Rheology and Processing of Paints, Plastic and Elastomer based Composites

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Lecture 42
Numerical problems related to various processing techniques

Welcome to NPTEL online certification courses on rheology and processing of paints, plastic and elastomer-based composites. We are on week 7 today and its lecture number 7.6 titled Numerical problems related to various process techniques. So, so far in the last week we have been I mean last lectures We have been talking about various processing as I promised today. We will come up with certain processing You know related numerical problems Say for example, start with the screw I mean, I mean with an extrusion rather and you remember I talked about total volumetric flow rate Which is actually if it is Q and Q is going to be, this is a resultant one equals to Q drag minus Q□ minus Q Leakage, so this is what the total volumetric output Looks like I mean, we are considering there is no constraint. It's a open discharge condition if you recall So now forget about this and we will try to Concentrate on the drag flow part of it.

Okay. So just try to read through the problem first a Polymer is extruded with a screw extruder, whose single metering section. We just consider the metering section only, Forget about the compression forget about the feed. So what's happening within the metering zone? Where from it's going towards the you know die land and followed by the die.

So a barrel internal diameter is given 150, So this is the D you can see the picture side by side. Okay, try to Interlink screw pitch is going given 150. So this is a screw pitch. Okay in one rated rotation it covers Okay and depth of the Screw flights it's consistent and constant since it's the metering zone Obviously, it's a 9 millimeter and width of the screw you see this is the width of the screw Okay, this is the width of the screw okay, so that is given as 15 millimeter and the length of the metering section is one meter say the screw is a Single start helix So I'll as a prerequisite or as a further study try to see the different Definition of a screw, starting from pitch a start a flight please read through it Okay, you must understand some definition about a screw right-handed helix, left-handed helix, helix angle, So in this case helix angle, you can see this is the helix angle phi. Okay.

So anyway, we will try to calculate What is the helix angle? so if the screw turns a hundred revolution per minute find the volume throughput of the polymer when no die is there, that's what is called open discharge condition, I elaborated last time also and you refer to this figure Correct. So this is the whole about that. So defining the problem Let's try to go to the solution straight away as I defined if you can recall from the earlier slides Okay, so your Vb, I mean rather we will try to define it Q Okay, which is rather than From Vb, I mean Q we have to calculate Vb you are trying to calculate okay pi into diameter into rpm of it, So you have calculated a Vb the velocity. Okay, remember? So the screw is going to the forward direction and then the melt is Sheared, and hence no net movement of the melt normal to the screw flight other way. It's taking way this way we are trying to see component of velocity in this direction.

$V_b = \pi D N$

So, in order to do that we must calculate the cost component of it. Okay and cos phi, phi is the helix angle Okay, so whatever you get it point seven five giving those parameters out for rpm you convert it Revolution per minute to revolution per second, of course, and then you can you have a diameter So straight away we calculate the Vb. So Vb is cost component is this, Now let's try to calculate cost component of it. What is the phi? Okay, phi you can calculate simply from the geometry you can calculate circumference You know that D value of it. So from that tan inverse this thing is 17.

V=0.785 cos ∅ m/s,

7 is a helical angle, So if it's 17.75 you can accordingly calculate the velocity cos phi of 17.75. And what is unknown here, you know? Width is given so width is that cost component. Remember your width is given in this direction helical angle direction So you have to see the component and minus 15, 15 is a flight width So this is the total so essentially H is the height of the screw.

$$\emptyset = tan^{-1}\left(\frac{150}{150\pi}\right) = 17.7$$

So essentially what we are calculating, we are trying to calculate volumetric flow rate So, area you are calculating W into H is the area and then you multiply with the velocity What you get is Qd. Qd equals to V H W by 2 and that way you calculate total volumetric flow rate Okay, so that is how you do it now think about a problem Where? You have a constraint got it constant means you have a die on that you don't have a open discharge So in that case there will be pressure build up. So if pressure builds up, There will be pressure flow back flow. So that you have to calculate, so total resultant volumetric flow rate is going to be then Okay, your whatever you calculated Qd or Q small d or capital does not matter, Minus Q pressure flow that is the back flow minus leakage flow So that way you can calculate pressure volume the total volumetric output. Remember I talked about pressure volume while designing it, combination of die with the screw design So that way you can calculate given a system Within the from the metering zone if you consider you can calculate out But of course if you have continuous diminishment of the you know flight either depth or flight width Then you have to take other complication comes into your consideration Okay, so we are not considering for this problem at least feed to compression However, your you know volume is constantly diminishing but in the metering zone you have a constant volume anyway So you just consider the simplest possible case and that's the solution you get it ultimately, So, problem number two is directed towards injection molding machine.

$$Q_d = \frac{VHW}{2}$$

Remember I talked about one thing, Once I am considering your screw has taken up to the reservoir, it got a short injected through the screw nozzle and you know gate, got it in the injected long return valve closes and it is pretty much into that mold, Now It's trying to take the shape. So at that juncture you have high pressure build up, As well as high temperature now what you are doing you are trying to cool it down. So while cooling continuously your pressure drops and You try to release it then the cycle goes you try to release it once pressure reaches one atmosphere You make pressure which is outside pressure of it Okay, then then you just open the mold and the whole thing will come out. Okay So let us try to calculate what temperature ideally, we should open the mold or in other words, What temperature pressure actually comes to one atmospheric pressure that's a problem. So, let's try to read through the problem, Question number two PMMA taken an I mean representative polymer to be injected in the mold, the cavity is will be sealed by freezing the gate, when the mass of the polymer cavity is at 165 degree centigrade it should be centigrade.

Okay and under the packing pressure of 40 MPa, Assuming the slow or uniform cooling, Okay. Predict the temperature of the melt at which the pressure of the cavity falls to the atmospheric pressure, So, one hitch you have to convert the unit 40 MPa given, Pressure during the injection when the mold is covered and then you have to convert it to atmosphere that can be taken up is a standard conversion factor 1.0 1 3 into 10 to the power 5 something like that. So, In order to solve the problem. I must get you familiar with one thermodynamic isotherm That correlates essentially the pressure Inside the cavity and the specific volume of it and with the temperature, so it's a I mean thermodynamic state equation, okay, so Interrelating pressure volume and temperature.

Okay. So this called Spencer Gilmore equation, This is very very important while calculating the temperature at which the pressure diminishes comes to atmospheric pressure So let's try to go through the problem, So if it is so, so what is I know the pressure is given Okay. pressure is during the injection 10^3, I mean its packing pressure is 40 MPa. So let's try to put that figure in Newton per okay in Pascal and Remember that unit was in Pascal and this is a figure and this specific volume is not known, I don't know the specific volume of it. Okay, so I know the temperature of course the temperature given in the Kelvin, Whatever centigrade you have 165 you remember we converted it plus 273 So 438 Kelvin so from there you straight away get a solution specific volume to be 8.763 into 10^{-4} m^3/Kg, the next step we are cooling it and while cooling it.

$$\left(10^{-3}P + 2.158 \times 10^{5}\right).\left(10^{3}v - 0.734\right) = 83.1\,T$$

temperature But I know that pressure has to come one atmospheric pressure with the proper conversion I made it Okay, and then I'm here. I'm sorry and the specific volume I put it here. So as a solution you get temperature to be 369 degree and which amounts to 96.5 degree centigrade, That's what I told you not necessarily, you have to come to the ambient temperature in the I mean hot condition itself, You just release the mold because most often engineering plastics has a very high Tg more than hundred or above So pretty much you can release that Okay, and then you have to think about how you dissipate, sometimes you Try to pull it down by air, sometimes you try to pull it down by sprinkling water or something like that. So on cooling See this 96.

5 degree the pressure comes to one atmosphere, That's the bottom line and the specific volume contracts and impression must put away from the walls of the committee, if the cooling is not slow. This is a comment I mean, this is not the absolute one These are the things you have to consider in a realistic injection molding cases slow and uniform Then the ideal treatment has to be modified but this is one of the things Spencer Gilmore equation that you can utilize, While deciding the processing conditions at what temperature ideally you should open the mold. So accordingly you program your Injection molding cycles as simple as it is. See, it is a simple one equation problem but it yields you, you can translate it straight away into the your warehouses in the production floor basically, This is interesting problem related mold shrinkage, okay mold shrinkage means polymer You know say rubber you put it in a cavity Okay, what happens you heat it at high temperature liquid flows fills the cavity Correct, and then what you do you try to reduce the temperature. So while reducing your rubber whatever liquid state it is there.

It will undergo volumetric contraction and metal mold also that also undergo contraction so how do you calculate then the result at contraction because rubber will expand more and contract more vice versa upon temperature cycling but metal will be less than that of that so as a result While you cool it down rubber will contract mold inside the cavity rather than the mold shrinks So that way you have a mold shrinkage. So that that is how you define a mold shrinkage Now, let us try to address this problem Okay, so a rubber to be injection molded in a cavity of 200 cc act at a pressure of 10^3 atm at 150 degree centigrade So that is the atmospheric pressure mold cavity volume is given, Pressure is given and you know the temperature now calculate the volumetric strain Assuming the bulk modulus to be 3 Gpa, I'll explain why bulk modulus is so important because bulk modulus you always often assume to be infinite So if it is infinite that means upon changing pressure there will be no change in volume But ideally I mean in realistic case is not so. So you have two effects, let me go through the problem first and come back, Assuming uniform cooling and predict the volume shrinkage of the plate when removed the mold at 20 degree centigrade, Say in a cold country Okay, where atmospheric temperature is 20 degree, room temperature is 20 degree and volumetric expansion coefficient of steel is 6 into 10^{-4}. Well, you see and rubber is 6 while steel is 0.

3. you can understand, You know expansion coefficient rubber is much more. Okay, so almost similar is the case for plastics and you know fibres. So also assume there is no change associated with the mold or steel due to the bulk compression, Bulk compression I am assuming bulk modulus of steel is infinite. So how to attack the problem. First let us let us try to see the definition volumetric strain that arises because of the pressure effect.

So you are pressurizing it, So your K is defined by P by del V by V Okay, so, you know the capacity of the V is known to you calculate del V_1 Let us define del V_1 del V_1 you are getting it from here now Further just simply calculating the from the equation of volumetric expansion You can calculate how much volumetric expansion del V_2 it undergoes just for the rubber sake or polymer sake Okay, and of course one thing I just neglected the metal case I neglected so you can calculate metal, How much it contracts the cavity volume so let us not take it into account. So you can very pretty well calculate two effects. One is contraction due to the polymer and second is contraction due to the bulk modulus effect from here. So if you have del V_2 here del V_2 minus del V_1, you will give you the resultant shrinkage Clear, However, you can see the figure 10^{-6} you can neglect it. So ultimately you you can calculate 15 percent is a shrinkage there.

$$\frac{\Delta V}{V} = \frac{P}{K}$$

$$\Delta V_2 = V - V_0$$

$$\Delta V_2 - \Delta V_1$$

there So, that is how that the basic fundamental of a mold shrinkage. Now all it depends that total volume you can you know, if it is a rectangular, if it is a square depending on the geometry Okay, you can assign to total. This is the total volumetric shrinkage and what it'll be manifested in all dimensions. Many a times if you have a very complicated mold Then it's it will be more like computational rather than numerical solution of it to be very practical Clear. so the bottom line is that, Unless you allocate that shrinkage factor into that, Say suppose if metal also undergoes same volumetric contraction that of the plastic what is the problem? You won't be able to release the mold tightens from the mold cavity, that rubber contacts more than the metal.

But what is important at the end you have to suppose if you are trying to make a six feet by six feet Okay, that extra shrinkage has to be allocated while designing the mold. Is it not very interesting and stimulating you can buy pen and paper calculate actually But when the design becomes little complicated of the mold Then that is why you have to go for computational way of mold designing taking into account. I just took two factors what is up, you know one factor is a volumetric expansion or contraction, another is a bulk modulus part, fair enough it gives you some idea about that, The fourth one is related to the internal mixture as I mentioned it to you, Fill factor is very important unless you correctly calculate a fill factor. There will not be enough space distributive mixing will be difficult even dispersive mixing will be difficult. Let's try to see one formulation of rubber.

See, this is a master batch formulation, master batch means incomplete formulation. No curatives Nothing, just we have a EPDM rubber lot of filler GPF, process oil and certain minor ingredients So Phr means parts per hundred gram, right? That means is the mass and other side you must know density of each ingredients Since I have taken minor ingredients I have taken average density. So what's the problem a laboratory internal mixture having capacity? 3.0 liter remember I talked about a commercial case internal mixture as a volume of hundred thousand liter.

Well, laboratory one is 2.5 or 3 liter here and determine the amount of EPDM you have to weigh for this and fill factor you have taken it assume it is 0.8. So I have to weigh how much ingredients are to feed in so it's simply okay, Rho equals to m by V that formula is a basic thing. You probably learnt in your seventh standard or eighth standard Okay, so that formula must be utilized.

This is the mass.   This is the volume and this is the density. So calculate the volume So you calculate volume of each ingredients? Okay, so net volume we can calculate now process becomes so total phr is 240. So it's a unitary process okay, In 214 cc you have a weight of 100 grams of rubber and you have remember you have 3 liter and 0.8 of it fill factor and calculate 3 liter as a available volume excluding the rotor volume. So that way you will be able to calculate how much EPDM ultimately you have to weigh for.

W= NV x SG x FF

W – Batch Wt [kg]; NV – Net Mixer Volume [dm^3]; SG – Specific Gravity (density) of the mixed batch [kg/dm^3]; and FF= Fill Factor.

For given this mixing phase So that way it's very simple only one formula that necessary rho equals to M/V not other than that. I'm not going into that how you because there are you remember internal mixer? I talked about there are other factors also you have to take it into consideration, Rather than the you know Fill factor alone, but of course the rotor speed plays very important role because that tries to increase the virtual volume of it Okay, so that is a very elementary thing one must learn while working in a rubber laboratory or even working in a rubber Factory because that way you have to program when your internal mixer how much each ingredient has to be put in correct? So I will not go into the many many problems Although I can show you many problems that I already taught about the theoretical part of it But let's try to see because I spend some time on two roll mill processing Okay, remember in the well talking about I talked about dispersion and distribution Okay, so dispersion I talked about onion model ultimately that accounts for millimeter to nanometer, how it goes the filler aggregates inside a rubber matrix Okay, here in I would like to talk about dispersibility factor, you remember from the stokes law I showed you a formula, dispersibility equals to 6 pi eta gamma dot by C what is what? Eta is a viscosity I assume Newtonian from the formula you can see gamma dot is the shear rate and Denominator C is the cohesion between the filler. So larger is the number this is dispersibility factor high will be the dispersibility. Obviously if you have a I'm sorry.

I missed out R factor here. R is the radius of the Filler, we are considering so smaller the filler size, K will be smaller. dispersibility so smaller the filler size, Okay higher will be the surface area. They will try to get united. So C will be higher. so unless you increase the viscosity or shear rate viscosity also given a rubber matrix.

You don't have much to do with that only thing you play with is a shear rate. And that's why I told you in the two roll mill or internal mixer in the nip action nip area, you try to generate very high enough shear rate to disperse, or ultimately you try to increase the dispersibility factor. That's the background theory. So let us go to the problem first Calculate the dispersibility factor of ISAF Okay, typical size of 20 nanometer average size, Here it is given 15 in the problem. In natural rubber at 30 degree centigrade the viscosity of the natural rubber at 30 degree centigrade is given.

So your eta is given correct and the here people try to when the problem is complicated by power law exponent, So this equation slightly gets modified as you can anticipate R into gamma dot Okay, K into gamma dot to the power n Okay, that's how it's modified n by C, Correct so you have to account for I am sorry. It should not be have the problem is wrongly taken ISAF Same filler the cohesive force C factor is given. So again, this is the formula So again, this is the formula, Forget about the power law fluid I am just considering for the timing as a Newtonian fluid If power law accordingly, this is nothing but eta into gamma dot is what? Tell me what the shear stress correct, so shear stress is tau and For power law fluid accordingly you get the modification like that it just gets modified So accordingly you have to replace those in place of eta into gamma dot and then finally calculate you get a dispersibility factor. So relative to two different, three different fillers you can calculate dispersibility. You can comment on which is more dispersible. $K = 6\Pi R_e \eta\gamma/C$

Which is less dispersible? Correct, so third one, Remember here we just considered the other part of it Taking into account that Newtonian fluid here, The last question, last numerical problem we will try to discuss here, It's about the Weisenberg number you remember Weisenberg number plays very critical role, while deciding whether it will go to, I mean region 1, region 2, region 3 and region 4. Region 1 and 2 are dominated by elastic responses while 3 and 4 are dominated by viscose responses(viscosity) ok, so we will try to calculate the Weisenberg number with the given Kinematic factor like geometry of the role. I mean its radius, the nip gap, and rpm of the roll. Simple so I am just ignoring the friction ratio part of it. So we have to comment whether elastic force dominate or viscous force dominates.

So let us go to the basic definition of Weisenberg number I taught already Okay, which is what the systems relaxation time theta divided by machines relaxation time If Weisenberg number is very very less than 1, That means system will try to flow so viscous dominant. What is greater than 1? Elastic dominance if it is just like 1, 1 is dangerous here in this case Neither elastic but nor viscous. So it's a quasi or mosaic. So it goes pretty much into the region 3 Correct. So that way just put in the numbers calculate it out.

$$
\left.\begin{array}{l}
W_e \ll 1 \rightarrow \text{viscous flow behaviour} \\
W_e > 1 \rightarrow \text{elastic behaviour} \\
W_e \approx 1 \rightarrow \text{flow instability}
\end{array}\right]
$$

What figure you are getting 2H0 is a 2 into nip gap. So we have to go to the H0 which is half of that and put it in the formula of Weisenberg number. You see you get a number 3.86 Which is what which is greater than 1 that means elastic dominant here at this stage. You cannot really comment on whether it's a region 2 or region 3 pretty much you want in region 2 only Okay, So normally Weisenberg number close to 1 or 2 or 3 Is within region 2 but it is more than that in 10, 12, 20 Then it's region 1 when you just put in the rubber and you remember I told you rubber bounces like a elephant.

$$W_e = \frac{\pi R N \theta}{H_0}$$

It doesn't want to go. It has all reluctance to go inside the nip. So this is another problem which which will give you a clue now why you do that? You can change this parameter say for example, you try to see your rubber is going to go. You know to region 3 you want to restrain it restrict it to region 2 so change the parameter accordingly, Okay either RPM Or nip, nip you have the liberty with the lead screw. You can always change the gap between the two roll and then you constrain it into the region, You know where you want that means two pretty much Another problem remained I couldn't give you because of the time constraint. Remember in the two roll processing I said whether it to go to front roll or back roll, It all depends on the nip gap as well as the friction ratio.

So you can expect in your examination problem related to that So hope this particular class on numerical problems and its approach will help you for better understanding what I taught so far regarding the processing that subsequent upcoming lectures. I'll try to take you through how we apply rheology in processing. It includes a simple example of wire coating by T head extrusion or cross head extrusion and Subsequently, we will try to see in general extrusion designing a die computational, Taking into account computational fluid mechanics, Remember don't get afraid of we will try to see very out of knowledge that you have so far. But we will be using one of the software tool to guide you towards that direction Okay, Once you do it go through and through practice yourself next time you will be an expert designer But remember one thing I'll tell you here, This course is not meant to make you an advanced learner or it's not meant for the advanced learner or expert. I'll take you to the intermediate level and next time when you try we will be able to be a expert.

I hope so With that. Thank you very much references all that I taught So two things I'll be covering in the 8.1, About the wire coating and this is another thing. I again I'll emphasize re-emphasize on extrusion because extrusion is the body of it in the Garvey die and profile extrusion will talk upon and then we will try to take you to CFD both demonstration and few of the lectures will be how to do CFD yourself or computational design of dies. I'm not taking care of the other part of its crew designer is outside the purview of this current lecture With that. Thank you very much