Introduction to Polymer Physics

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Lecture-48
Continuum Mechanics- I

Welcome so, so far in our discussion of Brownian motion and diffusion we have been talking about the motion at a molecular level and that will be true near equilibrium conditions that we have. So I want to take the discussion further looking into motion that happens at somewhat longer length scale a larger time scales that comes within the framework of what we know as continuum mechanics. So, let's say if we have like a polymer block or a polymer solution and if they are deforming or flowing then of course the molecules within them are also responding to the flow but what we see is not really a molecular level flow what we do see is like flow at a somewhat more continuum level where we can talk about the motion of control volumes or packets of fluid or a solid that undergoes a deformation or some sort of an averaged motion of molecules that we describe in terms of the control volume.

So, what I will do now is I will try to give you some quick background in continuum mechanics people of physics background may already have had it, so it is more for people from engineering backgrounds who did not have continuum mechanics and then using that particular background we will look at the flow and deformation in polymeric systems at longer length scales or I would say for microscopic systems as opposed to systems which are less than a micron or nanoscopic systems which are at a molecular level. For example when we looking at the Rouse model the higher modes refer to a very local kind of motion only for say 0^{th} mode we look at the motion of an entire polymer chain that the only the monster of the center of mass but if I look of like at a polymer block that is composed of a large number of polymer molecules actually moles of molecules then of course that description is not going to work that is one limitation to what we have done and second if we are looking at non equilibrium situations in which case diffusion is not the dominant mechanism then in that case to that description is not going to work. So, now we look at flow and deformation in a more general sense at along at a larger length scale than what we have been doing.

So, I want to do a quick review or tutorial of continuum mechanics, and I will begin with a description that does not differentiate between a liquid and a solid and then at some point on the derivation I will tell you like what will happen for the case of a liquid and what will happen for the case of a solid you will notice that it only happens when we come to the constitutive law the governing equations remain the same for a liquid and a solid of course we make certain approximations along the way and that may or may not be valid for the system that we have in mind.

But the idea the motivation here is the polymeric system can actually be in any of those states solid liquid is more likely gases of course less likely but more importantly they can even be between those two extremes. Let us say a polymer gel is both a liquid and a solid. It is somewhere between these two and therefore their flow or their deformation is between these two extremes that we have been used to and therefore we first build a general description and then try to start by looking at how the polymers respond after we are done with this descriptions what we also will do what will we will also do is to talk about the Rheology of polymeric systems where we take it from an experimental perspective of how do we characterize the flow behavior or extension behavior of polymeric systems that is the our agenda for the remaining of this course.

So, in the continuum mechanics we the first assumption we make is of a "continuum" and by continuum we mean that we do have control volumes or my system is large enough such that I can place many of these control volumes within the fluid or a solid, and the key idea is a control volume contains large number of molecule now the question is like how large is too large is it 100, is it 1000, it is 10,000 how large is too large when do we say that we have reached the continuum extreme and the answer to this is the following that it should be too large that we have variations that are significant within the control volume at the same time it should be large enough that we can take reliable evidence values.

Let us say when we define the velocity of a fluid packet or the velocity within the control volume this must be an average velocity over the large number of molecules because 1, 2 or 10 molecules will not give you a reliable evidence but if I say represent the entire beaker by one control volume of course we will have velocity variations within the control volume that will not be captured and that is the key idea of continuum. Continuum really means the notion that we have very large number of molecules within the system and any variation within the system can be explained by the notion of control volume were the control volume themselves contain enough number of molecules to get good averages yet not too large number of molecules that we have variations within the control volume.

So, of course if I have say a nanometer sized channel then within that channel across the diameter will have very few water molecules that is not a system where continuum approximation will hold but if I have say a channel of a meter size or a centimeter size diameter then in that case it's no longer an issue. So, the key idea is the length scales the sizes must be very high compared to the molecular length scales so why I say that the nanometer size channel will not work is because my water molecules are themselves like half a nanometer and therefore we will never have enough number of water molecules to represent a velocity within that nanometer size channel but that is no longer an issue if I have say a centimeter size channel or a meter size channel because we are very far or very high compared to the molecular length scale.

So, as long as this continuum approximation holds we can talk about the properties of any point with in the fluid or a solid let us call this point P in the continuum mechanics language this point is called a material point. And any material is composed of many, many of those points right. So, if the material moves all the material points also a move along the material and therefore the material point is not fixed in space, material point is fixed to the material itself. So, let us say here is a block and has my P and if I rotate the block like the like this way my P still remains there the relative position is unchanged of course if I look in any coordinate system the coordinate may have changed of P but the location of P within the material or a relative position of P within the material will remain unchanged.

So, if I look at any material point within the fluid I can talk about a small volume around that material point that I would refer to as control volume say V and which may have certain surface dS. So, just to illustrate the whole notion we can think of any small volume around the neighborhood of point P and that can serve as the continuum that P is a part of. When we say any property at P we do not really zoom in and try to look at what molecule is present there at that particular point, what we really mean is the property in the small neighborhood of the material point P that we can refer to as a control volume. So, now this point then experiences some body forces, let us say for example gravity and the position of this material point will change with time as the material deforms or flows so when I use the word deformation I typically reserved it for solid like materials when I use the word flow I reserved it for liquid like material but essentially the idea remains same both actually result in some deformation any change in the position of material point constitutes a deformation.

So, we normally talk in a language of the position of material point and let me represent as position of material point-

$$\tilde{r}(r_0, t) = position\ of\ material\ point\ P\ at\ time\ t$$

I am using the tilde here for the vector and the above thing is for the fact that it is a changing position or it is a function at time t and this is the position of P at t = 0.

$$\tilde{v}(\tilde{r}, t) = \left.\frac{\partial \tilde{r}(\tilde{r_0}, t)}{\partial t}\right]_{\tilde{r}=\tilde{r}}$$

We can also define the velocity of point P at time t again as a vector, so the tilde below represents that it is a vector the reason why we use a tilde then the arrow sign on top is because we soon will be needing higher order tensors and so on and therefore it is more convenient if I do it this way. At particular value of r I can find the velocity by simply taking a derivative with respect to time. So, then the r is also called by the way the velocity field. Just doing somewhat formal derivations that will set the ground for what we do next.

So, then we can define the equation of motion for material point P as something like-

$$\rho V \frac{\partial^2 \tilde{r}(\widetilde{r_0}, t)}{\partial t^2} = F_{tot}$$

There is simply mass times acceleration that is equal to total force which includes body forces such as gravity and surface forces such as stress. So, body force for example depends on the volume of the control volume that we have defined and this would depend on the surface that we have to find. So, far we have not differentiated between a solid and a liquid this is a general equation of motion for any kind of a material.

So, now let me define something known as the stress tensor that we use a lot in continuum mechanics and the stress tensor essentially amounts to the surface force or the force acting on the material point apart from the body force that is like acting on the entire material like gravity. In fact you can also include the body force within that stress tensor that is also a way but typically the body force is handled separately it is because of the molecules present in the system. So, in that sense stress do have a molecular origin but it is used within the continuum framework that is when we discuss it in the continuum framework we do not really resort to like a molecular origins or a molecular length scales but indeed the force acting on any point must be dependent on the molecules that constitute the material.

So, to understand what the stress tensor is what I can think of is around the material point I can draw a small surface around it and then that surface that contains the material point P, let us say this is my surface and a point can be anywhere on this surface then there are molecules below this plane and molecules above this plane and both the molecules above the plane and below the plane will interact with P that will give rise to a net stress in this plane okay. And I can draw the plane anyway. So, let us say my point is here I can think of a plane this way that way or any way the key point is the plane must contain the material point I am considering and depending on how I am drawing the plane the above and below represents the molecules that will exert a stress on the material point that I have.

So, let us say I am drawing in this particular way where the plane is normal to the Z direction. In that case I can think of the points below by this cube the plane containing material point P. So, now I have defined a volume around the material point keep in mind that this is really the cube that I have drawn is somewhat hypothetical in nature right. So, we may be looking at say a point that is lying in a beaker but we have drawn a small neighborhood around that point that is the cube that I have drawn here. And in that small neighborhood I cut a plane that contains material point and look at some volume above it and some volume below it, that is what we are doing here.

So, now I can also define a coordinate axis, let us use a different color this is my x this is my y and this is my z okay. So, in the way what we have drawn the normal to the plane is e_z . And for that particular plane we may have certain net force that is acting on that plane that I refer to as dF (z) that is the net force it is not the z component keep in mind. So, dF (z) is a net force acting on plane with outward normal ez.

So, now this plane will also have some surface area let us call it dS. We are talking about the force that is acting on the plane. So, if the plane would have had larger area the force must have been larger just because as I increase the area of the plane you will have more molecules above and below. So, whatever net force that acts on the step on the plane will increase as the area is increasing as the number of molecules is increasing so whatever interactions we have that results in the force will also be increased because we are talking about a larger area. And in fact it is not difficult to think that the force should be proportional to that because there is no other reason why it should not be linear right. So, as the area is increasing the force is increasing. So, instead of talking in terms of the force we can talk in terms of force per unit area and the force per unit area should be similar and therefore the force must be linear in the area.

So, then what it means is if I look at any particular component of this force let us say if I am looking at an α component then that also has to be linear of course so this also has a proportional to ds and there has to be a proportionality constant and that proportionality constant is what I refer to as the stress tensor $\sigma_{\alpha z}$.

$$d F_{\alpha}^{(z)} \propto dS \, so \, d F_{\alpha}^{(z)} = \sigma_{\alpha z} dS$$

This is the net stress that is acting this is the net, what I call stress that is acting on plane with outward normal e_z and of course we are looking at the component. So, it is the α component of net stress acting on the material and therefore the stress will have the units of force per unit area. So, although you may have temptation think of it like a pressure I will resist that by saying that the pressure in a material is typically same in all the directions they said is assumed to be as an isotropic. This stress need not be same in all the directions and we will talk about it later. So, although it has the same unit as the pressure it is not quite the pressure, pressure is typically assumed to be same in all the directions, pressure of course again has a molecular origin it is coming from the velocity of things and so on stress I would say is a more general concept that can include pressure but not vice versa. So, pressure and stress are somewhat different kind of concepts although both of them will have same units.

So, now although I have drawn in this particular kind of a way in practice I can draw a variety of planes with different outward normal. So, I can for example also draw a plane around P that for example maybe like that which have an outward normal along the y direction right. So, I can draw a variety of planes now that contains the material point P and for all those planes I can define the stress tensor and the components of that stress tensor.

So, in general using this kind of an idea what we can say that in general I can define a tensor with components $\sigma_{\alpha\beta}$ that are α component of force acting force acting on a plane of unit area. So, I have used a unit area here just to keep it force per unit area dimension normal to β axis. We can really find β as the as any of the plane depending on how I am how I am drawing the plane containing the material point P.

So, then it is it will be a tensor that in general will have components like this-

$$\sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$$

So, then it is it will be a tensor that in general will have components like this and we can define in any coordinate axis that we chose to work with. And then since I have said that dF αz is α σ αz ds I can write the statement that I have written right here in more general terms as dF-

$$d F_{\alpha}^{s} = \sigma_{\alpha z} dS$$

$$d \bar{F} = \acute{\sigma} \cdot \hat{n} dS$$

So, we will have something like σ αds the second term correspond to the plane which is at perpendicular to the normal that we have defined and the first component defines the direction or the component of the force I am interested in okay. So, this is like an intuitive way to understand it there is a more rigorous derivation that we can also do by drawing say a tetrahedron around point P that I will not go into right now. So, this in general I can also write as-

$$d F_{\alpha} = \sigma_{\alpha\beta} n_{\beta} dS$$

So, this is the definition of the stress tensor and we have defined the force acting on the plane on any plane that contains a material point P. So, in some sense this is a surface force that results from the interaction between molecules above and below the plane. Although we only say that we did not really go to the molecular description to get that forces will do that later. But right now it will suffice to understand that the molecules above and below a exert some force exert some net force in the material and that net force can be represented in terms of what is known as a stress tensor. So, of course it is possible that the net force is 0 in that case the material is just stress free. But it is also possible that the net force is not 0 in that case we say the material is under state of stress and it is that stress that give rise to the flow and deformation of the material.

So, with this idea I want to stop and in the next lecture we will take it further and talk more about the stress tensor for different kinds of material like solid, liquid and so on.

So, with that I conclude, thank you.