Polymers Processing and Recycling Techniques
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Lecture – 71
PolCoPUS: Flow Simulations

As we are getting towards the end of this course, we have transitioned into the 10th week and we have been at it in terms of discussion of various aspects of polymeric materials. The first half of the course was focused exclusively on looking at the structure and properties and in the latter half, we are focusing more and more on the processing aspect. So, we are continuing our discussion on polymeric processing materials and recycling of these materials.

In this lecture, we will look at an important component of industrial polymer processing these days, which is in terms of use of simulations in order to optimize and arrive at quick decisions as to how overall processing operation ought to be carried out. So, flow simulations have become quite common and there are several versions of flow simulators.

There are several types of flow simulators which are available and it is routine now in industries to actually use these along with the experimental trials to try to speed up the process of arriving at the best processing operation and the best formulation and the best part at the end.

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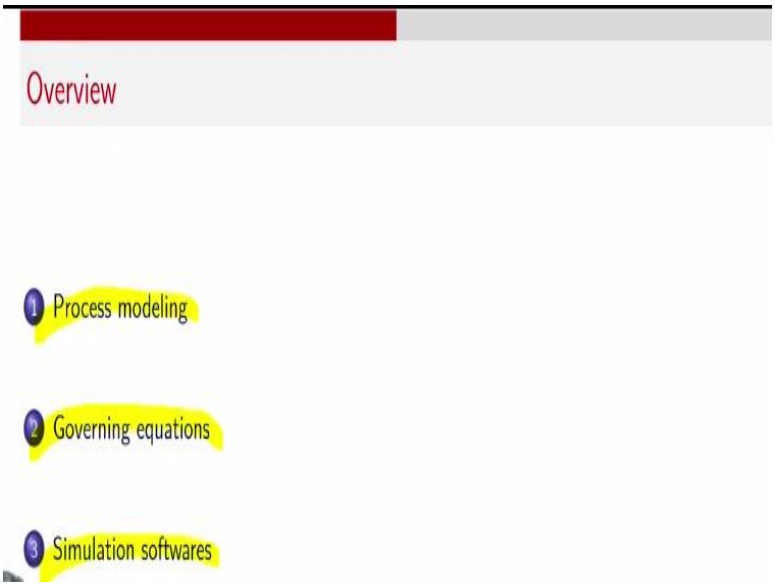

So, we will look at quickly what is involved when we try to do this process modeling, why do we need to do it, and we will look at the governing equations which are solved numerically by these simulation softwares. Given that this course, the emphasis was on polymeric materials, we will look at all of these from polymer processing point of view alone and then stop with just looking at a survey of what is the range of softwares which could be available or what is the basis behind many of these softwares without going into commercial aspects of what are the specific set of softwares available.

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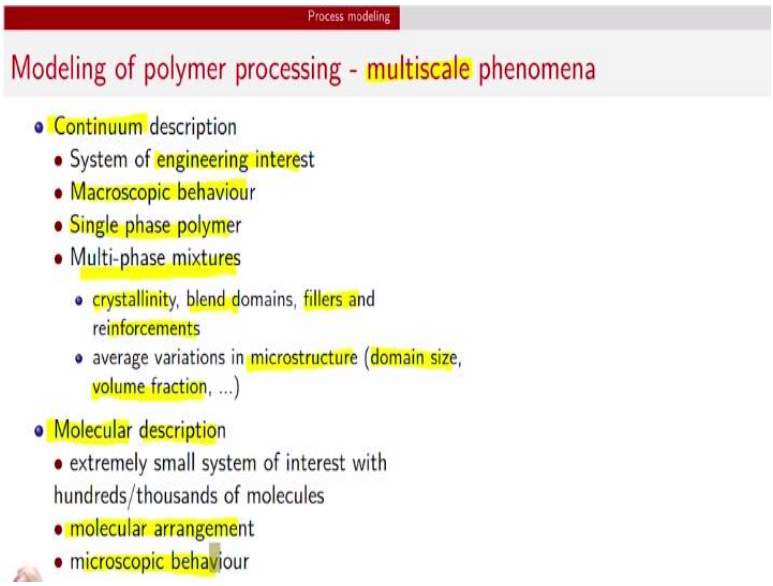

So, modeling of polymer processing inherently involves multiscale. This is a word which we have used quite often to describe the polymer themselves because from bonds all the way to macromolecular chain, there are several scales involved in terms of relaxation processes and we have even scales which are beyond were polymers are absorbed on surfaces which behave differently or maybe there is a blend and there are domains of two blends and so on.

So therefore, what we have is phenomena where macromolecular systems are multiscale. Because of this when we look at processing of these polymers, some of the features of multiscale nature feature in these processing operations also. So quite often when we are dealing with a system of engineering interest, we will follow a continuum description where we assume that the material is made up of these so-called material particles.

And they are distributed everywhere and between two material particles that are infinite, in fact uncountable infinite number of material particles. So that is the description of a continuum and this basically then let us get away with the discrete nature of atoms and

molecules and there is nothing in between and these atoms and molecules interact with each other. So instead of that, we make a hypothesis of a continuum.

And then we solve problems which with governing equations, which come from mechanics of continuum or continuum mechanics. So, this is very useful because in the end, we may be interested in looking at the macroscopic behavior in terms of what is the velocity and temperature profile, what may be the shape and so on. So, we could have a single phase polymer involved in a polymer processing operation or a multiphase mixture.

Of course multiphase mixture could be because we are having a crystalline and amorphous domains, it could be because there is a blending or it could also be that we have a composite material being processed. So not only do we need to know what are the multiple phases, so once we try to understand these multiphase mixtures and we are looking at their processing, we need to look at also the variation in microstructure, for example what may be the domain size of one blend component versus the other.

What could be if it is a miscible system, then what is the volume fraction or concentration of one species versus the other? And we need to do all of this as a function of space or the function of position within the part and this is quite necessary because sometimes if let us say the volume fraction of plasticizer increases too much in certain spot, the part may become too flexible or the reverse is also there that let us say plasticizer is absent or very low concentration, then that part becomes very rigid.

So generally, it is of interest to us to make sure that the distribution is good. Sometimes, we can also exploit this distribution to enhance properties in a certain range of the material, certain space of the material, but in any case, we need to know the description of multiphase mixture as a function of time and space. The other side of description is based on molecular description. So, this is by methods of statistical mechanics as opposed to continuum mechanics that we discussed earlier.

So, in this case, what we have is basically representing atoms and molecules, we have entities and these entities are interacting with each other. So therefore, we are looking at the molecular description. The problem of this kind of an approach is the fact that we have a very small system that we can deal with. Even all the advances of computations it is still not

possible for us to do a very large system with these things because the sheer number of molecules involved is extremely large.

I hope you recall that Avogadro's number gives you an idea of what is a number of molecules per unit mole and any engineering system will be having some moles of a mount. So you are looking at very large quantities of molecules to be stimulated. However, what is very helpful and why statistical mechanics has become such a powerful tool to simulate many of the systems is the fact that we can get a good average behavior even with the thousand or thereabouts number of atoms and molecules.

So, we do not need to really go to the 10^{23} atoms and molecules to represent a good realistic material. The advantage of doing molecular description is that we get the molecular arrangement and microscopic behavior as part of our solution. So therefore, given that using processing we will be modifying microstructure which will in turn influence properties.

If we can get a good description of what is the molecular microstructure by doing molecular description, then that is very helpful because that is what will determine the properties in the end.

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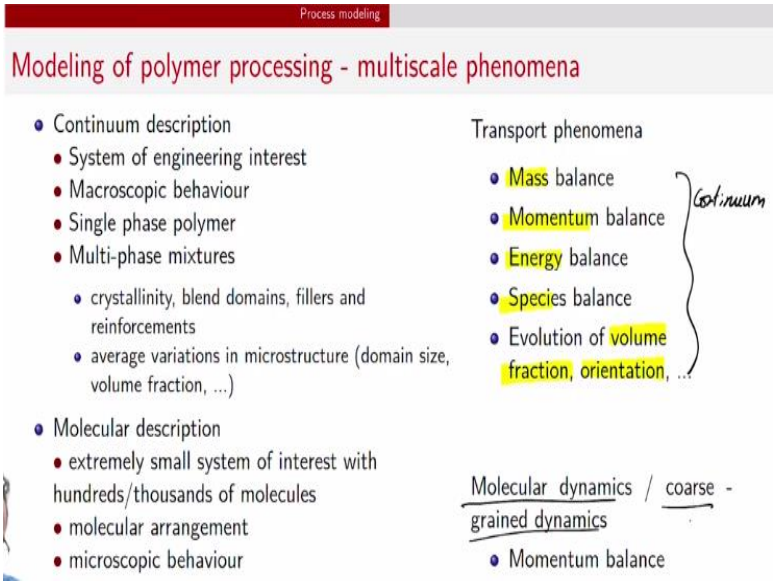

So generally, what is involved during a polymer processing operation is transport phenomena, which is taking the polymers away from equilibrium, making them flow, heating them, applying pressure on them, forcing them to flow through some narrow openings. All of this basically induces transport phenomena which is related to change of mass, change of

linear momentum, energy balance, species balance, or also if there are multicomponent systems evolution of volume fraction.

We may be also interested in knowing what is the orientation of macromolecular chains and so generally we can first write down and then solve many of these governing equations. This is again based on the continuum approach. On the other hand, we could also do molecular simulations or coarse-grained dynamic simulations in which case basically it is the second law of motion, only the momentum balance between all these atoms and molecules which are going around, they will interact with each other.

And keep on changing their position and their velocity also keeps on getting adjusted. So, we can write momentum balance at the level of these so-called particles which are molecules quite often and we can then try solving these equations. Given that there are hundreds and thousands of atoms and molecules representing particles, so the solution in case of molecular description is exceedingly slow and therefore to do large systems in such methods is not very feasible at the moment.

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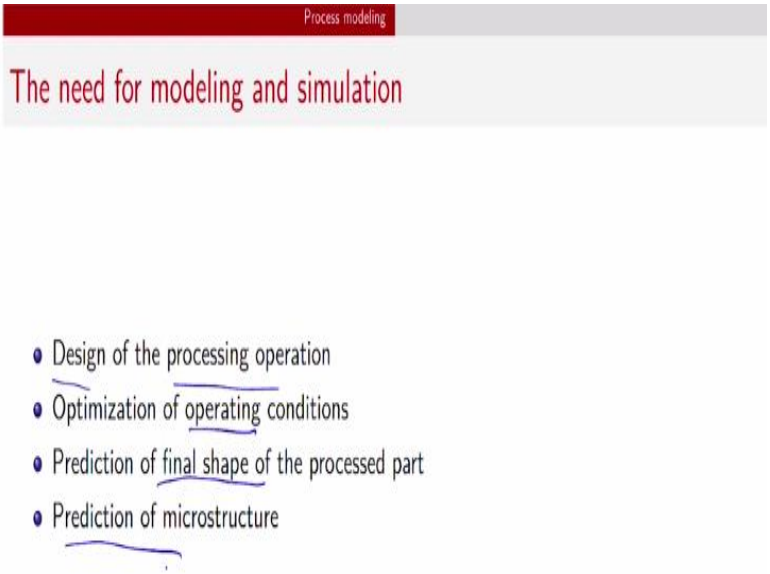

So why do we need to do all of this? Why do we need to do the modeling and simulation and probably all of you know the answer, but I have just condensed it here. We would like to design a processing operation and so that to see what kind of design will be needed. What kind of justifications do we give for the pressure that we are using? Where should we place the heaters? How will be the materials of construction of many of the components of the processing operation?

So various questions which are related to the design of processing operations. The other thing which goes hand in hand with the processing operation and its design is under what conditions will it be operated or using what conditions will this be operated? So the temperature, pressure and so generally we need to optimize, given a good design of a basic set up now we need to optimize for each and every material.

Based on the processing, the final outcome is the product, so is the product in the shape that it is required? And if any of these is not done properly, then in the end we may have a process where we get the fabrication done and but the acceptance rate and validation of the final parts may be lacking and so overall efficiency of the operations in this case will be compromised. Now, another important aspect of modeling and simulation is to predict the microstructure itself.

So, we can use this microscopic description to try to you know find out stresses in the material, velocity profile, temperature profile, concentration profile, so all of them can be solved. However, the description still remains at continuum level. Now, can we use this continuum level description to try to start predicting what is the microstructure? Now as soon as we want to go to microstructure, we need microscopic information and it may not be sufficient in terms of assuming continuum.

So quite often these days, simulations are also multiscale in the sense that they try to do simulations with molecular scale for certain things and they do bulk scale the simulation with governing equation with mass balance, momentum balance, energy balance to get the overall idea of the engineering process.

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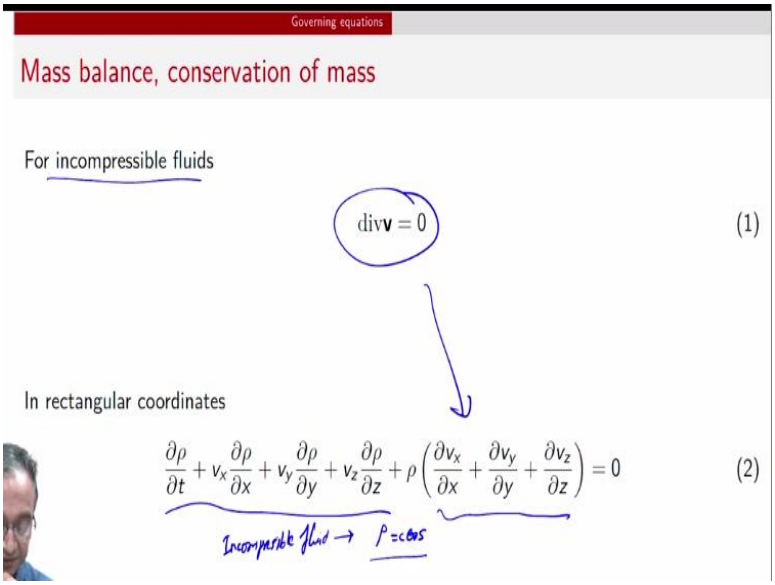

So, we will look at the equations which have to be solved and we will largely assume incompressible fluid as far as polymeric fluids are concerned and so divergence of velocity is pretty much the only expression that is required. So for example, in this you can see that for incompressible fluid any way all the terms will identically go to 0 because for incompressible fluid since ρ is a constant, you can see that all of these derivatives will go to 0.

And then we are only left with a divergence of velocity being 0. So this is one important component. So what this says is velocities are not independent in different directions as they depend on x, y and z, the variation is related to each other.

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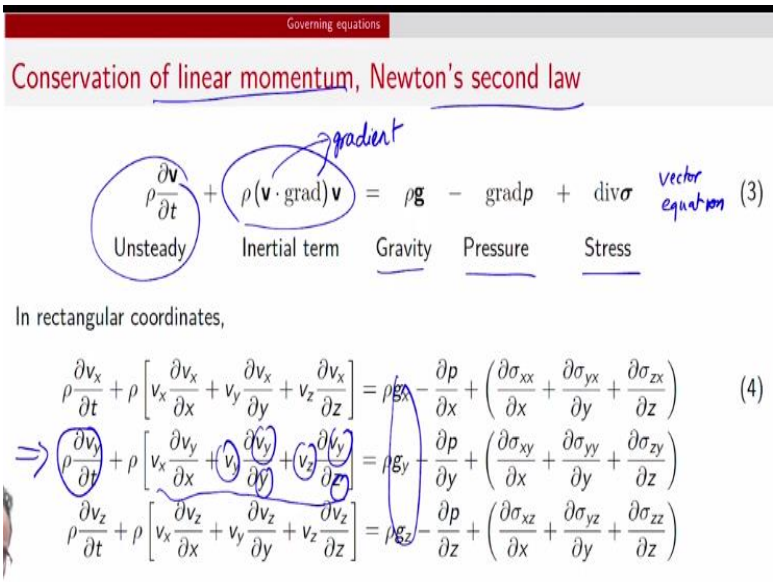

Now, the other governing equation is based on Newtons second law or we can say conservation of linear momentum or linear momentum balance and this is a statement where

we say that the unsteady change in velocity or velocity change at a given fixed point as a function of time. Then we have the inertial term which talks about variation in velocity as a function of position.

So the unsteady term is related to velocity at a fixed point, but change related to time, while the inertial term is related to as the material particle is moving, as the fluid element is moving, as the polymer is moving what is a change in its velocity. So that is why there is gradient operators being used here and gradient implies derivatives with respect to space. Many of these governing equations are far more complicated in cylindrical or spherical coordinates.

But the overall structure of the equation looks similar. So, you can see that the first time let us say, if we just focus on the v_y component, the first term is straightforward in terms of the derivative of v_y with respect to time. What you notice here is of course this is a vector equation, so therefore there are 3 components. Mass balance on the other hand was a scalar question and there was only one equation.

Now, the inertial and unsteady term are balanced by gravity, pressure and stress and generally there is a misconception that if I use the symbol τ it is shear stress, and when I use the symbol σ it is total stress, but you always have to look at the source and then try to make a sense of what is exactly being said. So do not go by symbols alone, so in this case σ is a total stress tensor, so the gravity, pressure and stress balance out the unsteady and inertial terms.

And this is the inertia term, you can see that if v_y changes with y or v_y changes with z, then these terms will be non zero provided v_y and v_z are also non zero. Depending on the coordinate system that we use maybe one of these quite often in school as well as other times we say z is where the action of gravity is. So, then $\frac{\partial p}{\partial x}$ and $\frac{\partial p}{\partial y}$ will go to 0 in that case.

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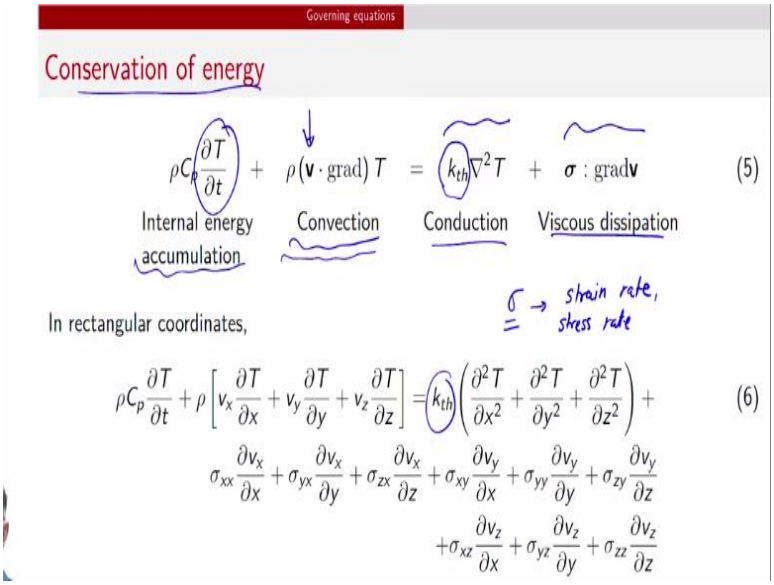

We have also to do the energy balance because of the associated heating and cooling that goes on in a polymer processing operation as well as changes in polymer that may take place due to the temperature change. For example, the conductivity of the polymer itself its specific heat may change, its viscosity may change as a function of temperature and so we need to know the overall behavior of the polymeric system under non-isothermal conditions when we have the energy balance as the key requirement.

Again, this can be looked at as terms of energy accumulated or energy getting convected, you can see that v is the velocity which is convecting in this case the thermal field. Then there is conduction mechanism and then you have viscous dissipation. So, the viscous dissipation in the material depends on the stresses that are being applied and how rapid is the deformation in the material in terms of gradient of the velocity.

So the strain rate in the material and stress determines the loss of energy or the dissipation rate of energy. And in case of polymers given that viscosity is very high, generally viscous dissipation will be very high. Additionally, in operation such as injection molding or several operations, the shear rates are also very high, gradient of velocity there is quite high. So again, viscous dissipation is dominant.

Over and above generally, the conductivity of polymer is not very high. In fact, we use polymers as both electrical and thermal insulators many times. So, the ability of the overall mass of polymer which is being processed to conduct the heat away is limited. At the same

time, even convection may not be always easy to achieve, especially because turbulent flow and rapid mixing is not possible in case of polymers.

So you can see why there is a very great relevance for conservation of energy in polymer processing operations. With heating, cooling and all the other processes where temperature is changing and we have high shear rates and very high viscosity the heat generated due to this viscous dissipation can lead to non-uniform temperatures in the material and non-uniformity can lead to a different set of properties at different spots in a part.

So therefore, the scalar equation which is basically a governing equation for temperature in material, basically the important parameters are the thermal conductivity and notice that this is an energy equation which is valid for all polymers, but we will have to choose a particular σ and how it depends on strain rate or a stress rate and variety of other variables to decide simulations to carry out.

And depending on the assumption of each and every polymer, sometimes we can say that look I will assume a certain type of fluid and then just get a preliminary assessment using a simulation.

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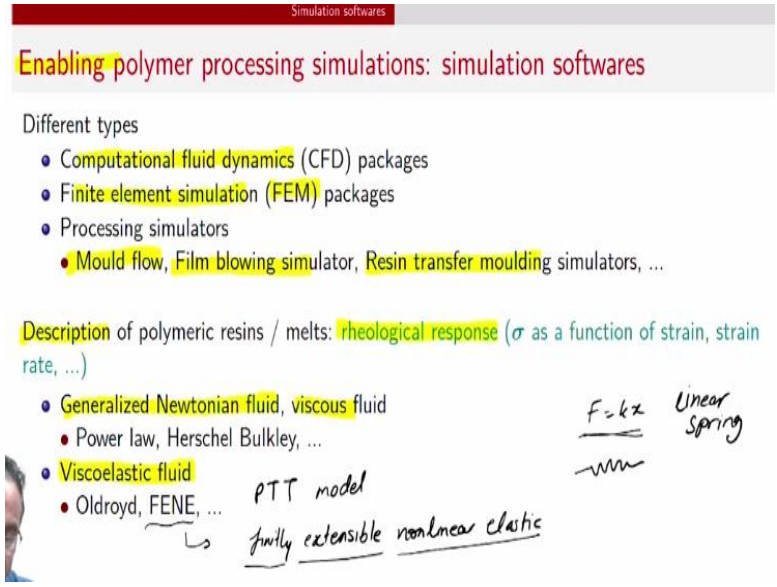

So, all this is possible. So generally, this can be enabled by commercial software which are available and these commercial softwares have to solve these partial differential equations with nonlinearities, nonlinearities I hope you can spot that in the same term we have basically

multiplication of variables. We also have nonlinear terms here, which are again there and of course we have partial differential equation.

So, these partial differential equations which also have nonlinear terms are quite tricky to solve and therefore we have either a finite volume-based technique which are computational fluid dynamics or finite element-based techniques, which are FEM packages. So options out there in both of them. Each package will have pros and cons depending on how it was designed, what kind of focusing was there in terms of problem solution, how many subroutines are available for the problem of your choice and so on.

So generally, these CFD, FEM packages are useful in R and D because they are a generic set of packages, you can solve any problem by suitably defining that problem in the overall software. However, there are trade based simulators also. So for example if a company is using only resin transfer moulding, then there are simulators available which can quickly give you again assessment of what flow rate to use.

What pressure to use or what could be the viscosity, which is appropriate for having a nice spreading throughout the fibrous bed in case of resin transfer moulding. So, the very specific questions which are related to resin transfer moulding will be answered by this kind of a simulation package. So, we can have injection mould flow or film blowing simulator and so on. So many of these specific set of software is also available today.

The key feature in all of these simulations will be how effectively do we capture the behavior of the polymeric materials. In other words, what is the rheological model that we choose, how close it is to the realistic behavior of the material? And of course, each of these packages will come with various options. So, for example, you could have a viscous fluid, which is called a generalized Newtonian fluid.

Where the overall model looks very much like Newtonian fluid but instead of viscosity being a constant, it is a variable and it depends on shear rate itself. So that is one class of material or you could also use viscoelastic fluids, which is like Oldroyd, FENE. One of the common polymers and this we will have a chance to discuss later on is called Phan-Thien–Tanner or PTT model. So, this is also used in polymer processing quite a bit.

This is a model which is finitely extensible non-linear elastic polymer. What this model does is based on molecular description, it imagines the polymer segment as a spring and the spring is non-linear elastic, which means this is F = kx, this is a linear spring. However, when we start stretching a segment as it stretches, the force required will be more and more. So it is not very good representation to show it as a linear spring that whenever you increase the stretching, the force will keep on increasing, but you can continue to stretch the polymer.

As you will lead to fully extended conformation for the polymer chain, there is no more further extension possible. So therefore, force must increase and eventually it should lead to the breakup of the polymer molecule. So therefore, we then use a nonlinear elastic spring in which case the force increases as you go towards the maximum extension possible for a given segment. So that is the reason for also calling it finitely extensible.

This implies that x can go on to infinity and only then force will become infinity. What we see is because of the finite extent of the polymer, it can be extended only up to that extent and therefore the force will go very high whenever this extension is reached.

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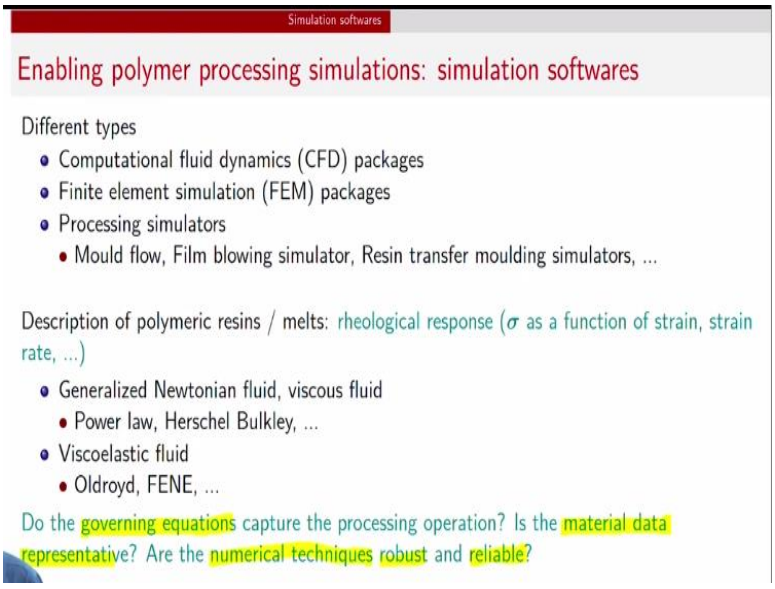

So those simulations are widely available and there are several packages and options available for us to do. Few broad questions that should always be at the back of our mind while doing these simulations and especially because simulation packages make it very easy for us to use them. With menus and clicks, we can basically formulate a problem. So the key question, and the first key question is really, I mean whatever governing questions we have chosen are they really appropriate?

Other very important aspect of a successful simulation is having a good set of material data because a polymer processing operation will use a very different range of shear rates, it will use a very different range of temperatures, compositions may vary from place to place and so it is very important for us to have the material data which can represent all these variations very nicely. One other aspect, which of course, we as users may not worry about and many times.

It is the software developers who worry about this, but as users we also need to know how to do checks and balances so that whatever is the result that we are getting it is within the robustness and reliability range of the software. So, there is always a good idea to try some simpler problems first and then look at the more difficult problem, and even when you are solving the difficult problem, look at some behavior which is easier to comprehend and easier to rationalize.

So many checks and balances have to be done for us to get a very good scope of results from these simulation packages. So with this, we will stop this lecture related to polymer simulations and in next set of lectures, we will start looking more on recycling related and sustainability related issues, still keeping the focus on polymer processing. Thankyou.