Basic Principles and Calculation in Chemical Engineering
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Module-11
Lecture-33
Process Degrees of Freedom

Welcome to massive open online course on basic principles and calculations in chemical engineering. So we are discussing about the computer aided balance calculations under module 11. Now this module we will continue that discussion on computer aided balance calculations.

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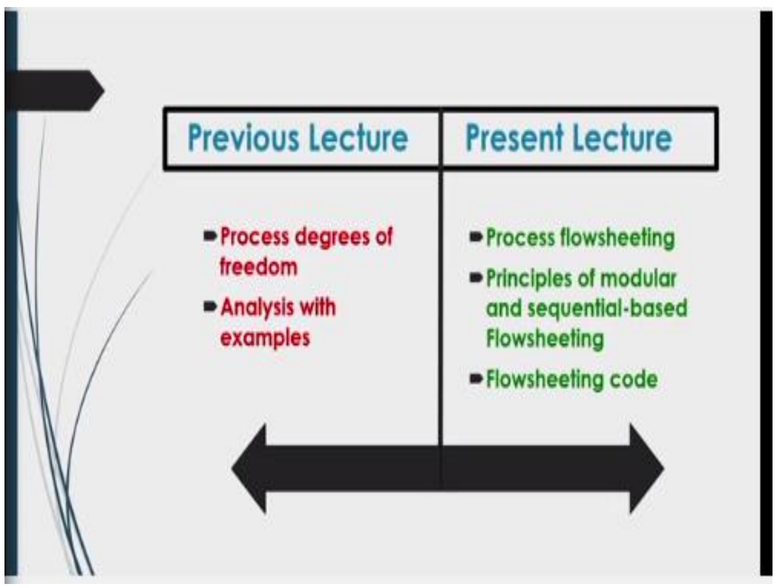

And in this lecture will try to discuss about process flowsheeting and it is principles and what are the different types of process flowsheeting and flowsheeting codes. Now for this flowsheeting based calculations you need to know about that process degrees of freedom. We have described in the previous lecture about that process degrees of freedom and it is analysis with various examples. And also we have described how to you know make a process flowsheet and just by mentioning different components and there that specifications of different variables.

And also how to you know analyze that number of degrees of freedoms, they are based on different variables and even different independent you know equations that is developed based on material balance and energy balance. Now based on those material balance or energy balance equations you can make it flowsheet. And that proceed maybe you know in terms of spreadsheet in computers screen where you can mention all those variables.

And those variables to be you know mentioned in (()) (02:16) that what is the actually material balance equation, what is the energy balance equation. Based on which you can note down in that you know spreadsheet for the solving of that linear equations or nonlinear equations whatever it is coming based on that material balance. And also after you know pointing out or you can say that specification of those you know process you know equations and you know variables.

And then you can solve those equations by you know of some codes or by you know that computer programs, so it will be called as flowsheeting code. So, we will show here that what are the different types of you know flowsheeting codes are being used for solving linear and nonlinear equations also or process optimization, you will see that there also there maybe some you know linear and nonlinear equations which is to be solved for optimization of the process.

Based on that you know material balance and also energy balance equation and for those you know solving of that optimization problems. Also there are several you know algorithms and you know codes are being used to solve those equation. And we will also show those codes also here. Now before going to that in details you have to what is that process flowsheeting.

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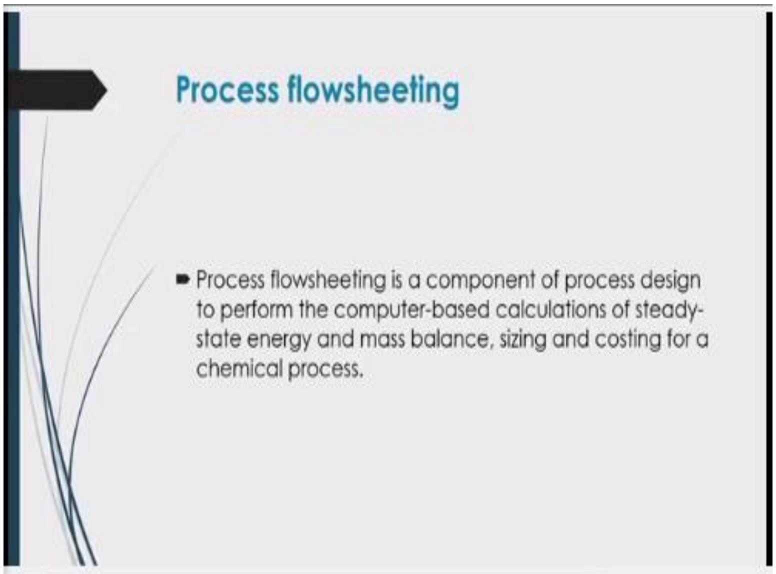

Now it is generally a component of process designed to perform the computer based you know calculations of steady state energy and material balance. And also you can asses by this flowsheeting, what is the size of that you know chemical process, equipment and also what are the costs or economy for that particular chemical process based on that optimization problems. You know that computer solved the problem that you know described the mathematically of a series of that operations.

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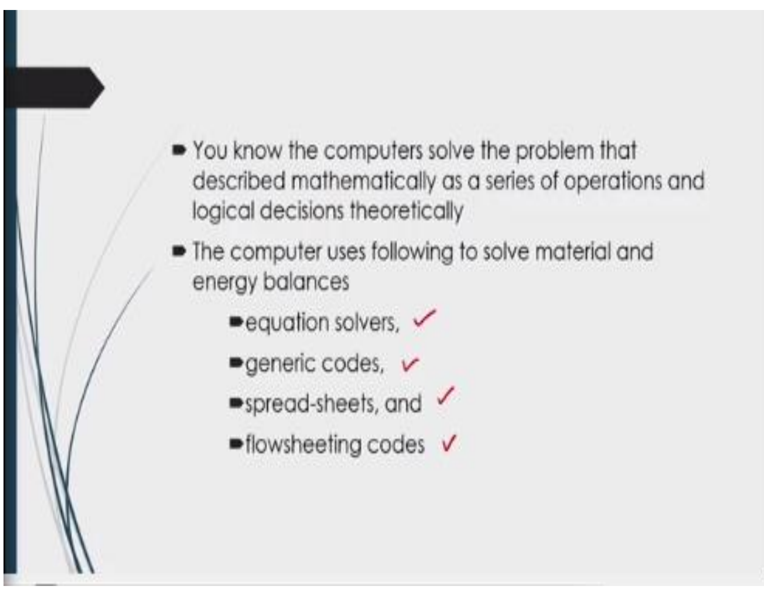

And you can say that some logical decisions or theoretically for the optimization of the process. And the computer uses some you know balance equations to solve those equations by certain you know course or like you know some other you know solvers like that.

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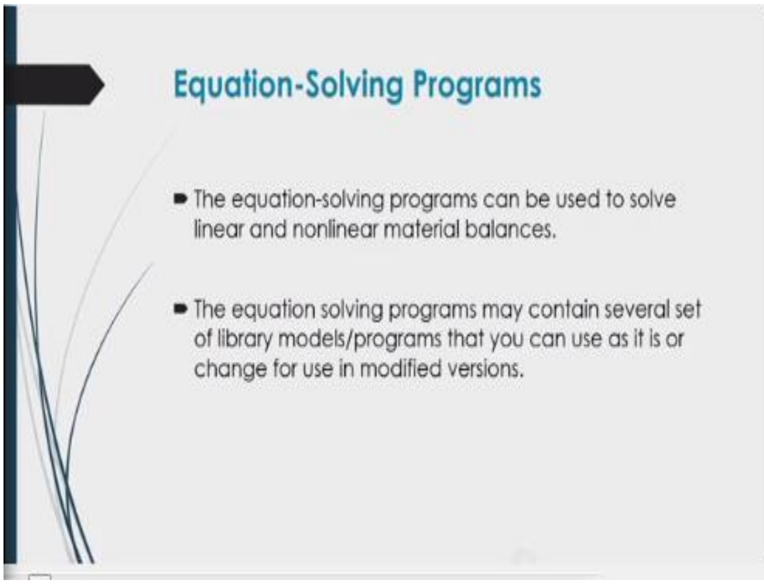

Now, the computer uses this following you know to solve material energy balances here you will see as given in the slides. Here some you know equation solvers can be used to solve that you know material and energy balance equations. Some generic codes can be used to solve that material and energy balance equation. Even you can solve that material and energy balance in a spreadsheets even some flowsheetings codes also available to solve with this material and energy balance equation.

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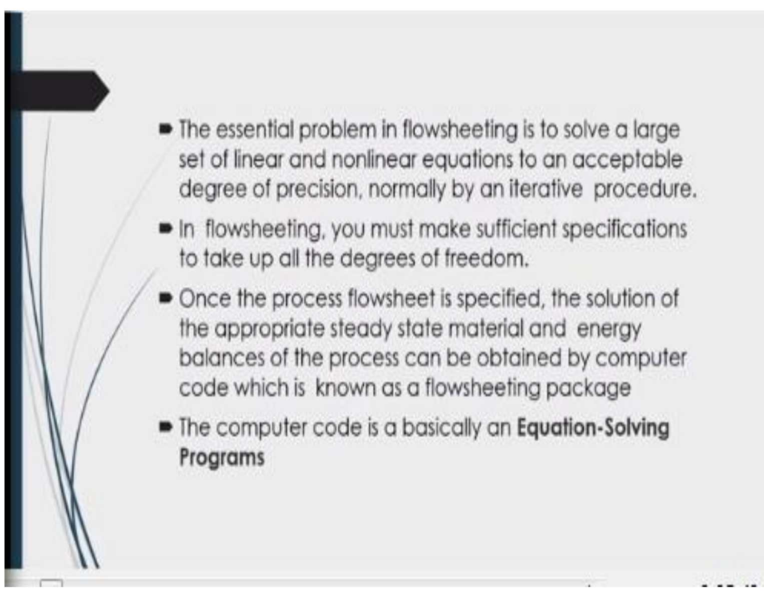

Now the essential problem in you know flowsheeting is to solve a large set of linear and nonlinear equations. And of course this you know solution to be an acceptable degree of precision just by iterative procedure. And in flowsheeting in that case you must make sufficient specifications to take up all the degrees of freedom. Once the process flowsheet is specified with process degrees of freedom and also processes specifications inlet outlet even specific specification of this inlet and outlet.

Streams, they are with different you know variables like thermodynamic variables even dynamic variables there. The solution of those you know specified flowsheet you know streams in that case you will see if you are considering steady state operation then you have to solve that steady state material and energy balances of that processes. And that can be obtained by computer code who is known as a flowsheeting package.

Now this computer code is basically an equation solving programs there and it is based on actually that energy and material balance equation. And some programs is made which is actually used for that solution.

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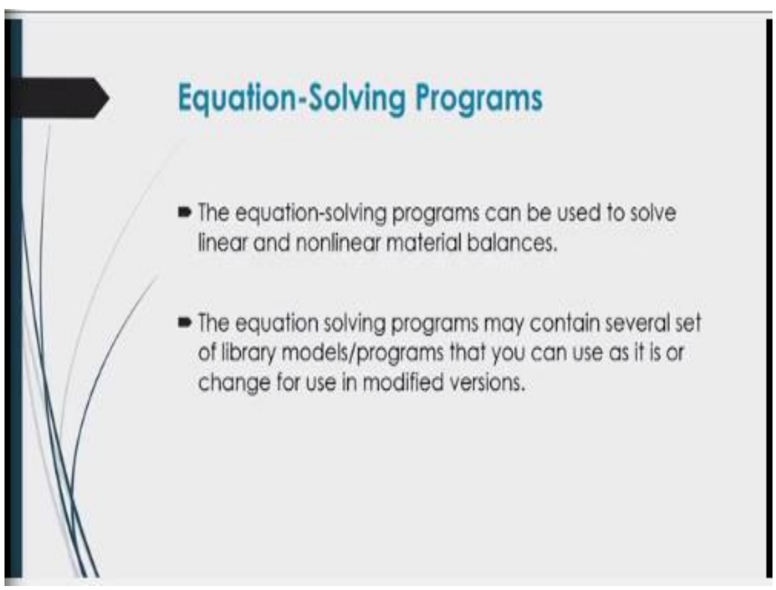

Now what is that equation solving programs, the equation solving programs can be use to solve linear and nonlinear material balance. The equation solving programs may contain several set of you know, library models of programs that you can use as it is or change for using modified versions. Sometimes you will see that code whatever is available commercially that you can use for solving that linear nonlinear equation.

But if you are having different type of you know linear equations or nonlinear equations for a specific problems there. So in that case you can modify those you know, existing you know programs or models which is available in a library. So, in that case, you can you know conventionally change that models and make a you know new you know modified versions of that programs.

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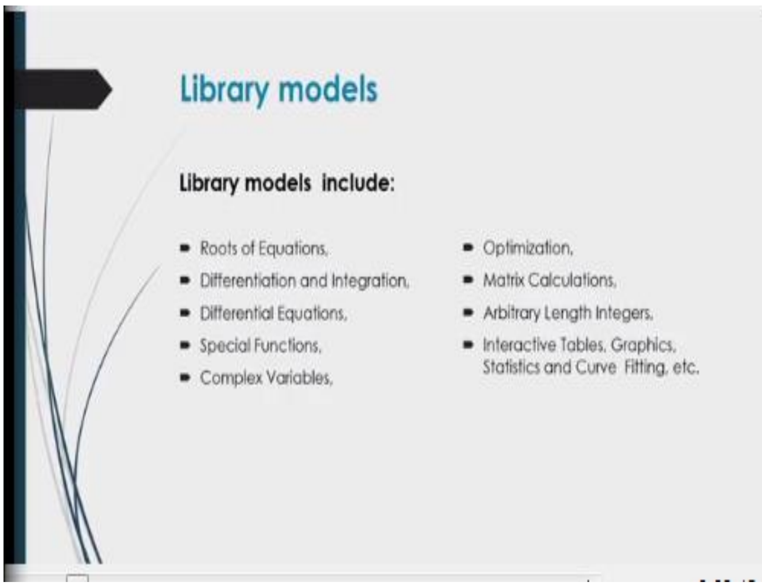

Now what are the you know existing library models generally available of commercially like you know that the roots of equations there is some programs available to solve these roots equations. And also some you know the library models are for differentiation and integration, differential equations you know special functions, complex of variables like optimization problems, matrix calculations, arbitrary length integers even you know interactive tables, graphics, statistics and curve fitting etc.

So, these are the library models that are available, you can use this library models to solve your you know linear or nonlinear equations. And also you can modify these models based on your problems. Now what are the techniques to solve that equations.

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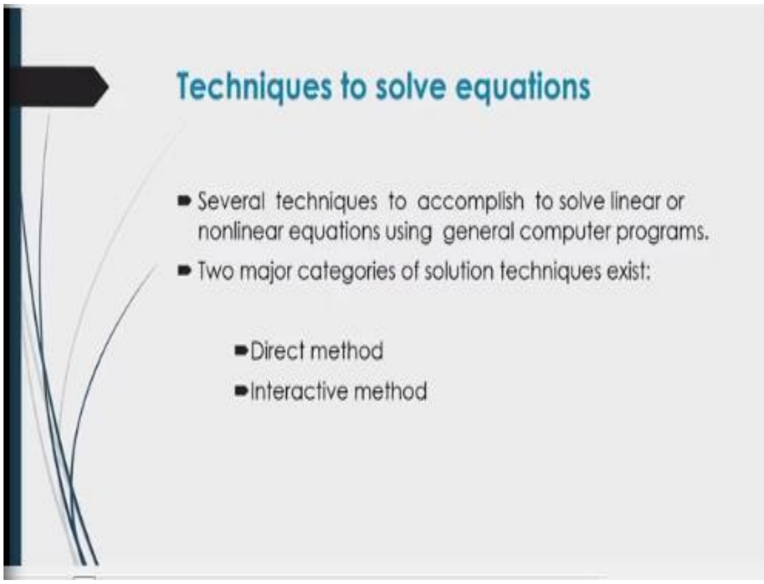

Now you will see that there are several techniques to you know accomplish to solve this linear and nonlinear equations using general computer programs. Two major categories are here like direct method and interactive method.

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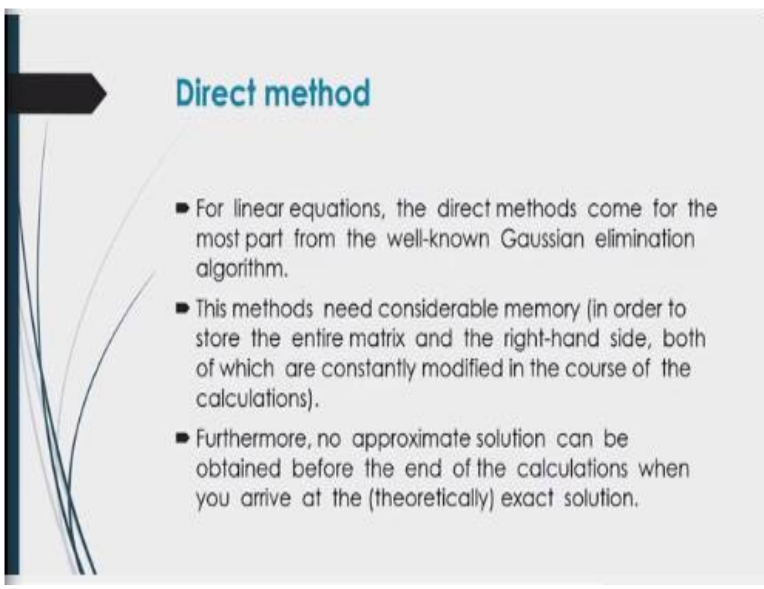

In the case of direct method, you will see that for linear equations the methods come for most part from the well known Gaussian elimination algorithm. And this methods need considerable memory in order to store the entire matrix and the right hand side both of which are constantly modified in the course of calculations. You will see that if you are having set up linear equations or nonlinear equations you will see that as per variables you can you know average you know those equations.

And you can write **a** you know a linear equation forms there as a matrix forms and then you can you know solve that matrix form of those equations by you know this Gaussian elimination techniques. There is the algorithm is available also, you can use that algorithm to solve those you know set of linear or nonlinear equations there. But Gaussian elimination algorithm is basically used for linear equation solving.

Whereas, you can use that Newton Raphson method or Newton's only methods to you know solve that nonlinear equation there. You will see that whenever you are getting that material balance equation or energy balance equations for different components in a particular process even for overall process also. You have to arrange all those equations as a matrix forms and then you have to solve that you know by computer codes.

Furthermore if suppose no approximate solution if it is you know obtained from your you know set of equations. Then you know that you have to modify that equations with some other you know auxiliary equations. So, that you can get that solution of there but sometimes you will see that without using that you know Newton's method or Gaussian elimination method you can solve that equation theoretically to get that exact solution there.

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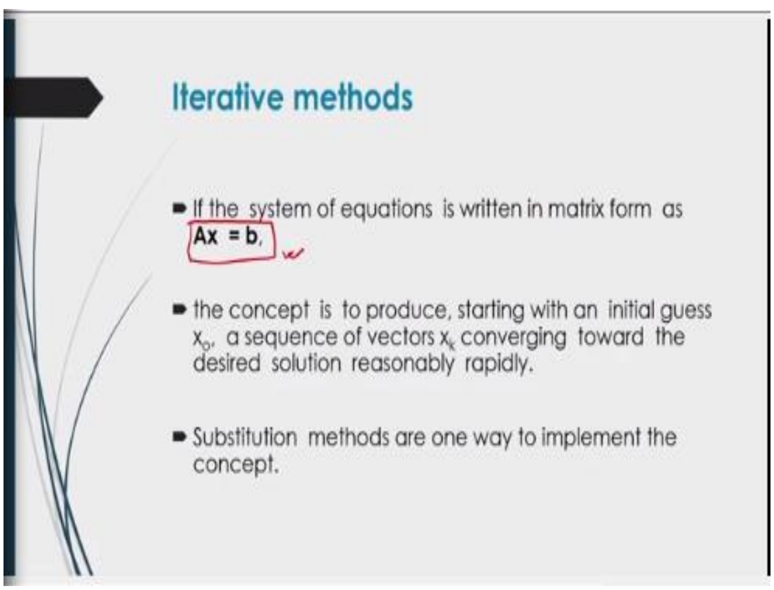

And iterative methods is basically if the system of equations is written in a matrix form like AX = b here A or here you know that coefficients and X is that set of you know variables, they are unknown variables and b is again that some coefficients there. So, if you are expressing this you know material balance equations as a matrix form then you can use this concept to produce you know of that solution just by an initial guess of that like X 0 a sequence of vectors X k that converging towards the desired solution reasonably and also rapidly.

Now substitution methods are one way to implement this concept also. So here, so in this form of matrix you can you know solve just by you know assuming that initial guess of that X value. And then successively you just you change that you know guess values based on that initial guess and then coming to that you know desired solution by conversing that you know assumptions there.

So, in that way you can solve these linear equations by iterative methods, even you can solve this by of you know computer programs there. And this can be used for linear and nonlinear equations but for only nonlinear equations there we have described earlier that you have to use modified you know Newton's method there just incorporating that inverse of your Jacobian matrix there, that we have described earlier.

Then another important points here that whenever you are expressing all those linear and nonlinear equations in a spreadsheet then you have to make a spreadsheet programs to solve all those you know equations there.

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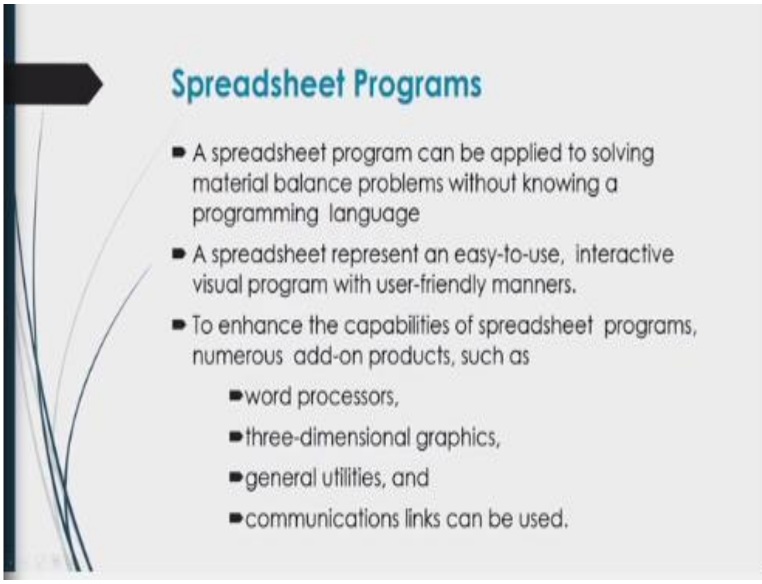

And that can be you know represented you know based on different you know aspects like you know whether it should be you know user friendly or not, whether it should be you know easily understood or not or whether it can be used for general utilities or not. Though there, is there any other you know tools can be used to reduce you know spreadsheet programs or not, all those to be actually considered there.

Now a spreadsheet program can be applied to solving only material balance problems without knowing a programming language. Here this is one of the important point here, a spreadsheet generally represents and easy to use and iterative you know interactive visual program with user friendly manners. And to enhance the capabilities of spreadsheet programs, numerous add on products such as you know word processors, 3 dimensional graphics, general utilities and communications links can be used.

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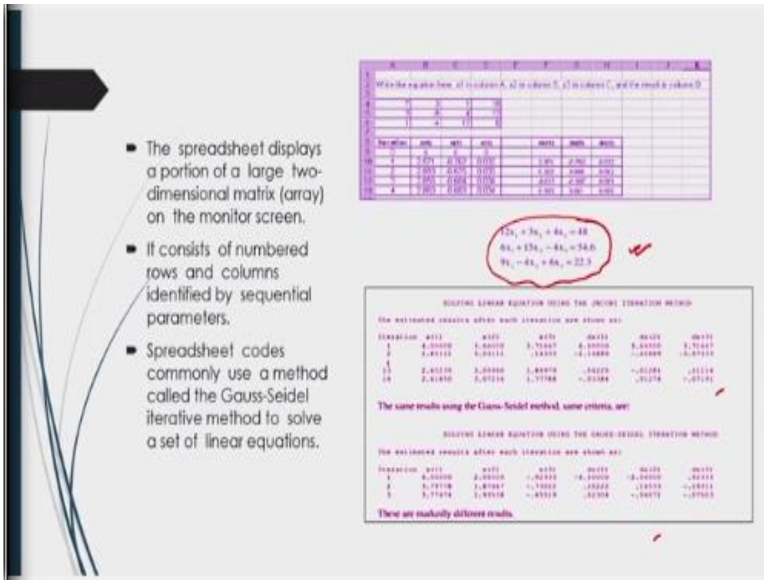

Here see that the spreadsheet displays a portion of a large 2 dimensional matrix or array on the you know monitor screen. As shown here in the slides that here how the spreadsheets are actually of seen in a monitors there. So, if you are getting here a set of linear equations and then how these set of linear equations can be expressed in a spreadsheet.

And how that is spreadsheet you actually being executed to solve this linear set of equation. So, in that spreadsheet generally consist of numbered rows and columns that identified by sequential parameters here. Like this here parameters or variables also parameters like here 12, 6, 9, 3, 15, 4, 4, 4, 6 like this, these are the you know coefficients here. Whereas you know that variables like here X 1, X 2, X 3 like this.

So, in a spreadsheet you have to mention all those you know variables like here these variables X 1, X 2, X 3 and also what is that, that coefficients there. For a number of iterative procedure you will see that that you can solve this linear equation in a spreadsheet. Now a spreadsheet codes commonly used a method called the Gaussian Seidel you know iterative you know method to solve a set of linear equations there.

So as per this here it is shown that here these equations are given, so as per this Gauss Seidel iterative method how to solve this linear equation in a spreadsheet it is given there. Like this here so how this you know linear equations can be expressed in a spreadsheet and how to solve this is shown here.

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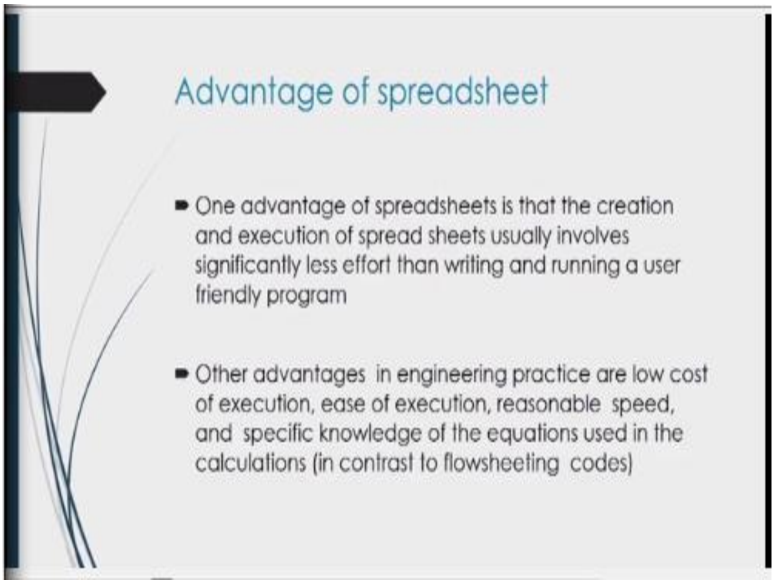

Now what is the advantage of spreadsheet, one advantage of spreadsheet is that the creation and execution of spreadsheets usually involves significantly less effort than writing and running a user friendly program. Other advantages like in engineering practice where you know that a low cost of execution and ease of execution reasonable speed and a specific knowledge of the equations used in the calculations. For those cases this you know spreadsheet programs or spreadsheet codes can be used for solving that set of linear equations.

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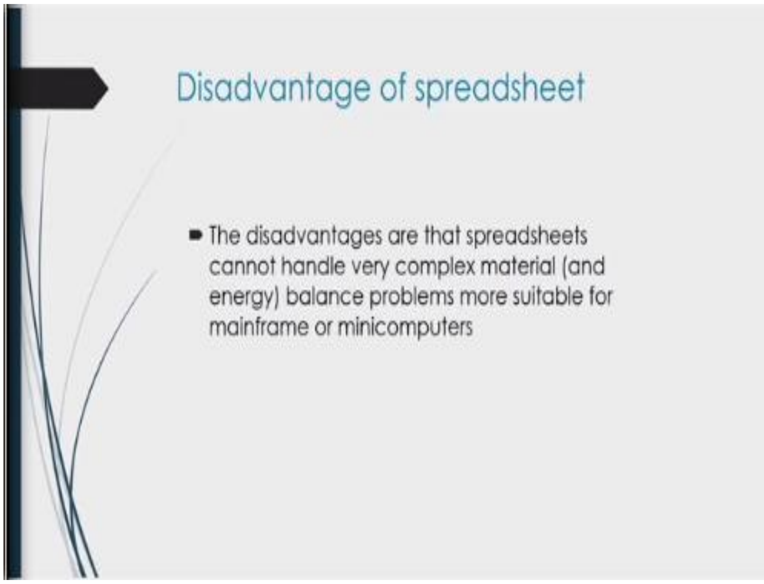

But here some disadvantage also there, in this case the spreadsheets cannot handle very complex material and energy balance equations. And also this spreadsheet actually is more suitable for maintenance and minicomputers. That is why it is of you know very tough to you know get the solution for you know very complex material energy balance in a simple computer. So in that case you have to use some you know of minicomputers no that you know minicomputers, and it cannot be you know used for this you know complex material and energy balance equations.

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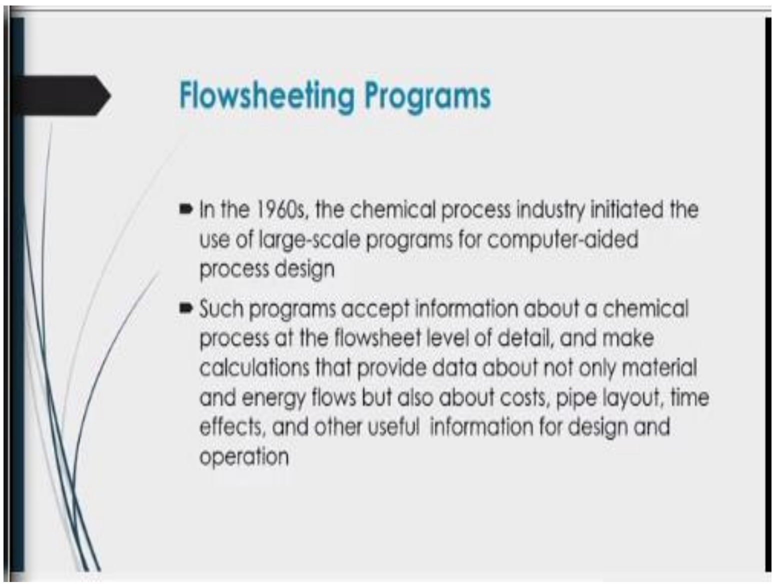

And flowsheeting programs, what is that actually in 1960s, the chemical process industry initiated the use of large scale programs for computer aided process design. And such programs accept information about a chemical process at the flowsheet level of detail and make calculations that provide data about not only material energy flows. But also about cost, even pipe layout, time, even effects and other you can say that useful information for design and operation.

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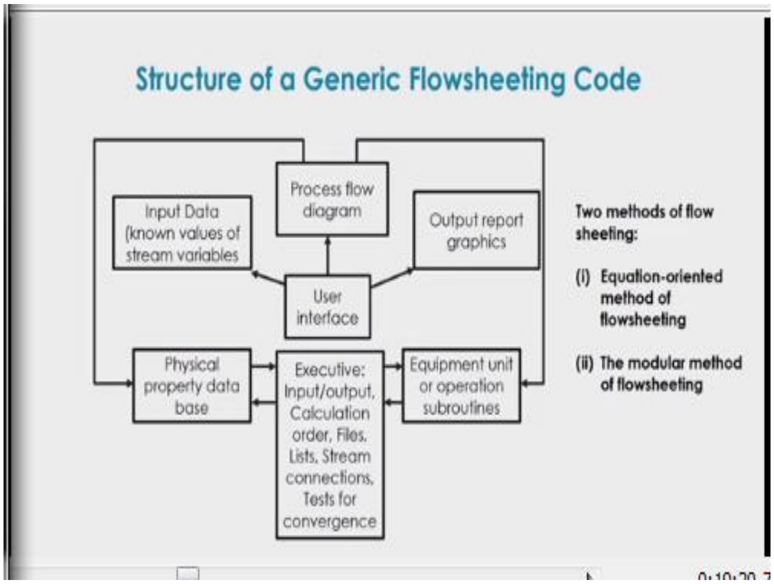

You can get the generic flowsheeting code based on that common structure like this here. If you are considering that user interface you know flowsheeting code. Then in that case you need that here input data, known values of stream variables, output report graphics and then process flow diagram. So, from this user interface you can get these 3 component and these 3 components basically based on that physical property data, and also that equipment unit or operation subroutines there.

And then you can you know interconnect this physical property data and equipment unit operation subroutines by executing that you know input and output calculations, order, files, lists, stream connection, tests for convergence like this. So, all those things will be you know incorporating here whenever you are using any physical property data for you know assessment of some equipment or process just by you know conjugating that subroutines of that you know individual equipment or process unit.

And after that you will see that based on this you can get that user interface to get that you know input data known values of stream variables. And also what would be the output report graphs there. And also process flow diagram based on which you can get that user interface incorporating with those you know of that calculation based on this subroutines of that process equipment.

Now 2 methods of flowsheeting here equation oriented method of flowsheetings are there and also modular method of flowsheetings are there. So basically under these 2 you know flowsheeting you know method you can you know do the flowsheeting codes and based on which you can solve that you know process input and output variables based on their material and energy balance equation.

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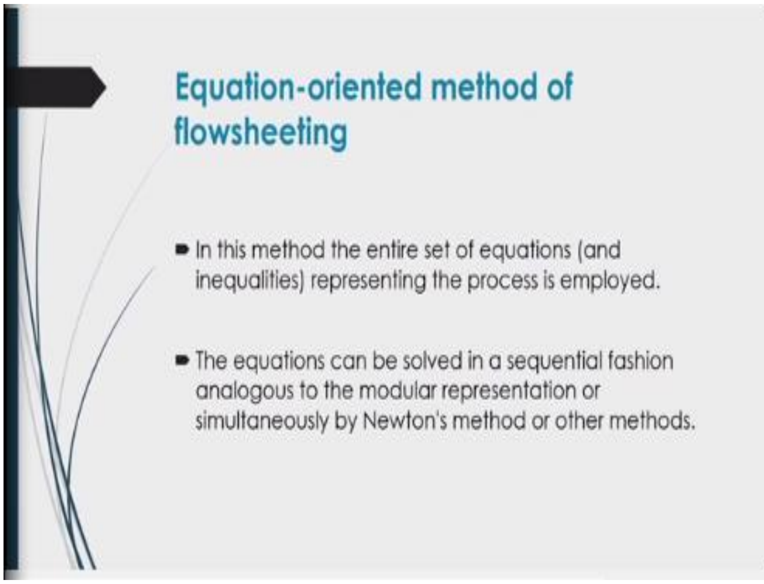

Now what is that equation oriented method of flowsheeting, you will see that in this case you know of the entire set of equations and inequalities that representing the process which is employed there. And the equations can be solved in a you know sequential fashion which will be analogous to the modular representation or simultaneously by Newton's methods or other methods.

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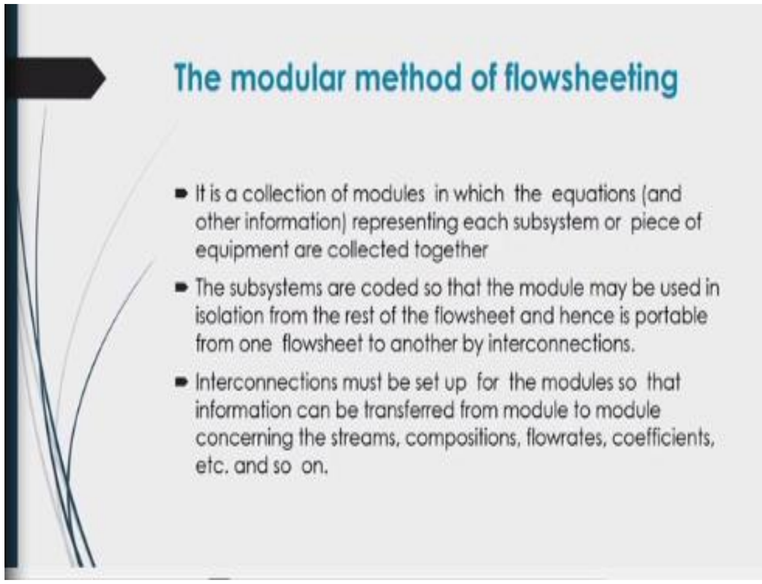

The modular method of flowsheeting is basically it is a collection of modules in which the equations and other information representing is a subsystems or piece of equipment are you know collected together. And the subsystems are coded, so that the module may be used in you know that isolation from the rest of the flowsheet and also it can be used as a you know portable from one flowsheet to you know another by interconnecting the streams there.

Now, interconnections must be you know set up for the module, so that information can be you know transferred from module to module and concerning the streams, compositions flowrates, coefficients etc and so on. So basically here in this case, there should be some modules this modular method of flowsheeting there. And in that case that modules basically subsystems will be there and those the subsystems as a module will be interconnected.

And that interconnections will be in such way that information can be you know transfer from one module to another module. And in that case you have to incorporate that information of the test streams, compositions, flowrates, coefficients etc. there.

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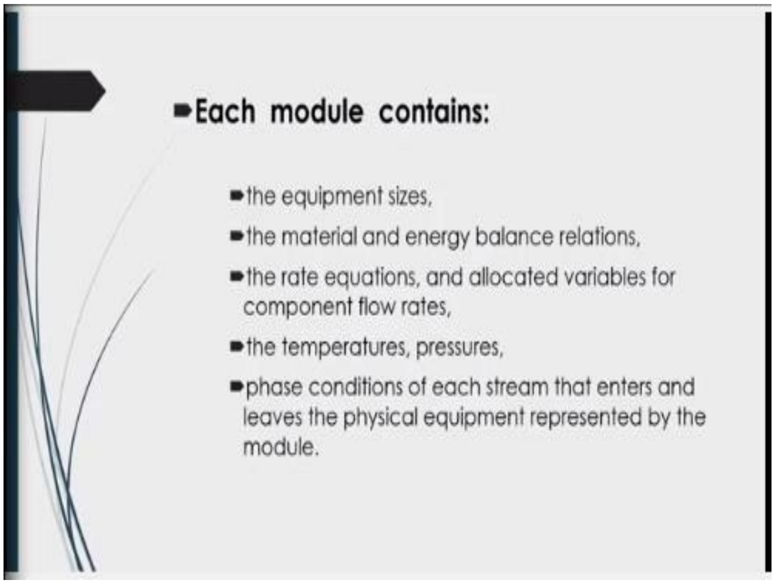

And each module will contents that you know equipment size, the material energy balance equations, even rate equations when you will see that what are the allocated variables for that component flowrates that also will be there. And the temperature and pressures that is called thermodynamic variables. The phase conditions whether you know that at a particular condition whether page will be that is converting into you know solid to you know liquid or liquid to solid or liquid to vapor like that.

So, in that case that phase conditions of the each stream that enters and leaves the physical equipment that will be you know represented in the module. So that is why the each module to be you know well arranged by this information, so that these informations would be you know transferred from one module to another module. Now other ways also you can analyze this module based flowsheeting.

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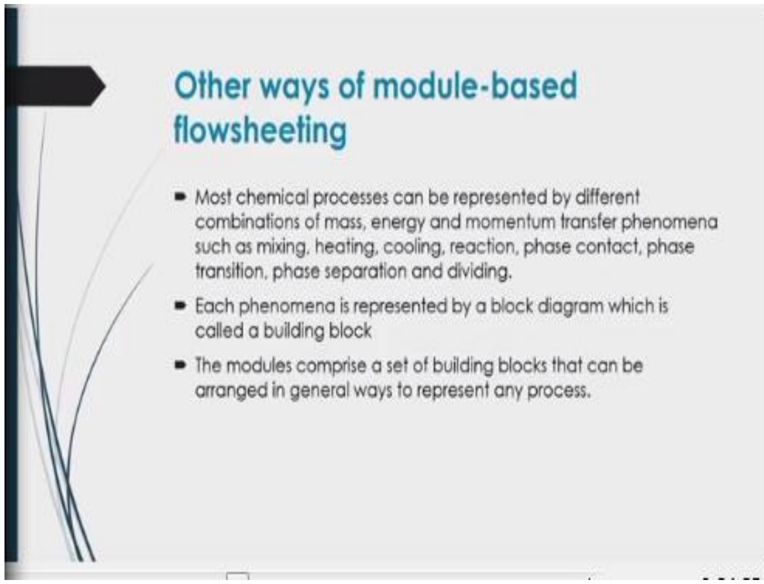

In that case you know that most chemical processes can be represented by different combination of you know that mass, energy and momentum transfer phenomena. Like you know that mixing, heating, cooling, even reaction, phase contract you know that phase transition, phase separation and also you can say that dividing up the streams like this. So, these are some you know phenomena based on which you can make a block diagram.

And based on this block diagram you can arrange this module and then you can you know assess that you know module and also you can solve that module by is particular module based codes.

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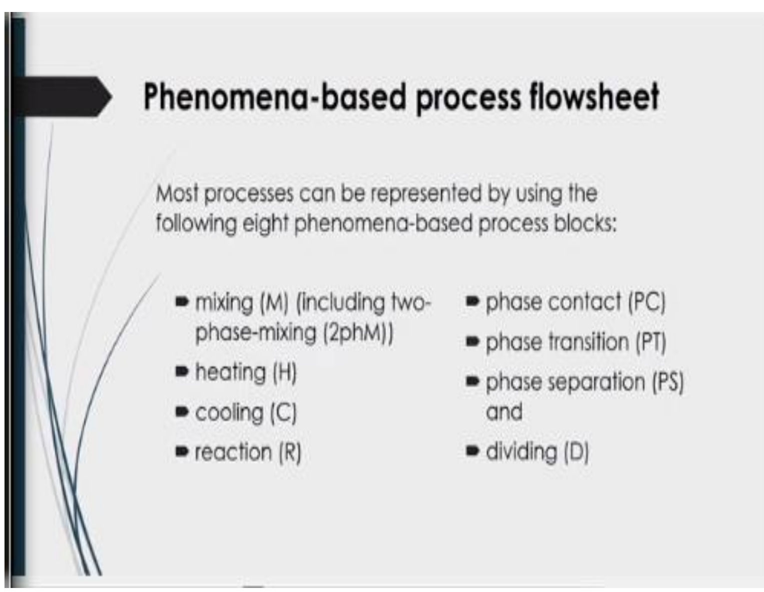

And this you know phenomena based process flowsheet, in that case most process can be you know represented by using the following 8 phenomena based process blocks. Like this you know mixing here including 2 phase mixing, even 3 phase mixing also be there if there is a multi phase flow systems in your chemical processes. Even heating one should be one module there or you can see that blocks.

And cooling reaction like phase contact, phase transition, phase separation and dividing. These are the you know different 8 phenomena based process blocks which are being you know incorporated to solve those you know linear and nonlinear set of equations that is based on your process problems. And also you can you know optimize those process based on this you know different you know phenomena based process blocks.

And then computers actually no computer codes are or you can say that phenomena based flowsheeting codes can be made based on these you know phenomena based process blocks.

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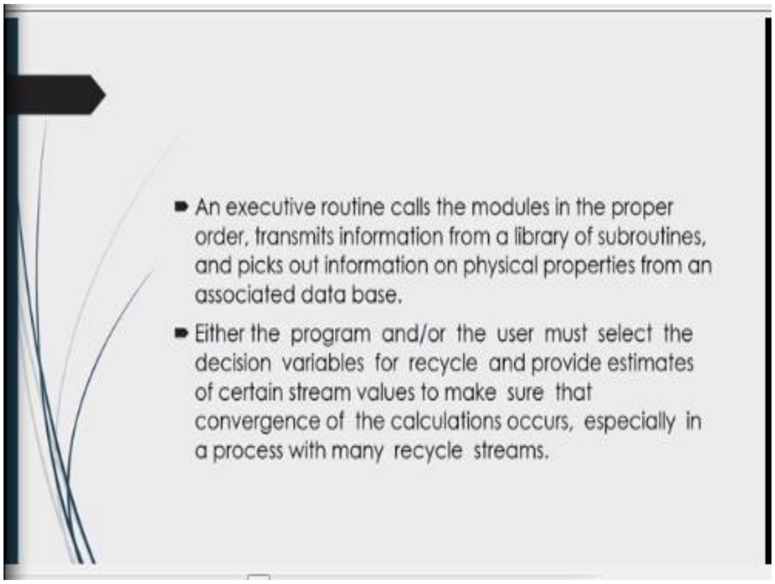

Now, an executive routine calls the modules in the you know proper order transmits information from a library of subroutines and picks out information on physical properties from an associated database. So if you have that data of that streams and modules or you can say phenomena based blocks from those you know associated database you can you know make a you know routine or programs.

And based on which you can transmits that information from a library of subroutines and picks out information on physical properties from the associated data and then execution of the of you know codes to solve that equations. Now either the program and or the user must select the decision variables to solve those for recycle and provide estimates of you know certain stream values to make sure that convergence of the calculations will be occurs.

Especially in a process with many recycled streams will be there. So it is very important, so interconnections of those information whenever you are using you know the process with recycled streams it would be required. Because in that case the informations from one output will be you know connected to the another input of another you know process unit.

So, in that case all the informations to be you know wisely you know selected and also what should be the you know of decision variables for that recycle or you know you can say that how that you know decision variables will be you know making that conversions of that calculation there. And it is important and it the code should be you know written in such a way that there will be some convergence of that you know solution whenever you are considering that transferring of that information from module to module.

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Now typical course that are used to execute that flowsheeting here given in the slides like ASPENPLUS you know CAPES CHESS, CONCEPT, even PROCESS you know SIMMOD SPEEDUP, even SYMBOL. These are some you know commonly used that codes to execute the flowsheeting calculations there.

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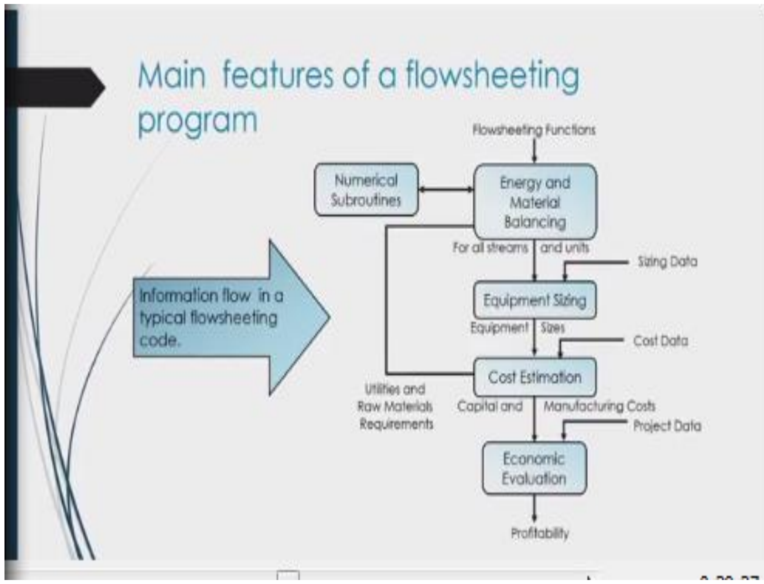

Main features of the flowsheeting program is that here given that information flow in a typical flowsheeting code is given here. Like flowsheeting functions that you have to first decide and then you have to do the manager and material balance equation and select those equations and write that equations there. And then it will be connected to that numerical subroutines, so that you can solve this energy and material balance equations.

For all the streams and unit is that you have to do this here and then sizing data to be incorporated for that equipment sizing. And then you know that cost data also to be you know incorporated for this cost estimation after that equipment sizing. All these you know energy balance equation when material balance equation, and then equipment sizing, and then cost estimation are interconnected with link information there.

And then after that you have to analyze that economic there, so that this process know that economically viable or not and then you have to analyze the profitability. So all for this finally this you know our feasibility of that process whether it will be economic or not based on that you know energy and material balance equation. Now you have to solve that energy and material balance equation sand for that you have to use some numerical subroutines.

And after solving those also you have to you know incorporate that equipment sizing, analyze that equipment sizing based on that sizing data. And then cost estimation based on that cost of data and then you know evaluation of the feasibility of that process based on that data. Now in this way you can say that how that you know flowsheeting programs can be made based on that you know raw materials data and also other informative of this process.

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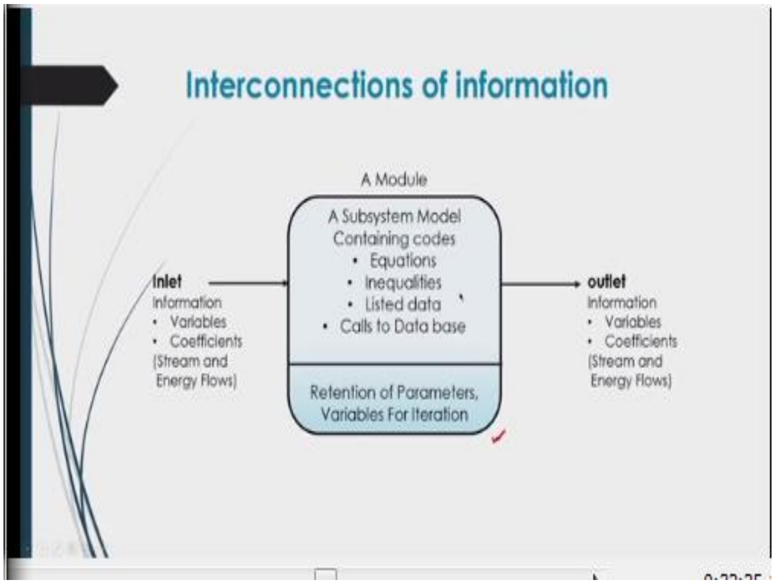

Interconnections of the information how it can be done, suppose there is a module here, so in that case some says subsystem module will be there. So, you have to use some you know subsystem model that contains equations, inequalities, you know listed data, calls of database. And then you know that you have to you know, know that inlet information there, what will be the variables, what will be the coefficient, what will be the streams and energy flows there.

In the outlet also that information should be there, variables coefficient streams and energy flows. Now this inlet and outlet will be interconnecting by this you know subsystem model and with those equations inequalities and listed data.

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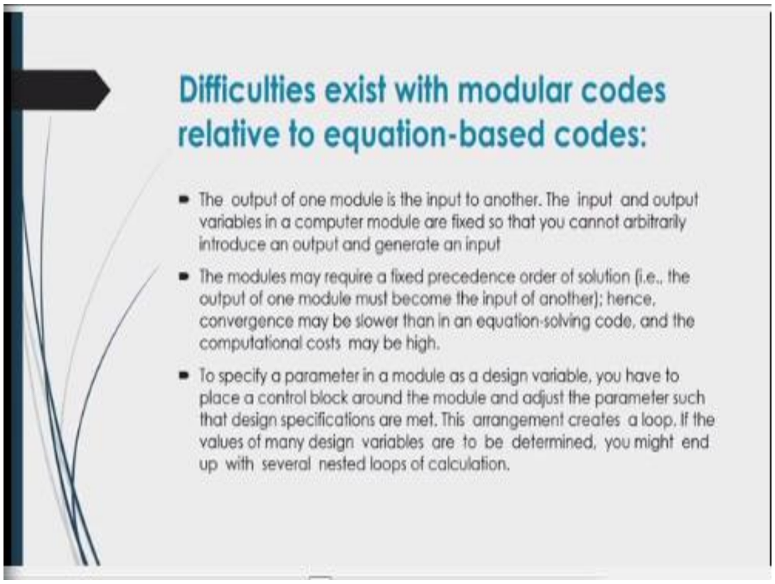

Of course you will see them some difficulties will be there with modular codes relative to equation based codes there. Now the output of one module is the input to another here in this case basically for modular based codes. The input and output variables in a computer module are fixed, so that you cannot arbitrarily introduce an output and generate an input.

The modules may require a fixed you know precedence order of solution that is the output of one module must become the input of another in this case. Hence convergence may be slower than in an equation solving code and the computational cost maybe high in that case. Now to specify a parameter in a module as a design variable you have to you know place a you know control you know block around the module.

And adjust the parameter such that design specification will be met there. And this arrangement of course will be creates a loop and in that case if the values of many design variables are to be determined, you have to you know end up with several you know nested loops of that calculation.

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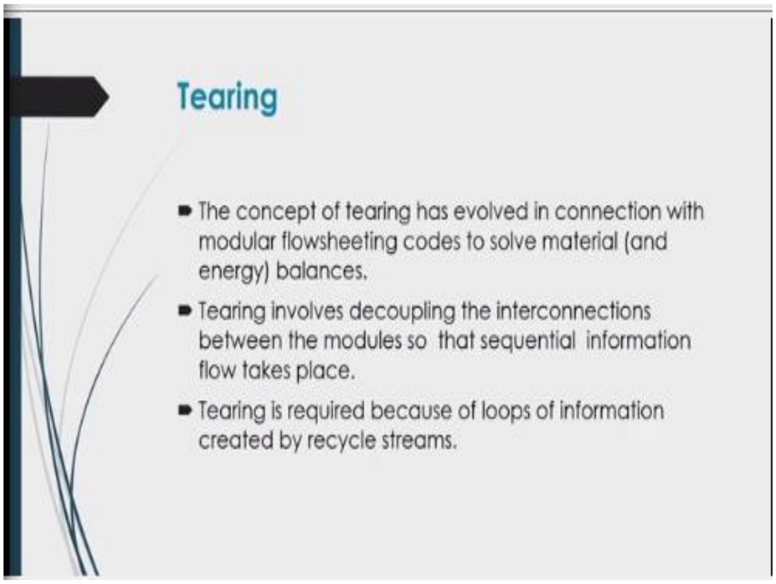

Now the concept of tearing is one important you know phenomena who is involved in connection with the modular flowsheeting codes to solve material and energy balance equation. In that case tearing will be involves for the decoupling the interconnections between the modules. So that you know sequential information flow takes place and also it is required because of loops of information created by you know recycle streams.

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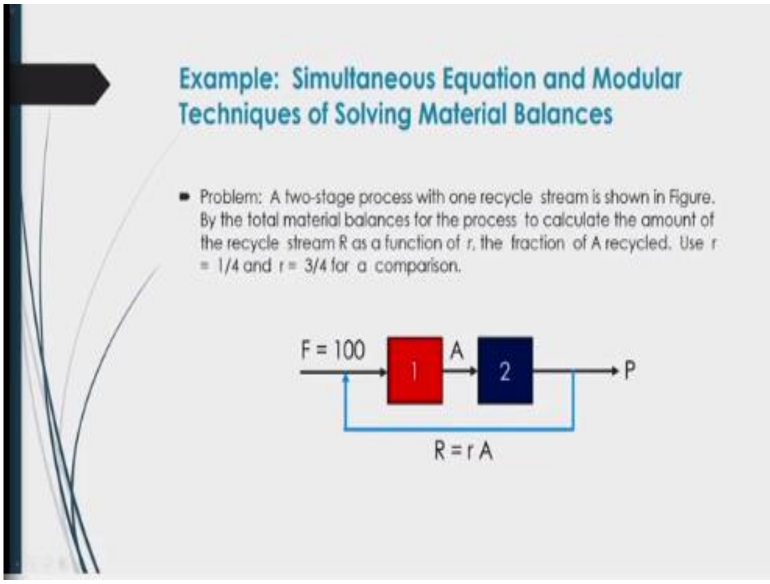

Now, let us have an example for this simultaneous equation and modular techniques of solving material balances. Now suppose a 2 step process with 1 recycle stream is shown in figure by the total material balances for the process to calculate the amount of the recycle stream r as a function of small r here. Now the fraction of a recycled use r = 1 by 4 and r = 3 by 4 for a comparison.

Now in this case you have to calculate the amount of the recycle stream r as a function of small r here. Now see here there are 2 models 1 and 2, 2 stage process here, so from this second stage there will be some recycle amount. Now that recycle amount will be you know that some fractions of this output of this process 1. So in that case you have to find out the what will be the amount of that recycled streams r as a function in that case.

And also you have to calculate that the fraction of A that is recycled, now in this case you can consider that fraction of A recycled is r = 1 by 4 and r = 3 by 4 for a comparison.

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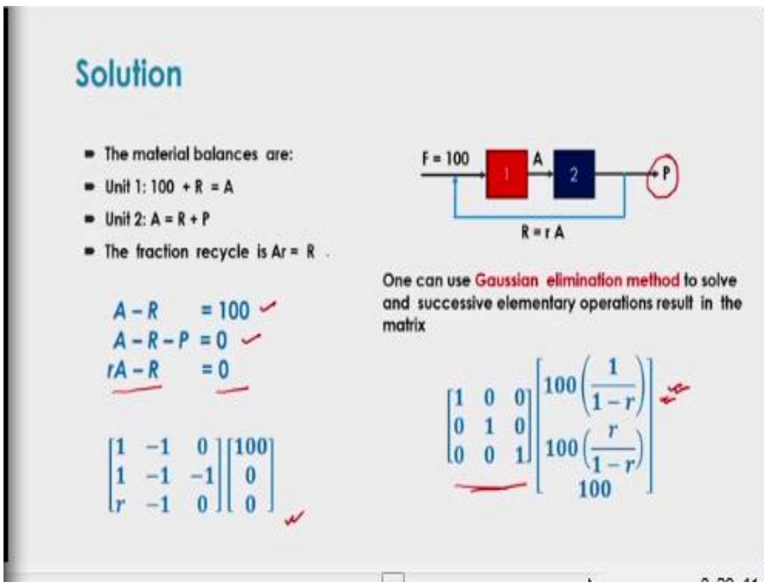

Now in this case if I considered that the material balance here for the unit 1 that will be 100 + R that will be is equal to A. And for unit 2 that material balance will be balance A will be equals to R + P. And the fraction recycled will be is equal to Ar that will equals to R. Now in this case if we write that you know linear equation set here. Like here we can write A – R will be equals to 100 and then A - R – P will be equals to 0 as per that unit 2.

And then from this rA - R that will be equals to 0, so these are 3 questions you can write. And if we express this linear set of equations as a matrix forms, we can write this matrix form here, 1 –

1 0 1 - 1 – 1 r – 1 0 100 00 here. Here this 1 1 1 these are basically the coefficients of that you know streams here of R A P like this. Then one can use Gaussian elimination method to solve and successive elementary operations that results in the matrix.

Like this here we can you know use this Gaussian elimination method and finally we can write these results as a matrix here. Like this here in this case 1 0 0 0 1 0 1 0001 you have to make like this as for Gaussian elimination method. And accordingly what will be this you know matrix of this write part of this you know formulation then it will be 100 into 1 by 1 - r 100 into r by 1 – r 100 like this.

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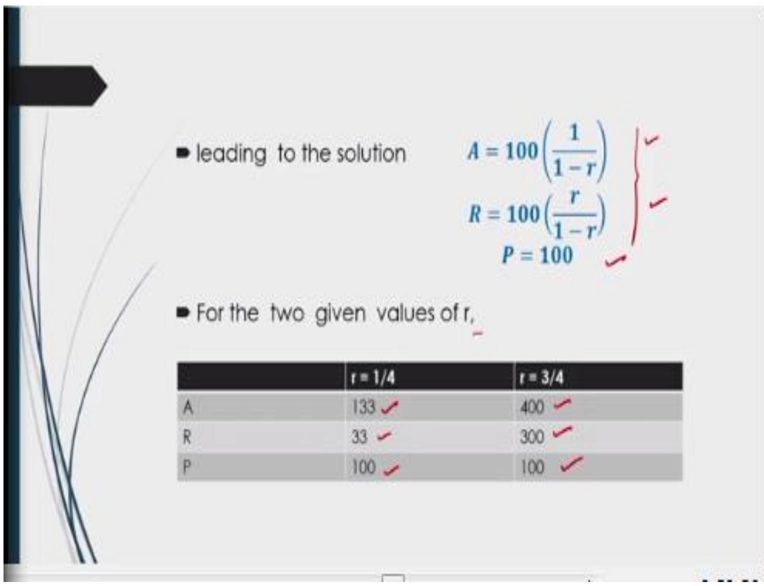

	r = 1/4	r = 3/4
A	133	400
R	33	300
P	100	100

So after that to get the solution what you can say that resolving this we can simply say that here A will be equals to here 100 into 1 by 1 – r.

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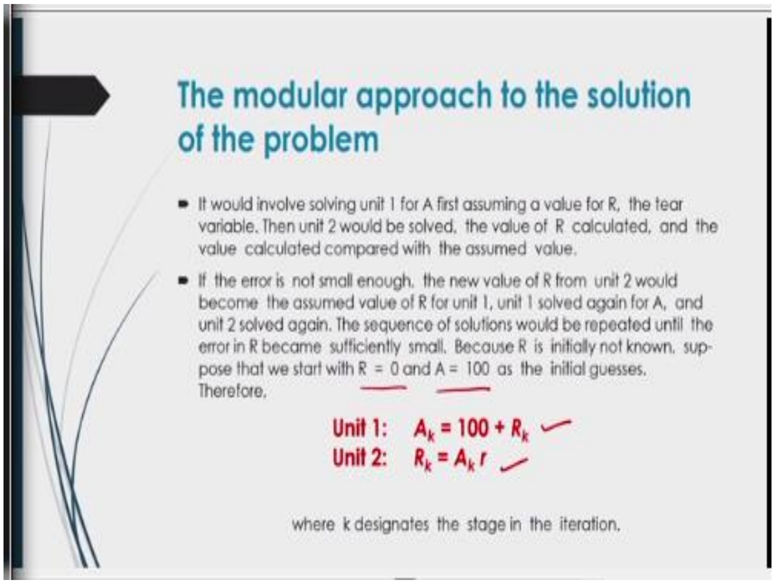

So here and then we can say that R will be equals to here 100 into r divided by 1 – r whereas P, here P will be is equal to what 100 there. So in this way we can solve this equation just ask for that formation of matrix from that linear set of material balance equation. Now for the 2 given values of R what will be the value of A what will be the value of R and what will be the value of P for that streams that can be obtained here.

Now for you know A if R is equal to 1 by 4 we are getting here 133, if suppose fractions is 3 by 4 A will be is equal to 400. And for r is small r is equal to 1 by 4 it will be recycled stream will be 33. And for fractions r is equal to 3 by 4 that recycled streams will be 300. And for products we can say that for the fractions r is equal to 1 by 4 this products streams will be of 100 and similarly for that fractions of r is equal to 3 by 4 it will be 100.

So here we are getting this solution for different fractions there, but for all cases we are getting that here same value of these products which is coming as 100 here. Because as per this you will see that overall material balance which will be giving as the heat 100 will be is equal to what is that output 100 here. Another examples of this modular approach to the solution of the problems like this.

It would be involved solve the unit 1 for A first assuming a value for r, the tear variables then you need to would be solved. Now the value of R calculated and the value calculated compared to the assumed value here. If the error is not small enough the new value of R from the unit 2 would become the you know assume value of R for unit 1. And unit 1 solved again for A and you need to solve again there the sequence of solutions would be repeated until the error in R becomes sufficiently small.

Because R is initially not known, suppose that we start with R is equal to 0 here and A is equal to 100 as the initial guesses. So in that case for unit 1 we can right here A k will be equals to 100 + R k and unit 2 R k take is equal to A k into r. So based on that you know initial guess how we are getting that different values of you know A and R there based on different iterations starting with initial guess.

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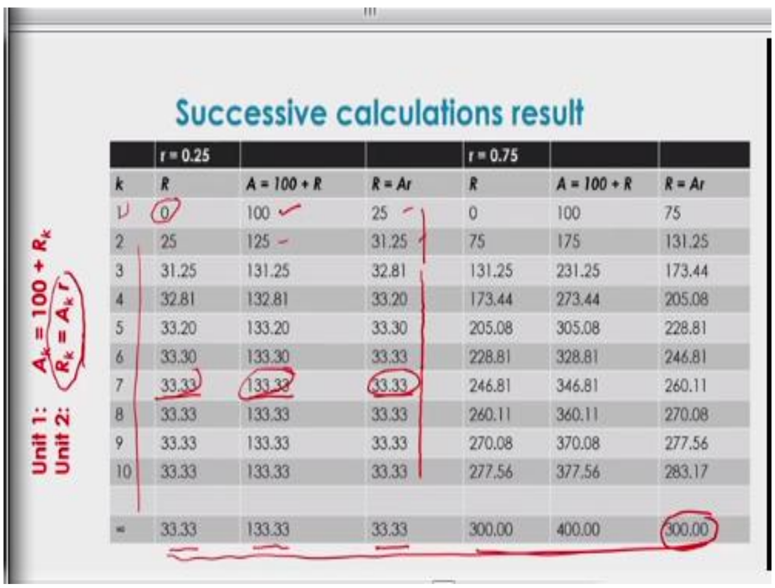

Successive calculations result

Unit 1: $A_k = 100 + R_k$

Unit 2: $R_k = A_k r$

	r = 0.25			r = 0.75		
k	R	A = 100 + R	R = Ar	R	A = 100 + R	R = Ar
1	0	100	25	0	100	75
2	25	125	31.25	75	175	131.25
3	31.25	131.25	32.81	131.25	231.25	173.44
4	32.81	132.81	33.20	173.44	273.44	205.08
5	33.20	133.20	33.30	205.08	305.08	228.81
6	33.30	133.30	33.33	228.81	328.81	246.81
7	33.33	133.33	33.33	246.81	346.81	260.11
8	33.33	133.33	33.33	260.11	360.11	270.08
9	33.33	133.33	33.33	270.08	370.08	277.56
10	33.33	133.33	33.33	277.56	377.56	283.17
∞	33.33	133.33	33.33	300.00	400.00	300.00

That is given here tabular format have of that successive calculations result. In that case if you are considering that r = 0.25 and initial case at you know first iteration here R = 0. And then A will be is equal to 100, and then for iteration 2 R is equal to you know 25, 125 it will be then, capital R is recycle will be accordingly there. So if we you know change the iteration here and changing that you know r value as per that you know this relationships.

Then we can have this you know a successive you know iterations just by guessing that initiation of the you know final value of the previous you know iterations. So, in that case finally we can get to that at R = 33.33 we are getting A is 133.33 and then capital R will be is equal to what will be that 33.33. And in this case you will see that this recycle streams are changing based on that iterations and it is changing from 25 and then 31.25 and 32.81, 33.20.

Once you will see that it will be not changing significantly, in that case we can stop that iterations there and we can select that final value of that R and respective A value and P value there. So here we are getting that this at R = 33.33 this you know the change of this R will be is equal to you know almost negligible. So, in that case we can decide that this R at this 7th iterations we are getting that final value of R and then A and then what is that capital R is equal to this.

Similarly for R = 0.75 that is 3 by 4, we can simply consider that iterations here and accordingly we can calculate. And you will see that infinite value of that you know iterations there. So we can say that there will be a you know R value of like this here where there will be no change of that you know of R value there accordingly. So, in this way we can say that just by guessing that initial guess and successively if we calculate that you know R k value.

And if you think see that there will be no sufficiently you know change of that iterations then you can stop that you know iterations and you can select that value of that particular that streams value there. So in this case since recycles we are considering that iterations based on these R value iterations value we are getting that at infinite you know iterations we are getting that almost negligible change of that R value.

So we can select that you know respective value of that R value and also respective for that stream other stream values.

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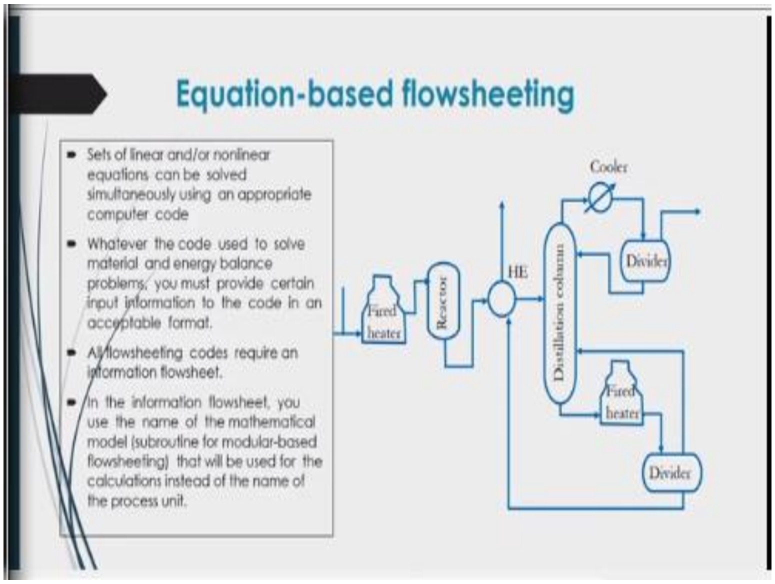

In this way we can solve this modular based approach to solve this type of problem. And equation based flowsheeting there, in that case you have to consider sets of linear and nonlinear equations which will be solved simultaneously using an appropriate computer code. Whatever the code used to solve material and energy balance problems, you must provide certain you know input information to the code in an acceptable format.

All the flowsheeting codes require an information flowsheet, like in the information flowsheet, you use the name of you know mathematical model maybe subroutine for modular based flowsheeting. That will be used for the calculations instead of name of the process unit there.

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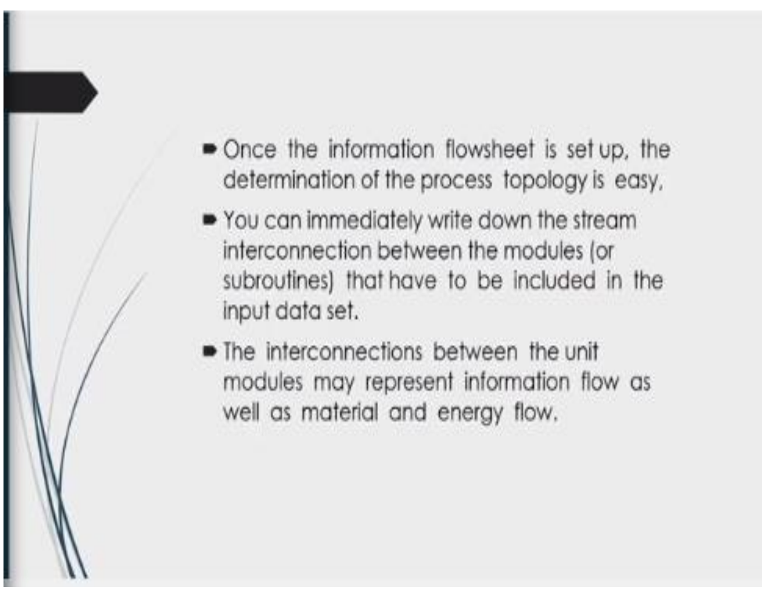

Now once the information flowsheet is set up then the determination of the process or topology will be easy. And you can immediately write down the stream interconnections between the modules or subroutines that have to be included in the input dataset. The interconnections between the unit modules may represent information flow as well as material and energy flow.

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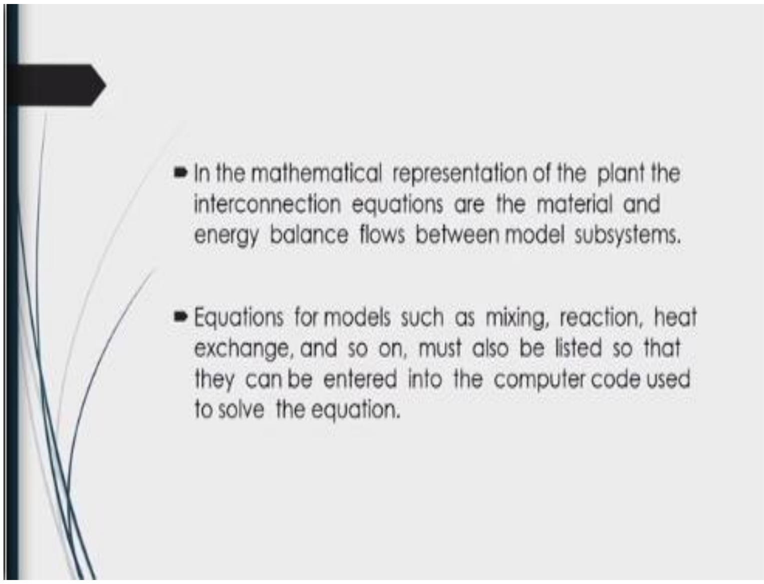

Now in the mathematical representation you will see of the plant the interconnection equations are the material energy balance flows between model you know subsystems. And equations for models such as mixing, reaction, heat exchange and so on must be listed, so that they can be entered into the computer code use to solve the equation.

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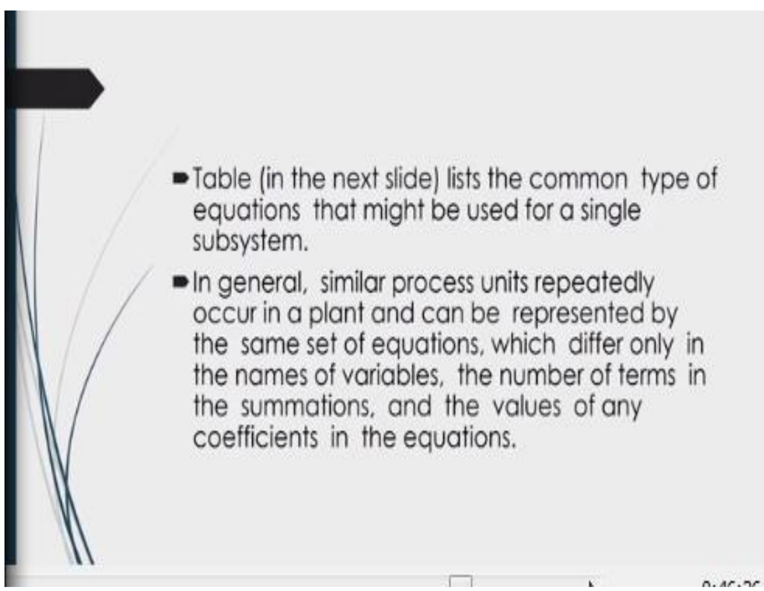

Now you will see that there will be a certain table which is shown in the next you know slides like this.

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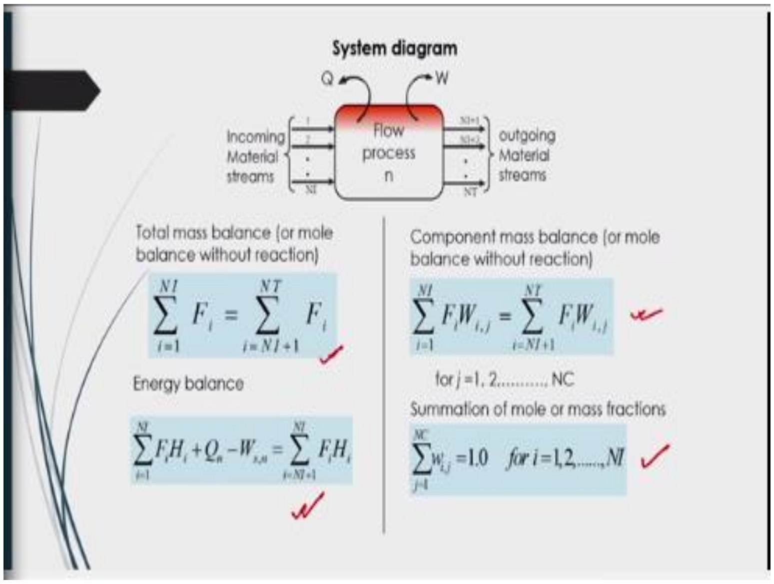

Some common type of equations that might be used for a single subsystem. In general similar process units repeatedly occur in a plant and can be represented by the same set of equations which differ only in the names of variables, the number of terms, in the summations and the values of any coefficients in the equations. Now there are several equations that are actually being used, some are you know material balance, some are you know energy balances.

Here it is given some material balance in general forms, in energy balance in general forms and component material balance also and summation of you know molar mass fractions to be there. So, for a particular flow process what will be the incoming material streams, what will be the outgoing material stream that you have to know. And based on which you have to do that material balance and energy balance and also some other equations that you have to note down.

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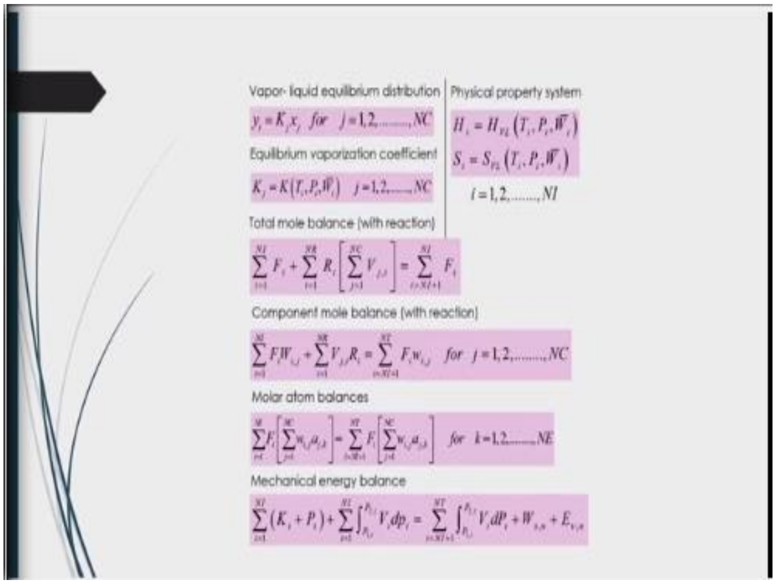

And also some other equations like you know vapor liquid equilibrium distribution is there or not, equilibrium vaporization coefficient or not how it will be related. And total mole balance, total you know component mole balance, molar atom balances, mechanical energy balance, all those equations to be incorporated there in equation based flowsheeting.

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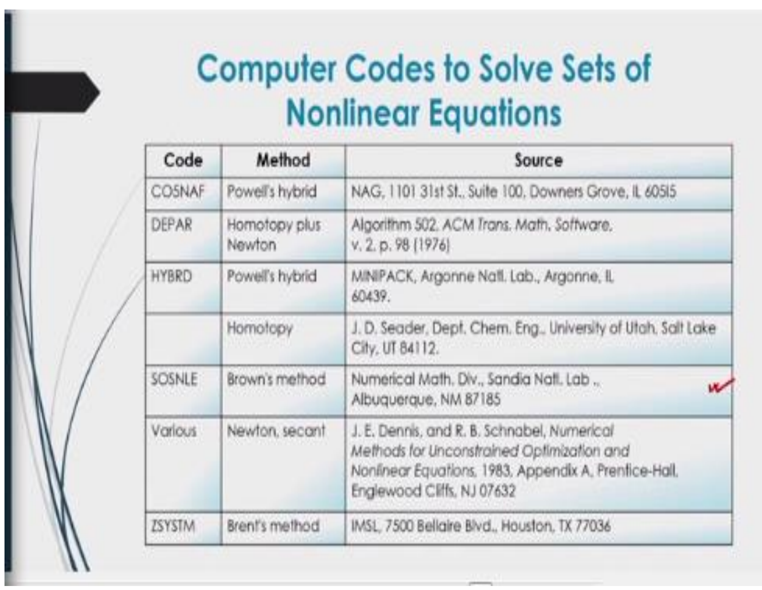

Code	Method	Source
C05NAF	Powell's hybrid	NAG, 1101 31st St., Suite 100, Downers Grove, IL 60515
DEPAR	Homotopy plus Newton	Algorithm 502, ACM Trans. Math. Software, v. 2, p. 98 (1976)
HYBRD	Powell's hybrid	MINPACK, Argonne Natl. Lab., Argonne, IL 60439.
	Homotopy	J. D. Seader, Dept. Chem. Eng., University of Utah, Salt Lake City, UT 84112.
SOSNLE	Brown's method	Numerical Math. Div., Sandia Natl. Lab., Albuquerque, NM 87185
Various	Newton, secant	J. E. Dennis, and R. B. Schnabel, *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, 1983, Appendix A, Prentice-Hall, Englewood Cliffs, NJ 07632
ZSYSTM	Brent's method	IMSL, 7500 Bellaire Blvd., Houston, TX 77036

Now, what are the general computer codes to solve the sets of nonlinear equations, there are several you know codes that are available thereof they are like this. Here in this slides it is shown here like Co5NAF in a deeper you know HYBRD SOSNLE and Various even you will see that ZSYSTM, these are the some you know, popular codes that are being used for solve the set of nonlinear equation.

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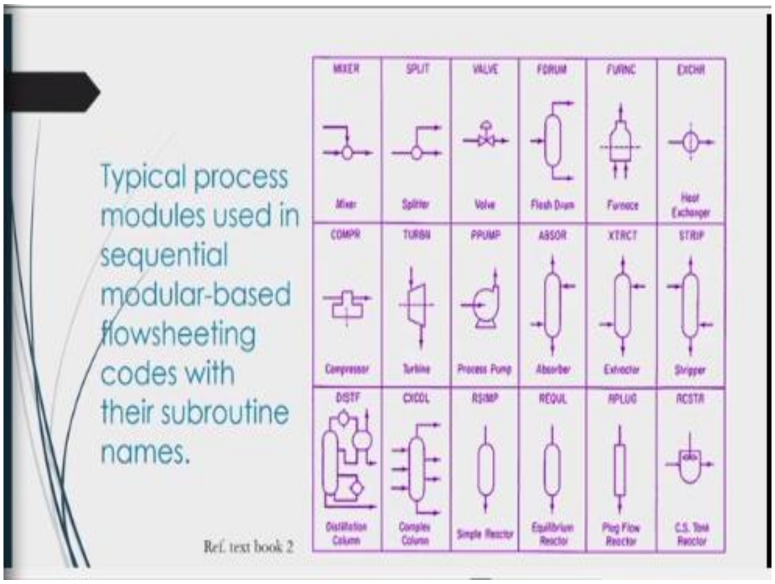

Typical process modules are given in the slides here in sequential modular base flowsheeting codes with their subroutine names here like mixer you know splitter, valve even flash drum when you will see that are furnace, exchanger even compressor, turbine, process pump, absorber, extractor, striper. These are you know commonly used chemical engineering process module there also distillation column, complex column there, simple reactor, equilibrium reactor, you can say that plug flow reactors, CSTR like this.

So these are the common you know process modules that is being used in chemical engineering process. And based on this there are you know flowsheeting codes are available with their subroutines names.

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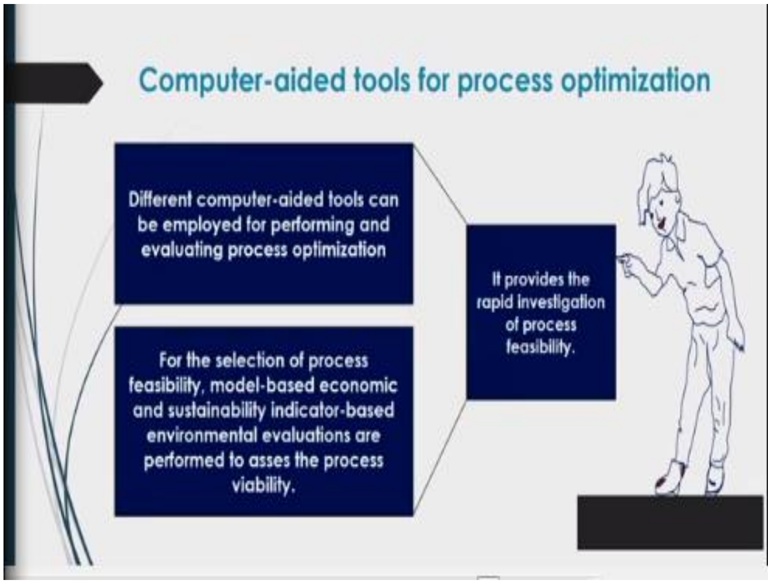

Now computer aided tools for this process optimization is also important there after you know of solving those equations and then you have to optimize also with a certain constants there. Now, different computer aided tools can be employed for performing and evaluating process that optimization. Now for the selection of process feasibility, model based economic and sustainability, indicator based, environmental you know evaluations are perform to assess the process viability. Now it provides the rapid investigation of the process you know feasibility.

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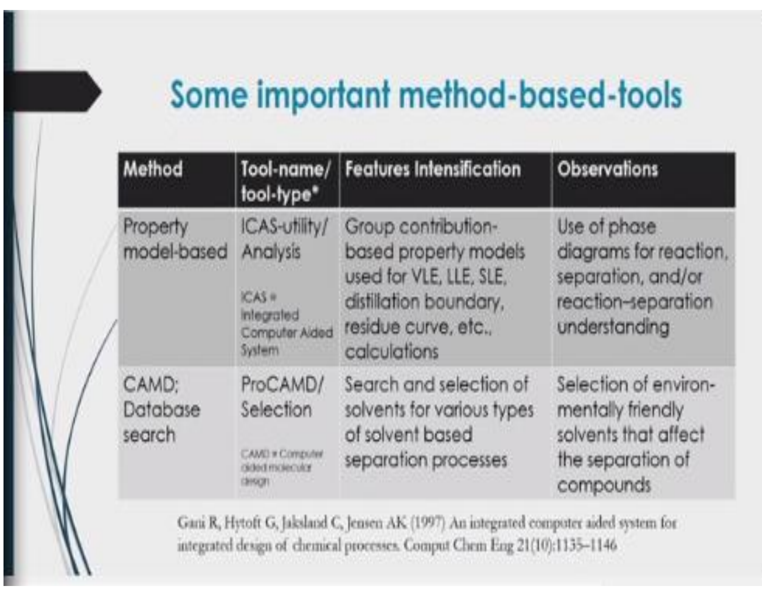

So, in that case you have to use some method based tools there, there are several methods are available and based on which respective tools also are available to you know assets that optimization problems. Now some methods like you know property model based methods there.

And based on that property model there are some tools are available like it is called ICAS utility tools or analysis tools.

Here ICAS it is called integrated computer aided systems there, they are you will see that group contribution, based property models used for you know vapor liquid equilibrium, liquid-liquid equilibrium and solid liquid equilibrium even you know distillation boundary, residue curve etc. For those things you know to analyze this you know codes are being used. Now, it is generally used for you know, phase diagrams for reaction separation and reaction separation process like this.

Like CAMD database search also one method based on which you know proCAMD or selection, computer aided tools of each you know developed. And in that case you will see that based on these CAMD tools you can you know search and you know select the solvents for various types of solvent based separation processes. And in this case the selection of environmentally friendly solvents that affect the separation of the compounds.

That is why you have to select that suitable solvents and various types of solvent which is useful for the separation process.

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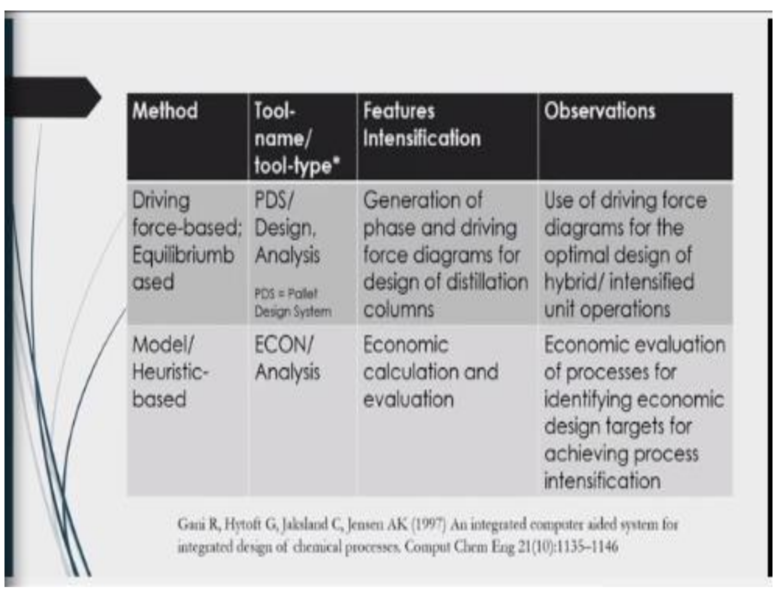

Method	Tool-name/ tool-type*	Features Intensification	Observations
Driving force-based; Equilibriumb ased	PDS/ Design, Analysis PDS = Pallet Design System	Generation of phase and driving force diagrams for design of distillation columns	Use of driving force diagrams for the optimal design of hybrid/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

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

Another important method like driving force based equilibrium of you know based methods. They are computer you know tools or they are like here PDS you know design analysis tools are there, generation of phase and driving force diagrams for the design of distillation column it is being used. And in that case how to use that driving force diagrams for the optimal design of the hybrid and intensified unit operations there.

Other tools like you know model heuristic based tools there, it is called ECON in that case economic calculation and evolution is being done based on this ECON.

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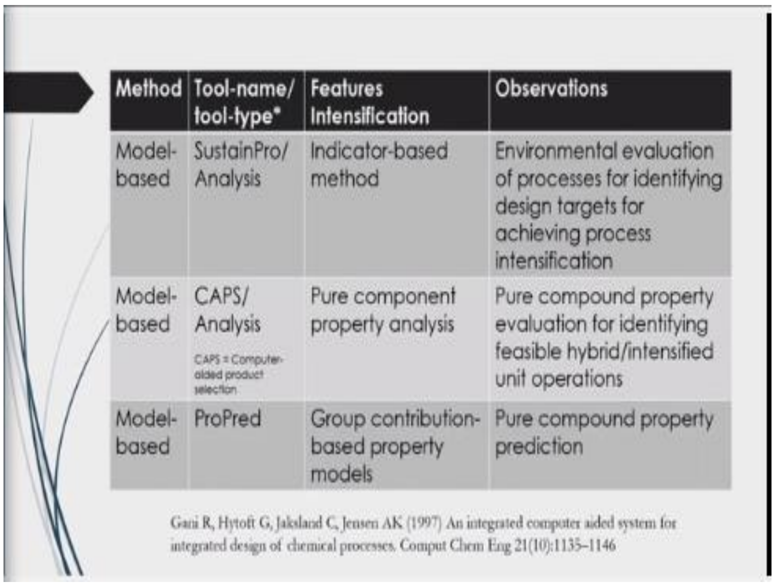

Method	Tool-name/ tool-type*	Features Intensification	Observations
Model-based	SustainPro/ Analysis	Indicator-based method	Environmental evaluation of processes for identifying design targets for achieving process intensification
Model-based	CAPS/ Analysis CAPS = Computer-aided product selection	Pure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

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

Other like model based here like this SustainPro or analysis it is generally used for you know environmental evaluation of process for identifying design targets for achieving process intensification. Another important model based it is called ProPred, this is generally being used for pure component property prediction. So for that particular process how to predict that property of that compound based on this tool.

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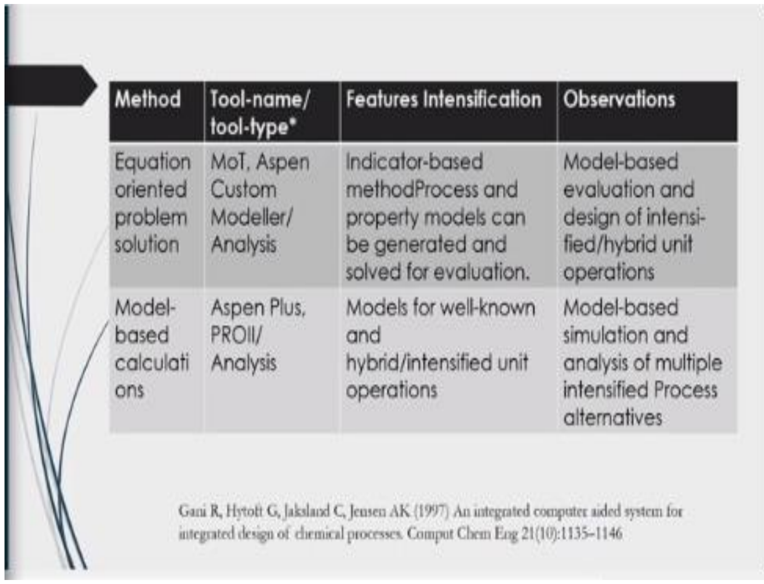

Method	Tool-name/ tool-type*	Features Intensification	Observations
Equation oriented problem solution	MoT, Aspen Custom Modeller/ Analysis	Indicator-based methodProcess and property models can be generated and solved for evaluation.	Model-based evaluation and design of intensi-fied/hybrid unit operations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

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

Equation oriented problem solution tool also available like Aspen, Custom Modeller there. In that case model based evaluation and design of intensified or hybrid unit operations are being done based on this tool. Even model based calculations also one method, in that case the tool is Aspen Plus or ProII there. And based on this you know tools you can assess the model based simulation and analysis of multiple intensified process alternatives.

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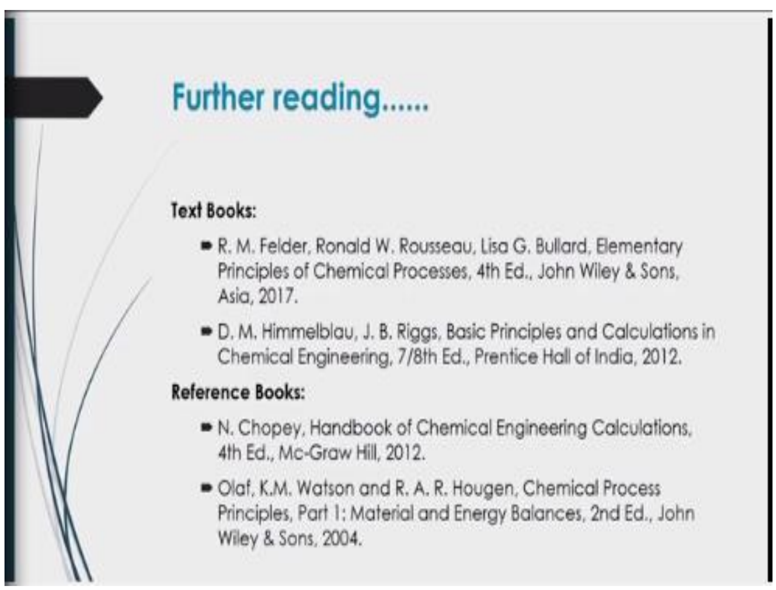

We have described the different aspects of that flowsheeting, even modular based flowsheeting and also equation based flowsheeting. And also how to you know solve that equation based flowsheeting, based on that codes. And also what are the other different computer based flowsheeting codes are available it is shown here. So these are very basic and fundamentals of this flowsheetings.

And further understanding of this you know flowsheeting codes there, you have to you know do another course for this you know optimization course where you can learn different codes by which you can solve that you know optimization problem based on that different tools and how it can be done it is the there. So this you know course only this much of scope is there to learn.

And I think it will be helpful for further understanding of the you know optimization problem based on these different codes, so it will be helpful for you. I would suggest you to go further for basic of this you know flowsheeting things from this you know textbooks . It will be you know more informative for you there.

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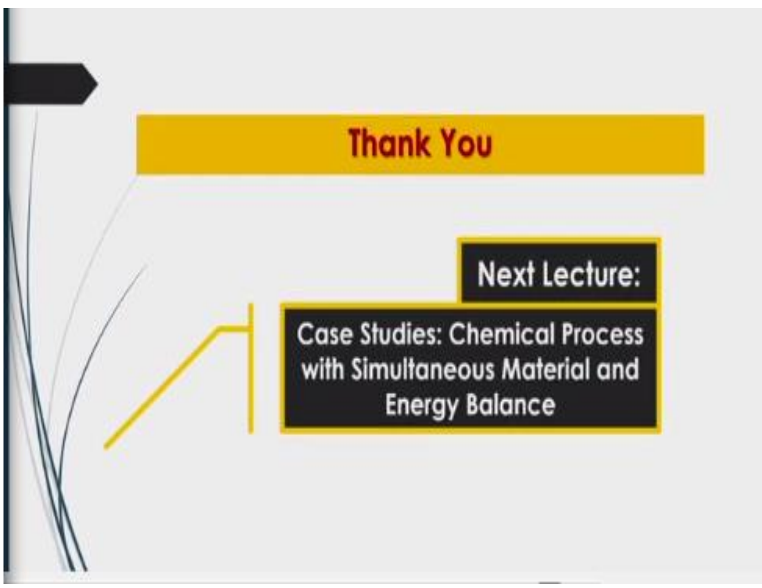

And in the next module we will try to you know discuss the case studies of chemical processes with simultaneous material energy balance equations. So, whatever we have learned till now that energy balance equation, material balance equation, even how to solve the equations they are. So, based on which we will describe one you know industrial process with multiple units, the complete processes.

And we will show that how to do that material balance and energy balance and based on which you will be able to understand that complete set of chemical process and it is material and energy balance. So thank you for giving your attention here.