Rheology and Processing of Paints, Plastic and Elastomer based Composites

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Lecture 45 : Introduction to FEA based computationalfluid mechanics on extrusion 2

Welcome to NPTEL online certification courses on Rheology and Processing of paints, plastics and elastomer-based composites. We are on week 8 today and lecture number 8.3 which encompasses introduction to FEA based computational fluid mechanics on extrusion and this in fact these are lecture number 2, same continuation where we talked about. So without going into the additional keywords and all let us come to the point first. So today I am going to give you today on basically. So far I talked about the rheometric experiment to understand the rheology and other physical property measurements.

I will show you how you can take those data to your computational platform and come up with a design of a die that is going to be our motto. And of course before I begin I must tell you one thing we do not expect you to be an expert end of the day but at least since this course is designed for beginner and intermediate I will give you the clues what is next and how you can effectively utilize all the knowledges you gain while attending the class till end. So now coming to the rubber we have chosen is a compounded elastomer. Basically it is a EPDM based one that I am going to exemplify.

So this is all about the profile extrusions to make seals to make you know weather straits etc for automotives. So the basic experiment you must perform before you go for designing a die for a particular given shape is first the capillary you know rheometry at constant temperature and as a you know complementary I mean as a another experiment you have to do side by side which is a you know parallel plate rheometry or cone and plate rheometry so that you can cover the whole range of shear rate small very low to very high that is not written here. I mean you read it like there is that will actually complement the total rheometry experiment. So two types of experiment you do it initially one is at constant temperature with varying shear rates and second one at constant shear rate varying temperature. The reason is why because you must understand one thing first of all you have to define the fluid type I mean you remember I talked about different fluid models you have to figure out exactly what model you get seen and those models has to be you know called or invoked into the computational platform number one.

Number two as I mentioned it to you it is not a very isothermal experiment I mean temperature does not remain constant all throughout the processing channels I mean right from the feed to the you know compression to the metering and even after metering also where your skin pack everything is there you have a die land and you know die leave up to that point and not only that after it extrudes out you have a continuous variation of temperature. So you must be able to your computer must know what is the rheological model and what temperature how it is going to change so that you come up with the solution in the post processing way you come up with the solution of what is the velocity profile going to look like. So is it not interesting so I am trying to give you one to one correlation what you learn and what you are going to do in application. And as I mentioned it to you it's a you know you have to concern little bit about the thermodynamics part of it. So you must know the you know heat capacity of that specific heat of it.

So you must have a measurement on the scanning electron I mean differential scanning calorimetry to understand to measure the heat capacity of it. Here it is mentioned dynamic mechanical analysis I am not say dynamic mechanical, it's more of a parallel plate geometry you read that way in a oscillatory mode basically or cone and plate mode. The next one is a thermal conductivity because your as I showed you set of equations I mean there are two condition one is the momentum part another is a thermal part. So in the thermal part your conductivity specific heat all are involved and also the density. So you must measure the thermal conductivity density and you know your specific heat from differential scanning.

So these two parameters will be fed independently into the platform. Platform means whatever simulation performance I am talking about otherwise you have to write the code accordingly for the solver. So here we will take the advantage of existing solver and here for this exemplification and what I used in my research was a ANSYS platform. And it is a registered platform and they have one software which can be plugging into the ANSYS platform is called poly flow. It deals with the designing dye etc etc understanding the flow behavior.

There are various commercial softwares but I am referring to them because we from the institute we are licensed we brought that. So I mean off and on I am referring to them so that in order to get rid of any conflict commercial conflicts there. So a non-Newtonian behavior easiest way as I told you earlier to look it from the power law point of view but hardly non-Newtonian fluids like rubbers they hardly follow that. I mean this probably fits in better with the models which has more parameters like maybe 4 parameter, 5 parameter like Carreau yasuda module, EPDM based formulation fits Well, natural rubber there are certain other recommendations. So I am not going into the details because since it is for a beginner.

So if I elevate this course to advanced level then I talk about what composition approximately feed with what constitutive equation of rheological equation. But this is what I am not going into the details you all know why now what is power law, what is Newtonian fluid, what is non-Newtonian fluid. So in order to characterize Newtonian behavior what you have to do the bottom line is that you have to do the rheometric measurements using two distinct rheometric technique. One is capillary which accounts for the higher shear rates and parallelly you have a low shear measurements that's parallel plate or cone and plate cone and plate and parallel plate comparison I told you. When there is a question of edge fracture you try to do it more like a cone and plate and for shear uniformity that I discussed I am not going again back there.

See here is the example you are trying to fit in a power law equation although I will be doing in a Carreau yasoda or Eyring other models. So just to give you a feel of it. First of all viscosity as a function of shear rate you try to have it. And then you try to overlay the result by superposition principle so that to capture from very low to high although it's so shown here is a capillary rheometric measurements already. But you can always do the superposition to have a master curve.

So here it fits in and you see a power law equation fits in with such a exponent. So you can obviously see that how much is going to be your exponent and pre exponent factors. Similarly, you can segment wise you can fit it in. Like I said a true or realistic polymer has a upper Newtonian in between some power law or other fluid and lower Newtonian sort of a lower and upper Newtonian. So that you can fit it in part by part also.

So I am not going into the regression part of it. Anybody can do it having a data and as any commercial software like origin or excel even you can fit in those data by the process of regression. So that is one component of it. But what is important here what I am going to talk about here little bit about computational fluid dynamics. See here in this example what we are going to exemplify, there are several ways you can have a solution.

As I mentioned it to you, you have less parameter more number of parameter less number of equation from the basics point of mathematics point of view. So you have to have a numerical solution and that numerical solution, one of the means is by finite element way. So what it is you have a you know big problem you split it into smaller and smaller you know mesh of it. And you try to actually have try to have those solution in the notes or small elements and then try to have a global solution from there. So it is something like breaking apart the problem to smaller segment and then try to solve it in every places and reunite it and have to have the final solution of it, that is how the finite element works.

Simplest example those who are not from that background I have given you a piece of cloth say. Then piece of cloth you have to make a hemispherical tent. So you have a hemispheric equation of a hemisphere say. So you try to how do you make a hemispherical tent then you have a basement ready with certain grids. And you have a adjustable you know bars or rods and first fix the midpoint and then second other places you try to adjust it.

So in finite element sense what it is going to do you have in your mind a equation of hemisphere and you try to really minimize the error and finally having a global solution. And then it is up to you to figure out where the tent you made by that process you understand what I mean. So suppose this is the basement of it you try to have some places like you are meshing it that way and every place you have a rod and try to overlay the cloth and you have a hemispherical try to have a central one first fix it here and then rest part of it you have a adjustable height and with that you adjust and finally to have it. So locally you are trying to figure out the solution with the minimum error and then finally try to reunite them having the final. This is the basics on for a layman that is the best way I can explain you.

I am not going into the details of the fluid mechanics but also designing a car when it appears to go at high velocity aircraft even a motorbike even a you know tire running on a slippy road which has lot of water and that water is going through so you have a drag from the you know air as well as from the you know water flowing through those channel you know cornering effect etcetera etcetera the classic example of fluid mechanical problem. So what we are going to give you a glimpse of that I am not going into the details itself demands three four such courses and they are expert I am not expert to be very honest here. But what I am going to give you a glimpse of that idea out of it. So let me read out what is written here computational fluid dynamics is a branch of fluid mechanics that uses numerical analysis of data structure to solve and analyze the problem that innovate fluid flows. Ultimately here unlike here we are dealing with the structure but here we are about the fluid flow try to see the you know velocity profile of it end of the day and after it flow is frozen what is going to be the resultant structure taking care of the basic problems of viscoelastic fluid that is the di-swell I mean that arises because of the first normal force difference surface irregularities that arises because of what second normal force differences that are going to be our point of concerns.

So computer used to perform this calculation as I mentioned nothing is doing the regression and solving it and simulate the interaction of liquid with the gases with surfaces defined by boundary conditions. So essentially you have three things first is preprocess that means you are giving essential inputs to the computer including the drawing, meshing giving the constitutive equation, governing equation, parameters and then actually you are trying to solve it you are simulating basically you try to solve it and try to see where the it is leading to the convergence with the I mean just monitor the Jacobian part of itself. So it is a kind of a once you get that the solution is a post process. So preprocess simulation that is how normally a finite element works. So now about the poly flow softwares is advanced general purpose finite element based CFD software product you can buy it commercially.

For analysis of laminar flow typical in the polymer processing as well as for the application this is good for person who is not actually from CFD background but still he knows where his material is going to be applicable. So just he has to use that platform and get it solved there otherwise an expert will always like to have his own code own solver ready so that you can fine tune it's a laminar you go for a turbulent flow. Say for example you are some few models or material models are there you try to embed more I mean make it more like universal. So those are the things and of course to me for a materials engineer the shortcut is use a platform like ANSYS, ABAQUS or whatever CATIA whatever you try to use it, and that solver you try to use it and if necessary you write your own subroutines eventually over the development. So here in the cartoons it shows some of the results that directly have been or people have been doing like making a say for example in a blow molding process or different-different unit processor and they try to make it what should be the typical design of the mold, design of the extruder etcetera etcetera.

So without going into the details let us try to be very specific as I mentioned I will show you exactly if you have a package how you are going to use it. I mean I am referring to polyflow because I used it I know that but otherwise you can refer to any any packages. Bottom line is that you are trying to solve your rheological problems and then try to come up with a design. In this case we are concerned about extruder die design nothing more than one of the design screw, we are not going to do other component of it because again that will be computationally more complicated problems. So poly flow accelerates design so I told you the motto of that if you try to design by iterative process you make something and then again you machine it, do it again try to see the profile match it if not again try to fine mesh it troubleshoot.

So that you want to get rid of this will help you in that essence. So poly flow accelerate design well shrinkage energy and raw material demands to make your manufacturing process more cost effective and environmentally friendly way sustainable way. And poly flow package has its unique inverse die design capability that is also important part. See one is given a geometry you try to see what you are going to get. Inverse is given a profile you directly feed in and it will just you know it is not actually happens in an extruder it is a virtual it comes out and your die as if it is deformable and it will show you what after deformation of the die, what is going to be your actual design that will give you that profile.

So that capability it has built in. So final die design is much faster I will elaborate both of the techniques. One is the direct extrusion that means you are given a geometry try to see what is going to be a profile structure is and second one is a inverse extrusion technique that means you are given a profile that profile is a kind of flashback I mean snapshot is it person is walking in a TV you see open action replay and then you try to take him back that kind of an action. So now let us try to go to the console directly. So console you have a ANSYS system design assessment many things are written here.

So it can do many things I mean it is electric is written IC engine is written but nonetheless let us go to the poly flow part of it. In that in the data entry you have number of things you have to geometry like I said whether profile geometry or die geometry you have to import from the AutoCAD or somewhere. Then you have to mesh it so there again you have to check the mesh optimization process whether the type of mesh there are different types of meshes 2D, 3D polyhedron sort of mesh. So if you increase the complexity in terms of the dimensions so 2D to 3D your computational time will be more as obvious but you have to really optimize it and also the number of meshes. See wherever you have a critical deformation or more contours you have to have more meshes so that you are ultimately you are solving in those nodes and trying to build it back.

So obviously there will be more number of meshes of this region of interest ROI you call it. So you have set up you have a solution you have a results. So it shows you the whole process that means preprocess simulating and debugging of course you have to debug that error if it does not converge really and then finally post process analyzing the results. So this is the flow chart of it roughly as I mentioned in solidus or catia or anywhere AutoCAD design of that die or that profile you have to import export and then export to mesh section then you do the mesh and there you can do modification, it is a iterative process. Then you have a specify boundary condition specific polymer properties I will mention you what are all properties step by step and then specify meshing technique and solver method.

So it is a mesh stability test it does internally. So it is a re-meshing part is also embedded and then specify evolution parameter there are different evolution parameter by which you just write you rightly check that whether that meshing or final thing you have given it is correct or wrong and then you have the processing starts simulation actual processing starts and polypore solves the conservative equation set of momentum as well as thermal equations and then of course you have given already boundary condition with that boundary condition it solves and then is the solution converge and sometimes it will show negative jacobian. Then you have to again check with the parameters and re-do it and then finally it stops yes and then you have a post process. So this is typically a process flow chart looks like logically the algo. So some of the geometries to mention you here you have some simple geometries here and actual geometries this is actually a nucleosil geometry that we try to solve it actually eventually in one of the project work with one of the government concerns.

I am not naming it because of some trade secrets and confidentiality and these are the some of the profile EPDM based profile extrusions actually they are really applicable in a car body that you are everyday riding actually. So now second thing is the 3D geometry construct you do it with the things. So you can see essentially this is your die land region and you have the actual die part of it. So exactly this is the die land and die leaf and then this is the extruded coming out. So that is how the exactly 3D geometry of it.

Remember I have to define up to which length of extrusion it cools down basically after that you do not get any solution I mean it is frozen in you do not get any changes. So that is how I mean I told you one thing you remember running die swell and equilibrium die swell it is almost like equilibrium die swell position where it after that it does not change in change in dimension or anything going to the die swell or second normal force difference surface irregularities which additionally gets created. So next important part is meshing it. Meshing is again you have to do mesh optimization and all you see this is the this is how my entire 3D drawing is meshed with certain sort of a of course you have to choose pick choose a particular element type of element it can be 2D, 3D and whatever it is and then you have to do mesh sensitivity test whether the number of meshes you have chosen is correct or not. So that is what as I mentioned it to you so as I say this contours if you consider a contour profile this particular region you have to choose more put more mesh elements so that your solution will be rather here you have a flat area you can afford to have less number of meshes.

So like that you do it as per the protocol. So general assumptions are made that that your solver has given the flow is steady here incompressibility as I mentioned it should del V equals to 0 inertia effect we have taken out of question and this thing specific heat that I measure from you know DSC thermal conductivity by guarded hot plate or by laser methods. So those are remain constant as a function of temperature that we are assuming otherwise it will demand more computational time you can of course solve it but it will demand more time. See again if you try to see the setup so you are trying to put in some material data density gravity is negligible here and flow boundary condition these are very important part of course the thermal conditions heat capacity whether you are going doing isothermal or adiabatic depending on that. So then about the this thing about the material part of it you try to fit in with some of the constitutive equation like Bird-Carreau law we try to fit in here or you can choose a cross law I mean it is as per you and you see whole lot of models few of them I already elaborated discussed. Now only one part remain is the temperature dependent viscosity there are many equations but Arrhenius is very popularly used but you can use you know Herschel equation or WLF type of an equation in order to say suppose if you have measured done the measurement or your extrusion is running at 100 degree centigrade.

So suddenly some reason the temperature goes to 110 how to account for that so automatically if you have that feed in data it will try to you know extrapolate or interpolate try to see what is going to be a behavior if the temperature fluctuation happens in any point of time. So this is the Bird-Carreau model and typically this is what it is, you see it has a lower Newtonian and upper Newtonian in between you have a exponential dependency specifically and everything is embedded in the constitutive equation. You have a cross law also let us not go into the model by model I already discussed so what you do bottom line is that you have a master curve that means overlaid low shear rheometric measurement high shear capillary measurement overlaid to a master curve and then from there you try to fit in the data and figure out which model it fits in if it fits in what are the coefficients see there are different coefficients lambda you know eta infinity n eta 0 this is a 5 parameter model you can see from here and those are to be fed in actually precisely. Now you have to put in boundary conditions see starting from entry to die land to where you give the equilibrium the entire range so from the die land to die leap to even the extrusion channel some length so every point you give certain boundary conditions here given. So inlet velocity is fully developed so we assume that whatever is peeping in from the metering zone it is already developed velocity is developed no slip condition at the die wall free surface this part 0 pressure because it already came out of the pressure release component of it and traction or shear boundary condition so force equals to 0 Fn equals to 0, Fs equals to 0, Vn equals to 0 and the convection heat transfer from the free surface to the surroundings happen here it was inside the you know die only and the normal stress condition.

$$\eta(\dot{\gamma}) = \eta_\infty + \frac{\eta_0 - \eta_\infty}{(1+\lambda^2\dot{\gamma}^2)^{(1-n)/2}}$$

$$\eta(\dot{\gamma}) = \eta_\infty + \frac{\eta_0 - \eta_\infty}{1+(\lambda\dot{\gamma})^{m}}$$

I am not going into the details actually do not get you know frightened looking at the equation but I already so continuity equation is that from the point of the velocity momentum equation in all x y z coordinate is there in terms of pressure and you know shear stress so these are the some of the equation. Now you have a additional energy equation as I mentioned it to you accumulation term is the first term getting heated up then convection term conduction term and dissipation term dissipation term because of the viscoelastic behavior of it viscoelastic dissipation so, this gives you the energy balance so this also have to be solved separately. Now let us see what happens in the solver you have to solve it in terms of velocity contours try to see all these three different you know die designs so you see velocity at the center position is more red is more blue is the less so you see the velocity controls for all this dies but what I told you, you have to make a design of the die lands or angles such a way that this velocity distribution has to be uniform but none the less given a die design we are getting this solution that is also good. Then in terms of pressure fluctuation you see same thing again red is the highest blue is the lowest so you can see the pressure contours you see as it releases it becomes 0 it comes to the atmospheric pressure so in that extruded part obviously the pressure is releasing you can see it from here you see velocity contour once again viscosity contour so viscosity contours obviously it is a other way round after it really goes viscosity becomes high because temperature it is losing and then also the shear rate contours where the shear as I told you the shear you can see for this area you have the maximum shear stress. So what do you expect you expect more deformation there because your die swell is directly related to the shear stress or shear rate there so you can see a animation frame by frame so, that is how your material is coming out from the die lip and going towards equilibrium out here.

$$\frac{\partial}{\partial x}(v_x) + \frac{\partial}{\partial y}(v_y) + \frac{\partial}{\partial z}(v_z) = 0$$

$$\frac{\partial P}{\partial x} = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z}$$

$$\frac{\partial P}{\partial y} = \frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z}$$

$$\frac{\partial P}{\partial z} = \frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z}$$

Where, P is the pressure,

τ is the extra stress tensor,

v is the velocity.

$$\dot{E}_{acc} + \dot{E}_{conv} = \dot{E}_{cond} + \dot{E}_{diss}$$

So whole facet frame by frame you can analyze where it is going wrong and where I have to re-do it in my design basically so that way direct extrusion gives you a clue about the entire fluid flow. So you can see the comparison of the product and die shape see a product always will give you a red one is showing you the your die and you see blue one the product how it is deviate particularly this you see this was the you know die shape and you have see at the contour positions narrow angle position you have most swell reason is that there was a stress concentration. So across all design you can see here you see because of this you know again you remember that thick circular flow and channel flow so that velocity discontinuity is reflected in terms of die swell here correct. Now you can correlate what I taught you and what you are getting after simulation I am not going into the more complicated design, but nonetheless this particular slides is animated version of swelling. First one what you are seeing it the die and then finally, its deformation is giving you this portion of it so that the deformities everywhere it is showing.

Even see the dimension is changing I mean it was supposed to be in this position is going lifted somewhere. So that you do not want your channel will not fit in if it happens so. So this is about the direct extrusion now so even if I do direct extrusion I have no clue what is going to be my die design like. So ANSYS provides you in a other way round so you have that you know profile and try to fit in with the same material parameter and try to see what is going to be your final design. So this is again by inverse extrusion process we have set in the boundary condition you see the velocity contours I am not going to repeat it pressure contours similar way viscosity contours and shear rate contours.

But end of the day what you get is other way round this is the profile actually and that is going to go into the die and it will show you what exactly but actually it cannot happen it is a virtual things everything virtual. And then here in the animated part you will be able to see this is the profile set the blue one and which is filled one and unfilled one is shows you what is going to be the die. So you are getting a ready solution one go then what all that you have to do you have to make a preliminary experiment making this die to your tool room and then try to have a single screw extrusion and check it small little precision patch up you have a final design done without much of an iteration. So that is the beauty of it so from the animation you can see it is exactly other way round your profile shape and die shape. So is it not very interesting guys so, to conclude at present extrusion industries are following traditional process of designing the die for particularly in indian context extrusion of this profile keep making physical prototype of the die tune its flow balancing do repetitive testing until the desired product shape is achieved in a practical commercial extruder extrusion this process usually involves lot of trials in the design.

And by understanding the rheology by understanding the simulation what you do we can shorten this product development cycle with more precision mind that and we improve the quality of the products by running trial and error process with simulation rather than the testing changes and production like. So this lecture gives you a glimpse of that again I will repeat I do not expect that after today s lecture tomorrow you will be able to design yourself but at the same time with this foundation you will have a courage to peep into that window. So this I aspire to give it in that I will plug in those lectures injection molding, blow molding, other mold design technique by computational fluid mechanics technique. And till that time I will come for the next lecture thank you very much bye bye.