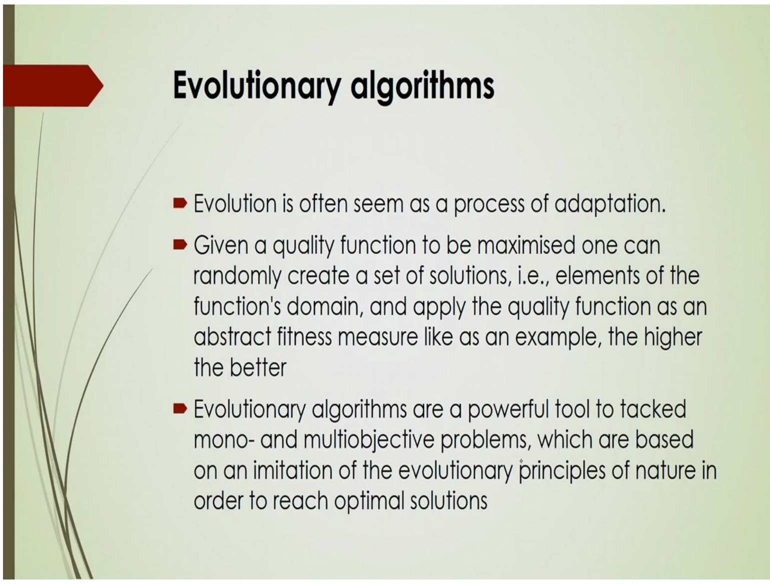


Now, as you know that there are several different types of algorithms that are being used for optimisation, here mainly we can classify these algorithms into two categories, like one called evolution algorithms and the other is called classical algorithms. And these two algorithms are actually coming under that stochastic algorithms. And in this case let us have some look of this evolutionary algorithms and also classical algorithms there.

So, in this lecture we are having this evolutionary algorithms, where it is actually seem as a process of adaptation, that you know that as like that features are being evaluated, adapting with the nature. So, here again that algorithm is actually created based on that adaptation of the process and based on which the algorithms is being actually procured. Now, in this case if we actually supply a quality function or consider a quality function to be maximised, then one can randomly actually create a set of solutions there.

That is elements of the functions domains and apply the quality function as an abstract fitness measure like as an example the higher the better. So, this is the actually the concept for that evolutionary algorithms there. We are always preparing that better one will be higher. So, in that direction this actually in a particular functions domain and also based on the quality function, that is being fitted for the optimal solutions. So, in that case that depends on the selection of the function that quality of a function that will be maximised just by creating a set of solutions there.

And in that case, elements of that function domain and the quality function to be selected based on that process criteria, even some different variables that are actually involved in the particular processes for the process based on that process intensification. Now, actually this evolutionary algorithms are actually seems to be very powerful tool to tack actually the mono and the multi-objective problems in the process intensification. And these are actually based on an imitation of the evolutionary principles of nature in order to reach that optimal solutions.

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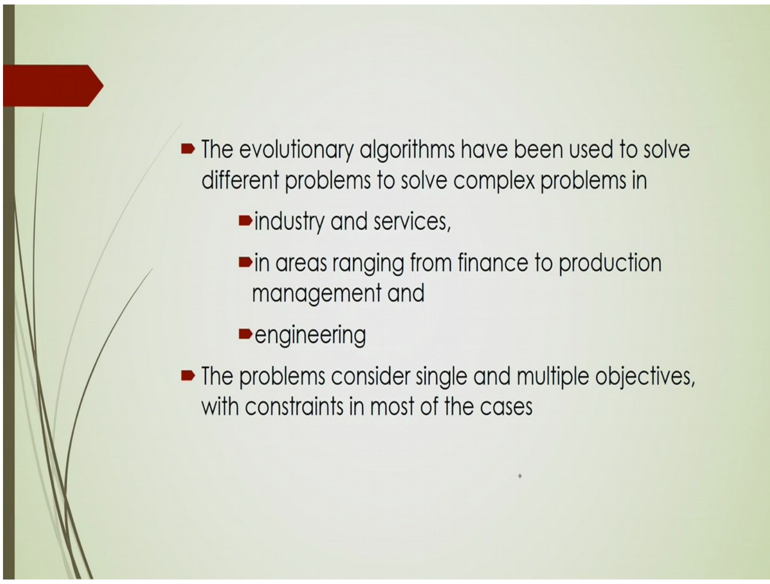


So, we can say that that is why these evolutionary algorithms have been used to solve different problems, to solve the complex problems also in industry and services, in areas ranging from finance to production management and also in engineering field. So the problems consider single and multiple objectives and there will be certain constraints in most of the cases, based on the process variables, even some process conditions. So, that is why these evolutionary algorithms are mostly used in several sectors, like industry, engineering and other, you know that finance also Department they are using these evolutionary algorithms there.

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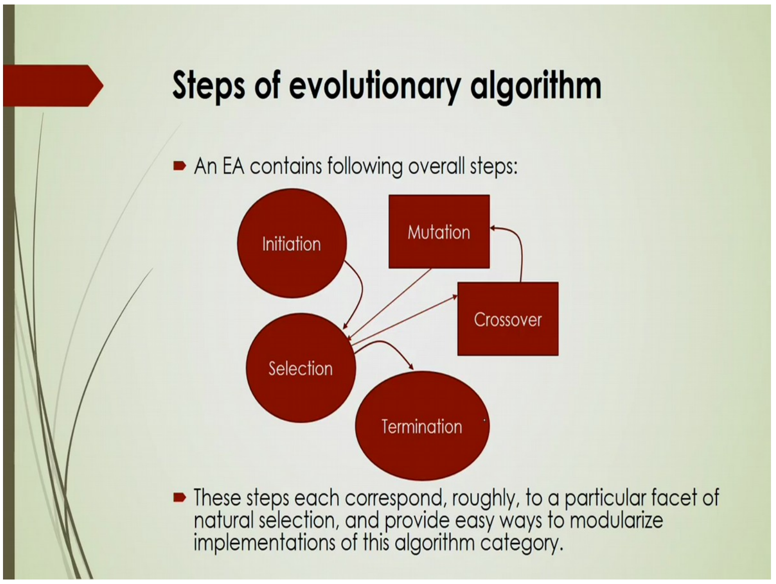


What are the steps of that evolution algorithms? We will see that and evolutionary algorithms contain these following steps here like initiation, then selection, selection based on that mutation and crossover because based on the crossover some mutation also depends. And once this mutation obtained, then how it can be selected, that is also important. So, after initiation, then selection should be there. After selection, then you have to have some termination steps. So, these steps actually corresponds roughly to a particular facet of natural selection and provide easy ways to modularise implementations of the algorithm category.

So, that is why these steps are actually preliminary that based on which that evolutionary algorithms are procured.

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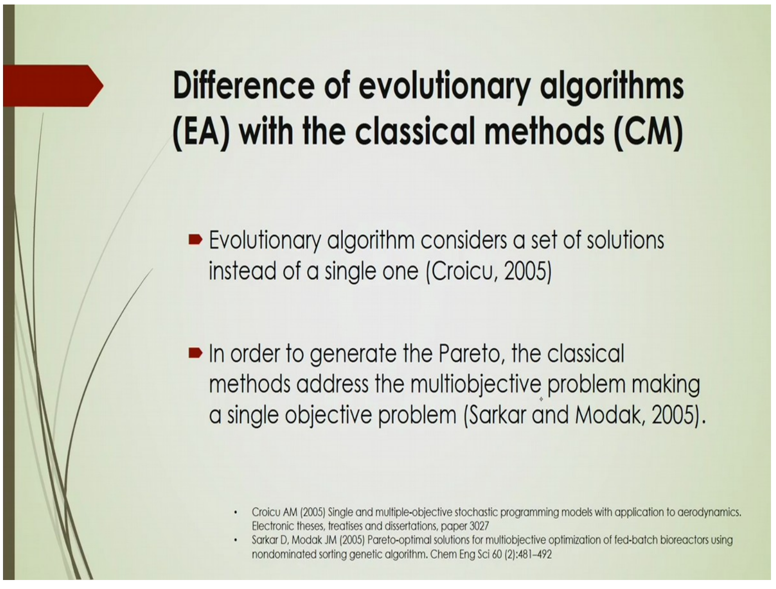

Now, there are other methods called classical methods. In this case these classical methods actually adjust the multi-objective problems that making a single objective problem there. So, a lot of multi-operative problems will be making a single objective problems. So, in that case main objective is to generate a Pareto optimal. So, that is why classical methods will address the multi-objective problem which will be actually an ultimate single objective problem there.

And evolutionary algorithms consider the set of solution instead of single one there. Whereas these classical methods there, it will generate that multi-objective problem making a single objective problem.

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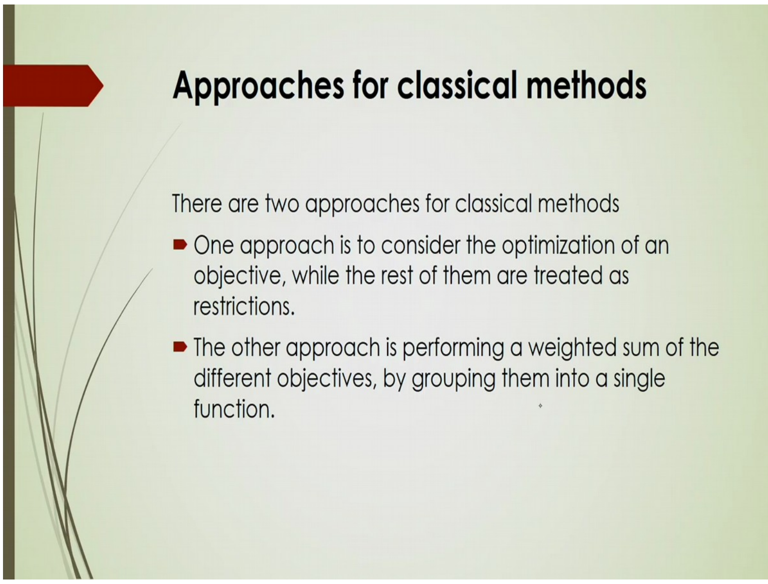


Now, what are the approaches for the classical methods? There are generally two methods or approaches for the classical methods. One is to consider the optimisation of an objective, while the rest of them are treated as the restrictions there. And the other approach is performing a weighted sum of the different objectives by grouping them into a single function.

So, if there is different objectives upcoming, so you have to group them and you have to consider a single function based on that grouping. So, that is why these 2 actually approaches are very important to actually execute these classical methods there. So, in this case you have to consider that often objective first optimisation of an objective and rest of them are, will be treated as the restrictions there. So, this is the first approach and then other approach is that you have to perform a weighted sum of the different objectives by grouping them into a single function.

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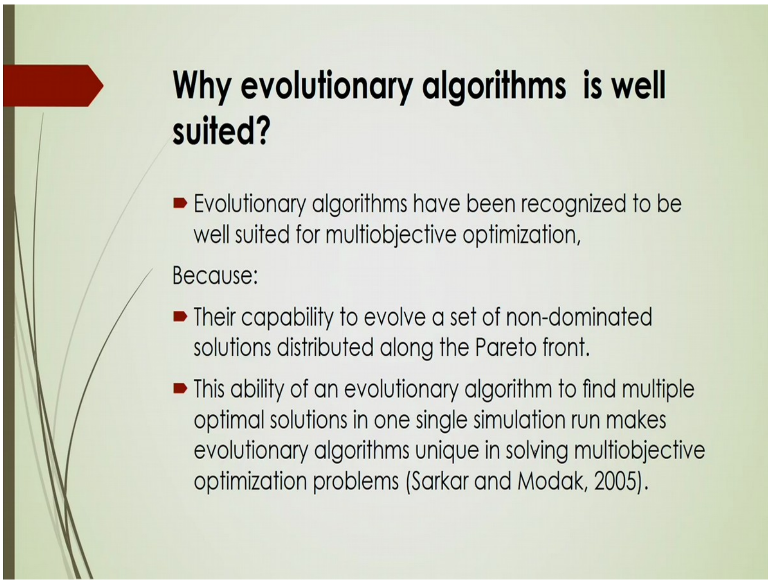


Now, why evolutionary algorithms is well-suited? That is also important to know here because you know their capability to evolve a set of non-dominated solutions that is distributed along the Pareto front. So, in this case whenever you are selecting some set of objective functions there and in that case based on that different objective functions, which one will be that actually feasible and that capable of you know that feasible, you know that set of functions and it should be, it will have that non-dominated solution and it will distribute it along the Pareto front there.

So, that is why it is actually, these algorithms are being recognised to be well-suited for multi-objective optimization. And also these evolutionary algorithms, it has some ability of such cases where it can find multiple optimal solutions in one single solution that will run evolutionary algorithms that is unique in solving multi-objective optimisation problems. So, that is why it is very important.

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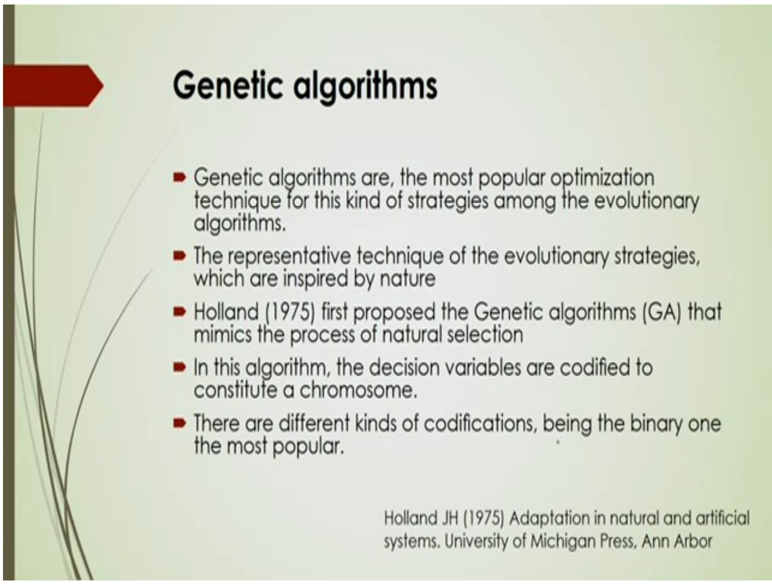


So, under this evolutionary algorithm, there are several different types of algorithms. Now, genetic algorithms are one of the most popular and useful optimisation techniques for this kind of strategies among the evolutionary algorithms. And the representative technique of this evolutionary strategies, which are clearly inspired by the nature as per the genetic algorithms.

And these genetic algorithms actually first proposed by you know that Holland in 1975. And they actually propose that these genetic algorithms will mimic the process of natural selection. And in this algorithm, the decision variables are to be codified to actually constitute a chromosome there. So, based on that these actually algorithms are being considered, where that, how that chromosomes is being constituted.

And there are different kinds of codifications actually, being binary one the most popular one in that case. Because we are having different kinds of codifications there. So, in that case binary one will be the most popular there. Other different types of courses will be there.

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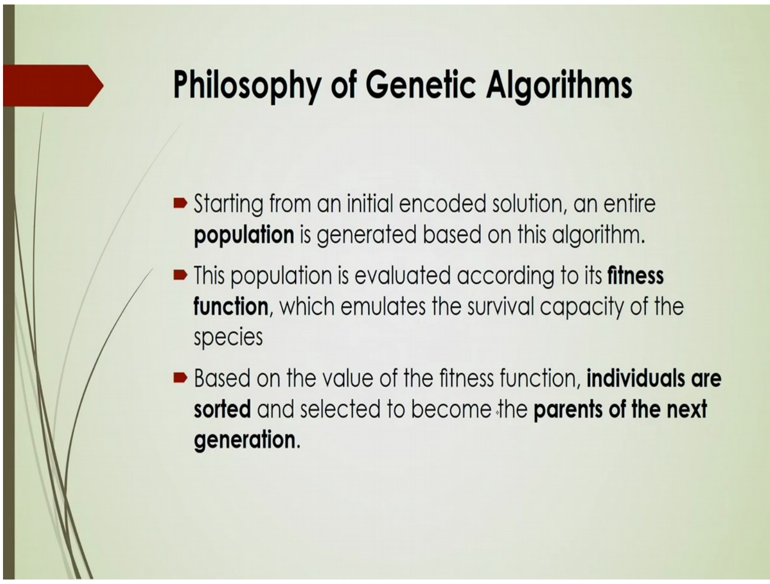


Now what is actually that philosophy of genetic algorithms? From where actually it has come? Now, if we start it from an initial you know that encoded solution, an entire population is generated based on this algorithm. So, encoding a solution like that, that total population will be generated based on these algorithms there.

So, in that case just population is evaluated according to its fitness, function which you can say that it will emulate the survival capacity of the species there. So, that is why you have to select that fitness function where it will say that okay, there will be some survival capacity of the species or entities which have actually created that population there.

And based on that value of the fitness function, that individual, that is species should be sorted and also selected and actually to have a superior or you can say that to have a well-being which will become the parents of the next generation there. So, that is why based on the value of the fitness function, that you have to identify individuals and it will be sorted, all species or entities and then you have to select in such a way that selection to become the parents of the next generation there.

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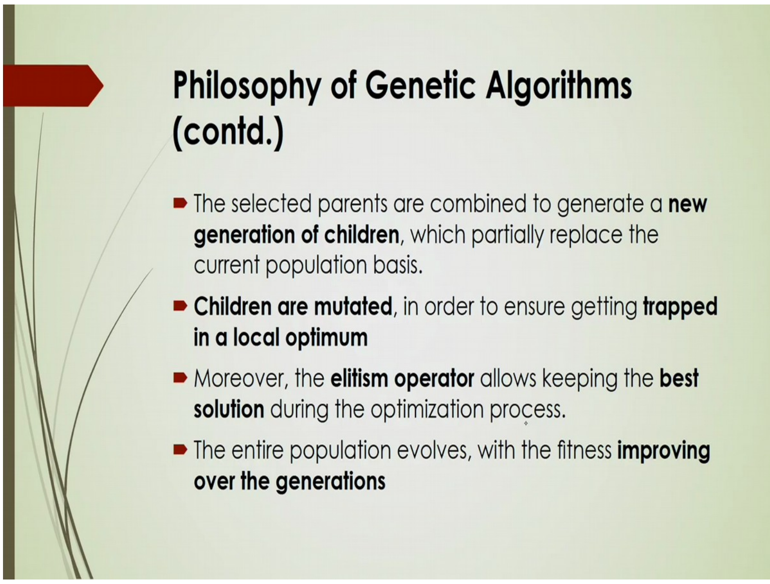


And then after selection, the selected parents are actually combined to generate a new generation of those children. So, which partially replace the current population basis. So, this is simply that you know that finding out the better to better, then better, than best, like this. So, that is why the selected parents are combine to generate a new generation of children. And then after that this will partially replace the current population basis, based on that survival or you can say the fitness of that function.

Now, children are later mutated and in order to ensure getting trapped in a local optimum, so you have to make a set of optimal solutions, where the children are to be mutated. So, after that mutating you have to ensure that you are getting them trapped in the local optimum. So, in that case you have to select some elitism operator, which will allow you for keeping the best solution during the optimisation process. And then the entire population will involve for that trapping in the local optimum and which will evolve, so the fitness improving over the generation there.

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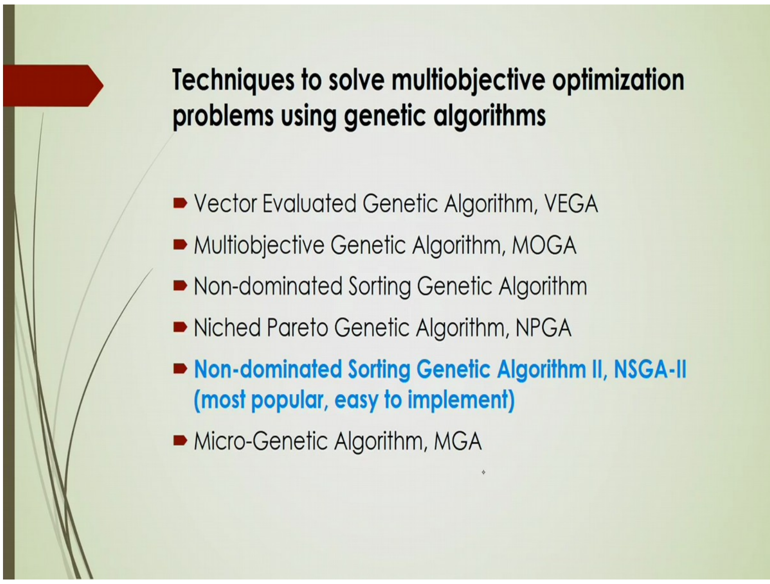


Now what are the techniques actually to solve these multi-objective optimisation problems using genetic algorithms? Now, there are several techniques are available like vector evaluated genetic algorithm, multi-objective genetic algorithm, even non-dominated sorting a genetic algorithm and Niched Pareto genetic algorithm, NPGA it is called. And also this non-dominated sorting genetic algorithm, this is actually a very important and most popular and also this is very easy to implement to get that optimal solution of the multi-objective optimisation problems.

And also another important one it is called Micro genetic algorithm, nowadays are coming, but among these different techniques here are non-dominated sorting genetic algorithms are the most and easy to implement.

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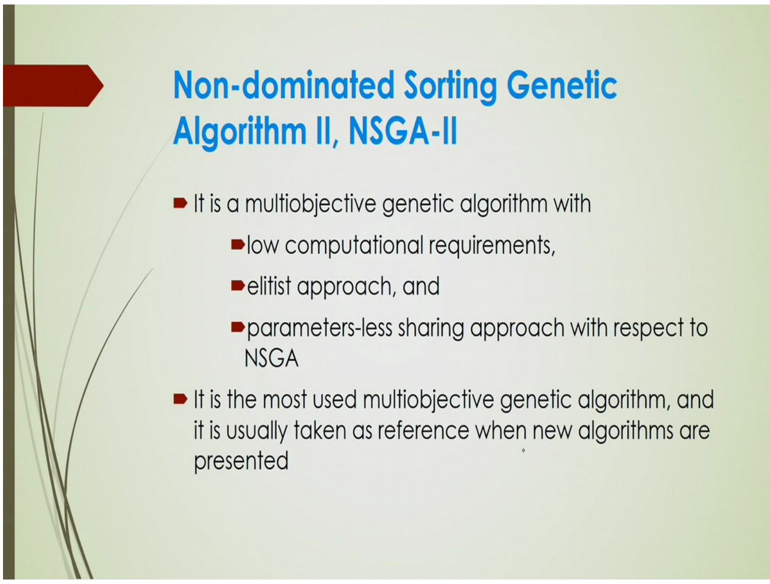


Now, what are these actually non-dominated sorting algorithm? It is actually denoted by NSGA, it is a multi-objective genetic algorithm with low computational requirements. Even you know that elitist approach also the parameters less sharing approach with respect to NSGA.

Also it is the most used multi-objective genetic algorithm and it is usually taken as, you know that reference when you are actually devising new algorithms and which will be presented for that optimisation problem.

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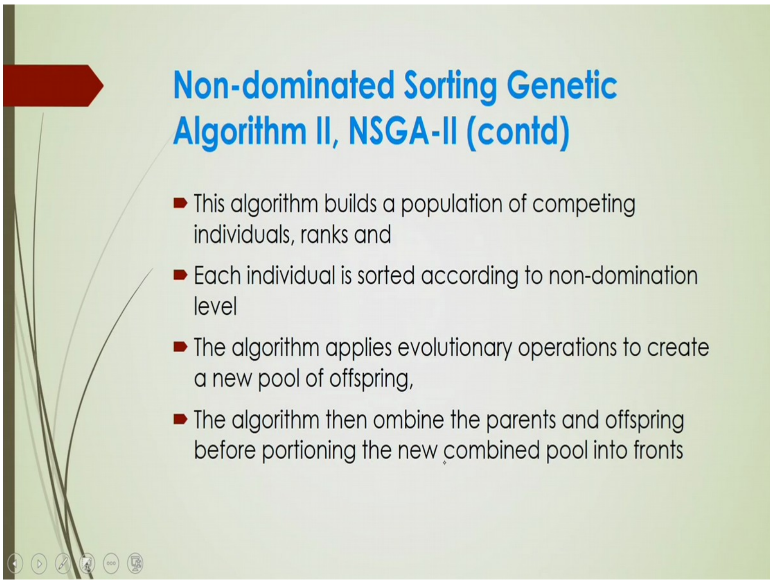

Also, we will say these algorithms builds based on the population of competing individual ranks and also each individual is sorted according to non-domination level. So, the algorithm applies evolutionary operations to create a new pool of offspring and also this algorithm combines the parents and offspring before partitioning or portioning the new combined pool into the fronts.

So, that is why this algorithm based on the competing individuals ranks and also sorted out of the each individual, based on the non-dominated level. And also it is actually creating a new pool of offspring and whenever you are just going to combine these parents and offspring, then you can combine a new pool into the fronts of that Pareto where you can get that optimal set of solutions there.

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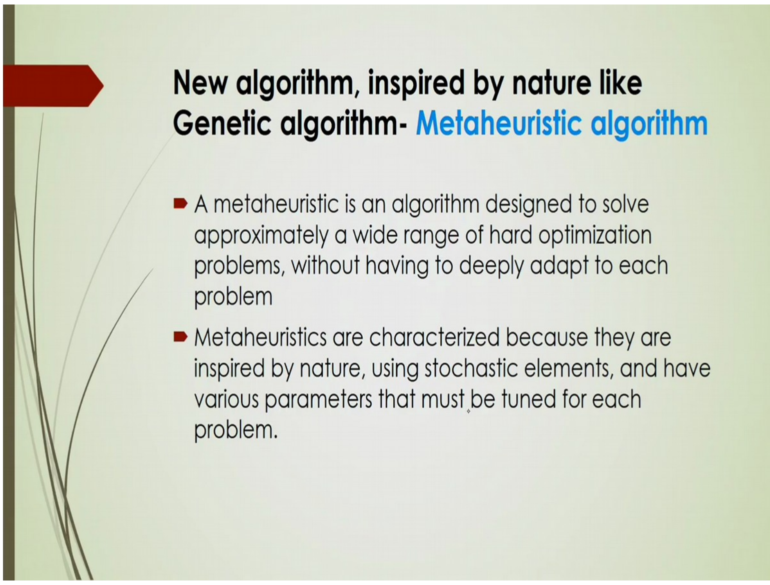


Now, new algorithm inspired by nature like genetic algorithm, there are several other different types of that under this genetic algorithm. One is important, that is called meta-heuristic algorithm. In this case it is an algorithm designed to solve approximately a wide range of hard optimisation problems without having to deeply adapt to you know that is problem there. And also these types of algorithms are characterised because they inspired by the nature using stochastic elements, even have various parameters that must be tuned for the problem.

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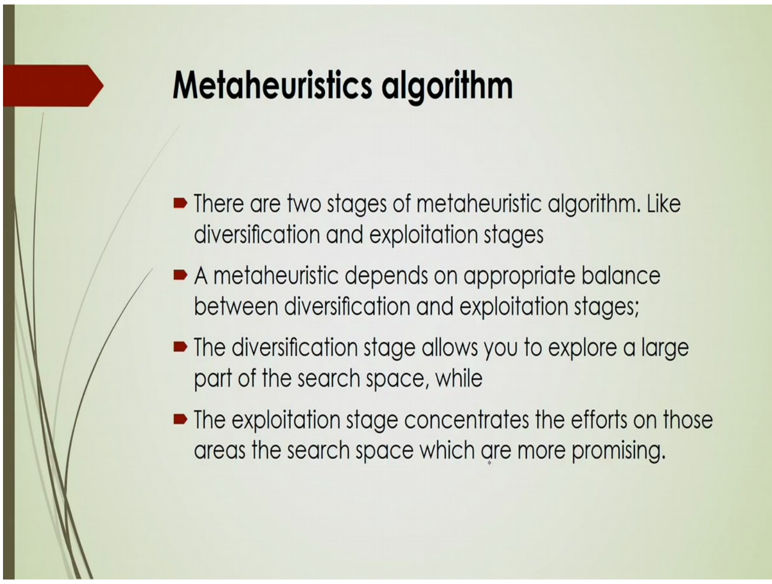


And there are 2 stages of that metaheuristic algorithms like you know that diversification and exploitation stages. A metaheuristic depends on appropriate balance between diversification and exploitation stages. The diversification stage allows you to explore a large part of search space, while the exploitation stage concentrates the efforts on those areas of the search space which are more in this case promising there.

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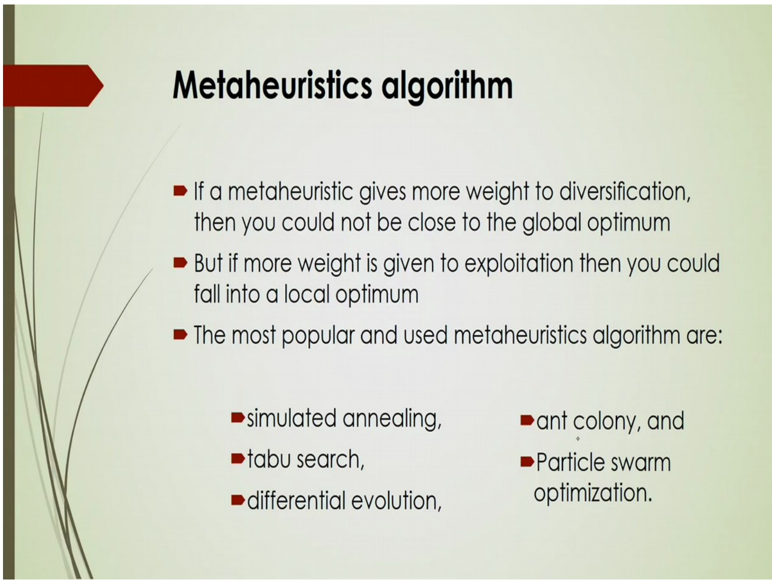


And also if a metaheuristic algorithms gives more weight to diversification, then you may not get the close to the global optimisation solution. But in that case some more weight is given to exploitation than you can have a fall into a local optimum solution.

So, the most popular and used meta heuristic algorithms are in that case simulated annealing, tabu search, differential evaluation, ant colony and particle swarm optimisation.

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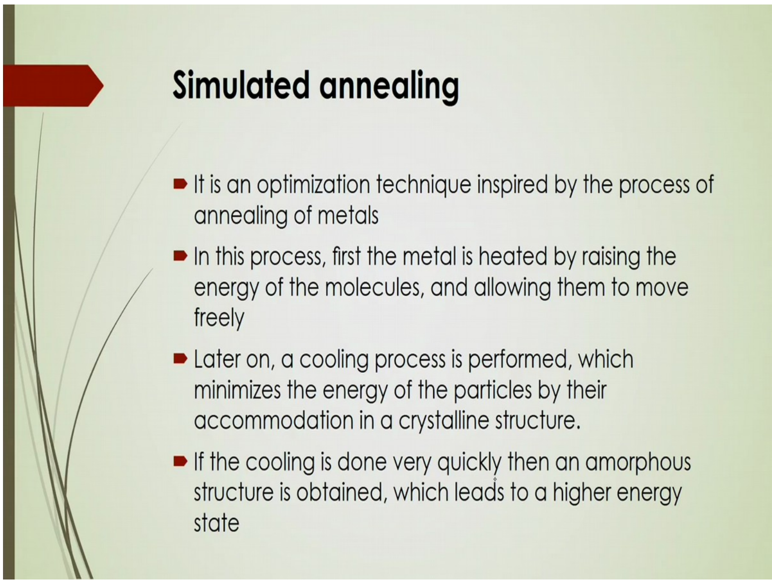


Now, what is that simulated annealing optimisation algorithm? So, it is an optimisation technique that is inspired by the process of annealing of metals. In this process first the metal is heated by raising the energy of the molecules and then allowing them to move freely. After that a cooling process is performed, which minimises the energy of the particles by their competition in a crystalline structure.

So, that is why you will see that if the cooling is done very quickly there, then an amorphous structure is obtained, which leads to a higher energy state. So, this is called annealing. So, this concept of annealing of the metals, the algorithms is actually procured or you can say that optimisation is made. So, that is why this is based on the, you know that how metal is heated by raising the energy of the molecules and allowing them to move freely and also cooling process how that minimises the energy of the particles by the accommodation in a crystalline structure. And also how quickly then an amorphous structure is obtained and which will leads higher energy state.

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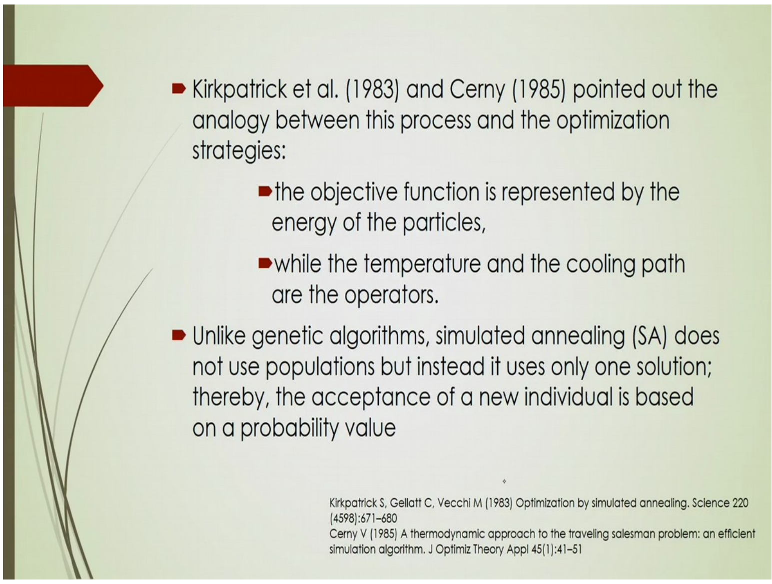


In this case, you know that Kirkpatrick et. al. and Churney 1985 has pointed out that this analogy between this process and the optimisation strategies, like the objective function is represented by the energy of the particles, while the temperatures and the cooling path are the operators here. So, very interesting that energy of the particles here where that you know that based on that energy, that annealing of the metals have been happened. So, in that case the objective function will be considered, the energy of the particles where the temperature and the cooling path will be considered as an operator.

So, unlike this genetic algorithm, this simulated annealing does not use that populations, but instead it uses only one solution, thereby the acceptance new individual is based on a probability value. So, that is why in this case an annealing optimisation algorithm does not require any population. Whereas this, you know that genetic algorithms are there, it requires in that case, you know that population based. In this case also annealing uses only one solution, thereby the acceptance of this new individual is based on a probability value is very important for this consideration of this algorithm.

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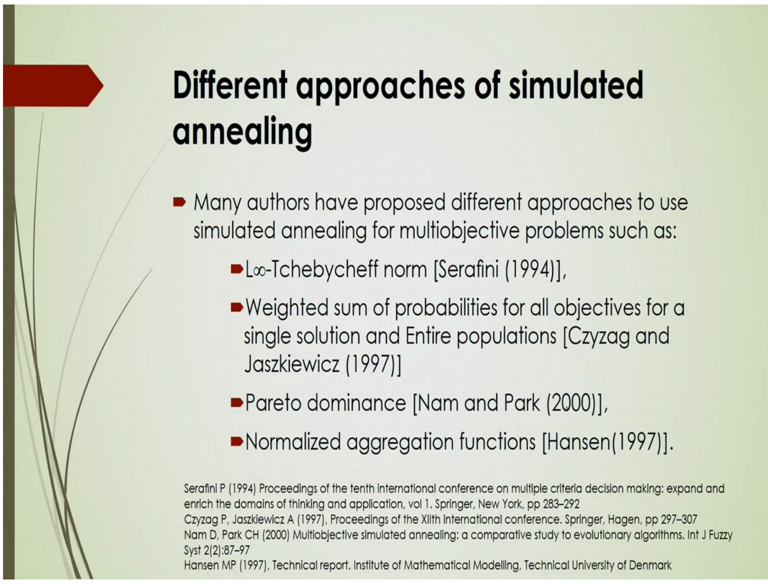


Now, a different approaches of similar type of annealing, many authors have proposed different approaches to use simulated annealing for multi-objective problems such as $L_\infty$ - Tchebycheff norm, even weighted sum of probability for all objective for a single evaluation or single solution and entire populations. And also Pareto dominance is there, normalised aggregation functions to be considered there. So, these are different approaches for this having a solution by this simulated annealing.

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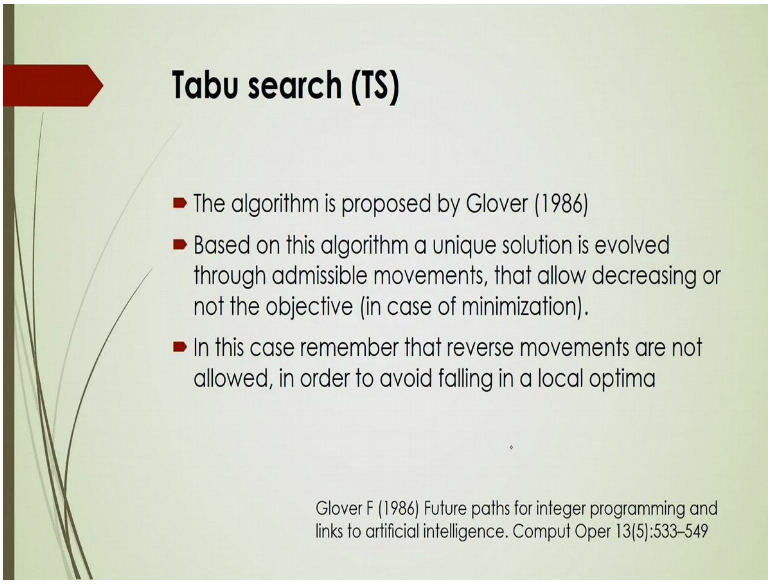


And taboo search is the algorithm where it is proposed by, this is Glover based on this algorithm, unique solution is evolved through admissible movements, that allow to decreasing or not the objective here in case of minimisation, in this case. So, in this case remember that reverse you know movements are not allowed in order to avoid falling in a local optimal solution there. So, that is why this algorithm will give you that unique solution through the admissible movements and which will allow the decreasing or not the objective in this case. So, reverse movements are not sometimes allowed in order to avoid the falling in a local optimum value.

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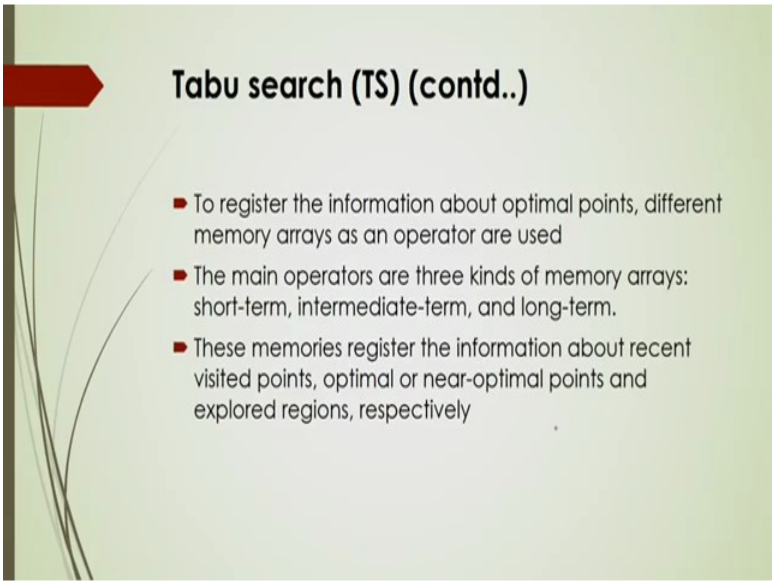


And to register the information about this optimal points different, you know that memory arrays as in operators are to be considered or used and in this case the main operators are generally three kinds of memory arrays are considered, one is short-term, another is immediate intermediate term and then long-term. And these memories register the information about recent visited points and optimal or near optimal points and also it will explored to the regions accordingly.

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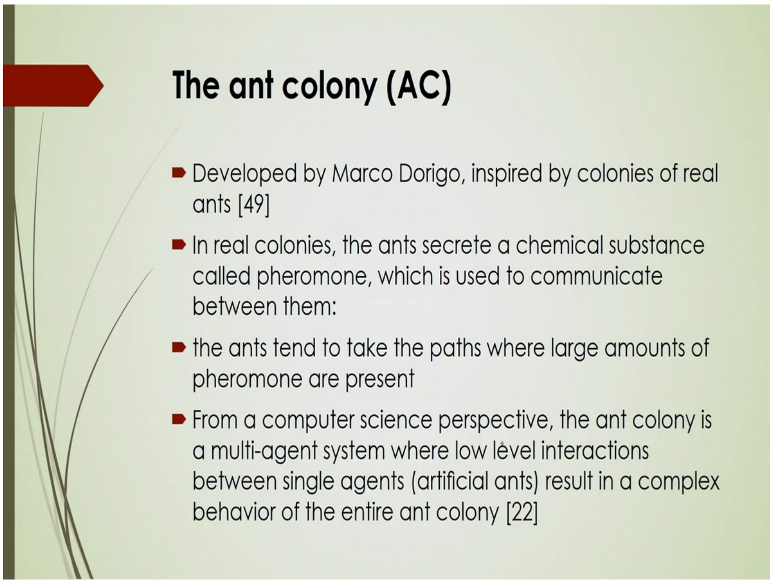


The ant colony is developed by Marco Dorrigo, that is inspired by colonies of you know real ants. In this case that real colonies, the ants secret chemical substance called pheromone which is used to communicate between them. And also in this case the ants are tend to take the parts where large amounts of pheromone are present there.

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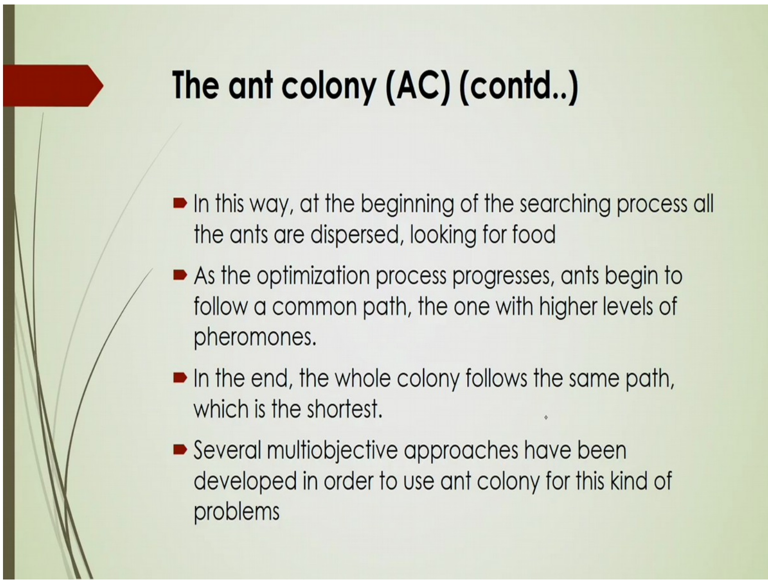


So, in this case you will see that at the beginning of the searching process, all the ants are dispersed looking for food. And as the optimisation process, if it is progressed, then ants begins to follow a common path, the one with higher levels of pheromones. Also in the end, the whole colony follows the same path which is the shortest there and also several multi-objective approaches have been developed in order to use ant colony for this kind of problems as per literature we are having there.

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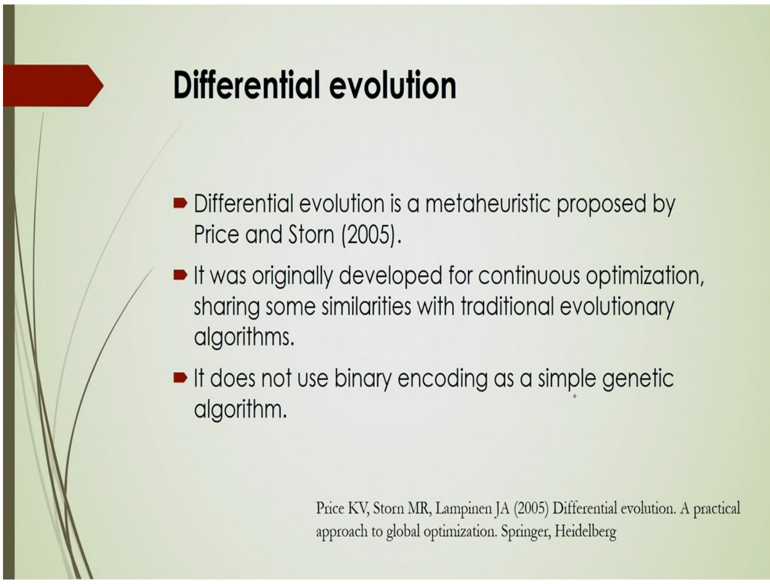


Now, what are differential evaluation, the differential evaluation is a meta-heuristic evaluation which is proposed by Price and Storn in 2005. And it is generally developed for the continuous optimisation and it shares some similarities with traditional evolutionary you know algorithm. Also it is not giving the means for using that binary solution according to a simple genetic algorithm there.

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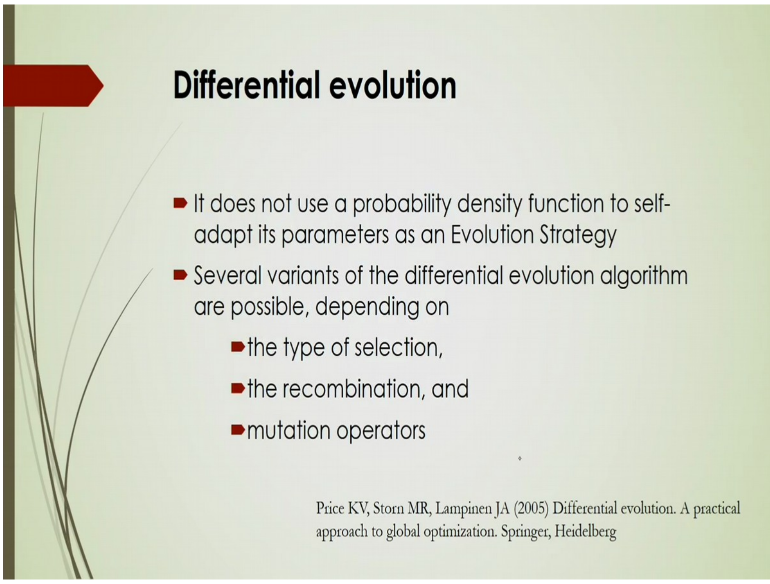

And also it does not use a probability density function to self-adopt its parameters as an evolution strategy. And also several variants of the differential evolution algorithms are to be considered and which is possible they are depending on the type of selection, the recombination and also the mutation operators.

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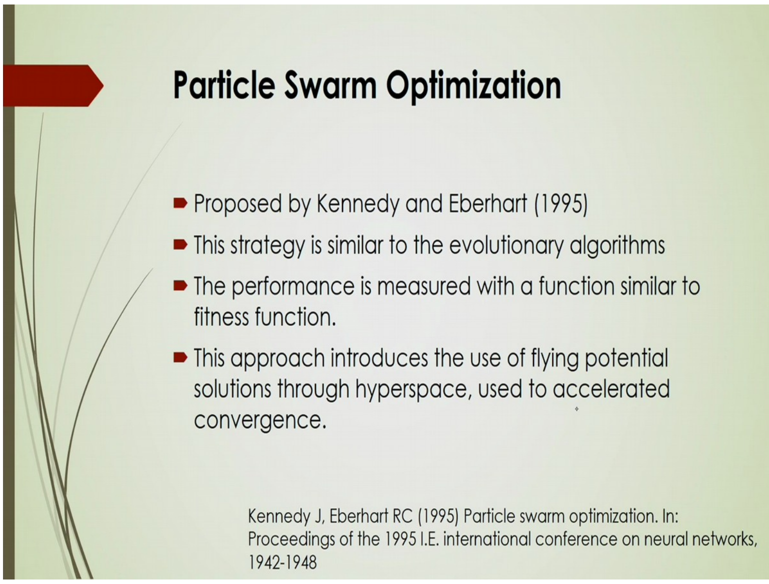


And particle swarm optimisation, that is proposed by Kennedy and Eberhart in 1995 there and according to this approach you can say that the use of flying potential solutions through the hyperspace generally used for accelerating that convergence there. And in that case you have to measure the performance with a function that will be very similar to the fitness function. So, that is why the strategy should be similar to the evolutionary algorithm and that is why this approach, giving the use of flying potential solutions through the hyperspace. And by generating the accelerated convergence.

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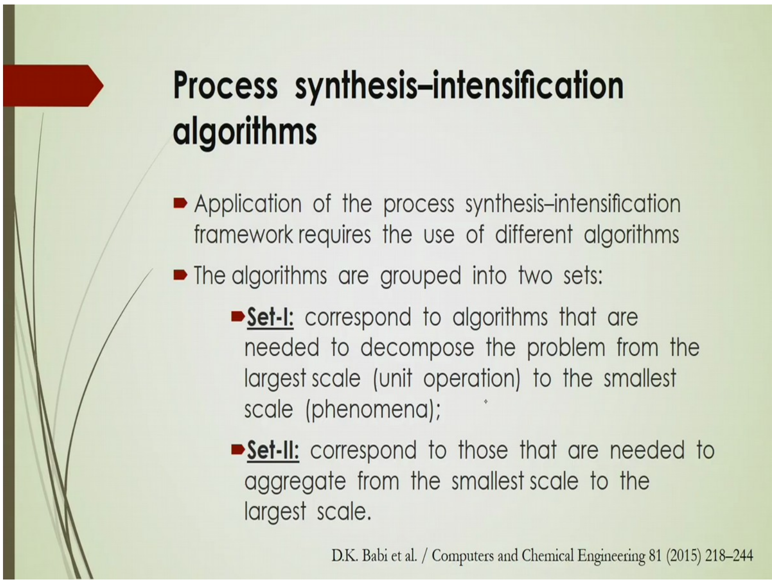


Now, let us have some look of process synthesis intensification some algorithms there. Now, in this case Bobby et al in 2015 they have given you know different types of algorithms and also there are different you know that sets for that algorithm which are being applicable actually for the process synthesis intensification. Now, in this case if we apply this process synthesis intensification, of course this one framework is required. Now, this framework requires the use of different algorithms like this these algorithms can be grouped into two sets like set 1 and set 2.

So, in this case set 1 generally corresponds to algorithms that are needed to decompose the problem from the largest scale, that is called unit operation and to the smallest scale, that is called phenomena. So, very important that unit operation to the phenomena, scale to be considered in the first set. And the 2nd set, they told that this corresponds to those that are needed to aggregate from the smallest scale to the largest scale there.

So, this is your very interesting that this one is going from you know that smallest scale to the largest scale. Where in the set 1, in this case that decomposing the problem from the largest scale to the smallest scale there.

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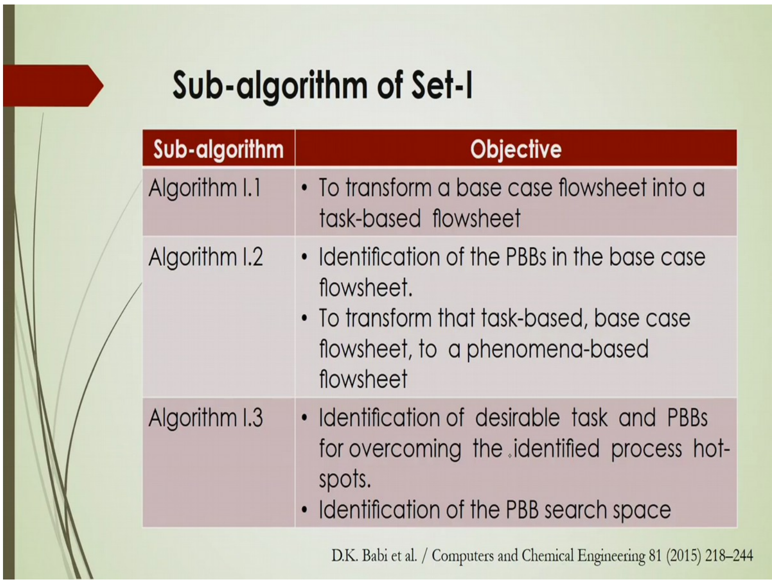


And sub algorithms also, set 1 and set 2 are there. So, in this case some sub algorithms of that one are being given here, that is in table, in the slides like sub algorithms here, like algorithm 1.1, that is set under this, that is 1 and to transform a base case flow sheet into a task-based flow sheet, then you have to you know consider this sub-algorithm there. This is actually under this objective to transform a base case flow sheet into a task-based flow sheet there.

And algorithm, that is 1.2 here, in this case identification, what are the objectives, their identification of the PBBs in the base case flow sheet and to transform that task-based, base case flow sheet you have to consider that you know phenomena based flow sheet. So, that is why you have to transform that task-based flow sheet to the phenomena based flow sheet here.

And under this algorithm of 1.3 of this sub algorithm of set 1, in this case the main objective is to identify the desirable task and also phenomena based building blocks for overcoming the identified process hotspots there. In that case you have to also search the phenomena based building blocks search space there. So, this is to be remembered.

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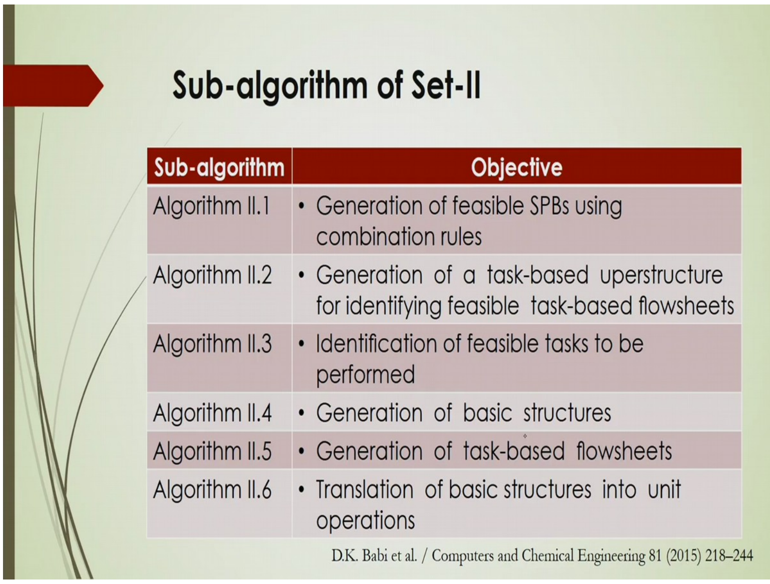


Also, some sub algorithms also to be considered under the set 2 there. In that case you know that some objectives like generation of feasible you know simultaneous phenomena based building blocks is considered which are being used for combination rules there. So, in that case you have to use this algorithm 2.1.

And algorithm 2.2 here, generation of a task-based upper structure for identifying you know that feasible task-based flow sheets to be considered there. And also an algorithm 2.3 here, you know that identification of feasible tasks to be performed and also under this sub algorithm offset 2, here the generation of basic structures to be considered. Algorithm of 2.5, in this case the main objective is to generate the task-based flow sheets. And then sub algorithm this 2.6 here, the main objective is to translate the basic structure into a unit operations there. So, these are the various objective is under this sub algorithm of set 2.

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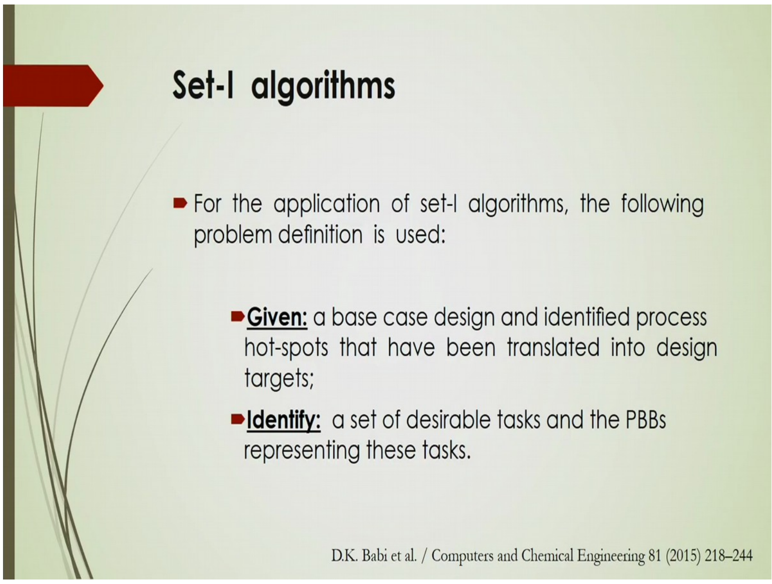


Now, what are those that set one algorithm for that, for the application of set 1 algorithm, the following problem definitions are to be considered here. And in this case some given and also identified criteria should be there. What is that given? A base case design and identified to know process hot-spots that have been translated into design targets that should be considered in this case. So, that is why given as a base case design and the identified process hot-spots to be considered there.

And then after that you have to identify a set of desirable tasks and also the phenomena based building blocks that will represent this to know that tasks. So, that is why you have to consider this you know that problem definition before going to that using of the set 1 algorithms.

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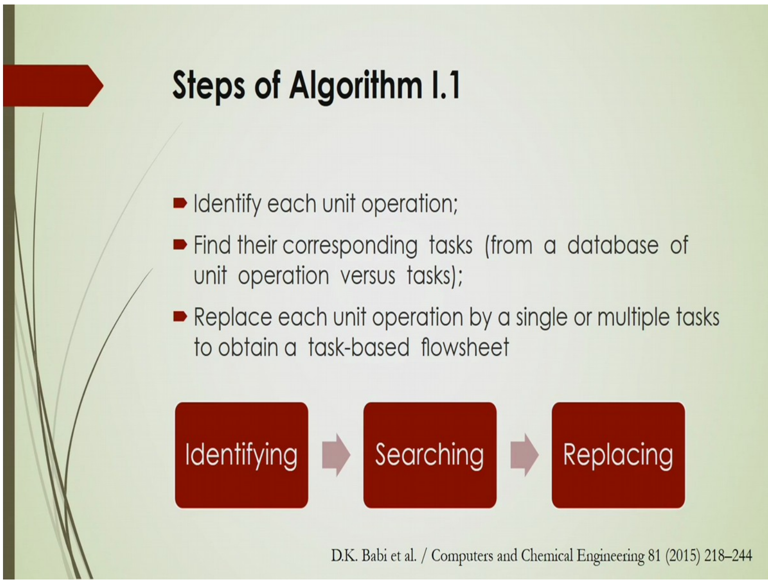


And what are the steps of that algorithms 1.1, in this case identify each unit operation and after that you have to search that corresponding tasks from the database of unit operation versus various tasks. And then replacing of that each unit operation by a single or multiple task to obtain a task-based flow sheet. So, these are the identification and searching and replacing, these 3, you know that steps to be considered whenever you are using this algorithm of 1.1.

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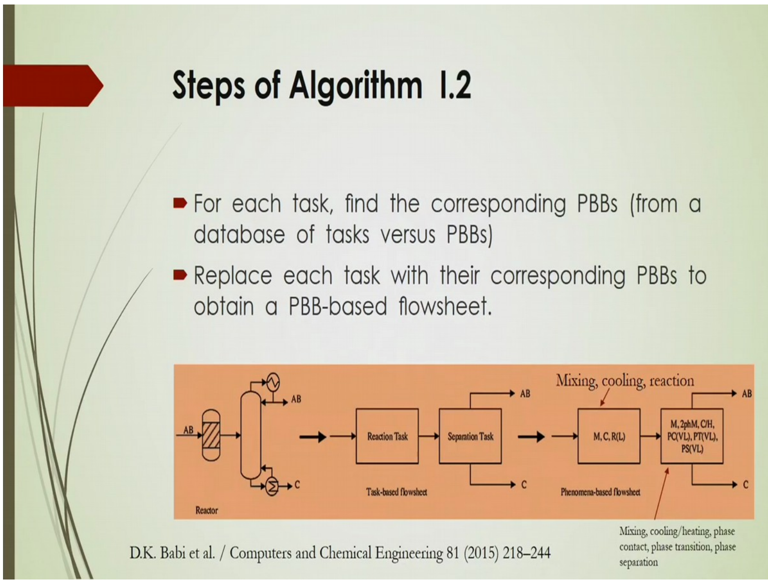


Now, what are the steps of those algorithms of 1.2? In this case for each task, you have to find a corresponding PBBS, that is phenomena based building blocks that will be from the database of task that is versus PBBS.

And then you have to replace each task with their corresponding PBS to obtain a phenomena based building block-based flow sheet there. Here in this case it is given in the slides that according to that Bobby et al in 2015, that there is you know that reactor, after that there will be separation. And in this case task-based flow sheet is the reaction task and then you know that the re-separation tasks. After that phenomena based flow sheet to be formed based on this phenomena based like this, mixing, cooling and reaction. Based on this that is called phenomena based flow sheet here.

And after that you have to, you know that consider that based on this mixing cooling reaction and how to separate those things by this flow sheet. So, this is the actually that task to be converted to that flow sheet there. So, that is why for each task you have to find the corresponding phenomena based building blocks there whether it is mixing, cooling or reaction. After that you have to replace each task with their corresponding phenomena based building blocks to obtain that phenomena based building blocks related or based flow sheet there.

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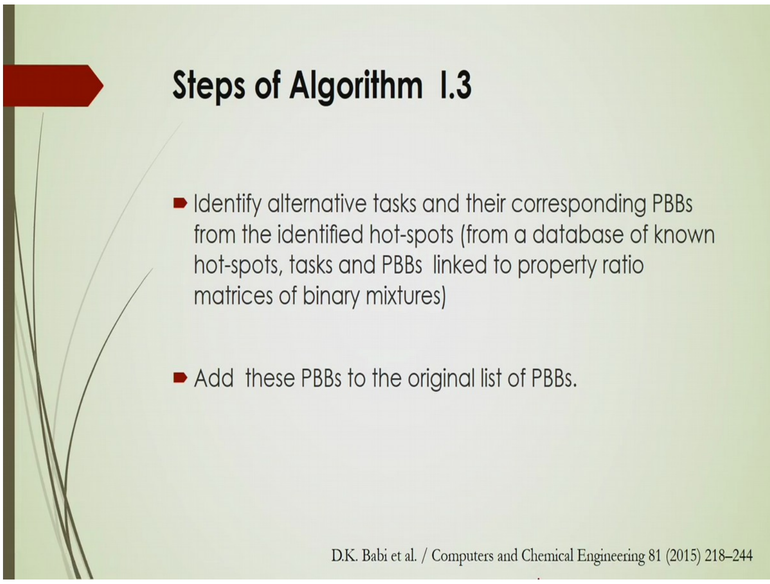


And then steps of algorithm 1.3, in this case also you have to identify that alternative tasks there and their corresponding phenomena based building blocks, from the identified hotspots there. This is also again from the database, that is known hotspots, tasks and phenomena based building blocks linked to property ratio matrixes of the binary mixture is there. And then you have to add all those phenomena based building blocks to the original list of phenomena based building blocks there. So, this is the case where that identification of the tasks and their corresponding phenomena based building blocks is required at the steps of building blocks algorithm 1.3.

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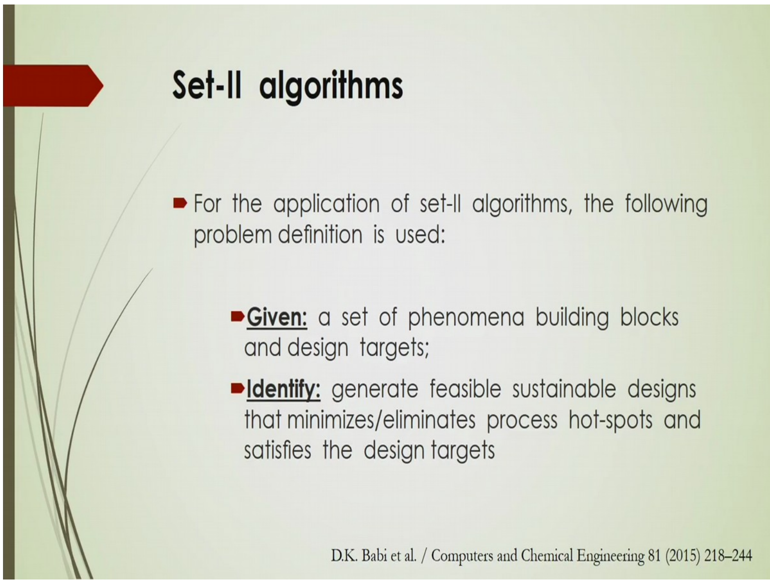


Then what are those steps 2 results and what are those conditions and also in this case of set algorithms, again that you have to have some condition like given and identified, what are the given set of phenomena building blocks and design targets to be given there. And for the application of set 2 algorithms, then you have to use these set of phenomena based building blocks and design targets. After that you have to identify and then in that case what is that generate feasible, sustainable design and also that minimises or eliminates the process hot-spots and also satisfies the design targets there in case of that particular process synthesis.

So, that is why as per that 1, also set 2 will have that given and identification tools there. So, as per given you have to have that set of phenomena based building blocks and designs to be considered, and identification in that case you have to generate the feasible sustainable design that will minimises all eliminates that you know that process hot-spots also and also satisfies the you know that what are the targets of your design there.

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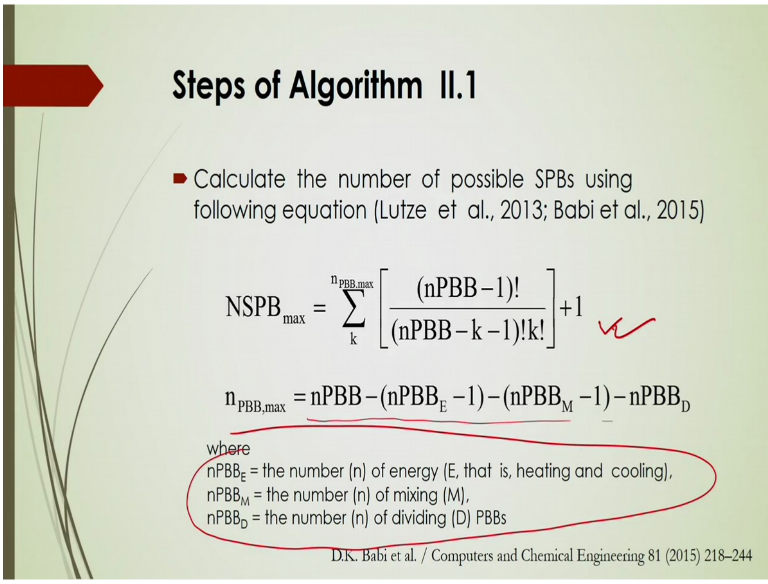


And in this case for the algorithm that under the set 2, the first algorithm, you have to calculate the number of possible simultaneous phenomena based building blocks. These possible, the simultaneous phenomena based building blocks to be calculated based on that phenomena based N number of phenomena based building blocks. So, this equation, here can be used to maximise the NSPB, here for this maximising problem in this case you know that it can be calculated by summing up these phenomena based building blocks. If it is N number of phenomena based building blocks, then it will be here as

$$NSPB_{max} = \sum_{k}^{n_{PBB,max}} \left[ \frac{(nPBB-1)!}{(nPBB-k-1)!k!} \right] + 1$$

Where this nPBB can be calculated based on this equation here

$$n_{PBB,max} = nPBB - (nPBB_E - 1) - (nPBB_M - 1) - nPBB_D$$

What is this $nPBB_E$? $nPBB_E$ is the number of energy, that is heating and cooling like this. And $nPBB_M$ is the number of mixing, you can say that is phenomena based building blocks of mixing and $nPBB_D$ is the number of phenomena based building blocks for the dividing. So, these are the things, these are the parameters that you have to use to calculate these number of simultaneous phenomena based building blocks to maximise it.

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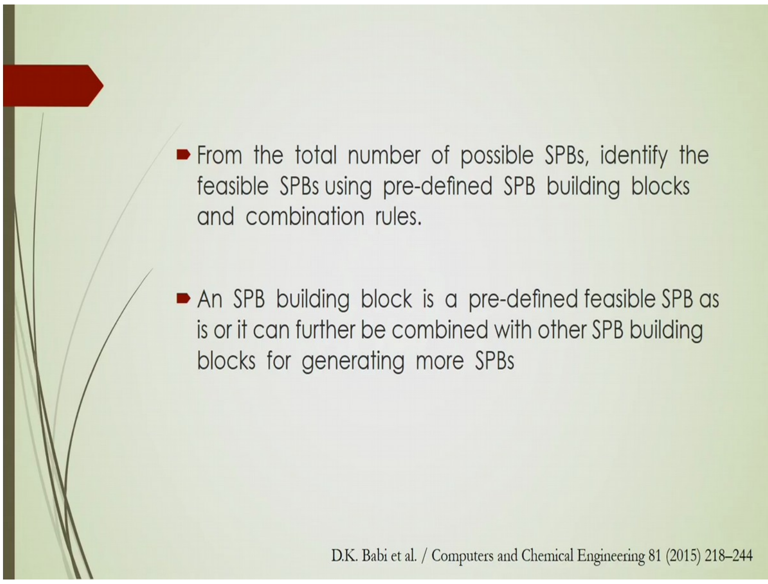


And from these total number of possible SPBS, that you have to identify the feasible SPBS. Now, among the SPBS you have to then segregate which one will be the feasible SPBS using the predefined SPB building blocks and also combination rules.

Now, after that what you have to do that an SPB building block should be predefined feasible SPB as is or it can further be combined with other SPB for the building blocks for generating more simultaneous feasible phenomena based building blocks there.

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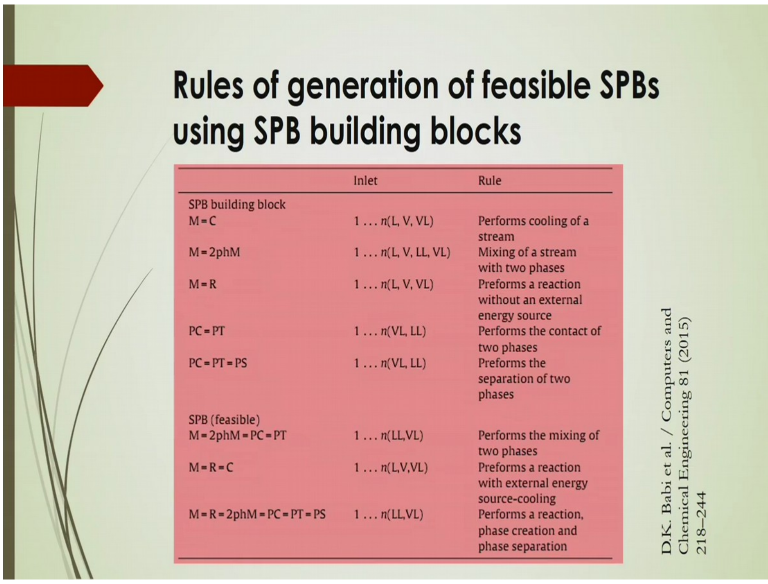


Now, what other roles of generation of feasible is PBS there? So in this case you can use this SPB building block for the generation of feasible SPBs here. Now here some inlet and some rule is given there. SPB building blocks if it is M and C, that M mixing and cooling will be used there, in that case inlet should be 1 to N there, based on that you know that liquid vapour or vapour liquid. In this case you have to perform the cooling of a stream there.

If suppose mixing based on that two-phase mixing, what will happen, in that case your inlet again will be 1 to N, there of that stream, you know that liquid-vapour, liquid-liquid, even vapour-liquid there. So in this case mixing of a stream with two phases will happen. And to be considered also and also here this like M is as reaction, in this case you know that again N number of inlet to be considered, inlet us seems to be considered here like liquid-vapour and vapour-liquid mixture there.

So, in this case a reaction also to be performed without an external energy source. And then after that you know that phase contact and phase transition, in this case again that vapour-liquid and liquid-liquid mixture to be considered as an inlet stream. And in this case also you have to perform the contact of two phases for this phase contact and phase transition.

Again that phase contract and phase transition and phase separation, if you are considering as a SPB building block, in that case again here you have to perform the separation of two phases under this inlet of a vapour-liquid and liquid-liquid streams there.

And what are those feasible then SPBS based on these SPBS building blocks? In that case if you are considering that this M2 PSM, PC and PT, that means you are mixing, two-phase mixing and face contact and phase transition there, between the liquid-liquid and vapour-liquid phases. So, in that case you have to perform the mixing of two phases. And if you are considering that feasible simultaneous phenomena based building blocks for this mixing, you know that reaction and cooling, then you can consider here that again liquid-vapour and vapour liquid as streams, as in any bet of 1 to N.

And in that case the performance will be as a reaction with external energy source that is called cooling. And if there is a mixing for the reaction, for two-phase reaction, even phase transition, phase contact and phase separation simultaneously happen as a feasible simultaneous phenomena based building blocks. In that case again that you have to perform reaction in this case phase reaction, phase separation under the phase of that liquid-liquid and vapour-liquid there.

So, these are the different rules based on that inlet and also that simultaneous building blocks. And several simultaneous phenomena based building blocks may form their sand out of which you have to select the feasible one of SPBS that is called simultaneous phenomena based building blocks.

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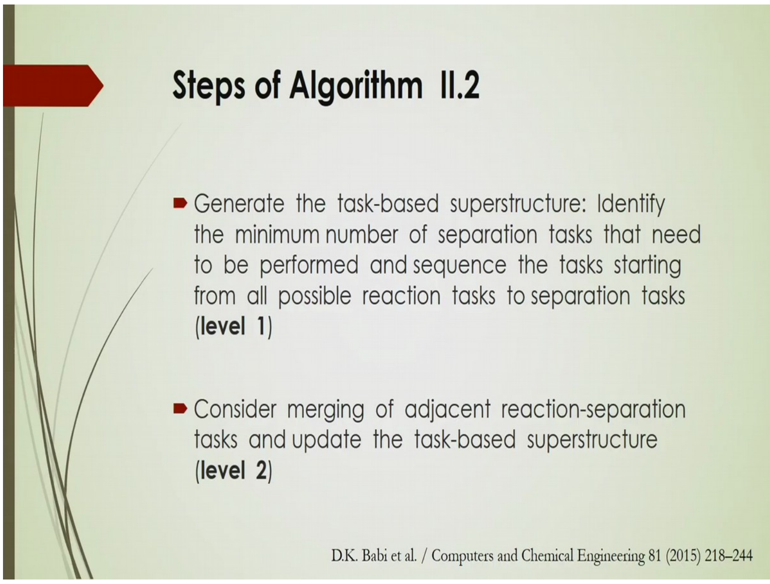


After that this algorithm II.2 will be followed. Now in this case there are two levels to be considered here and the first level you have to generate the task-based superstructure, in that case identify the minimum number of separation tasks and that will actually need to be performed and sequenced the task starting from all possible reaction tasks to separation tasks there.

So, in the level I, that you have to consider these things and in the level 2 you have to consider the margin of adjacent reaction separation task and also you have to update parallelly the task-based superstructure there at this level.

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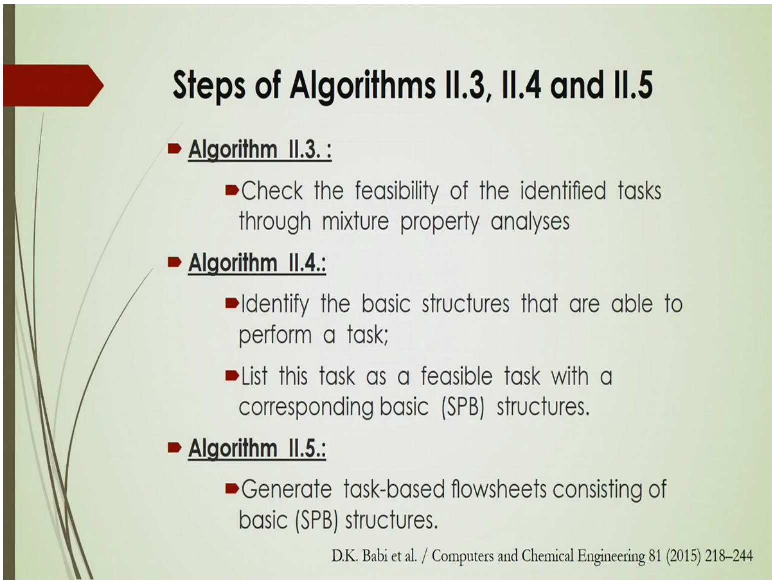


And what are the steps of then algorithms II.3, II.4 and II.5, there in algorithm II.3, that you have to check the feasibility of the identified task through mixture property analysis. And in the algorithm 2.4, in that case identify the basic structure and also in that case you have to make a list of that task as a feasible task with a corresponding basic structure also.

And in that case you have to identify the basic structure, those will be able to perform a particular task. And in the algorithm II.5, after that you have to generate the task based flow sheets that will consist of the basic structure there.

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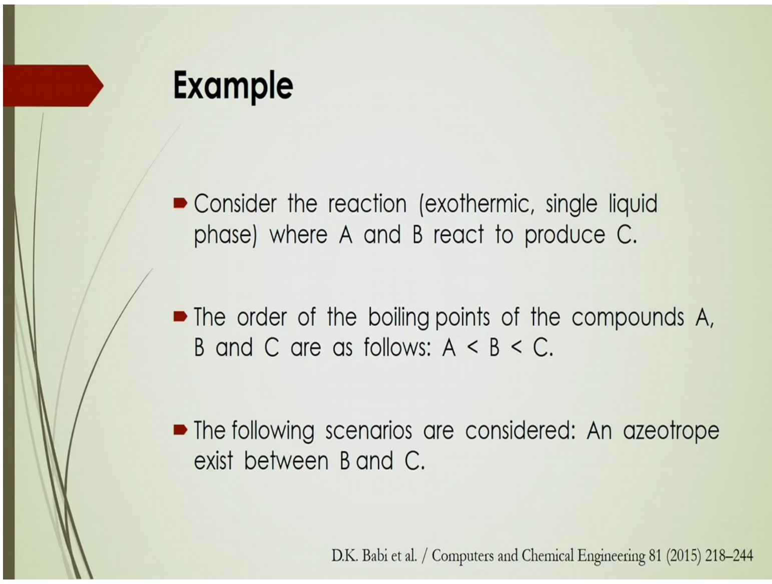

Now, let us have an example for those algorithms there. Now, if we consider the reaction, if it is suppose exothermic, single liquid phase where A and B react to produce the option C there. So, in that case the order of the boiling point for those streams, that is our components A, B and C should be considered in well manner, otherwise that whatever you know that mixing or reactions will be there, that separation of that by-products will be very difficult. So, you have to select that components will be well difference in their boiling point.

So, that is why boiling point sequence to be maintained in this case like this A should be less that B should be less than C. So, if it is considered then, you have to find out whether is there any azeotropes will be formed between those components of A, B, C or not because those by-products, whatever will be coming, that may have that azeotropes. Because these azeotropes maybe, they will have that similar kind of boiling points after products. So, that is also to be considered, whether the products will be forming any azeotropes or not.

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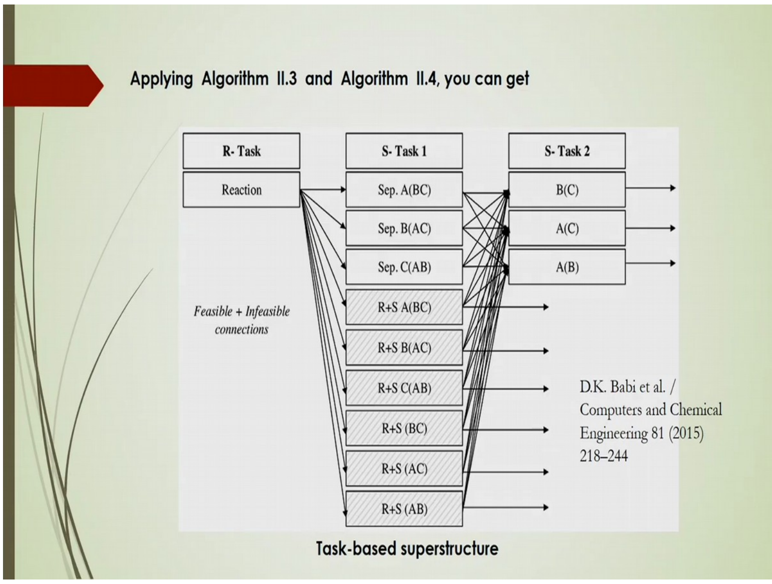


Now, based on that algorithm II.3 and algorithm II.4, you can get this type of task-based superstructure of simultaneous phenomena based building blocks there. So, here we are having these R-tasks and then S-task 1 and S-task 2. So, if we consider that R-tasks, that is reaction task as here reaction and S task as separation task and again S-task as separation task 2.

So, if we consider that reaction separation, both will happen simultaneously, then we are having these building blocks of reaction separation. Now separation maybe between that A or BC, there will be competition, there will be several possibility of that phenomena based building blocks will be there. Based on that may be either mixing or based on that maybe either heating, based on the cooling, based on the phase transition, based on the face contract, like this.

So, there may be a combination of like this separation of A, B and C, separation of B from AC, separation of C from AB and separation of that A from BC. Along with that reaction also, if there is a pure, if you are considering the separation and reaction separately, then there will be a building block.

If you are considering reaction, then reaction plus separation will be another building block, then you can consider it as R Plus S and S should be again different combination like separation of A will be from the BC mixture and you know that B should be separated from AC and C should be separated from AB. And like only BC may be separated and A should be totally nullified, it will not count the by-product. And also AC may be separated, and also AB may be separated from that reaction separation mixture.

So, there is a combination of that operation and task there. So, here feasible and invisible connections to be in the state and which one will be feasible, that should be considered. Now, from this you can consider that BC as a suppression task and AC and AB, like this. So, these are the different superstructures can be formed based on the task. Now, what are the different tasks that can be there?

So, this, here is maybe you know reaction and separation, maybe some other things like extraction or distillation, even you know that extraction and also crystallisation, those are the things may come there. So, this is a simple example reaction as well as sample separation which are being mostly actually happening in chemical engineering process.

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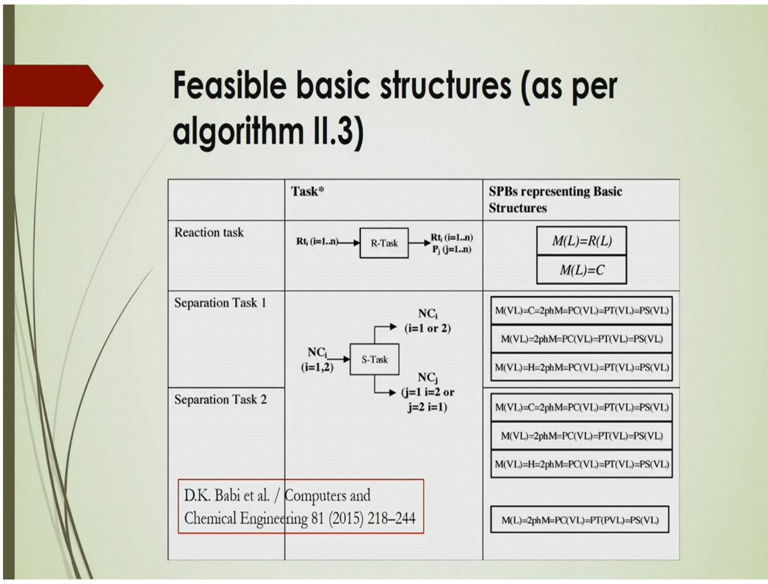


Now after that, what are the basic feasible structures that are formed as per that algorithm II.3, that you can form like this reaction task, like these are the building blocks to be formed for this task can also here simultaneous phenomena based building blocks which will represent the basic structure like this.

Similarly for separation tasks, and separation task 1, separation task 2 the corresponding tasks are actually made here based on that contact and also that other components also, what components is coming to the task and what the components to be separated out are.

And based on this there are several combinations of phenomena based building blocks to be formed and based on that simultaneous phenomena based building blocks can be represented from this basic structure there.

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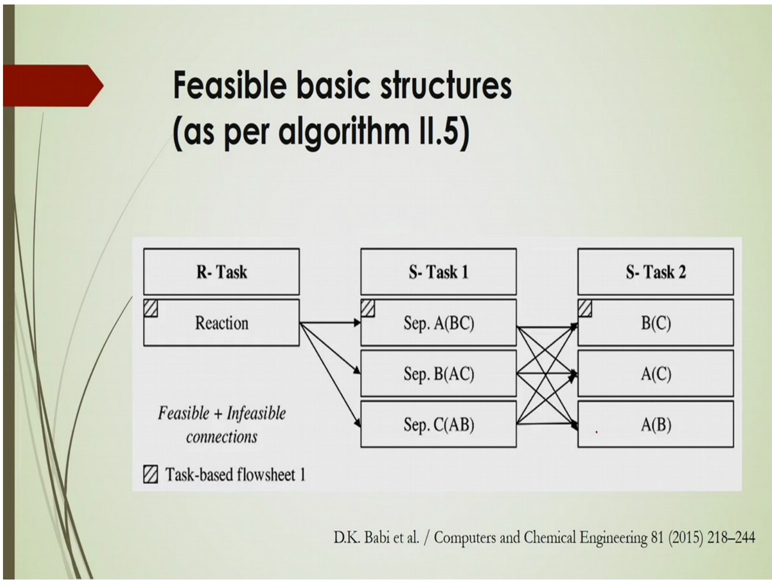


And after that feasible basic structure as for algorithm II.5, it can be also generated based on this R-task, here reaction and the S-task 1 and S-task 2, like this here, separation will be ABC, separation B from AC and then separation of C from AB, like this here as task 2, here BC, AC and AB so these are the task-based flow sheets, which are feasible and sometimes not feasible. So, that you have to identify or segregate the feasible basic structure as per algorithm II.5.

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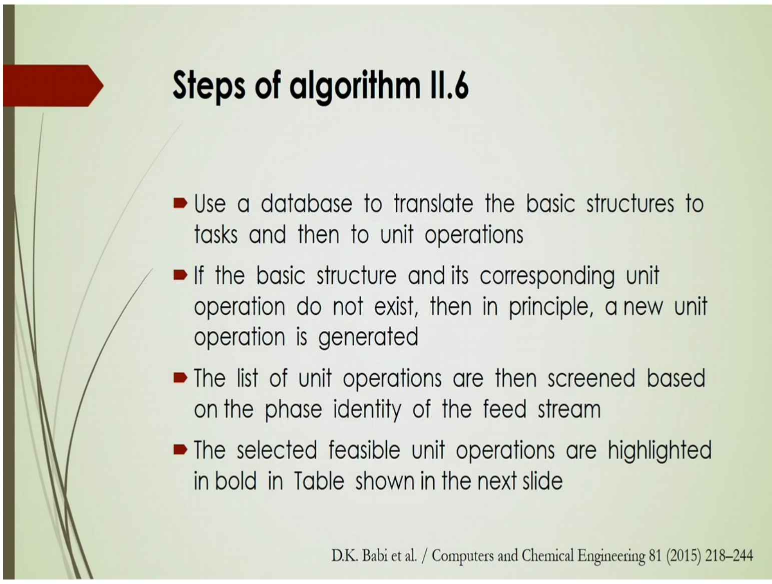


Now, what are the steps of algorithm II.6, there in this case you have to use some database to translate that basic structure to task and then to unit operations there. And if the basic structure and its corresponding unit operations do not exist, then you have to generate a new unit operation there. And after that a list of unit operations to be screened up and identify the feed stream based on that phase identity there.

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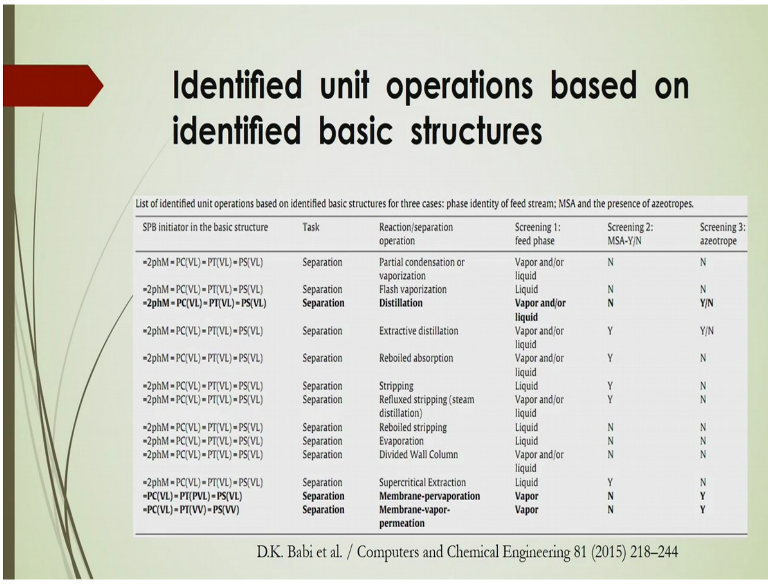


List of identified unit operations based on identified basic structures for three cases: phase identity of feed stream; MSA and the presence of azeotropes.

| SPB initiator in the basic structure | Task | Reaction/separation operation | Screening 1: feed phase | Screening 2: MSA-Y/N | Screening 3: azeotrope |
|---|---|---|---|---|---|
| =2phM=PC(VL)=PT(VL)=PS(VL) | Separation | Partial condensation or vaporization | Vapor and/or liquid | N | N |
| =2phM=PC(VL)=PT(VL)=PS(VL) | Separation | Flash vaporization | Liquid | N | N |
| **=2phM=PC(VL)=PT(VL)=PS(VL)** | **Separation** | **Distillation** | **Vapor and/or liquid** | **N** | **Y/N** |
| =2phM=PC(VL)=PT(VL)=PS(VL) | Separation | Extractive distillation | Vapor and/or liquid | Y | Y/N |
| =2phM=PC(VL)=PT(VL)=PS(VL) | Separation | Reboiled absorption | Vapor and/or liquid | Y | N |
| =2phM=PC(VL)=PT(VL)=PS(VL) | Separation | Stripping | Liquid | Y | N |
| =2phM=PC(VL)=PT(VL)=PS(VL) | Separation | Refluxed stripping (steam distillation) | Vapor and/or liquid | Y | N |
| =2phM=PC(VL)=PT(VL)=PS(VL) | Separation | Reboiled stripping | Liquid | N | N |
| =2phM=PC(VL)=PT(VL)=PS(VL) | Separation | Evaporation | Liquid | N | N |
| =2phM=PC(VL)=PT(VL)=PS(VL) | Separation | Divided Wall Column | Vapor and/or liquid | N | N |
| =2phM=PC(VL)=PT(VL)=PS(VL) | Separation | Supercritical Extraction | Liquid | Y | N |
| **=PC(VL)=PT(PVL)=PS(VL)** | **Separation** | **Membrane-pervaporation** | **Vapor** | **N** | **Y** |
| **=PC(VL)=PT(VV)=PS(VV)** | **Separation** | **Membrane-vapor-permeation** | **Vapor** | **N** | **Y** |

D.K. Babi et al. / Computers and Chemical Engineering 81 (2015) 218–244

And also the selected feasible unit operations are then highlighted in bold, in table, as shown in the next slide here. The feasible that here unit operations are shown here like this like I have highlighted there. Now, there are several basic structures, you can form and also from that basic structure you are identifying the feasible unit operations there. So, this one will be the feasible unit operations based on your total reaction separation process there as per process intensification. And also here this is also another feasible unit operations based on that identified basic structure there.

So, these tables also, you have to go through that what are the different simultaneous phenomena based building blocks can be formed and these building blocks based on the task on that here are given different separation, separation, and all those things. And also reaction separation combinations are also there. And then you have to do the screening of feed phase, and screening the structure and also screening the azeotropes is there is there any formation or not. So, these are the case based on this table you can identify the unit operations there.

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So, I think we have discussed that preliminary based idea of that algorithms, how it can be used and what are the different algorithms that are given based on that phenomena based building blocks and also how that algorithms can be used by basic examples of that reaction separation, how this SPB can be formed and how to segregate that feasible unit operations based on that algorithm.

So, I will suggest you to go further about these algorithms, I think it will be very much useful if you follow this Juan Gabriel Segovia Hernandez textbook there, Chemical Engineering Design Optimisation and Control. These books will be very useful for this more information of stochastic algorithms which are being used for the Chemical Engineering Process Intensification. So, thank you for this lecture.