Rheology and Processing of Paints, Plastic and Elastomer based Composites
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Lecture 24

Numerical Problems related to basic rheology

Welcome to NPTEL online certification courses on rheology and processing of paints, plastic and elastomer based composites. Today we are in week 4 and lecture number 6 that is the last lecture in this week and we will be trying to brush it up with the theory I taught you so far with the numerical problems I mean related to basic rheology of course. So, without giving a content I will just target here 5 problems and we try to solve and try to understand essence of it ok. See the problem number 1 you can write it down the master curve of polyisobutylene in the below figure, indicates the stress relaxes to a modulus of 10 to the power 6 dynes per centimeter square and in at about you know 10 hours at 25 degree centigrade. So, you know stress relaxation experiment where you monitor modulus as a function of time that means stress as a function of time strain is essentially constant ok. So, as I mentioned it you in a realistic you know experimental setup you can do the test at different discrete temperatures ok and ultimately using WLF all if you know this discrete graphs can be overlaid in a single graph, that is you call master command that is the essence of WLF equation and you try to calculate the shift in this scale and this shift factor is actually is the time ratio basically ok or inverse of frequency ratio ok with respect to a reference temperature of course.

$$\log\left(t_T / t_{T_g}\right) = \frac{-17.44\left(t_T - t_{T_g}\right)}{51.6 + \left(t_T - t_{T_g}\right)}$$

So, in this step problem statement if you try to see see it takes 10 hour at 25 degree centigrade and what is asked you using WLF equation you try to monitor the same thing same relaxation to a you know modulus at minus 20 degree centigrade how much it is going to be time the 10 hours at 25 degree centigrade corresponds to you know which hour at minus 20 degree centigrade. So, as I mentioned it you to have a you try to understand you have a T1 that means, this is temperature this is a time and that is equivalent to at a different domain temperature T2 the time T2 you do not know. So, you know the T1 which is 10 degree in when 25 degree centigrade plus 25 degree centigrade here and your time is 10 hour. Now, your change temperature domain is minus 20 degree centigrade and you have to really calculate using WLF what is the T2 as simple as it is and basic experiment is a stress relaxation experiment in this case you can do for creep as well, and dynamic experiment also let us try to see how we can solve it.

So, Tg is given for your information is minus 20 degree centigrade for poly isobutylene for this problem. So, you can you know WLF equation log T by Tg Tg is the universal reference temperature is minus 17.44 plus T minus Tg by 51.6 you know T minus Tg. So, that way if you just put this first set of values means what you knew was you know this 25 degree centigrade is the temperature and then of course, this T should be capital I am sorry this should be T the temperature this axis is a small t.

So, now if you put it these are read it as a temperature here temperature is Tg. So, 25 and 70 that way minus minus 70 is plus 70. So, you get to see this C factor here is minus11.3 log of that. So, actually time required at minus 70 that is unknown this was known 10 hour.

So, you put it you get to see 2 into 10 to the power 12 hour required. So, now, what you do not know is minus 70 was not asked in the question. But what you can do you can use it as a reference time at minus 70 degree centigrade and put it once again in the WLF equation and try to calculate the. So, what is unknown here T minus 20 degree centigrade and if you solve it you get to see 5140 hour. See although this has been done in 2 steps the same problem you can solve it in single step itself because anyway essentially if you write 2 equation this is equation 1 this is equation 2 if you just subtract T minus 70 cancels out basically.

So, for a beginner it is better to do in step1 step2 like I said first to try to calculate what is the time required at minus 70 degree centigrade that you put it back in WLF equation once again because your reference temperature remains the same minus 70 degree and try to solve it out and you get to see it is 5140. Now remember see the apparently at plus if you go back at 25 degree centigrade which was taking you only 10 hour the same relaxation will take you 5140 hour. So, time is delaying as your temperature reduces that means your relaxation becomes sluggish. So, this is one of the basis although I am not going to show you the entire range of data you can always by the way before I forget for understanding you know time temperature superposition principle in this course MATLAB is one of the you know things which we expect that you should know you can use MATLAB to do the superposition. So, you already are aware of the you know transformation that means horizontal shift and vertical shift of the data experimental data you get it and you can always do yourself in a more automated way in a MATLAB as a.

$$\log\left(\frac{t_T}{t_{T_g}}\right) = \log\frac{t_{25^\circ}}{t_{-70^\circ}} = \frac{-17.44(25+70)}{51.6+25+70} = -11.3$$

$$\frac{t_{25^\circ}}{t_{-70^\circ}} = 5.01 \times 10^{-12} \quad \text{and} \quad t_{-70^\circ} = \frac{10}{5.01\times 10^{-12}} = 2\times 10^{12} \quad \text{hr}$$

$$\log\frac{t_{-20^\circ}}{t_{-70^\circ}} = \frac{-17.44(-20+70)}{51.6-20+70} = -8.59$$

$$\frac{t_{-20^\circ}}{t_{-70^\circ}} = 2.57\times 10^{-9}$$

$$t_{-20^\circ} = (2\times 10^{12})(2.57\times 10^{-9}) = 5140 \quad \text{hr}$$

This shows how lowering the temperature maintains mechanical "stiffness" for much longer periods of time.

And not only that this related problems the books I referred already some of the problems are given, the same problem you try to do in you know MATLAB. Say for example, I talked about several rheological models starting from 2 parameter, 3 parameter, 4 parameter. So, in those particular books specially by B. R. Gupta's book you will see this set of data- shear stress and shear rate data and that you can actually use MATLAB and you can fit it in and with the carreau-yasuda I mean which is a 4 parameter model you can fit it in other models also that I uttered.

So, that will give you some sort of a hand on experience in solving problems. The problem number 2 is meant for getting you more familiar with the conception of storage modulus plus modulus storage viscosity plus viscosity namely eta prime eta double prime g prime and g double prime. As I mentioned it to its very relative for a dynamic or oscillatory experiments whether you define modulus or viscosity all that matters it how your look out I mean, what is your perspective you looking at that. If you look at the material from the point of view of solid always try to assign its g prime and g double prime as the properties. While you try to consider its more of a fluid because it is a viscoelastic material it is all relative.

So, when you are trying to look at it from the point of view of fluid your eta prime and eta double prime becomes apparent. So, using a generalized Newton's law will you try to see the significance of it try to read out I am reading out the problem for you here. The behavior of a viscoelastic material subjected to oscillatory perturbation may be treated by generalizing the concept of viscosity as I mentioned rather than the modulus and separating into both in phase and out of phase terms. And then if I write Newton's law then you know that stress which is a complex term becomes viscosity into rate of shear.

Now, the what is eta prime is eta prime minus eta double prime eta complex viscosity and eta prime and eta double prime and similarly you know storage modulus is also you can write it g prime, g star composite modulus is g prime plus i g prime i g double prime.

$$\eta^* = \frac{\sigma^*}{d\epsilon^*/dt}$$

For a dynamic experiment, $\epsilon^* = \epsilon_0 e^{i\omega t}$

$$\therefore \frac{d\epsilon^*}{dt} = \epsilon_0 i\omega e^{i\omega t} = i\omega\epsilon^*$$

$$\eta^* = \frac{\sigma^*}{i\omega\epsilon^*}$$

So, now let us find out this relation this is the relation eta prime equals to g double prime as I told you also by omega omega is a you know angular velocity of that experiment oscillatory experiment and eta double prime is g prime by omega how do we get it let us try to see the solution. So, if I can mention eta star equals to sigma star by d epsilon star by dt, for a generalized Newton's equations. Now, for a dynamic experiment let us take the strain in a generalized term you know epsilon star equals to e 0 into i omega t that is how you always do it rather than doing it in sine or cosine terms basically. So, now if it is so what is d epsilon star by dt just differentiate it its i omega into you know epsilon star and now what is again eta star equals to epsilon star by i omega epsilon star. Now, what is g star equals to sigma star by epsilon star.

So, you put it here this by this is nothing but g star by i omega now you try to multiply it with the complex conjugate then your eta star turns out to be as I mentioned its already eta prime minus i eta double prime and you just multiply it with the complex conjugate and then you try to see it turns out g prime is g prime by i g double prime and then it becomes this by this that means g double prime by omega minus i g prime by omega. So, obviously your eta prime is nothing but g double prime by omega and you get eta double prime is g prime by omega just opposite way storage viscosity is related to loss modulus loss viscosity is related to storage modulus. So, this is the conception and that I have told you so far while talking the view you know generalized conception of you know dynamic experiments.

But

$$G^* \equiv \frac{\sigma^*}{\epsilon^*}$$

and

$$\eta^* = \frac{G^*}{i\omega} = \frac{-iG^*}{\omega}$$

$$\eta^* = \eta' - i\eta'' = \frac{-iG^*}{\omega} = \frac{-i}{\omega}(G' + iG'') = \frac{-iG'}{\omega} + \frac{G''}{\omega}$$

Thus

$$\eta' = \frac{G''}{\omega} \quad \text{and} \quad \eta'' = \frac{G'}{\omega}$$

Now, we will try to solve another problem, another two important conceptual problem related to capillary extrusion like one of the what I am trying to do quickly get you familiar with different rheometric problems. How do you extract the corrected data basically in capillary viscometry if you mention I mentioned two things one was you know entrance correction because of the fluid vortex that it forms during the entrance that actually demands additional L by D ratio that is what I told you that has to be corrected.

And second thing while flows in a capillary you essentially while calculating, you estimate that at wall velocity is 0 and that is how you see parabolic velocity distribution. But is it really it happen there will be definite amount of wall slip and that wall slip will be higher and higher if your shear rate becomes higher and higher. Of course, at a very low shear rate, you can neglect the wall slip parameter, but point is that how to calculate how much wall slip happening on the you know on the wall basically. So, first let us try to take one by one let us try to you know focus on L by D Bragley correction which is entrance correction. Then we will go to the next which is you know wall slip correction the second this is the first part.

$$\tau = \frac{\Delta P_T}{4\left[(L/D) + (L/D)'\right]}.$$

So, what you have to do you have to do a separate experiment to take care of the Bragley correction or entrance correction what you do, you try to do capillary experimentation using different L by D ratio capillaries, but same diameter. So, what you generate pressure difference versus L by D ratio try to generate a plot. So, if you do it so you can really at different you know shear rates you can do the experiments and you can get to see this sort of a plot. So, given a plot given a particular L by D given a particular you know shear stress and shear rate, if you just extrapolate it or interpolate it you see here in the negative x axis you have a intersection and that L by D ratio is the additional L by D ratio that has to be taken care of in the calculation of shear stress basically. So, let me go back and show you exactly what you are doing, see shear stress is del p by 4 into L by D ratio that derivation I showed you already, In that this additional L by D what you get it from the intersection in the negative x axis that has to be added on that is the one way.

$$\tau = \frac{\Delta P_T - \Delta P'}{4(L/D)}$$

Second way you probably have not I mean given lot of attention here, it is not only had a intersection, but intersection on the y axis also. So, that additional del p has to be subtracted otherwise and in that case L by D you have keep it unchanged. So, what is essentially happening while extrusion either you are doing a correction because of the extra vortex it's forming in the terms of additional L by D ratio or else you are trying to taking it care of that additional L by D ratio corresponds to, how much of additional pressure drop. So, that is how you take care of so these are the respective terms you can see it from here. So, this is how you do the you know corrections for L by D ratios I mean entrance corrections.

$$\dot{\gamma}_{wa} = \frac{4Q}{\pi r_0^3} = \frac{4u_{r_0}}{r_0}$$

Similar so wall slip can be estimated also how much wall slip it happening it is all together a different, little different experiment what you do you again run the capillary viscometry. And then you try to do for I mean same L by D ratio you do it, but different diameter other way round. So, if you try to do it first try to plot shear stress versus shear rate. And you try to add a given shear rate, shear stress you try to see all this intersections. And then try to generate this type of a plot this gamma 1 gamma 2 gamma 3 in a axis and x axis you try to plot 1 by diameter.

Then what you have to do finally, you see all this wall slip parameters I already have depicted you this you know different integral form of it. And finally, what you get it this is the wall slip and this the second integral parameter it vanishes basically. It actually becomes you know at a constant shear stress if you do the experiment this term will vanish. So, this additional 4 u r 0 by r 0 and that is exactly what is the wall slip parameter that ultimately you get it, this kind of a plot the corrected one wall slip. And then from there with the shear rate, shear stress you see as I mentioned with the shear stress at higher shear stress you have a higher and higher wall slip possibility.

$$\dot{\gamma}_{wa} = \frac{4Q}{\pi r_0^3} = \frac{4u_{r_0}}{r_0} + \frac{4}{\tau_0^3}\int_{\tau}^{\tau_0}\left(-\frac{du}{dr}\right)\tau^2\,d\tau$$

So, that way you can calculate again all these things sources are given this is from applied rheology of by B.R Gupta book. So, earlier one you might have not noticed, the problem number 2 was taken from a Aklonis book the source is given here. The first problem which is related to you know WLF it's taken from very fundamental polymer books written by Stephen. So, far you have seen 4 different problem, In 4 different direction first one was related to WLF equation.

Second one was a generalized conception of storage and loss viscosity storage and loss modulus in between that relationship assuming a generalized Newtonian model Newton's model. And the third problem we try to understand the correction factors, corrections that we have to often make in the capillary rheometric measurement say for example, bragley correction and related to a estimation of wall slip for the details, you always please refer and ask me in the question I mean 2 times I will be appearing online. So, if you have any problems whatsoever first you refer to the book, if you cannot solve yourself you raise the question that time we will we will be happy to clarify you. Now, problem number 4 once again it is a bit related to the rheometric experiments it's a cone and plate rheometry. So, you just try to see this is a cone your sample is placed between the cone and plate here it is placed and this is rotating oscillating basically, With angular frequency omega and a measure torque that rheometry is given m and this is the geometry typically you see this is alpha is the angle and every now and then on a cone you have to really see to estimate, what is the vertical height from that plate basically.

So, this is the problem. So, again we try to what we are going to do actually calculate out shear rate and shear stress, with reference to this geometry and this kinematic parameter including the geometric parameter like angle radius as well as the kinematic parameter like your you know angular velocity. See, again a tangential velocity v of a point on a cone let us try to realize it is v equals to omega into r cos alpha, From the geometry if you realize at the distance as I mentioned it you if it is a d is the distance is alpha into r. So, obviously your velocity gradient or rate of shear, rate of shear is related to what it's actually velocity gradient. So, velocity by vertical distance. So, it will be roughly about omega by alpha.

The tangential velocity v of a point on the cone relative to the plate is $v = \omega r \cos\alpha$. Fluid is sheared between that point and the plate over a distance $d = \alpha r$:

$$\dot{\gamma} = \frac{v}{d} = \frac{\omega r \cos\alpha}{\alpha r} \xrightarrow[\alpha]{\text{small}} \frac{\omega}{\alpha} \qquad (\textit{independent of } r)$$

*At first glance, it might seem that there is a gradient component in the r direction because tangential velocity increases with r. However, material points in a cone at constant ϕ do not move *relative* to one another; that is, they undergo rigid-body rotation, and so there is no shearing in the r direction.

So, it is depending on the how you then increase the you know shear rate simply you have no option when a given geometry alpha is fixed you can change the angular velocity. So, as you increase the angular velocity your shear rate is going to be high and high. Now, let us try to understand how much is shear stress to do that first try to realize the torque, torque equals to shear stress into area the force into momentum. So, dM equals to tau into 2 pi r dr from the geometry r cos alpha and then if you try to put and integrate and calculate you end up having an expression, tau equals to 3M, 3M is a measurable parameter as I told you already you the direct measurement is a torque into 2 pi r^3, r is the diameter of the you know plate basically. So, that is how you calculate similar.

$$\text{torque} = \underbrace{(\text{shear stress})(\text{area})}_{\text{force}}(\text{moment arm})$$

$$dM = (\tau)(2\pi r\, dr)(r \cos\alpha)$$

Integrating over the cone face

$$M = 2\pi\tau\cos\alpha \int_0^{R/\cos\alpha} r^2\, dr = \frac{2\pi\tau R^3}{3\cos^2\alpha} \xrightarrow[\alpha]{\text{small}} \frac{2\pi\tau R^3}{3}$$

$$\tau = \frac{3M}{2\pi R^3}$$

So, let us try to divert our attention to a parallel plate geometry what happens how do how can you calculate. So, here unlike a Newtonian fluid, which was the easy to realize we are assuming a power law fluid, Power law fluid once again what is power law fluid, shear stress equals to what. So, that way you calculate basically with the two parameter model. So, in a disc and plate viscometry obtained an expression for torque related to maintain a steady rotation. So, this is the geometry everything is clear omega is here you have the x term here and r term here ultimately this what I told you remains same, d is the distance between the two plates stationary as well as moving plates.

So, now consider a ring of the disc. So, it is a disc is a ring of radius r and try to imagine a area element I mean thickness element in the perimeter dr then area will be obviously 2 pi r dr and dM equals to r into tau into d into A. So, 2 pi r^2 tau into r now this is your power law fluid, tau equals to k into you know gamma dot to the power n that is what. So, you try to substitute here and then you got to see Rw by d to the power n and then accordingly you can calculate out you know respective terms say for example, here you can easily calculate out here the shear rate gamma dot equals to r into w by d. So, that is how you got to calculate that this problem was only about to calculate the shear rate, for a power law fluids up to that point I have given it to you for any further details, any type of a fluid a similar sort of a problem in a parallel plate geometry can be taken forward. As I mentioned it to you for this sort of a problem you get yourself familiar with using MATLAB.

Consider a differential ring of the disk (or plate) surface, at radius r with thickness dr:

$$dA = 2\pi r\, dr$$

$$dM = r\tau dA = 2\pi r^2 \tau\, dr$$

For a power-law fluid, $\tau = K\dot{\gamma}^n = K(r\omega/d)^n$,

$$M = 2\pi K\left(\frac{\omega}{d}\right)^n \int_0^R r^{2+n} dr = \frac{2\pi K(\omega/d)^n}{3+n} R^{3+n}$$

or,

$$M = \frac{2\pi K R^3}{3+n}(\dot{\gamma}_R)^n \qquad \text{(power-law fluid)}$$

where

$$\dot{\gamma}_R \equiv \frac{R\omega}{d}$$

So, to understand the MATLAB you go to you know MATLAB help files and try to see start from how to write a you know equation how to plot a data enter a data that you as a beginning after this you know numerical session problem solving session, you try to slowly yourself into the MATLAB get you acquainted with. So, we will come back again we just try to cut it short only five problems we came up with from three four different books, but we'll try to come back again with similar sort of a numerical problem challenges after we finish the processing. So, with that thank you very much.