Indian Institute of Technology Madras

NPTEL

National Programme on Technology Enhanced Learning

COMBUSTION

Lecture 14 Combining Chemical and Thermal Processes 4

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This summarizes what we have done so far on the well stirred reactor, where basically we have considered a global mass balance over a control volume and global energy balance, so effectively now get a set of n equations which you can now say okay one equation is a sample for high species, there which contains your Yi which could now be just simply called as Yi as the n variables okay or the one sample variable, for this equation but then we also understand that ω Ri is going to be a function of temperature.

Therefore we need another equation to close this which is now the global energy balance and the global energy balance again involves the Yi okay so it is it is now coupled with, this one so unless you solve this we cannot solve this unless we solved as we can solve that and then we now see that the hi are the ones that are containing the temperature sitting on top here okay. So course you could you could make a calorically perfect gas assumption and say this is like linearly in temperature and so on if you want to simplify your life.

But if you want to do the hardest work then you keep the integral do polynomial fifth 50° 60 ° polynomials for CP and go on integrate and all those things and so okay. So that is the two equations and two unknowns but however I would like to point out or maybe you should be asking this question to yourself, ω Ri is not only a function of temperature but it is also a function of concentrations okay, whereas concentrations of species okay.

So it is actually a function of CI, T okay so but ω is a function of CI comma T but we do not we have not really had see eyes as our on our unknowns, we have been having Yi as our unknowns okay. So we need to supply Ci hear right so there must be some sort of a relationship between Yi and Ci to close that set, so you could look at this you are now actually having Ci as another set of fun own, so it is actually 2 n + 1 unknowns and equations. So you need to have other n equations that relate Yi and Ci.

So that is basically given by Yi = Ci Wi / by σ j = one to n c f/c I am sorry C_J capital Wj okay, so this is like you any time you try to find out why you have to find a C_I out of it and then plug it back in the deck ϖ i and use it there and so on so this is this is i equals 1 to n as well okay. So previously i mentioned that in some of the problems where we want to size the combustor right we want to know the volume, rather than input the volume.

So that the volume is now like the square lead the thing in question, so therefore you now try to redo this problem a little bit by saying sometimes, sometimes a residence time is defined as residence time is defined as $t_R = \rho_V / m$. How do you get this m. times the time it takes is like the mass, mass flow into it complete the total mass flow into it that should be equal to the density of the mixture times the volume the mixture occupies.

Okay that will be the mass that is contained in it so if you have a m dot kind of mass flow rate that is coming into this volume over a time of TR during which it is supposed to reside in this volume m dot x TR is the mass that is into this volume that should be equal to ρ v right so with of course row given by the equation of state where we now say this is equal to P times w mix / or UT you now begin to see the molecular weight a lot more okay previously we were dealing with moles.

And we were always looking at the universal gas constant but now the molecular weight kind of tags along because we are now beginning to do things in a mass basis okay so here w mix is the mixture molecular weight that is defined as it is not really defined you can actually calculate this but this way so this is this is obtained by amass weighted approach so this is like one over sigma i equals 1 to n why I /WI this is again a statement of mass conservation okay so if you take like

one mole of the mixture and look at its mass constituents each of which has different molecular weights okay how will the number of moles of each of those pan out and then you now add the number of moles and so on okay so that is how we are trying to do this is this can be derived but I am NOT going to derive this for you stated it.

So if you do all these things then here in this problem in this problem we are given we are given m dot that is like the throughput that we want to achieve V or TR okay and Q dot okay so if you now have a TR you can try to find out V and so on course I guess we also given P so in NP so the pressure at which you want to do the work to do this do this problem and then you can actually have a relationship between T is a variable get him to be evaluated and so you can actually have relationship between TR and V okay and what else that is about it okay so if we get M dot given this is given the so you just have to go ahead and solve this okay.

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So we have so if you want to now count one let us say two and three okay one two and three actually gives you 2n+ 1 equations we are interested in obtaining why I comity that is n+1 quantities right that means if it is possible for you to eliminate your sea ice okay for 2n+1 equations for why I see I and T that is 2 n+1variables just as well but we are interested in these

say I and why I they do not really give additional information okay but you just have to go through that.

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So what typically happens in this case is you could you could do this problem in a multiple ways depending upon what you are looking for as I said the other day okay so essentially these are algebraic equations did you notice that right so 1 2 & 3 are all j brick equations but they are nasty algebraic equations okay so this is this is going to be a very nasty looking expression in temperature okay first of all and then you have this T sitting on top of this integral and all that stuff so this is this is not going to be a very easy equation to a set of equations to solve okay so what would we do with this we can do a couple of different things one for example you now say let us let us look at Jesus parameters in the problem all right and if I am now allowed a certain m dot I fixed that and in certain p and I.

Now say I will allow a certain Q dot that is fixed okay that is like a heat loss to the surroundings if you want or if you want this, this reactor to be heating something else like, like let us say in an a in an external combustion engine where you have a combustion chamber that is giving heat to like I said let us say a water to get converted into steam or something like that you want certain Q dot ok so let us suppose that you can put that there and on now but you want to make sure that your combustion is complete okay so what you then do is you now start varying your TR okay so as you now keep on varying your TR you now get for each value of T are you now get your why I and T.

And then you now can plot your YI and T as a function of T are okay why I aunty are actually not functions of pretty much anything there, there are no independent variables here we are not looking at time or space nothing okay these are parameters in the problem so you know very your TR you can now get your species and temperature to, to be calculated as function of TR and then plot this what you should find is beyond a certain value of TR are these things will stop varying right you could also think about it like it is as if like giving more and more volume is it essentially it is like you know how like a little large pipe.

And then you are basically looking for how long this pipe should be for your reactants to become products larger the longer the pipe larger the volume and greater the residence time so if the reactants had actually become products somewhere here but your pipe is still longer okay the products are going to continue to remain that way and what you are going to get out will be the same as if you were to add truncated your pipe somewhere here you see.

So if you were to increase your TR your answers are not going to vary further on right that means you, you can actually decide what should be the right residence time by the time these things now level off to some value beyond which you do not have to worry about so that is like the way you, you sighs your combustor you now say this corresponds to a certain volume and therefore I will now get my length for this diameter.

And so on okay we cannot distinguish between diameter and length that is that there is a no-no because we do not know how what is happening inside okay so you fix the diameter by some other consideration or the lateral distance then you can get a length out of it and so on because you can estimate a volume for complete combustion okay so one of the ways of doing.



This is by beyond, beyond a certain, certain TR or v why i and t stop wearing this means no further change no further change in the in the reactor for the extra volume or residence time provided right so this is used to size the combustion or okay we will just stick to the word reactor as a pure chemical engineers okay that is fine another thing that you could do is let us suppose that I had a reactor all right let us suppose that I had a reactor and my question is how much MDOT can I can this reactor handle can I dump more and more reactants at it alright so that is another way of looking at it so essentially the point basically these are parameters you could vary them.

And you can now fix a few things you can vary one of them to see what is the effect of it so another meaningful variation is to actually keep varying your m dot given other things okay so beyond a certain m dot I mentioned this earlier beyond a certain m dot the equations do not converge to a solution when you say converge it implicitly means that you are going to solve these things numerically okay with an iterative approach it is like this is like chicken and egg problem I do not know ω i I cannot get my why I so I do not know my why I so I cannot get my tea and so on right and do not even think about solving this simultaneously like you used to do in your middle school simultaneous simple algebraic equations to equation to a known system.

Right so obviously what you are going to do is say it if we start with some guess right and then plug that in there and then see well you get an answer for the next iteration and then and so on and of course if you keep doing this blindly you are probably going to go haywire okay so you are starting guess must be pretty smart okay and then you need to look at things like method of steepest descent towards see solution and so on so you have to adopt even other matter of fact Newton rap son method kind of thing is sometimes too simple for these kinds of solutions gated that are required here.

So ultimately but basically what I am saying is you how you are looking for a numerical solution that means you have to converge to, to a set of answers for you so you may not converge all right so that that simply means as far as this model is concerned is a blowout that means these equations just simply cannot be satisfied for the set of parameters that we are looking at all right the typically the way you do this is you, you start with some m dot and then keep varying okay until you hit a point where you cannot get a solution then you know that beyond this point the flame would not sustain is essentially what it really means okay.

So that that becomes a meaningful exercise it is it is like it is not like you just took some set of parameters here and then just juggle with aware being them dog taking like 2m dots and let us say take two pressures and all those things that is not the way you do you see how to systematically do so that you approach the no solution situation and then you know that you are approaching m dot am in a physically meaningful manner right.



Okay I would like to point out a couple of things in what we have done here which are which are somewhat unique or interesting one the notion of residence time is a very powerful idea okay regardless of how complicated an analysis that you want to do or not this gives you this gives you a first good idea so for example one of the problems with the scramjet combustor is like supersonic combustion okay is lack of residence time or inadequate residence times because you are looking at a very fast flow that is coming in which is decelerated to let us say Mach 1.6 to something like that 1.62 to something of that sort still you are looking at supersonic flow.

And then you, you now have to inject sometimes if you are unlucky you have to inject liquid fuel and then that has to actually get atomized and then get into droplets and then vaporize and then mix and then burn okay so keep doing all these things you are out of the combustor the flow just does not want to stop all right or if you really stop the flow for all these things you are not going to fly okay.

So the residence time is one of the key ideas in most of the combustor designs that you want to think about okay so this is a powerful idea that comes out of the misanalysis the second thing that I would like to point out before we get to the next thing which is the plug flow reactor is in whatever we have done so far in combining the thermal and chemical processes so far which is constant fixed mass reactors both constant pressure and constant volume.

And the will stirred reactor on a open flow system is we have primarily considered only to conservation laws one is energy conservation the second one is species mass conservation okay in some sense you will find this approach recurring as are curing theme in most combustion problem approaches run other words they always think about doing the combustion part what is special about combustion in addition to just a flow a situation is primarily two things one first of all you have to deal with multiple species and therefore you have to conserve the mass of each of those species so you now are having to deal with a species of a set of species conservation equations in addition to that you it is directly coupled to the energy balance because the reaction rates depend on temperature.

And you need to know what the temperature is through the energy balance which in turn will depend on the species for the heat release so they get coupled okay many times you will find that it is possible to decouple this set of equations from the flow set of equations therefore then you will now be able to identify that they flow equations or like a standalone and the combustion equations can be solved after you have solved the flow equation and plugged in the velocities here for the convective effect of the species and the temperature and the enthalpy okay so in some sense that you can now say that is a flow problem.

And this is the combustion problem right so if you were to basically look at something like convective heat transfer of incompressible flows you will understand that this kind of thing happens there and there you would say is you can solve for the flow which is decoupled from the energy balance and you can now plug the flow field that has been solved from the flow into the energy equation to get the temperature field and from there you can get the heat transfer that is heat transfer kind of approach this is similar here except that in addition to the energy equation which is going to be complicated by the presence of multiple species and reactions.

And so on we also have to take into account the species mass conservation equation set and this constitutes the combustion problem mostly so most of the time we will always be worrying about

two things species mass conservation equations and energy equation this is like pretty much the combustion problem there are some occasions where this will get tightly coupled with the flow problem there are lots of other occasions which we will be looking forward to where it gets decoupled therefore we do not worry about the flow problem we outsource that to a fluid mechanics person okay so to speak you get the flow field and then you can solve the combustion problem.

So what we have been doing is the combustion problem the reason why we I am stating that now is the moment you actually step into the plug flow reactor we are now going to actually keep it keep track of what is happening in space and what is going to happen in space will all will primarily be influenced by how the velocity of the flow is going to change in space roll it up in relation to how like let us say a quasi one dimensional manner the deduct area changes okay so we will go back to something that is familiar in our gas dynamics where if you now have like a area decrease the velocity increases and so on so the velocities change so the velocity now comes into picture the means we have to bring in a momentum equation okay whereas we have never bothered about momentum.

So okay so typically this is combustion where we do not have to worry about momentum equations but the plug flow reactor we will do that okay so let us now look at the plug flow reactor so as I said if you wanted to have PFR rhyme with the well stirred reactor you would want to call it perfectly start reactor and call it PS are okay but this is PFR no changes in how we want to do this so here the model that we are looking at is you now have as variable cross-sectional area situation so a equals a of X where X is going in the predominant flow direction we do not want to entertain any other flow direction the flow is actually turning around and all those things to go along with the walls.

And so on we are oblivious to it we would we will keep our eyes shut okay instead we will actually be looking at a velocity which is a quasi one dimensional velocity the quasi one dimensional velocity is not area velocity okay it is not directly it is not the same as the axial component of the actual velocity because in reality when the flow turns there is a certain mass that's associated with going that way okay but we will conserve mass as if things are all going only this way okay so our quasi one dimensional velocity will have to conserve mass only in one direction so that velocity is not the same as the axial component of the actual velocity okay so this is the way we will do this of course many times I find that gas dynamics teachers who actually deal with this do not emphasize did this particular point.

And then we always get confused when we want to get back to our reality comparing experiments and so on okay we will get discrepancies the reason is we will have to keep this in mind okay so what we will do is again look at like local control volume and look at something like a Q dot double prime notice the double prime that is coming up we never had a double prime so far okay so what this really means is this is the heat flux so far what we have had its own the Q dot is, is in is in vats okay this is basically the rate at which heart goes out this duels for a second there is vats this is like the power okay this is heat flux that means it is vat per meter squared so since it is meter squared you have double Prime okay.

So directly goes with the number of linear dimensions over which you want to normalize so if you had a Q dot triple prime you can imagine it is like a volumetric heat loss or heat release whatever okay that is typical of this trade this, this is the way we would notate the heat flux okay so here we are saying that you now have a velocity that we will have to worry about keep in mind we are now introducing a V this is velocity okay previously we have been using a small way that stood for 1 over Rho that was like specific volume we now change okay the same symbol is used as we very, very rarely do you come across a formulation that uses both the specific volume and the velocity when you are now getting into things like velocity you are looking at a open flow system.

And you will always use rope okay you do not have to worry about a specific volume at all and things are all done in a mass basis you would not really use the equation of State on a molar basis and so on so we should not have any confusion from this point on so similarly we now say p equals P of X T = T of X ϱ = ϱ X Y i = y X ki =1 to n we have to keep track of spatial one-dimensional spatial variation of n species along okay that is how we want to do this okay.

So assumptions first a steady flow what goes in should come out right away right away is the key point that means there is no accumulation or depletion okay K watts 1d flow that means the V velocity is equal to V of X I vector so this V effects that we are talking about is aquasi one dimensional velocity it is not the axial component of velocity in the real flow we now assume no mixing in the axial direction all right that is to say yeah of course we are keeping track of things as a function of X right.

So if you now had as a function of x and y I changed as a function of x then you will have why I gradients in why I okay so you will have gradients in concentration so if you have gradients and concentration does this mean that it is going to drive some mixing as we will see soon okay because mixing is driven by concentration gradients similarly temperature gradients will lead to conduction a velocity gradients will lead to viscous effects we would not worry a monster okay we would not worry about any axial transport processes in this formulation transport processes me meaning species mixing viscous effects and heat conduction okay.

So that is for mass momentum and energy transport we would not worry about any of those and since we are actually saying that the velocity is only in one direction we are also assuming that there is an instantaneous mixing that is going on in the perpendicular direction all the time that means we are oblivious to any variations of anything in the transverse directions let alone concentrations that means the concentration that you are looking at is supposed to be represented representative of the entire station it is supposedly the same along the entire station that means it is all got mixed gay no gradients okay.

So that means this actually assumes instantaneous mixing in the transverse direction right this is what I said right at the beginning when we are neglecting mixing it is because we say that it is not there or too much of it is there either way okay so you can you can neglect something if it is now there you are not neglecting there is nothing to neglect gay it is not that so you can even neglect okay essentially as far as the axial mixing is concerned you are saying it is almost negligible why would you say that that is because we are looking at a conductive situation okay. So even if you are thinking that for example you had a gradient and therefore you will have a species that is trying to actually mix okay you have the convective effect that is bringing it back. So Axle if you axial diffusion at x0 mixing typically lose this when you now have a reasonably large convection and this is given by pellet number similar to how you would use Reynolds number to decide between inertial effect and viscous effects okay for the momentum balance okay.

So when you now have a significant amount of flow we do not have to worry about this that is to say it is small it can be neglected the other thing where you are saying that you are having an instantaneous mixing and therefore your mix you are neglecting is to basically assume that you have too much of it okay so you do not worry about it so this is also true in our lives when we have too much of something you take it for granted you do not even think that it is there okay.

So if you have like Wi-Fi everywhere you do not realize it until it gets shut off right or you have electricity all the time you do not realize it until it get it gets shut off so it is sort of like that ok so these many of these assumptions you know are very intuitive you just have to think about how it compares with your day-to-day experience and you will understand that this is not this is not far-fetched at all ok so I thought you would feel it that's what you are trying to do course.

As I said the fourth assumption would be a in viscid flow in viscid flow and fifth is perfect gasps I think by now you never question the perfect get assumption you have been brainwashed into supposing things a perfecto as far as the gases are concerned yeah actually that is quite true it is if somebody would have a question I mean is it really perfect most of the time yes the answer is do not worry about it okay most of the time in whatever we are dealing with the gases are indeed perfect this is one of the perfections that is relatively true in reality so this is actually a good assumption okay so as I said earlier we do mass conservation and energy conservation as part of them as part of the combustion problem but here we also have velocity okay.

So we have to worry about momentum conservation so mass conservation we simply have to say d over DX of ρ to 0 quite familiar to most of us okay from, from some things like gas dynamics okay and notice that we are using ordinary derivatives okay it is as if like we do not even know how to write a partial derivative of this change okay so we go step by step we are like with regard to learning combustion we are babies.

So we take baby steps toward spatial derivatives just wait for a few more classes then you will find too many partial derivatives for you to stomach okay so let us be happy with the ordinary derivatives at the moment so X momentum conservation okay this is simply boiling down to your one-dimensional ruler row you I should say thank I met a we will just say okay this is fine this is fine we will call this that say that essentially says the velocity is only a function of X we will now call that as new okay.

So that is what you are using you row you d you over DX=0 energy conservation row you a h + u squared over 2 plus q dot double prime time p this is capital p not the small p which is pressure so this is equal to zero where capital p is the local perimeter okay that is P= P of X okay the parameter here refers to whatever happens here we are only keeping track of one dimension it could be like a box could be like a tube circular tube whatever it is so you have a parameter there that goes with it or in other words you are saying that the heat transfer is happening only along the walls we need to have an idea of how the parameter happens the wall then we have the species conservation that is a row you.

So let us just fix this up like this row you do why I /soy d dy / DX + ω i w= 0 this should have been likes this together should have been small WI that is for the source okay the source essentially is like the number of the DD I am sorry the amount of mass per unit volume per unit time is what we are saying so this is mass flux times a mass fraction derivative alright so the mass flux times a mass fraction derivative will give you a volumetric rate of flow okay so this is eventually volumetric rate of flow ω i is the number of moles per unit time per unit volume times its molecular weight will give you the mass per unit time per unit volume okay notice something here we are not okay. (Refer Slide Time: 40:36)



I have not derived this for you okay I am just writing this out and I am not going to worry about how to divide this okay we will derive a the general species conservation equation in 3d pretty soon okay taking in the count diffusion and all those things that at the moment I just assumed that you can figure out how to derive this let us not worry about it what I told you was what we were here I said typically be worried only about these two the energy and species okay and then I said because we are interested in the flow we have to worry about the momentum what is this and how is it different from this right is mass conservation for an individual species.

So this is actually going this i=1 to n this is n equations anytime you look at a species conservation equation keep in mind it is actually n equations okay this is one equation for the mixture alright and that does not really have any production terms it does not worry about this kind of a term why is that because and chemical reactions mass is conserved so whatever is getting produced there must be something that correspondingly gets consumed in the mixture all right therefore we should not have to worry about we will come back to this much more specifically when we do the detailed three-dimensional species conservation and derive the mixture of mass conservation from there okay.

But ultimately what would what would mean is the mixture does not even know that reactions are happening inside okay it is as if like for example when you were doing when we were doing aerodynamics let us say okay let us say you go to an aerodynamics class and then the ER on apex professor is talking about flow past and our foil and all that stuff and then he writes equations for mass conservation continued equation and so on you cannot say stop you are doing aerodynamics that means is this air flow past at our foil air contains oxygen nitrogen all these things these are all individual species where is the individual species conservation equation should really do that would not you do not have to the mixture does not know that it has it is actually a mixture even if nitrogen.

And oxygen were to react that is a point ago so, so it is very interesting there this is like this actually says something like a collective behavior okay as if the mixture did not exist this is collective behavior with a mixed with taking cognizance of the mixture so it becomes part of the combustion problem okay so there is a difference between taking cognizance of the mixture and not taking cognizance mixture so well so how can we do this how can we now deal with this so we can we can write we now have to actually do some more jugglery and I hope we can do this now pretty soon we could write some of these equations as let us say you want to pick the first one you open up these brackets there.

And so you write this 1 over Q D Q over DX+ 1U DX+ 1 over 8 over DX let me go a little further out and that right equal to 0 you are not begin to get the drift of why I'm having the zero right at the far end I want to point out that row and you are unknowns here but a is not an unknown it is given so 1 over a DA over DX is like a source term okay it is it is known to you it is not an known okay then the next equation you can now write this as Q u 2 u over plus okay I am just going to write DP over DX = 0 why am I spacing things out I am beginning to see if i can write all the like derivatives one below the other and I am going to now form a matrix okay so the next equation you could write this as UD u / DX +DH / DX = 0 right but for the other ones you have to do some jugglery so let us try to do that quickly this is a lot of algebra so not much point in spending time.

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So we notice that h is equal to $\sigma y_i h_i$ how are you using small catch use why I when you are using capital catch you have to use on a molar basis so the h / DX= ω dy over DX times H I plus σ Y I DHI over DX this is equal to Σ D dy over DX times H I plus σ Y I partial do divided by partial Tat constant P times DT over DX.

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We want to bring in temperature okay so not contented with gentle p therefore we can write this as Sigma D why I over DX h I+ σ Y I small CPI dt over DX the dt over DX can be pulled out of \sum and then you have a \sum Y I CPI so this together is basically CP for the mixture ok so this is equal to σ H I dy over DX + CP DT over DX keep this then you have another problem p =Q are you T developed by WM x so this means that 1 over P DP over DX= to 1 over 0 0 / DX+ 1 over TDT over DX- 1 over w mix d w mixed over DX oh my god can you now, how to worry about how the molecular rate of the mixture changes with space okay terrible well of course we know how it changes its supposed to change with the composition and the composition is given by Y ice.

So we should simply be able to write the variation in the molecule herb mixture molecular weight in terms of variation in the composition therefore but w mix is equal to Sigma YI / WI whole to the - 1 so DW mix /DX can be written as minus W mix squared ρ 1 / WI DYI / DX so therefore DP over DX is 1 over ρ D ρ over DX +1 over T DT over DX plus the negative signs get together so you get a +WM x σ 1 over WI DYI over DX all right therefore what happens is you can plug this DP over DX over here okay DP over DX but it is going to now contain zero over DX DT over DX and DY I over DX right.

So and of course the species equation for you I already had a DY over DX and this acts as a source term okay involving y is and T of course therefore it is coupled and we can write so we obtain equations in terms of in terms of wealth simply say Q u T and why I.

Plug Flow Reactor(PFR)	
• We have $\frac{dh}{dx} = \sum_{i=1}^N h_i\left(\frac{dY_i}{dx}\right) + \sum_{i=1}^N Y_i C_{p,i} \frac{dT}{dx}$	(181)
$\frac{dh}{dx} = \sum_{i=1}^{N} h_i \left(\frac{dY_i}{dx} \right) + \sum_{i=1}^{N} C_p \frac{dT}{dx}$	(182)
$P = \frac{\rho R_{\mu}T}{W_{mix}} \Rightarrow \frac{1}{\rho}\frac{dP}{dx} = \frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{T}\frac{dT}{dx} - \frac{1}{W_{mix}}\frac{dW_{mix}}{dx}$	(183)
\bullet where $rac{dW_{mix}}{dx} = -W_{mix}^2\sumrac{1}{W_i}rac{dY_i}{dx}$	(184)
$\frac{1}{P}\frac{dP}{dx} = \frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{T}\frac{dT}{dx} + W_{mix}\sum \frac{1}{W_i}\frac{dY_i}{dx}$	(185)
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So these are like four unknowns but keep in mind why I is actually a set of n unknowns and so you need to have a four-set four equations where the last one being a set of equations that is exactly what we have okay so solve this and live happily ever after I will see you Monday.

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