Rheology of Complex Materials
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Lecture - 59
Strain, convected rates and non-linear models

In these segments of lectures, we are looking at the definitions of strain and some examples of derivatives which are useful in describing the non-linear response of materials looking at non-linear rheology or the rheology at large deformations. And we are also quickly going to review a couple of non-linear models. So, we have already define the strain and we saw that how strain reduces to infinitesimal strain tensors for small deformations, but for arbitrarily large deformations, the overall finite strain tensor should be used.

When we use when we work with largely fluid like materials, quite often strain does not appear in the overall governing equations, only when we look at the integral type models then the strain might appear in the overall governing equations. However, if we are working with solid like materials and if you recall we had discussed standard linear solid model, where strain was involved in the overall governing equation. So, in such cases if we are looking at the overall model for large deformations, we will have to replace the small infinitesimal strain tensor, which is valid for small deformations with the finite strain tensors that we defined.

So, therefore, generally in rheological discussion, the overall finite strain tensors may not be as common as they are in let say discussion of non-linear response of solid like materials. So, in this lecture continuing on we will define the convected rates and then look at some examples of non-linear models and then finish up with the overall governing equation for Giesekus model as well as its response.

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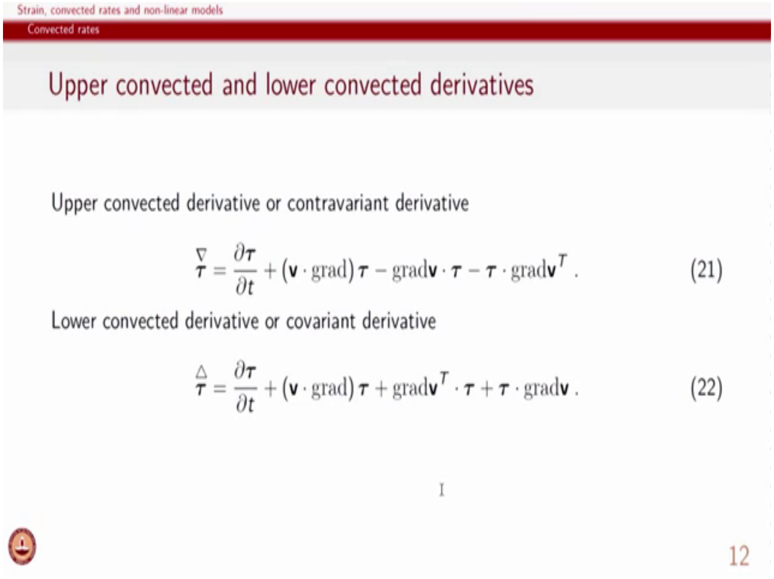

So, let us look at the convected rates, as we had looked earlier the given that the overall description of the material for deformation or for rheological analysis can be done using convected base vectors and convected coordinates and so, when you evaluate the rates of change of these quantities in the convected frame, they are related to the derivatives that we otherwise know. So, for example, the upper convected derivative which is indicated usually by this triangle which is inverted, I we should also remember that depending on the source that is being used there are multiple notations which are possible and so one should be careful in terms of looking at what is the derivative and look at the notation and its relation to one another.

So, this is one of the commonly used notations, but not the only one. So, the overall convected rate of stress is related to the rate of change of stress with time alone and then this is like the convective term which is there in the navies stokes equation also or the inertial term that we call. This is rate of change of tau with respect to the position itself the gradient and this term arises as we have seen in acceleration also this is these 2 terms put together are the material derivative. And then finally, some terms which are related to the deformation in the material.

So, if the material is not deforming gradient of velocity would be 0 and therefore, in that case we will not if we want to evaluate the rate of change of stress, we will not have any contributions due to these terms. So, these 2 terms put together are the terms due to convected rate and so to summarize again the overall convected rate is based on the rate of change of stress with time, rate of change of stress with position and then contribution to the convected rate based on the deformation that is that the material is accounting for. And given that we had seen that there are two sets of base vectors that could be defined in convected coordinates, we had seen that we could define either the covariant or contravariant base vectors therefore, we also have covariant or contravariant derivative. If you recall we had also called these set of base vectors as one set was called tangent base vector and the other one was reciprocal base vector.

So, therefore, we have 2 possibilities of defining convected rate also. Generally the upper convected rate is far more common in case of rheological analysis, from a mathematical point of view there is no way to choose one over the other as to which is more appropriate, it is through experience and through our working with models and its description and comparison with whatever are the results for specific materials we choose one or the other. And we have found generally that of the upper convected models seem to give results which are more according to our experience in terms of rheological response of real materials.

But lower convicted derivative can also be defined and again it has 3 similar terms rate of change of stress with time alone rate of change of stress with due to spatial variations and then the contribution to the convected rate of stress due to deformation in the material it is also possible to define other non-linear other derivatives which are also frame invariant each of the derivative is based on slightly different physical interpretations.

So, these are what we have defined in this slide are convected.

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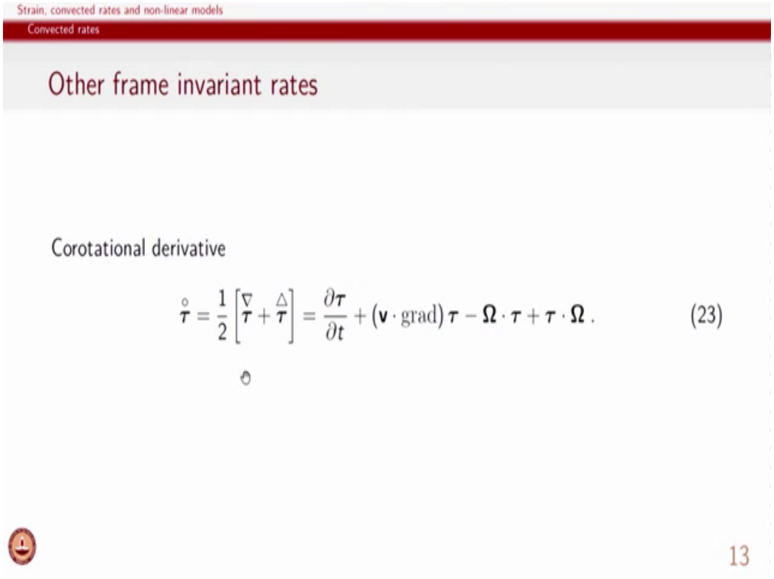

However we could also define for example, a co rotational derivative in fact, you can also construct these derivatives by combinations of these derivatives. So, if I add these 2 or if I subtract these 2, I can get alternate set of derivatives. So, therefore, if we add the two then we get what is called a co rotational derivative, because instead of the velocity gradient what is involved here in the terms which are due to deformation of the material are the spin tensor or the rotational and that is why it is called a co rotational derivative. And so this derivative is also frame invariant and can be used.

So, therefore, what we have is the wherever in linear models, we had the partial derivative that has to be replaced with one of these non-linear frame invariant derivatives for us to get a model which can describe the non-linear rheological response of materials. So, generally if we look at the types of models which are there to describe the non-linear rheological response, we could think of these models in terms of what is the overall form of the governing equations.

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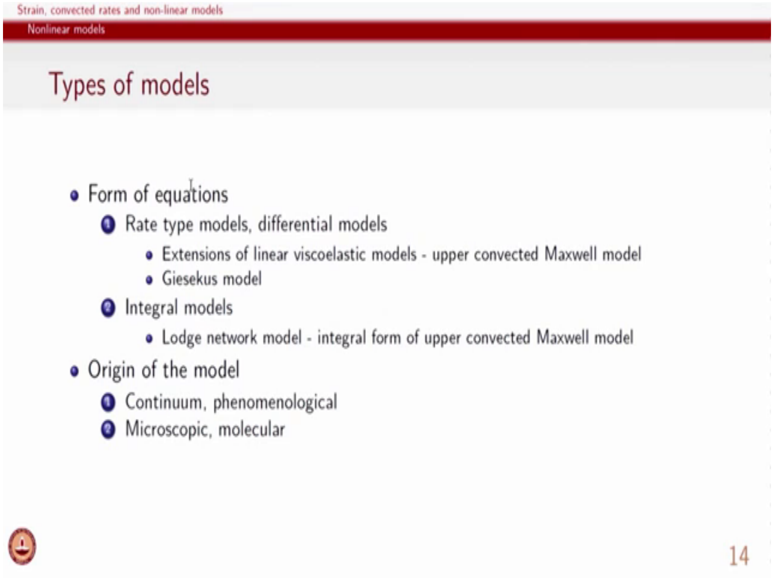

So, generally there are 2 broad type; one is the rate type equations or the differential models and then we have the integral models. The idea in rate type models is to say that at each and every instance of time how are the rates of different quantities and quantities themselves are related to each other. So, for example, Maxwell model that we have seen where we just wrote it in terms of stress and stress rate related to strain rate at each and every instance of time is an example of a rate type model. We also saw that the Maxwell model can also be written in an integral form.

Any differential equation can all be transformed to an integral form and similarly in a rate type model could also be transformed to integral models. A depending on the overall development of the model itself sometimes based on the physical arguments that are being made while developing the model, we may end up getting integral model as the beginning stage and so therefore, a corresponding differential form can also be found from the integral form.

So, generally depending on the history of how the development of the model took place, we have some of the models which are more commonly used in the rate type form and some other models, which are used more in the integral type form. For example, the Maxwell model more often than not is used as a rate type model. So, upper convected Maxwell model we will see is an example of a rate type model and its also an extension of a linear viscoelastic model. So, linear visco elasticity we used Maxwell model quite extensively if we replace the partial time derivative with upper convected derivative we have the extension of linear viscoelastic Maxwell model to a non-linear viscoelastic model called upper convected Maxwell model. Similarly we will also look at another example of a rate type model which is Giesekus model. On the other hand we have several integral models and one example is large network model, which happens to be an integral form of the upper convected Maxwell model, but in originally when it was derived it was derived as an integral form. One most commonly known integral form of governing equation is to account for reputation in polymer melts. So, given that macromolecules are entangled with each other in any description of rheological response of a polymer melt requires description of entanglement and repetition of the macromolecules, to account for the reputation dough adverts developed a model which is an integral form model.

And so, as I mentioned earlier quite often we may have a model, which has both integral or rate type expressions some other times it is not possible for us to transform them based on the complexity of the equation. So, when we say form of equations is important this is only for us to know the phenomenological basis for how the governing equations were arrived at and also intuitively for a given rheological problem we may choose one over the other depending on the application. The other thing that we could sort of look at is in terms of how is the model motivated and how was it derived. So, if it was derived based on continuum and phenomenological macroscopic arguments, then we will have one type of arguments and leading to the overall governing equation. The same governing equation could also be reached starting from a microscopic or molecular picture.

So, in one case we use continuum mechanics, in the other case we use statistical mechanics or molecular theories to arrive at these equations. So, quite often it is important for us to traverse back and forth between these 2 types of models or these 2 types of understanding to get the overall picture. It is important for us to look at the continuum scale and look at the overall macroscopic behaviour, because for many engineering applications we need that. However, at the same time since many of the physical mechanisms are at the molecular and microscopic scales, it is important for us to understand the material constitution as well as material response at the molecular or microscopic scale.

So, generally we use both of these approaches to try to understand the overall rheological response. In this course so, far we have focused mainly on the continuum and phenology phenomenological description of rheology for advanced learners it is very important to look at the microscopic and molecular response as well.

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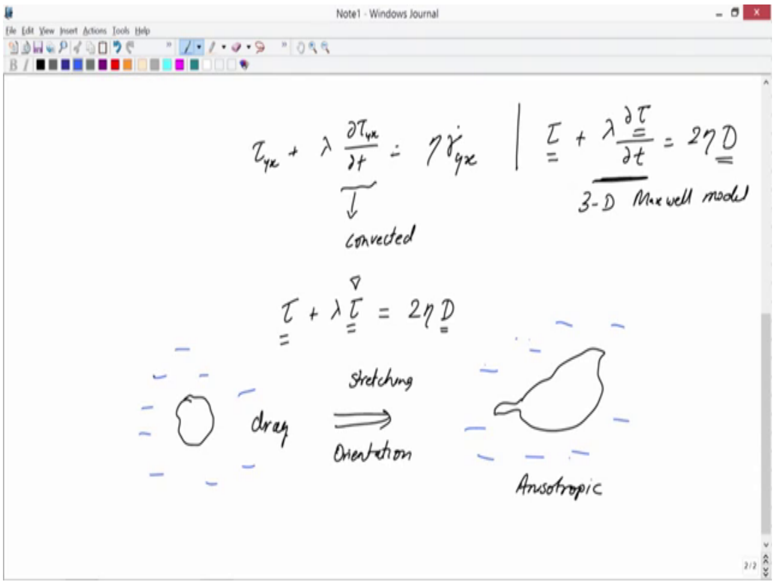

So, now looking at the upper convected Maxwell model since we are quite familiar with the overall Maxwell model which we have used several times in the course so far.

So, we have been the one dimensional version of it we have been always writing it like this as this is let say valid for the simple shear case and so when we write the upper convected model, what we are doing is this time derivative which is partial derivative has to be replaced by convected rate. And so the just to remind ourselves the 3 dimetional version of this model will be just where we replace the single component model with the tensor and therefore, this is the overall 3 D version of Maxwell model.

But this is valid only for small deformations because the rate quantity which is being used which is the partial derivative of stress is only valid when we have deformation small. However, for a convected Maxwell model what we do is we replace the partial time derivative with the convected rate and in this case this is upper convected Maxwell upper convected derivative of tau and therefore, this becomes the upper convected Maxwell model. And so given that the upper convected derivative itself is algebraically complex, the overall governing equation of the Maxwell model therefore, now becomes algebraically more complex. If you look at it in the boldface notation its very similar to the Maxwell model itself except that we are using the convected rate.

So, we could again in this description physically intuitively say that Maxwell model basically relates stress and stress rate to the overall strain rate tensor in the material. And given that there are nine components we can write each and every component, and for example, in this slide we have written the yx component which would be very important for many of the simple shear type of deformations in the material.

And these two terms are of course, from the earlier Maxwell model itself, this is the inertial term which arise when we have material derivative being incorporated and you can see that this is now variation of stress with respect to position. So, that is why we had said earlier that this is variation of stress with time alone, and this term incorporate variation of stress with position or spatial variation of the stresses and then the last term which is the convected rate contribution due to deformation itself.

So, if any of the velocity gradient terms are non zero then only this term would contribute. Of course, we know that if lambda itself is 0, then we have only the Newtonian fluid model and in that case the overall convected rate itself is not immaterial and the stress is only related to the current value of the strain rate tensor in the material. So, therefore, we can now use this overall governing equation instead of using the Maxwell model that we have done, and the results of this model will be valid for arbitrarily large deformations.

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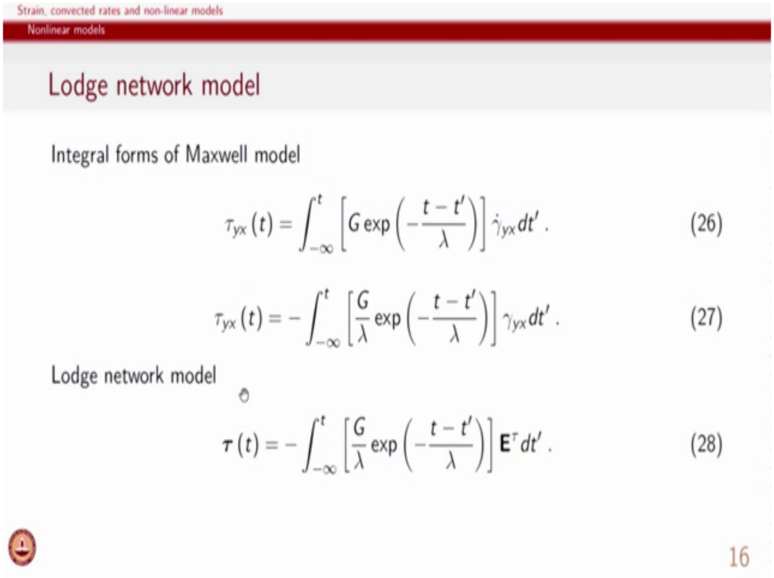

Now, going on we can look at the integral counterpart and we had seen earlier that the Maxwell model could be written in integral form using a relaxation modulus. So, if you recall G into exponential t minus t prime by lambda is nothing, but the relaxation modulus and if we integrate this equation by parts, we can get the overall stress in terms of strain.

So, we have one integral statement where we define it in terms of strain rate, the present value of stress depends on present the integral of strain rate, which the material is subjected over all the history. Similarly by integration by parts we could arrive at the present value of stress as a function of past history of strain that the material has been subjected to. And this gamma yx is only valid when deformations are small and so we replace this infinitesimal strain tensor component in the 3 dimensional version with a strain tensor. So, this is now the large network model which is integral form of the upper convected Maxwell model and one can show that this form is equivalent to this form.

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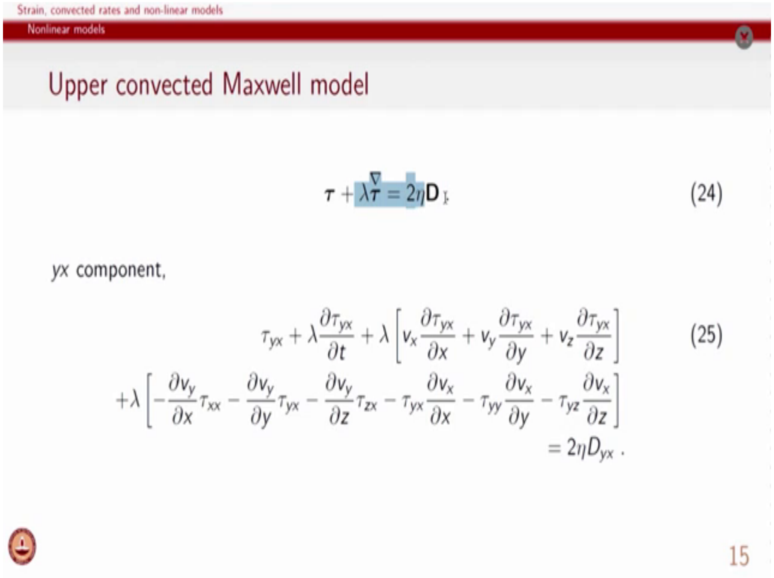

So, this is the differential form of the model and this is the integral form of the model, but we choose to call it at large network model, because the origin of its derivation our integral and large network model is a specific case of large rubber like liquid model where instead of if you instead of the exponential relaxation modulus which is due to Maxwell model, if you use any other form then we have what is called the large rubber like liquid model.

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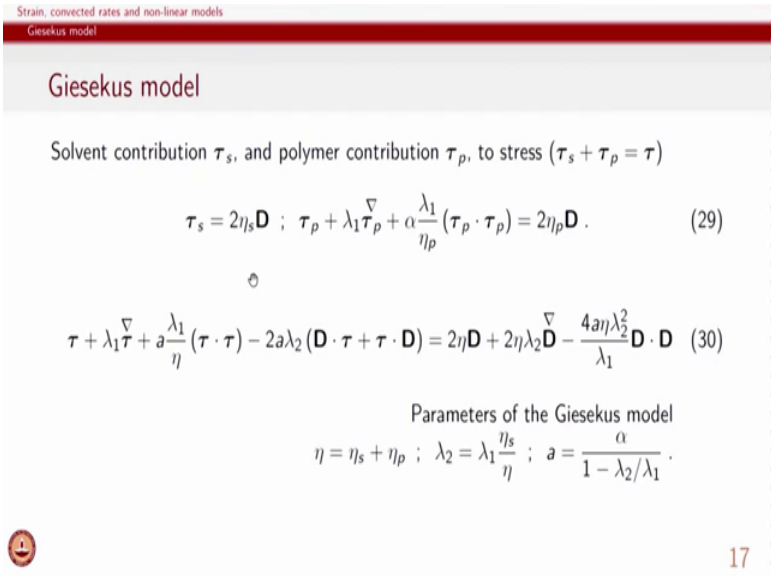

So, now going on we will finish up by looking at an example of a non-linear model, Giesekus model has been very useful in terms of non-linear rheological response of materials originally it was again derived for polymer solutions.

So, therefore, it can be used for a specific set of materials, we have discussed in course worm like macular systems, supramolecular systems and polymer solution. So, many of these systems Giesekus model is a good starting point. It is a good starting point for non-linear logical response because it has all the reasonable response that is expected from a non-linear rheological response of realistic materials. We have seen earlier that if we look at this upper convected Maxwell model it shows in fact, no shear thinning or shear thickening.

So, viscosity is constant in steady shear. Similarly we saw that the normal stress difference for upper convected Maxwell model was proportional to strain rate squared. While we know that the proportionality is not at all related to gamma dot squared, but it is far more complicated. So, therefore, upper convected Maxwell model shows certain features of non-linear response of materials, but it is grossly inadequate. On the other hand Giesekus model seems to have a reasonable set of non-linear responses, which many of the realistic materials also show. Originally it is derived it terms of polymer solution. So, the overall hypothesis was that there is a stress contribution in terms of solvent and there is a stress contribution in terms of polymer and both of these added together give us the overall stress in the material.

So, now the question is to derive each of these and the contribution due to solvent is just a Newtonian contribution where eta therefore, is the solvent viscosity. The polymer contribution which includes viscoelastic response is basically related to the upper convected Maxwell model. So, if we say for the time being ignore this term and say alpha is equal to 0, then you can see that the polymer contribution here tau p plus lambda 1 times convected derivative of tau p is equal to 2 eta p D will be nothing, but the upper convected the Maxwell model of tau p.

So, basically what this model incorporates are the mechanisms of stretching and orientation of the macromolecules. So, whenever a polymer solution is being deformed the macromolecules can stretch and macromolecules can orient and therefore, we have the upper convected Maxwell model of polymer contribution stress arising. Now additionally we have the term which is due to what is called the non-linear term, where alpha is the most important non-linear parameter. In fact, it is called the non-linear parameter because if alpha is 0, then the overall governing equation reduces to the Oldroyd-B model this governing equation will reduce to upper convected model this is already there. So, when you add the two we get what is called the Oldroyd-B model and again Oldroyd- B model is only very qualitative descriptor of the overall rheological response it has many of the same limitations as the upper convected Maxwell model. However, the Giesekus model response is realistic predominantly because of this non-linear term.

And so, for nonzero values of alpha, we have the overall stress appearing as a non-linear term effectively stress squared. So, this is like saying tau squared terms which are there. And the origin of this term was based on the fact that when we have stretching an orientation of macromolecule, the drag that it experiences there is an isotropy in it. So, if you remember we have been talking about Stokes law and drag for macromolecule what macromolecule experiences and so between the solvent, solvent and the overall macro molecule we have the drag and because of stretching and orientation.

So, if we have stretching and orientation basically the macro molecule ends up being a much more anisotropic object and therefore, now the drag which is experienced by this macro molecule will be have to be found out for an isotropic object and the term due to alpha is due to this. So, alpha is called the non-linear mobility parameter or the non-linear parameter itself. Now when we substitute the value of tau p and tau s in this equation and simplify, we get a algebraically complicated governing equation for Giesekus model. And in terms of overall description of these terms in words we can see that stress and convected stress rate in combination with the non-linear stress square term, and stress and strain rate multiplicative term is related to the strain rate, convected rate of strain rate, and strain rate squared.

So, now this is evident enough for us to see that how Giesekus model is an example of non-linear model. The convicted rate of course, contains non-linear terms, but we additionally we have non-linear terms which are involving stress squared, we they are involving multiplication of strain rate with stress we also have convected rate of strain rate itself and then we also have multiplication of strain rate with itself. So, you can see that the parameters are eta s, lambda 1, alpha, eta p. So, these are 4 parameters of the overall Giesekus model. Sometimes it is useful to rewrite some of these parameters in terms of additional more parameters. So, then we have eta, which is eta s plus eta p lambda 2, lambda 1 and a as the overall set of parameters using which we can use we can describe the Giesekus model. Given that these models end up being algebraically very complex, sometimes they are tedious especially to an uninitiated or if you are not familiar.

So, the best way to get familiar with these is to actually work with these models and see their response. So, for example, in class we had seen earlier that if you want to see the response of Maxwell model to let us say stress relaxation then we say that strain is constant and therefore, we substitute that value in Maxwell model saying that gamma y x is constant and therefore, gamma dot yx is 0. So, similarly what we will have to do in each of the case for Giesekus model also, is to substitute the working condition. So, let us say if it is steady shear then we will have to say that since it is simple steady shear only d yx will be nonzero d xx and everything will be 0 and that substitution here we will give us a governing equation for components of tau and then those have to be solved for us to get the overall response of Giesekus model.

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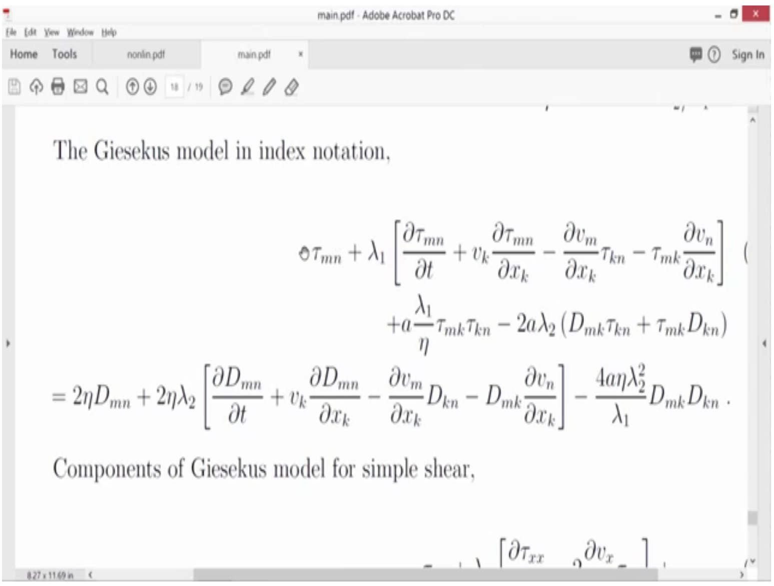

So, this is the overall description of the Giesekus model in index notation and we can see that it is fairly complicated. And so each and every term one has to carefully calculate if we have to work with the Giesekus model in general and so we will finish up by looking at the components of Giesekus model for simple shear.

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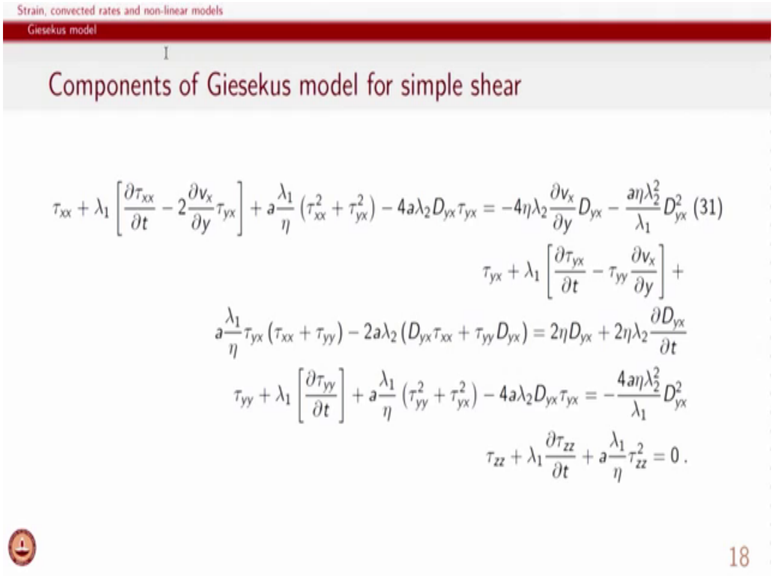

So, here d yx is related to gamma dot yx as we have seen in the class earlier and so, the overall governing equation for Giesekus model we still have 4 terms of stress tensor which are nonzero, we have seen that for for any general viscoelastic material in simple shear flow we can have 4 components the 3 normal stress and the shear stress nonzero and therefore, we have governing equation for tau xx for tau yx tau yy and tau zz. So, it is these 4 equations which have to be solved depending on what is the d yx that is being imposed.

So, if it is a simple steady flow then d yx will be constant. if it is stress relaxation then d yx will be 0. if it is creep then tau yx will be constant and we will have to solve for d yx and also strain. So, therefore, these set of governing equations are for simple shear alone, analogously we could find the governing equations for extensional flow or any other flow for which Giesekus fluid or a material, which is described very well by Giesekus model response can be derived by such equations.

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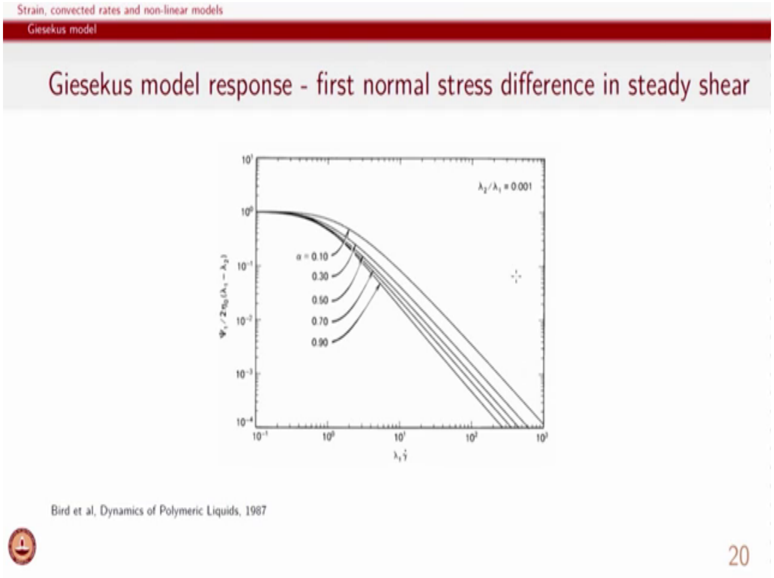

And looking at the overall response of some of these some of this example.

So, looking at steady shear response, we can see that the Giesekus model response describes shear thinning there is a Newtonian Plateau in the beginning of the at low strain rates and so therefore, this is quite useful for many of the polymeric system and as the strain rate increases, the overall material is shown to exhibit shear thinning behaviour. And alpha which is a non-linear parameter as we have seen that when it is 0, it will lead to in fact, no shear thinning and as alpha increases more and more shear thinning is shown by Giesekus model.

So, Giesekus model shows more and more shear thinning when alpha the non-linear parameter is higher and higher. And the first normal stress difference also in terms of the coefficient is a function of strain rate itself. Remember that for upper convicted model or for Oldroyd model the stress first normal stress different coefficient is constant. So, only when we have alpha non zero we have actually first normal stress difference again varying as a function of strain rate itself and again this is qualitatively observed for many of the polymeric system.

So, the Giesekus model describes both shear thinning as well as variation of first normal stress difference, qualitatively reasonably for many polymeric systems.

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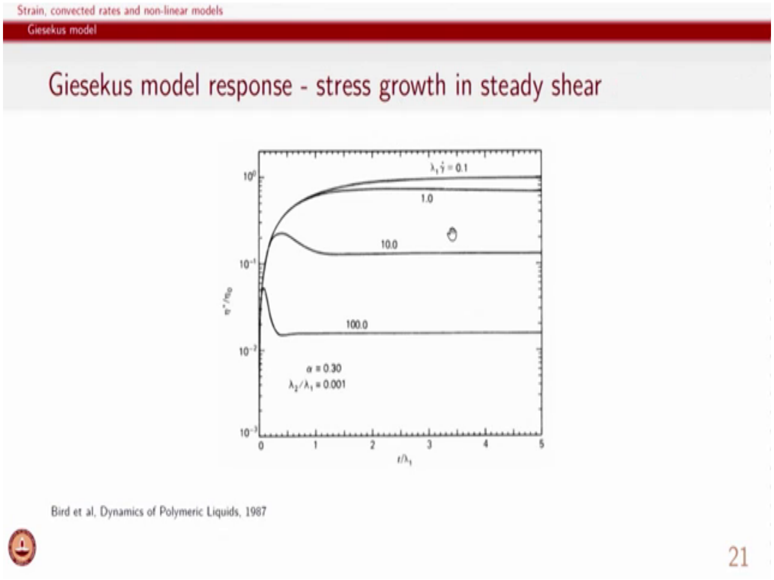

If you look at stress growth in steady shear again we have a very reasonable response from a Giesekus model. At very low strain rates we have the predominantly exponential type increase of the stress growth viscosity and whenever we go to higher strain rates then we have this stress overshoot and then reaching the steady state and if you look at the steady state values themselves you can see the apparent shear thinning also because for low strain rates the steady value which is reached is much higher and when you go to higher and higher strain rate you reach lower and lower values of steady state viscosity.

So, therefore, Giesekus model is very useful in terms of describing the non-linear response of various materials, and familiarity with it would involve working with the governing equations, which we showed in terms of index notation and simplifying them for a set of specific rheological characterization.

So, with this we have reviewed the overall non-linear models, which are useful for the characterization of rheology of complex materials. However, we should remember that these are very simplistic models that we have discussed even though they happen to be very complex algebraically; there are far more complicated models which are useful in today's world to describe the rheological response of materials. There are of course, also a set of models which only are developed using microscopic theories or in terms of computer simulations, and those the discussion of such models will be there for the advanced learners.

So, with this we will now close the discussion related to the non-linear response of complex materials.