Advanced Mathematical Techniques in Chemical Engineering

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Lecture No. # 08
Matrix, Determinant

Well, in this class, we will be looking into one more example of contraction mapping, then we will seal the topic and move over to the next topic that is the matrix and determinants.

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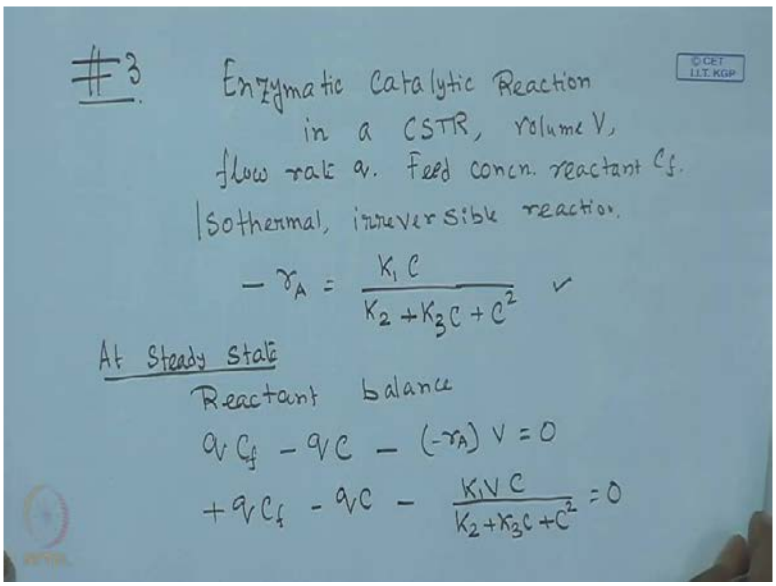

So, the third example on contraction mapping that we are looking into this class is that again we will be considering enzymatic catalytic reaction; reaction occurring in a C S T R, with volume V, flow rate q. Feed concentration of reactant as earlier is C f, again it is an isothermal, irreversible reaction, but the rate constant is different in this problem, the rate expression is different in this problem. The rate expression is given as K 1 times C divided by K 2 plus K 3 C plus C square; this is the rate expression.

At the steady state, again we proceed the same way as we have done in the earlier problems. We write down the reactant balance in the C S T R, so it will be q time's C f minus q time's c minus minus rate of reactant A times volume, is equal to 0. At the steady state, rate of accumulation is 0, is the net mass that is coming into the system, net mass per unit time going out to the system and the amount of material of reactant that is consumed in the reactant volume per unit time. So, we write down the expression of r a there, so it becomes plus q c f minus q c minus K 1 V times C divided by K 2 plus K 3 C plus C square must be equal to 0.

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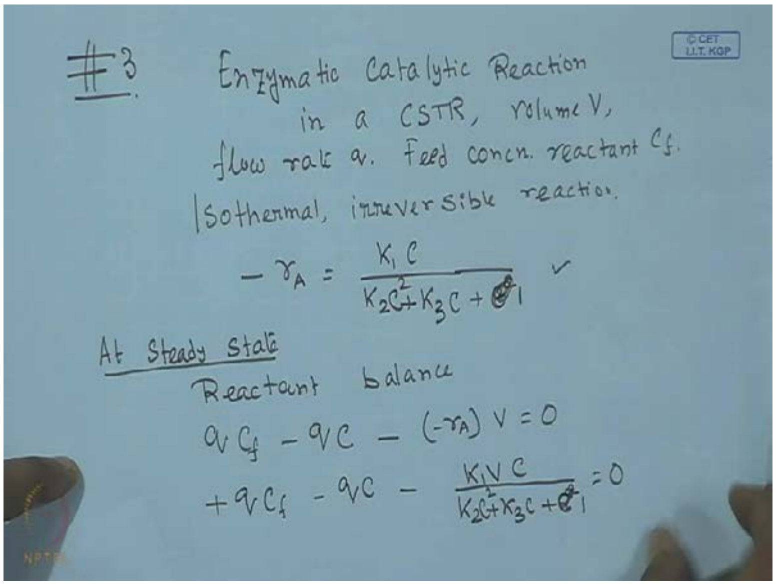

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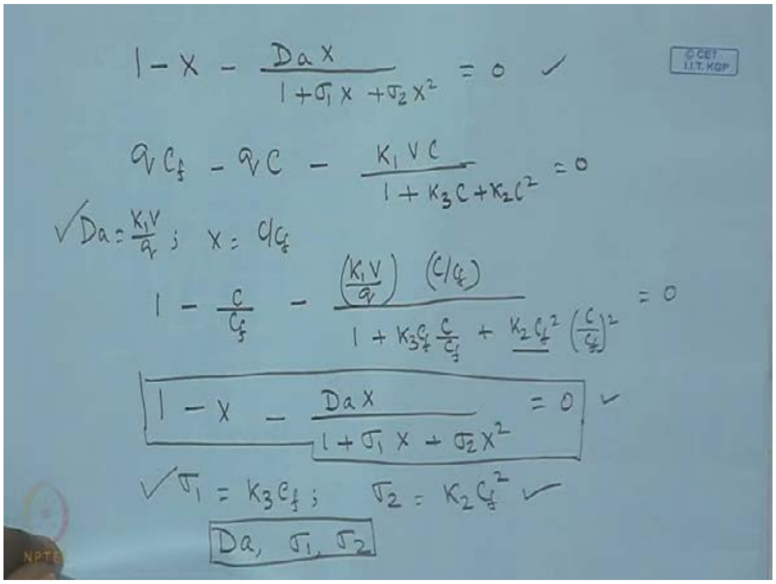

Again, we were non-dimensionalize the governing equation, after non-dimensionalization, we will be getting 1 minus x minus Da times x divided by 1 plus sigma 1 x plus sigma 2 x square is equal to 0. The rate expression is slightly different, we put it as k 1 C K 2 C square plus K 3 C plus 1, So K 2 C square plus K 3 C plus 1 and it is basically 1 plus K 3 C plus K 2 C square. If you write down the governing equation, then this becomes q C f. I am just reading the whole thing for you, minus q c minus K 1 V C divided by 1 plus K 3 C plus K 2 C square is equal to 0. Make it non dimensional, we define x is equal to c by C f, so divided by q and C f, this becomes 1, minus c by C f minus K 1 V divided by q, it is also divided by C f, this becomes c by C f, the dimensionless concentration. Then, we make these things also non-dimensional, so 1 plus K 3 C by C f plus into C f , this will be K 2 C f square c by C f square that will be equal to 0, put x is equal to c by C f, damkohler number is equal to K 1 V over q.

In the non-dimensional form, this equation becomes 1 minus x minus damkohler times x divided by 1 plus - we call this as sigma 1 x plus this is sigma 2 x square is equal to 0. So, we get the - we land up to the same equation, where sigma 1 the non-dimensional parameter sigma 1 is K 3 times C f and sigma 2 is nothing but K 2 time C f square.

Therefore, we have three parameters in this system Da, sigma 1 and sigma 2. All of them are non-dimensional, the definitions are Da definition of damkohler number, is K 1 V by q.

Definition of sigma 1 is K 3 times C f and sigma 2 is K 2 times C f square. So, we must be having - we are looking for a relationship between these three parameter Da, sigma 1 and sigma 2, so that there will be existence of a unique steady state to this particular problem.

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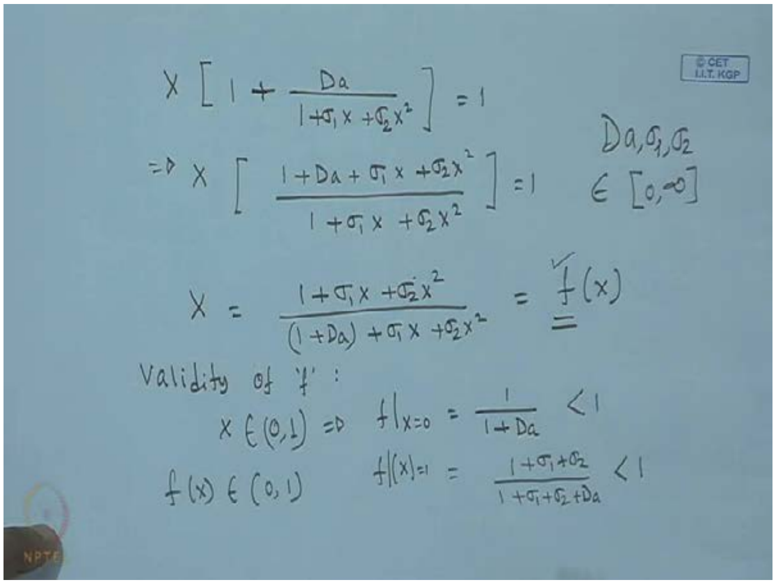

This is our governing equation, we are going to cast this equation in the form of x is equal to f x. Like the previous problem, we rearrange that equation, we will be getting x 1 plus Da 1 plus sigma 1 x plus sigma 2 x square is equal to 1. So, x 1 plus Da plus sigma 1 x plus sigma 2 x square divided by 1 plus sigma 1 x plus sigma 2 x square that should be equal to 1. So, x is equal to 1 plus sigma 1 x plus sigma 2 x square divided by 1 plus Da plus sigma 1 x plus sigma 2 x square. This is the form, x is equal to f x, where f x is given by this expression. If we look into the validity of this map f, so let us check the validity of map f. x lying in between 0 and 1, let us put the minimum value of x as 0, so f at x is equal to 0 becomes 1 divided by 1 plus damkohler number. All these three parameters Da, sigma 1 and sigma 2, they are lying between the positive real half plane.

So, 1 by 1 plus Da is always less than 1, f evaluated at x is equal to 1 will be 1 plus sigma 1 plus sigma 2 divided by 1 plus sigma 1 plus sigma 2 plus Da, since Da is a positive real number, so denominator is always greater than numerator, so this will be always less than 1.

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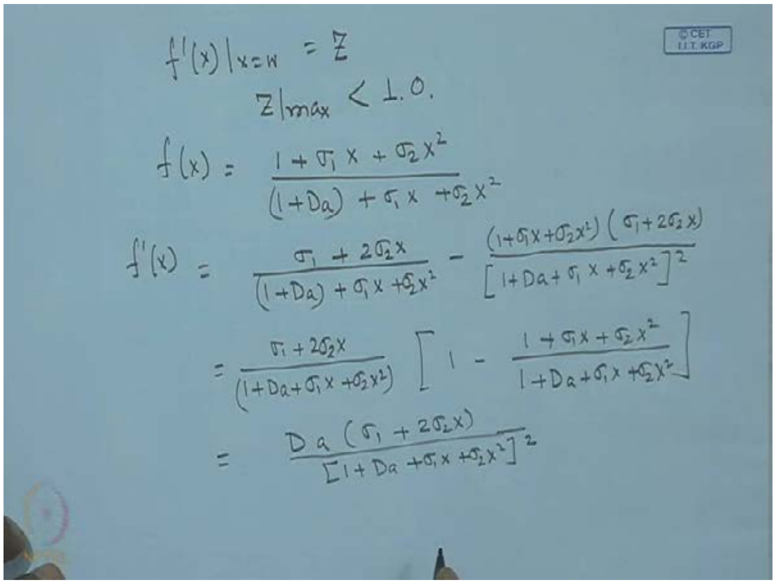

f x is also lying in the domain 0 to 1, therefore choice of this map is appropriate and this map has every quality to be a contraction map. Then, we look into the next steps, you have to evaluate a prime x at x is equal to w, we term that as Z. Then, Z will be a continuous function of w; we look into the Z max - maximum value of Z that has to be less than 1 for this f to be a contraction map.

Let us evaluate f prime x, so f x is equal to 1 plus sigma 1 x plus sigma 2 x square divided by 1 plus Da plus sigma 1 x plus sigma 2 x square. So, f prime x is equal to - we just differentiate it, exactly the same way you have done earlier. 2 sigma 2 x divided by 1 plus Da plus sigma 1 x plus sigma 2 x square minus 1 plus sigma 1 x plus sigma 2 x square constant. Then, we differentiate this one, so this will be sigma 1 plus 2 sigma 2 x divided by 1 plus Da plus sigma 1 x plus sigma 2 x square square of that.

We simplify this equation, we take this thing as common, sigma 1 plus 2 sigma 2 x divided by 1 plus Da plus sigma 1 x plus sigma 2 x square. So, this is 1 minus 1 plus sigma 1 x plus sigma 2 x square divided by - one will be remaining, 1 plus Da plus sigma 1 x plus sigma 2 x square, bracket close. Therefore, once you simplify in the numerator, only Da will be remaining, all the three quantities will be vanished. It will be nothing but Da sigma 1 plus 2 sigma 2 x divided by 1 plus Da plus sigma 1 x plus sigma 2 x square square of that. So, what is f prime w, so that is our Z.

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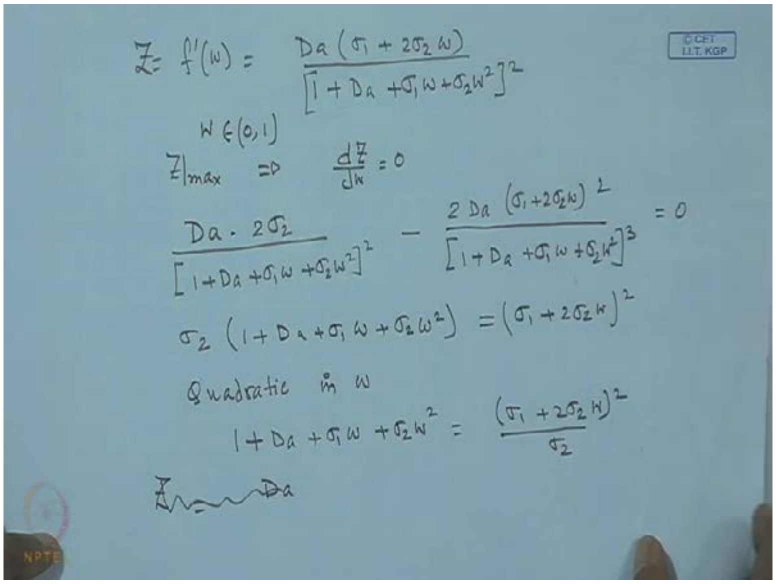

So, Z is f prime evaluated at x is equal to w, so Da sigma 1 plus 2 sigma 2 w divided by 1 plus Da plus sigma 1 w plus sigma 2 w square then square of that. Now, Z is a continuous function of w, where w is a variable lying in the domain of x that is from 0 to 1. So, we evaluate the Z max - maximum value of Z, so maximum value of Z will be obtain if we evaluate d Z d w and put it to equal to 0.

If you do that then this becomes Da times 2 sigma 2 divided by 1 plus Da plus sigma 1 w plus sigma 2 w square square of that minus 2 Da sigma 1 plus 2 sigma 2 w. On the differentiation of this, this becomes sigma 1 plus 2 sigma 2 w, so this becomes square of that divided by cube of this one plus Da plus sigma 1 w plus sigma 2 w square, cube of that should be is equal to 0.

Now, if you one can simplify this whole thing, so Da - 2 Da will be cancelled out simply, it will be gone. So, will be getting sigma 2 multiplied by 1 plus Da plus sigma 1 w plus sigma 2 w square. After simplification, this should be is equal to - Da will be cancelled out, this will be remaining, sigma 1 plus 2 sigma 2 w square. You will be having relationship between this one; so there are two ways to solve this problem, you just look into this problem. This is a quadratic in w, So you can identified that this whole thing 1 plus Da plus sigma 1w plus sigma 2 w square, that is appearing in the denominator, should be is equal to this. We can substitute that one, if we do that this becomes 1 plus Da plus sigma 1 w plus sigma 2 w square, is equal to sigma 1 plus 2 sigma 2 w divided by sigma 2 square of that.

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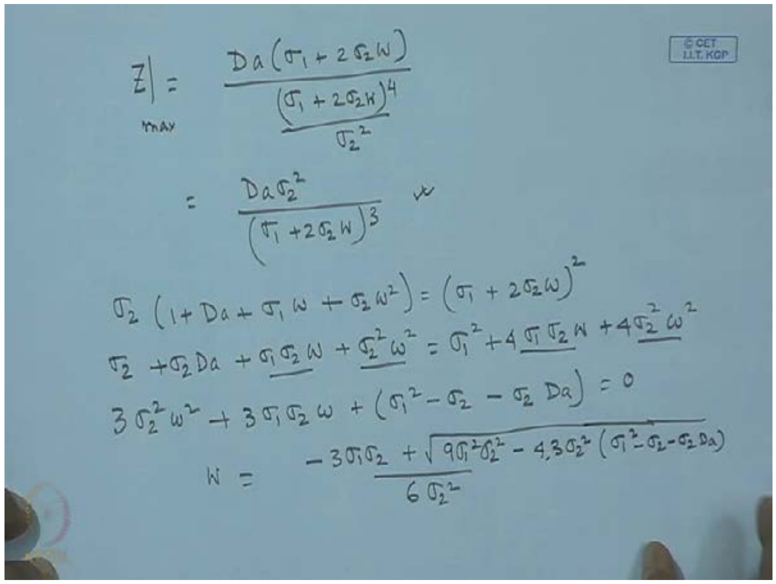

If you are going to substitute it over here, Z becomes - we will just write into the next one. Next page, so if you look into the expression of Z, Da sigma 1 plus 2 sigma 2 w. We have already obtained 1 plus Da plus sigma 1 w plus sigma 2 w square as sigma 1 plus 2 sigma 2 w square divided by sigma 2, therefore this will be sigma 1 plus 2 sigma 2 w square of that. So, it will be 4 divided by sigma 2 square. At the maximum value of Z, this will be Da sigma 2 square divided by sigma 1 plus 2 sigma 2 w to the power 3.

Now, we are going to put the value of w, where that will be satisfying the earlier equation in here, to get an expression of Z maximum. Therefore, if you go back to the earlier equation that becomes sigma 2 into 1 plus Da plus sigma 1 w plus sigma 2 w square is equal to sigma 1 plus 2 sigma 2 w square of that. Just open up this square and see what you get, sigma 2 plus sigma 2 Da plus sigma 1 sigma 2 w plus sigma 2 square w square.

Here, you will be getting sigma 1 square plus 4 sigma 1 sigma 2 w plus 4 sigma 2 square w square. So, you get all this term on the right hand side, so w square will be here, it will be 3 sigma 2 square w square. Sigma 1 sigma 2 will be here, so it will be plus 3 sigma 1 sigma 2 w, you have plus, this is taken care of, this is taken care of, so the rest terms will be sigma 1 square minus sigma 2 minus sigma 2 Da is equal to 0.

We solve this equation for w, at this w Z is maximum, so w is obtained as minus 3 sigma 1 sigma 2 plus - you should not take the - I will come to that later on, plus this square that is 9 sigma 1 square sigma 2 square minus 4 3 sigma 2 square - 4 into 3 sigma 2 square algebra by sigma 1 square minus sigma 2 minus sigma 2 Da divided by 6 sigma 2 square.

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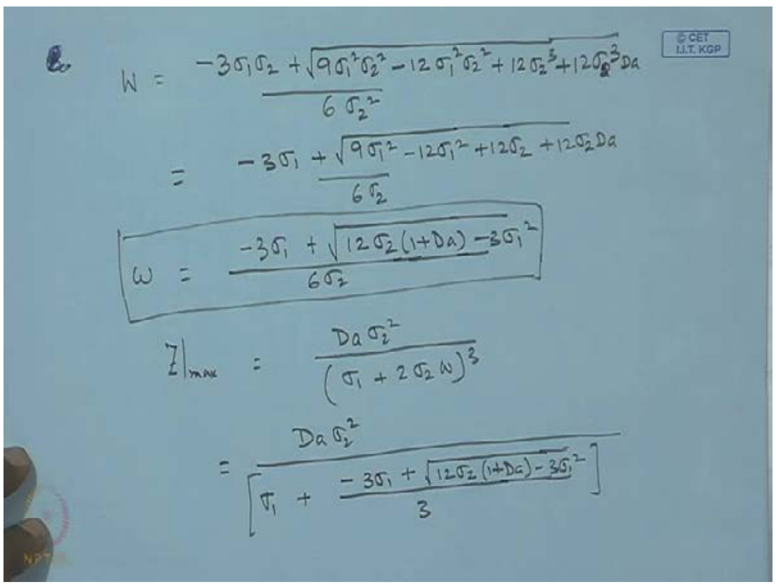

So, you can further simplify this equation probably to a little bit. You will be getting w is equal to minus 3 sigma 1 sigma 2 plus under root 9 sigma 1 square sigma 2 square minus 12 sigma 1 square sigma 2 square, minus minus plus, so 12 sigma 2 cube, minus minus plus, so is to be 12 sigma 2 cube Da divided by 6 sigma 2 square. In fact, we can take 1 sigma 2 square out of this that will be cancelling out. So, minus 3 sigma 1 plus root over 9 sigma 1 square minus 12 s igma 1 square plus 12 sigma 2 plus 12 sigma Da divided by 6 sigma 2, 1 sigma 2 will be canceling out. So, this will be 6 sigma 2 minus 3 sigma 1 plus root over 12 sigma 2 1 plus Da multiplied minus 3 sigma 1 square.

We should not take the plus minus root here, we should take only the plus sign, minus cannot be the thing, because if you take the minus sign, then w turns out to minus and w is ever positive a fraction lying in the mid domain 0 to 1. For this value of w, the Z is maximum, we can put that and see what you get. So, z max, if you remember, is equal to Da sigma 2 square divided by sigma 1 plus 2 sigma 2 w (( )) over 3.

So, we are going to substitute this value of w here, so it will be w sigma 2 w sigma 2, is nothing but 1 upon 3 right, it will be become sigma 2 w is equal to this thing divided by 3. So, you will be having Da sigma 2 square divided by sigma 1 2 sigma 2 w, so it will be minus 3 sigma plus root over 12 sigma 2 into 1 plus Da minus 3 sigma 1 square.

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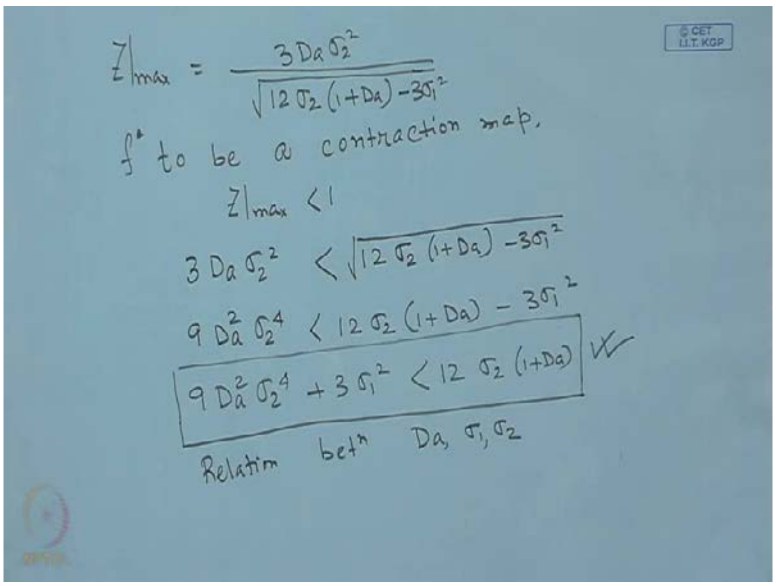

So, it becomes a bit more complicated, so we write down that equation once again in a neat compact form. Z max should be is equal to 3 Da sigma 2 square divided by 3 sigma 1- in this equation, 3 sigma 1 and minus 3 sigma 1 it will be simply cancelled out, so that makes our life simpler. This becomes root over 12 sigma 2 into 1 plus Da minus 3 sigma 1 square.

So, f to be a contraction map, Z max should be less than 1, therefore the whole equation turns out to be 3 Da sigma 2 square divided by whole thing. This should be less than 12 sigma 2 1 plus Da minus 3 sigma 1 square, square root of that. You just square it up, so it becomes 9 Da square sigma 2 to the power of 4, so less than 12 sigma 2 into 1 plus Da minus 3 sigma 1 square. Therefore 9, make it more amenable form Da square sigma 2 to the power of 4 plus 3 sigma 1 square should be less than 12 sigma 2 into 1 plus Da. This is the equation, this is the inequality between the relationships, between the relations, between the parameters Da sigma 1 and sigma 2, should satisfy in order to have a unique steady state for this particular problem. This has become very important. If you look into the - see the complexity of the problems, as you have gone up from problem example 1, 2 and 3, we have kept everything constant. In one case, we have to assume a reactant reaction rate expression; in another case, we have changed the reactions rate expression slightly. In the third case, we made the reaction rate expression more generalized form and see how the condition for have being - having a unique steady state changes from problem to problem.

For the last problem, whatever we have seen, that a rate expression - the generalized rate expression, this is the relationship between the parameters sigma 1, sigma 2 and damkohler number. So, you have to select q and C f, these are the actual operating conditions, you are controlling as an operator on the other hand. This kinetic parameters K 1, K 2 and K 3, they are being specific, fixed by the rate expression. You do not have much control over them.

So, the control you are having over the feed concentration and volumetric flow rate, this non dimensional numbers are the combinations of these, so that these equations have to be satisfied in order to get a unique steady state in your problem. Therefore, we finish the contraction; we complete the contraction mapping stuff. Next, we go to the next topic that is the matrix and determinants.

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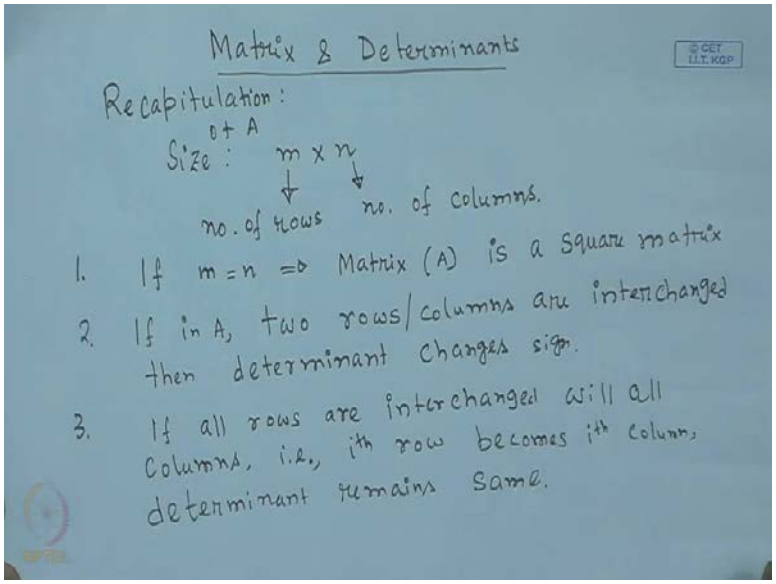

Matrix and determinants are again, will be discussing some of the important properties. They are extremely important as far as the chemical engineering problems are concerned; they are useful tool to analyze the chemical engineering system. As we have seen you have done in the last few lectures, regarding the contraction mapping and the matrix basis. We will try to develop the basic theory and the concepts of matrix and determinants, how they will utilize for the chemical engineering systems in real life. We will be looking into couple of examples, also before that we will be rebrushing - recapitulating some of our definitions and the properties of - basic properties of the matrix and determinants.

So, let us do that - let us look into what is the size of a matrix. Size is writen as m into n, so let us see what m stands for and what n stands for. m stands for number of rows and n stands for number of columns; let us look into the various properties. If m is equal to n, then the matrix A, let us say this is size of matrix A, the matrix is A square matrix. If in A, two rows or columns are interchanged, then determinant changes its sign.

Then, next property is that if all rows are interchanged with all columns that is the I th row becomes I th column, determinant remains same; these are the some of the properties. Then, we look into some more properties of determinants and matrices.

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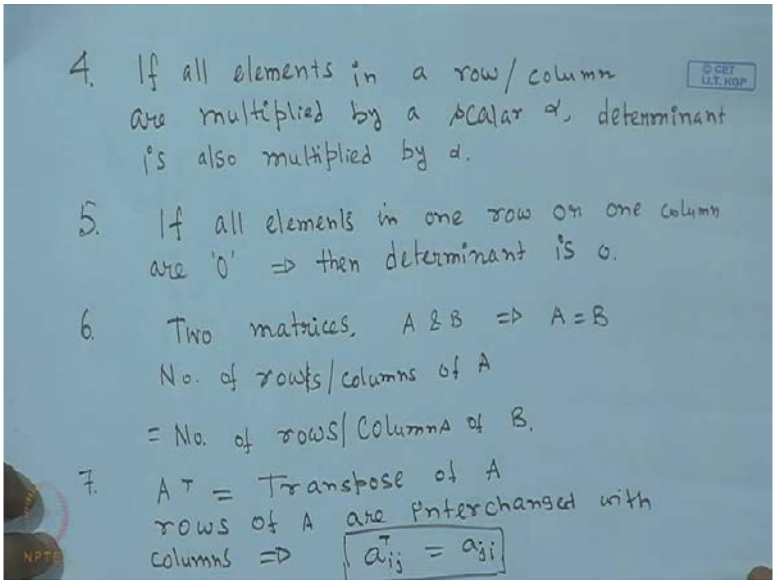

The fourth one is that if all elements in a row or a column are multiplied by a scalar alpha let us say, determinant is also multiplied by alpha.The next property is that if 1 row or 1 column, if all elements in 1 row or 1 column are 0, then of course determinant is 0. Next property is that if A and B, if 2 matrices - 2 matrices A and B, they are equal - A is equal to B, then number of rows and columns of A should be equal to number of rows columns of B. So that is quite obvious.

Next one is a transpose, it is the notation, is a superscript t, which represents transpose of matrix A. This simplified - this simply says that rows of A are interchanged with columns of a transpose or the other way round, does not matter rows of A are interchanged with columns. So, that becomes a transpose matrix, so the rows are now becomes columns. So there are three rows, let say three into three matrixes, they become now columns for the columns of a new matrix.

The new matrix that is generated by interchanging the rows with the columns is called a transpose matrix. So, if t represents the transpose matrix superscript, then a i j superscript, t should be equal to a j i. So, that is the relationship between the elements of a matrix A and it is transpose version.

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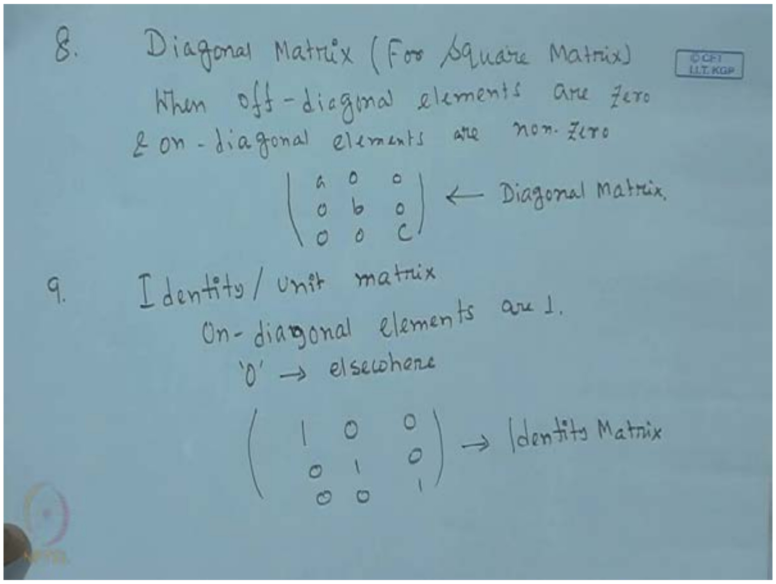

We go to the next property that is property number 8. We define a diagonal matrix; remember diagonal matrix is defined only for a square matrix. What is a diagonal matrix? When off-diagonal elements are zeros and on diagonal elements are non zero, then the matrix is called a diagonal matrix. So, if you talk about this matrix, let us say a 0 0 0 b 0 0 0 c, then this is a diagonal matrix. If on diagonal elements is one, then we call it is an identity or unit matrix - on diagonal elements are 1 and 0 elsewhere. This will be 1 0 0 0 1 0 0 0 1, so this is an identity matrix, so we look into some more definition of the matrices and determinants.

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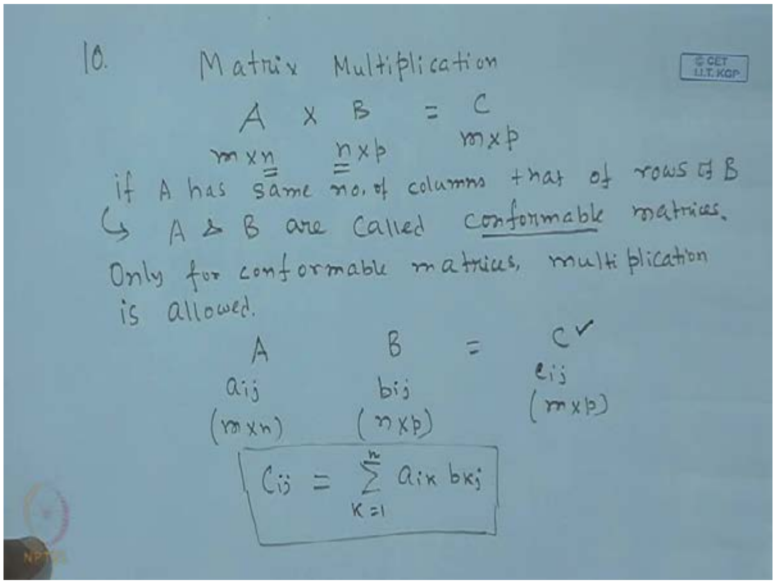

Next property is the matrix multiplication. Let say two matrices, A which has a size m into n, B which has a size n into p, then a multiplied by b should be is equal to C which will be having a size m into p. That means, if A has same number of columns that of rows of B that means number of columns of A should be matching with the number of rows of B, then these two matrices are called conformal matrix - conformable matrices, then A and B are called conformable.

Two matrices, if two matrices are conformable, then their multiplication is allowed. Only for conformable matrix, matrices multiplication is allowed, otherwise not. So, if the number of rows of one matrix is equal to number of columns of the other matrix, then these two matrices are multiplicable. So, A we are - which will be having unit elements a i j with the size m into n, B which as elements b i j size n into p, should be equal to C, which will be elements having elements c i j and size m into p.

So, c i j can be expressed as sum multiplication - summation of a i k multiplied by b k j, where K is equal to 1 to n. So, by following this rule, one can get the elements of the product matrix, will be getting the elements of the product matrix by following up this rule of the corresponding conformable matrices.

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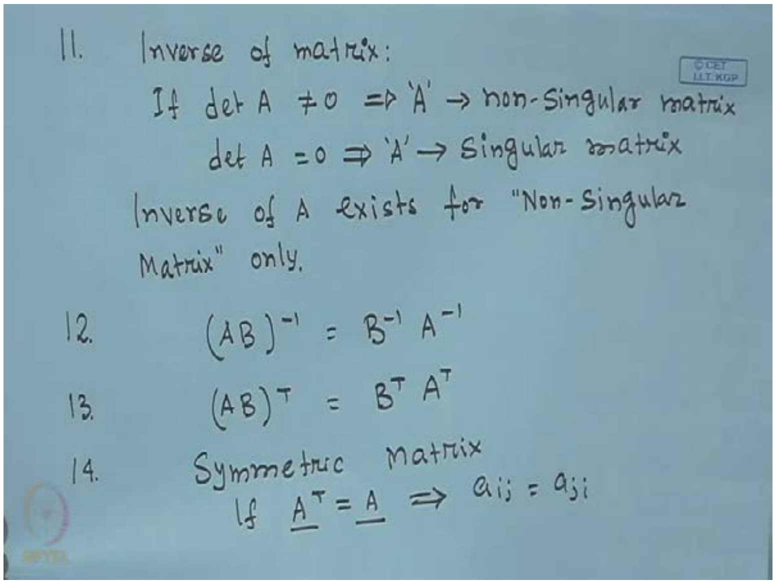

Then we talk about inverse of matrix. If determinant of a matrix A is not equal to 0, then A is called a nonsingular matrix. If determinant of matrix A is equal to 0, then A is called a singular matrix, inverse of matrix exists if A is nonsingular, inverse of A exists for nonsingular matrix only. Next, we look into some more properties, A B inverse is nothing but B inverse A inverse.

A B transpose is nothing but B transpose A transpose. Then, we called about - we talk about the symmetric matrix, if A transpose is equal to A, then a i j is equal to a j i, we call the resultant matrix A as the symmetric matrix. So, if A transpose is equal to A, then we are talking about a symmetric matrix. That means, rows and the columns, even if they are interchanged, there is no difference between the two and they are absolutely symmetric matrix.

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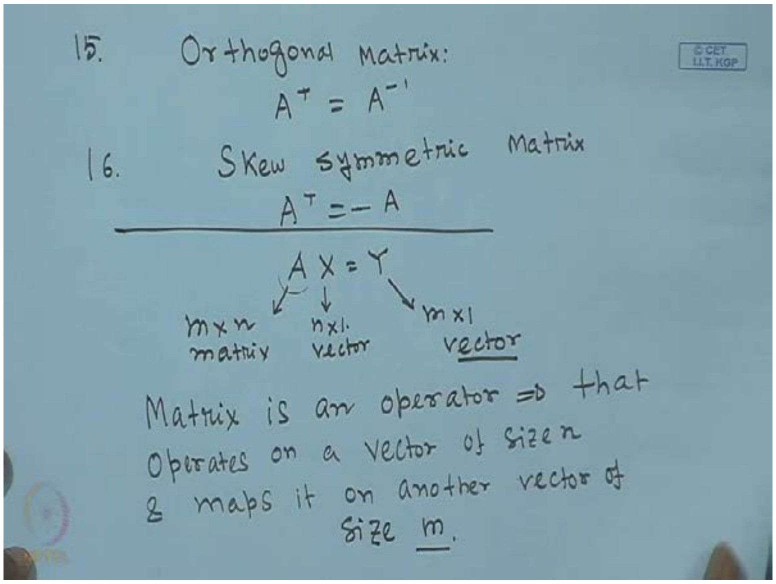

Next one is the orthogonal matrix. If A transpose is equal to A inverse, then we call the matrix A as orthogonal matrix. Then, we talk about skew symmetric matrix, A transpose is equal to minus A, then it is a skew symmetric matrix. If you remember the definition of a symmetric matrix, a transpose is equal to A and for the skew symmetric matrix A transpose is equal to minus A. So, let us look into the matrix - so these are the basic definitions and properties of matrices and determinants, then let us look into any matrix operation.

Let us let us say A X is equal to Y, where a is a m cross n matrix, whereas x is n cross 1 vector, then Y is nothing but m cross 1 vector. So, this vector is basically nothing but a special matrix, where the number of columns is 1. When you talk about A and X, see number of columns is equal to number of rows. Number of columns of this matrix and number of rows of this vector, they are conformable, so their product is - their multiplication is allowed and then you will be getting another vector of size m cross 1.

So, it becomes a vector, it no longer becomes a matrix, so it becomes a special form of matrix known as the vector. So, what is A? It is like Y is equal to f x, so A is an operator, matrix is an operator; it operates on a vector of size n and maps it in a vector of size m. So, matrix is an operator that operates on a vector of size n and maps it on another vector of size m.

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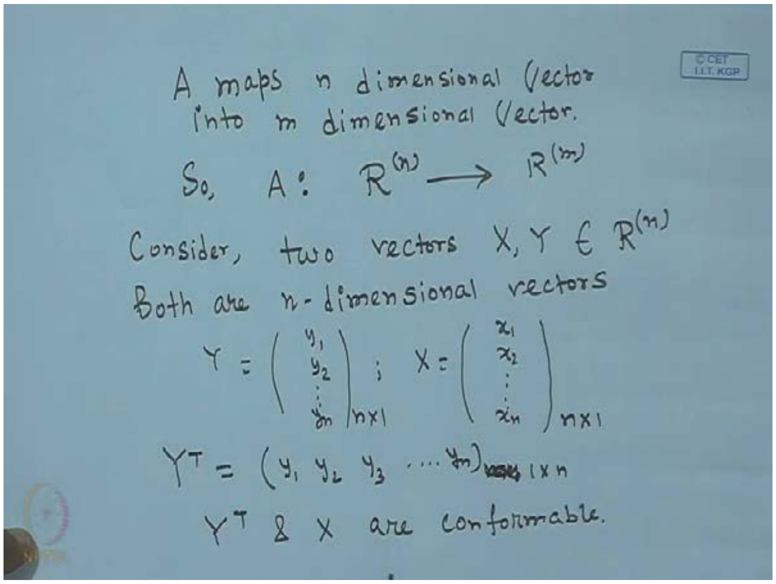

Matrix is nothing but an operator and it is A map, it is nothing but an operator or a map. A maps n dimensional vector into m dimensional vector, so it maps n dimensional space into m dimensional space. In a short form, we can write A is map, where which basically takes of the n dimensional map into m dimensional map in real space.

Consider another property of the vectors; consider the two vectors X and Y, both belong to n dimensional real space, so both are n dimensional vectors. So, Y is nothing but y 1 y 2 up to y n, x is x 1 x 2 up to x n, then what is Y transpose? Y transpose is y 1 y 2 y 3 up to y n, the column becomes row in case of transpose, then it has a size, n into one, there will be n number of rows, this will becomes n into 1. This will be a size of 1 into m, so this is Y transpose and X is also having a size n number of rows and 1 column, so n into 1.

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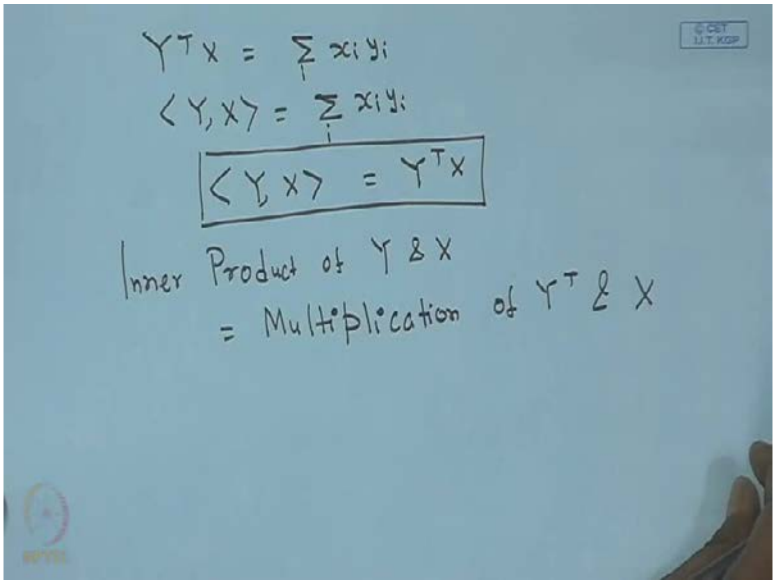

Y transpose and X they are conformable, Y inner product of Y transpose and X are conformable. Matrix multiplication is allowed. If you multiply Y transpose and X, then it becomes summation of x i y i. So, if you take the inner product of Y and X, if you remember the definition of inner product of vectors, we take up the corresponding elements of the vectors, multiply them and add them up, so that also becomes multiplication X summation of x i y i.

Therefore, inner product of Y and X is nothing but Y transpose multiplied by X, so this is very important relationship, we will be utilizing this relationship quite often in our - as we proceed in our course. Inner product of Y and X should be equal to multiplication of Y transpose and X. We have looked into several properties of matrices and vectors, looked into some special form special relationship of the transpose matrix, the operators like how they will be connected to the inner product space.

Then, we will be able to position, to move on further for an eigen value problem, we will see various theorems those are varied for the eigenvalue problems and how eigenvalue problems are quite important in various chemical engineering applications. We can solve so many of chemical engineering problems by elegant eigen value eigenvector approach.

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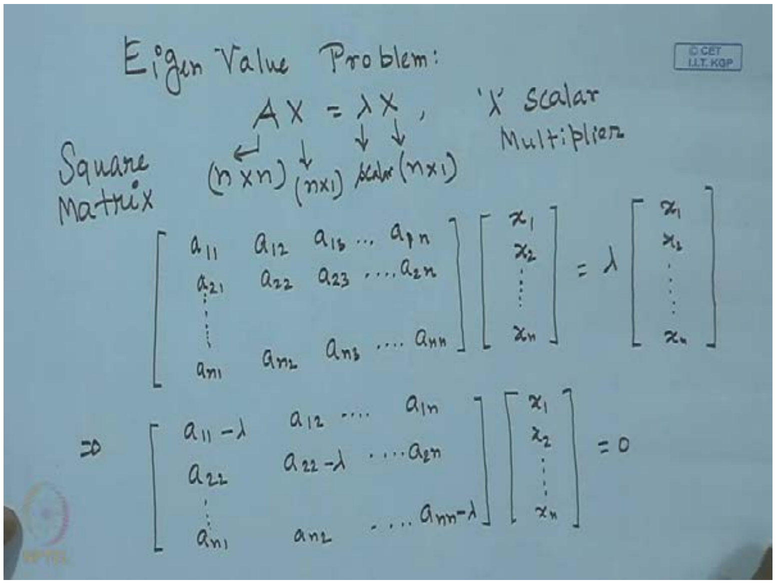

Next, we talk about - move forward for the eigen value problem. If the form of the matrix, A X is equal to lambda X, where lambda is a scalar multiplier that is the form - that means A is A matrix of size n into n, so we are talking about a square matrix. This is a vector of size n into 1, so these two are conformable, so it will be returning a vector n into 1. So, n into n matrix, it will be operating on a vector n into one matrix, number of rows and number columns are identical.

Then, it will be returning a vector, so they are conformable and multiplication is allowed. They will be returning the vector in of size n into 1, so this vector of size n into 1, this is a scalar. If we write an equation like this, then we called this problem an eigen value problem. If we write different, you know elements of A matrix, a 11 a 12 a 13 up to a 1 n, a 21 a 22 a 23 up to a 2 n, then this will be a n 1 a n 2 a n 3 up to a n n multiplied by - we write different elements of X vector x 1 x 2 up to x n, is equal to lambda times x 1 x 2 up to x n.

Then, we just subtract, we just bring the right hand side into the left hand side and write in the form of x 1 x 2 x 1. So, we can write it as a 11 minus lambda a 12 up to a 1 n a 21 a 22 minus lambda up to a 2 n, like that a n 1 a n 2 up to a n n minus lambda, this becomes same as x 1 x 2 x 3 up to x n, this is equal to 0.

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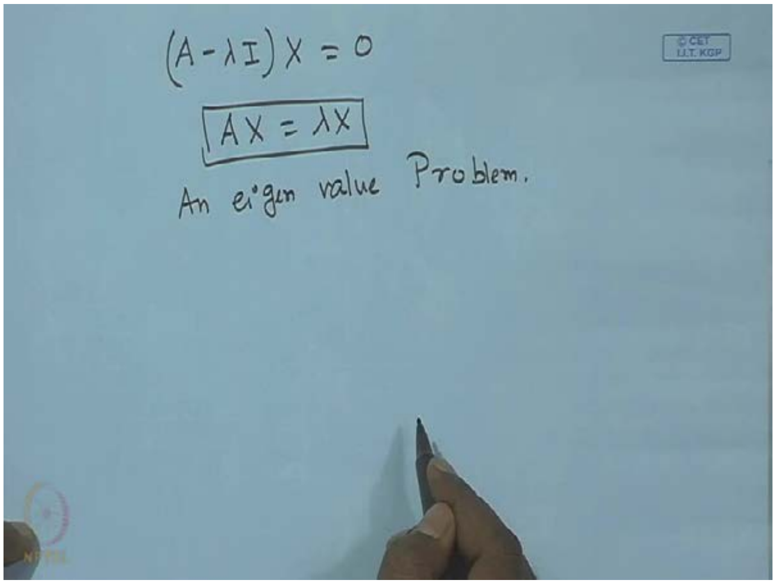

In a compact form, we can write down that a minus lambda I that is the identity matrix multiplied by X, should be equal to 0. Therefore, the form A X is equal to lambda X, is called an eigen value problem. We will see in the next class how the eigenvalue problems are so important for the chemical engineering applications? What are the different important properties of the eigen value problem, which will be exploiting to solve the chemical engineering problems? Thank you for your kind attention.