Indian Institute of Technology Madras

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National Programme on Technology Enhanced Learning

COMBUSTION

Lecture 22 Schvab-Zeldovich Formulation 2

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We have been looking at the derivation of the Schvab-Zeldovich formulation leading up to formation of these coupling terms of a linear operator working on both the energy and the continuity. So the steps that we have followed so far is to have the overall continuity taken in account in the simplified energy equation where we are having the relevant terms based on the assumption that we have made.

And then we add this term which is having essentially amounting to zero to the energy equation. So that we can now group these two terms together and we now have a V + VK, so this is actually amounting to the species velocity. So this is sort of like saying recall this is actually the mixture averaged convection of enthalpy of the mixture averaged enthalpy. This is actually the enthalpy convection due to diffusion.

So if you now try to put these two together this would actually be like the species velocity conducting the species enthalpy right. So effectively we are having like a species specific convection of enthalpy grouping together that is actually happening at the from these across the surface of a control volume, this is conduction happening across the surface of a control volume.

So obviously we are having like a divergence of both equal to 0, because when you now have surface defects the cause of divergence theorem shows up this divergence here. So you can clearly see the physics of the manipulation also that is going on, but here what we then do is well if you now have something like a species specific enthalpy convection, can I now use the species specific mass consumption, a mass convection right, that is equal to these.

So if you now look at this is like a species velocity a vk vector then the diffusion is embedded in it. So we do not have to worry about diffusion explicitly, so then it would be like species convection equal to a reaction okay, the order the production or should have actually had a WK here right. So of course you do not have the unsteady term because you assume steady state.

So whatever is conducting in and out should be based on how much is being produced or consumed inside the control volume, that is how the species conservation looks like which is now possible for us to plug this into this okay. And then we do the expansion of the enthalpy species enthalpy, and say this is like standard heat deformation plus the sensible enthalpy, you now plug that in there, and what you will find this for example for that term with the standard heat deformation alone you now try to use this equal to WK.

If you did that then you would get this to be taken to the right hand side with a negative sign and for the remaining you now keep it as it is, but then notice that this is going to be mixed averaged anyway, therefore, you could go ahead and sum overall cpks and then you get a kcp right. So here $CP = \Sigma = 1$ to n YK cpk right.

So that is what being is being used to over here, but you cannot do that here because you have a DK that is waiting it, so you have to have a YK VK cpk within this integral so you cannot get this YK alone here and then have the summation DK is interfering there. And then we had the K gradient T coming from here as it is, and I told you how we got this right hand side. Now I would like to point out which I did also previously is this is the chemical heat release rate term that has now been identified explicitly for you.

What I would like to think what we should leave I would like to think about is, so how does this really work Δ hf K0 actually means the standard heat deformation of species K right, so that is going to be in terms of something like J/Kg or J/Kg of species K, and WK is actually the net rate of production or consumption of species k in terms of something like kg/m³/sec right. And if you now add up this product over all of all of the species, you are not going to get the net heat release that is being produced out of this chemical reaction.

There is an alternative way of doing this, so this is actually per species right, so you now take heat release per species and then add up across species. Of course in the Schwab-Zeldovich formulation, I think I guess the 9th assumption is assuming a single step chemical reaction. But what if you had multi-step chemical reactions right.

So we know that for a chemical reaction which is not necessarily a formation reaction any chemical reaction you will have a heat of reaction, let us say standard heat of reaction. So if you know h ad a standard heat of reaction for one reaction, but you know or looking like a multi-step reaction scheme each of these reactions having a standard heat of reaction associated with it, which could be in endothermic or exothermic right.

So if you now have all these reactions happen and each of these reactions has a reaction rate associated with it right, which is not specific to any particular species it is participating in the chemical reaction in those reactions. So on the one hand you have a heat of reaction, on the other hand you have a reaction rate. So from there you should be able to find out what is the rate at which heat is released in a particular reaction.

And then you can now look at all the reactions together and find out what is heat release the net heat that is released per unit time, there is a heat release rate per unit time for all the reactions happening. So there you sum over reactions, so one of the exercises that you would like to work out is, is it possible for you to show that the heat released from the chemical reactions on the whole is the same, regardless of whether you actually some do with the species and their heats of formation, or some do with the reactions and the reaction rates right.

So that is something that we will not really pursue here, because we make an assumption about single step chemical reactions okay, but that that is not going to actually stop us from writing another expression for multi-step chemical reactions in terms of reaction rates and heats of reactions are supposed to be heats of formation of species that we are doing here. So where are we actually going to use the single step reaction assumption is yet to be seen, we have not really utilized it yet okay.

So that is one thing that I wanted to point out, so while we have now dealt with the this term there are three terms that we want to now deal with on the left hand side, and let me just number them as 123, so that we will actually try to work on some of these terms identified by the numbers. (Refer Slide Time: 08:04)



So now let us let us first for example take term three right, so we now take term three that is like k grad T that is the simplest looking term and in all this. So let us now take this and then hear what I am going to do is to I am going to write k and then multiply and divide by pcpd or with pd put over there and a CP put over here and then write the grad T right, that looks like a lot of cosmetics that has been done around without any effect.

But what is in here now what do we have, so this is our Lewis number right, this is our Lewis number that is equal to K/pcpD, and we have assumed it to be one right. And therefore, so this is assumed, therefore, this is now nothing, but pD CP grad T all right. So that is what you a re going to get for the third term. So effectively what you are basically saying is the conduction is going to happen pretty much based on the diffusivity because the Lewis number is equal to one yeah okay.

Now the second term is a little bit more complicated to deal with. So term three all right, so term three is $\rho\Sigma$ k=1 to n YK VK vector integral T super script T0 to T cpk dT all right. Now we will have to actually show why what this amounts to, and so I am going to I am going to try to show

that for you. So this is I am going to show that this is like $-\rho D\Sigma$ k=1 to n grad YK integral T0 to T cp dT.

This is actually coming from, so I will open parenthesis here multi-component diffusion equation right, simply boils down to D gradient X K = XK Σ k = 1 to n, Xj Vj vector – Xj Vk vector K-1 to n. This is to say in the multi-component diffusion equation only the first term on the right hand side survives and all the other terms are though all the other terms vanish, because of the assumptions that we have made exclusively to get rid of them.

And we also have made the assumptions that all the binary diffusion coefficients are equal to D, so you just have to unwrap the left hand side on the right-hand side together in the multi component of fusion equation to get this. Now you can further, so what you can actually do here is now we are not really interested in having XK we are interested in having YK that is what we are dealing with right.

So one way of actually trying to get rid of this is divide by Xk and multiply by Yk. So if you do that then what you will find is you have a grad Xk/Xk right that gives you something like a grad natural logarithm Xk right. So you get into those kinds of things, so what you whatever I would say is a multiply I am going to skip steps here multiply by Yk/Xk and Σ K=1 to n right, that means you add over you should okay.

So you now get a D gradient natural logarithm $Xk - \Sigma J = 1$ to n, Yj gradient natural logarithm YJ should be XJ I guess, XJ = - Vk right, k=1 to n. Now so you can show this okay, so show as in I cannot try to do this, and then you can further simplify this if you now try to write it out for all the species you can say further show Vk vector is equal to simply minus the gradient natural logarithm YK k = 1 to n right.

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Schvab-Zeldovich Formulation	
• Unity Le $k\nabla T = \rho \mathcal{D} \underbrace{\frac{k}{\rho C_{\rho} \mathcal{D}}}_{\substack{le=1}} C_{\rho} \nabla T = \rho \mathcal{D} C_{\rho} \nabla T$	(252)
$\rho \sum Y_k \vec{V}_k \int_{T_{ref}}^{T} Cp_k dT = -\rho D \sum \nabla Y_k \int_{T_{ref}}^{T} Cp_k dT$ • Multi-Component Diffusion Equation	(253)
$\mathcal{D} abla X_k = X_k \sum_{j=1}^N X_j ec{V}_j - X_k ec{V}_k ~(ext{i} = 1 ext{ to } ext{N})$	(254)
Multiply by Y_k/X_k and sum over	
$\mathcal{D}\left[\nabla \ln X_k - \sum Y_j \nabla \ln X_j\right] = -\vec{V}_k \text{ (i = 1 to N)}$	(255)
NPTEL $\vec{V}_k = -\mathcal{D}\nabla \ln Y_k \ (i = 1 \text{ to } N)$	(256)

This is actually retrieving Fick's law, so the way we have actually made the assumption that DIJ will be equal to D and also getting rid of all the other terms except the first term on the left-hand side of the multi-component diffusion equation should essentially amount to being able to retrieve Fick's law for a multi-component system right.

So if you now say Vk is equal to minus the natural log, gradient of natural logarithm of YK this amounts to saying gradient Yk/Yk so this Yk can actually go over here to the left hand side and then you can now see how this Yk Vk can be written as –D gradient Yk. So we also had a ρ , so the negative sign and the ρ will go there then Σ k=1 to n gradient Yk integral T0 to T cp, so we can use this above okay.

So that closes this parenthesis then let us now consider, but gradient of T0 to T cpdT right, the reason why we want to do this is, we now find that gradient Yk shows up here right, and then you now have a CP integral CPdT. Let us look at what we have over there, we have a divergence of pd CPdT right, and I am sorry no, no, no that you see here you now see pd Cp grad T okay. So there the gradient is actually on the temperature and here the gradient on the Yk, so is it possible for us to see if we can combine these.

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So if you now consider this particular term out of the bloom to seemingly out of the bloom gave you just we just consider this term, then gradient of the blooming. We can now write this as gradient of Σ K=1 to n Yk integral T0 to T cpk dT not a problem simply writing what CP is starting from here it is only CP that needs to be integrated with respect to temperature not Yk, so you can pull the Yk out of the integral, but with the information.

So let us now try to get the gradient inside the summation and see what happens, so this is k=1 to n gradient Yk all right, integral T0 to T cpk dT+ $\Sigma k=1$ to n Yk gradient integral T0 to T cpk dT right. So this is equal to $\Sigma k=1$ to n gradient Yk integral T0 to T cpk dT, then we now have to see what is going on, here t is a variable right.

So we are looking at actually taking a gradient of temperature this is always been in our minds all right we always found that temperature is actually the variables sitting on top of this integral so if you want to look at any gradient that needs to be taken very bit, if that needs to be taken with respect to temperature what we what do we need to do, we will have to apply Leibnitz rule, because Leibnitz rule is where you now are looking at derivative of an integral whose limits or functions of what you are going to take differentiation with respect to okay. So that is where the problem is and so that is going to yield for us plus Σ k = 1 to n Yk cpk(T) grad T the way it works is Leibnitz rule, so this is actually coming out of Leibnitz rule, the way it works is you evaluate the integrand at the at the limits and then multiply that by the gradient of the limits or the differentiation of the limits. So in this case T0 is a constant, so the second term which is having a gradient of T0 is going to vanish.

So you do not have to worry about evaluating the integrand as T0, so the only term that is going to actually, and then of course what you done then can do is you will also have a another term which is like an integral of gradient of cpk okay, so that is not going to contribute, so what is going to contribute these three terms from Leibnitz rule is only that term where the gradient of t is there with the CP evaluated to the T that is how it goes.

In fact in my notes I am a little bit more particular about pointing out that you can say this is actually this is T' dT' okay, so where we are now saying T' is like a dummy variable of integration, whereas here we are evaluating the temperature that is going to be there as unknown okay. So if you know okay with this, then what happens is we now get Σ k=1 to n, gradient Yk integral T0 to T cpk dT+ grad T does not depend on species.

So that can be pulled out of the summation and all you have a Σ Yk cpk which is simply CP right. So this is like cpk CP grad T right. So what are we trying to do, we are now trying to look for this term in here okay. So from the third term we got this by applying the multi-component diffusion equation reducing to Fick's law to get this term right and this term can be identified here as what we started out with minus this okay.

Therefore, $\Sigma k = 1$ to n gradient Yk integral T0 to T cpk dT let us also do this a little bit better. If you want to now look at this as a negative sign therefore, -pd right, then what happens, you now throw in a –pd over here. So you now have a –pd, pd at integral T0 to T cpdT that is here. And then this goes to the left hand side with a negative sign, but you have multiplied by –pd, so you get a +pd cp grad T right.

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Schvab-Zeldovich Formulation	
Consider	
$ abla \int_{\mathcal{T}_{ref}}^{\mathcal{T}} C_{p} d\mathcal{T} = abla \sum Y_{k} \int_{\mathcal{T}_{ref}}^{\mathcal{T}} C_{p,k} d\mathcal{T}$	(257)
$=\sum abla Y_k \int_{\mathcal{T}_{ref}}^{\mathcal{T}} C_{p,k} dT + \sum Y_k abla \int_{\mathcal{T}_{ref}}^{\mathcal{T}} C_{p,k} dT$	(258)
$=\sum\nabla Y_{k}\int_{\mathcal{T}_{ref}}^{\mathcal{T}}C_{p,k}d\mathcal{T}+\sum Y_{k}C_{p,k}\left(\mathcal{T}\right)\nabla \mathcal{T}$	(259)
$= \sum \nabla Y_k \int_{\mathcal{T}_{ref}}^{\mathcal{T}} C_{\rho,k} d\mathcal{T} + C_{\rho} \nabla \mathcal{T}$	(260)
$ \sum \rho \mathcal{D} \sum \nabla Y_k \int_{\mathcal{T}_{ref}}^{\mathcal{T}} C_{p,k} dT = -\rho \mathcal{D} \nabla \int_{\mathcal{T}_{ref}}^{\mathcal{T}} C_p dT + \rho \mathcal{D} C_p \nabla T $	(261)
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So right, good then what happens try to put all these things together right. So we have the first term as it is just keep the first term as it is ρv integral T0 to T cpdT okay, the second term has been the one, the one that is been giving us a little bit of a problem, and that is now looking like effectively two terms okay. So that is $-\rho d$ grad integral T0 to T cpdT + ρd cp grad T okay. The third term is coming with a negative sign k grad T which is also written as ρD cp grad T.

So we now have this subtracted from the second term you can clearly see that this gets cancelled with this right away okay, and this appears with a negative sign along with the first term and of course the last term on the right-hand side remains as it is. So we now can assemble all these different pieces of the energy equation. So therefore, the energy equation becomes gradient sorry, divergence of ρV vector integral T0 to T cpdT that is exactly the first term.

We need to borrow only this term for the second term, the other one is going to get cancelled with the third term. So we have $-\rho D$ integral T0 to T cpdT = $-\Sigma = 1$ to n, whatever we had on the right hand side there we will just copy here, so Δ HfK0 WK all right, what is just like. So last 5 to 10 minutes we have to be like, so what we got finally, there are something that we can think about yeah.

This is the mixed or average velocity right this is the sensible enthalpy of the mixture. So this basically means this is the convection of the mixture enthalpy all right, and this you can clearly see is divergence of gradient of something right with a pD sticking there. So that is actually the diffusion term it is effectively coming from a combination of species convection of enthalpy and the conduction okay.

So this is acting like the diffusion term and of course that's a chemical reaction with term. So we now see that there is three effects that are now coming together convection of the mixture diffusion and chemical reaction. So whatever we talked about right at the beginning of the course where we are now talking about a interplay of three processes convection, diffusion, reaction. So for all the shake-up that is happen we finally come down to only these three right.

So that is the physics involved in this equation, we call this the Schvab-Zeldovich energy equation right. So we also want to work with the species equation right, so let us get back to how the species equation looks like equation B, so equation B is now divergence of ρ YkV+Vk=Wk, we do not like VK, we do not want to look at Vk in fact what we decided here was we wanted to throw out VK, that is how we got this ρ D grad Yk Σ right.

So that is coming from how the Fick's law looks like, so we want to be able to now substitute Vk=-D grad Yk/Yk or in other words Yk Vk = -D grad Yk, if you are able to now substitute it over here right, then what happens divergence ρV Yk plus or sort of negative sign – D grad Yk right, that is what you are going to get. Do let us try to write it out.

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Species equation B becomes applying the simplified form of multi-component diffusion equation right. We simply get divergence of $\rho V Yk = \rho D$ grad Yk = Wi, this is what we want to call the Schvab-Zeldovich species equation right. So here again you can see no clearly this is convection of species, this is diffusion of species, this is reaction of species right. So in species conservation also you are having convection, diffusion, reaction three terms.

The other interesting thing is this is ρV times something Yk in this case and $-\rho D$ grad that thing which is Yk in this case. Here we have ρV times something which is a little bit more complicated than that integral T0 to T CPdT and $-\rho D$ grad is the same thing which is integral T0 to T cpdT. And what do we want, we wanted our left hand side to look like some sort of an operator that is operating upon a quantity like α i or α t.

We are now beginning to think, we are now beginning to see the contours of that both the lefthand sides of the Schvab-Zeldovich energy and species equations are actually the same operators, operating upon two different quantities in this case Yk the other one is integral T0 to T cpdT right. So we are beginning to achieve this goal, but what is the original goal, our original goal was we wanted to have a operator script L of $\alpha i = \omega$ and operator script L of $\alpha t = \omega$. That means we wanted the right-hand sides to be the same okay well X off the case now have a w WK over here right and you have a you have the WK within a summation over all K how is that how do we deal with it, so this is actually this is a first for this is n equations k = 1 to n right, that is one equation summing over all Wk weighted by the Δ hfK0, so how do you deal with this situation.

So you now try to form here, so you and you are not quite at the α yet we have identified Yk and integral T0 to T cpdT as potential candidates for our α K and α T, but the right-hand sides are looking good right. So let us do something here, so for a chemical reaction of the form Σ i equals we can say you can keep it K=1 ton μ k' = Mk gives Σ k=1 to n μ k'' = Mk that is a single step reaction okay.

So you are now beginning to stop start thinking about why single step reaction as opposed to a multi-step reaction scheme we may write ω =Wk/Wk µk''=µk' k=1 to n.

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Schvab-Zeldovich Formulation
• Schvab-Zeldovich Energy Equation

$$\begin{aligned}
\overline{\nabla \cdot \left[\rho \vec{v} \int_{T_{ref}}^{T} C_{p} dT - \rho D \nabla \int_{T_{ref}}^{T} C_{p} dT\right] = -\sum \Delta h_{f,k}^{0} w_{k}} \quad (262)
\end{aligned}$$
• Schvab-Zeldovich Species Equation

$$\begin{aligned}
\overline{\nabla \cdot \left[\rho \vec{v} Y_{k} - \rho D \nabla Y_{k}\right] = w_{k}} \quad (263)
\end{aligned}$$
• For a chemical reaction

$$\begin{aligned}
\sum_{k=1}^{N} \nu_{k}' \mathcal{M}_{k} \to \sum_{k=1}^{N} \nu_{k}'' \mathcal{M}_{k} \quad (264)
\end{aligned}$$
• $\omega = \frac{w_{k}}{W_{k} \left(\nu_{k}'' - \nu_{k}'\right)} (i = 1 \text{ to } \mathbb{N}) \quad (265)$

This is how we defined our ω which is the molar rate of reaction okay, the fact that we are not bringing in moles is because we are now dividing by the molecular weight WK right. Now this can be done obviously only for why single step reaction, if you had multi-step reaction then you had many ω themselves it is not possible for you to write a single ω right. So a single ω can be written only for a single step chemical reaction that is where we have to bring in the single step chemical reaction assumption.

And what you are essentially saying is let me now try to look for something that is common for all WK, so that I can just have that alone and pull everything else to the right hand, left hand side and keep only the ω on the right hand side. I can easily achieve that with the species conservation equation, because I have this definition that relates two Wk to the ω , the single chemical reaction rate.

So if you know, so what would you do if you now were to divide your equation your K species conservation equation by Wk times $\mu k'' - \mu k'$ right, the right hand side becomes ω , the left hand side you do not really have a Yk in itself, you have a Yk/Wk times $\mu k'' - \mu k'$ right, that is your αK . So then that $\alpha k = Yk/Wk \mu k'' - \mu k'$ right, good.

Can you also substitute $Wk = \omega$ times $Wk \mu k'' - \mu k'$ okay, can we now substitute that we were here, if you did that then you are going to get this term as $\Sigma k=1$ to n $\Delta hfK0$ Wk times $\mu k'' - \mu k'$ times ω , ω does not have any code any subscript K. Therefore, I can pull that out of the summation and keep it as a factor, and whatever is there in the summation, the summed up quantity I would now try to divide that throughout.

If I divided this equation throughout by that some depth quantity leaving only the ω on the right hand side I have only ω on the right hand side and I am going to get ω on the right hand side for here as well. So now I am beginning to look at α T, so α T is originally we thought our candidate was integral T0 to T cpdT, but now it is actually divided by Σ k=1 to n Δ hfK0 Wk μ k" – μ k'. So what if I use these α now in the Schvab-Zeldovich energy in species equations.

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Then we can write $L(\alpha) = \omega$ right, where $\alpha = \alpha k k=1$ to n gives species equation, I should say SZ species equation and $\alpha = \alpha T$ gives SZ energy equation. So what is $L(\alpha)$, and here L effectively is $L(\alpha)$ is divergence of ρV vector $\alpha - \rho V$ gradient α right. So there is divergence $\rho V \alpha - \rho D$ gradient $\alpha = \omega$ and this is convection, this is diffusion, this is reaction pretty much achieved our goal right. All we have to do now is to notice that this is a linear operator.

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Schvab-Zeldo	vich Formulation	
• Dividing the	species equation by $W_k\left(u_k''- u_k' ight)$	
	$\alpha_{k} = \frac{Y_{k}}{W_{k}\left(\nu_{k}^{\prime\prime}-\nu_{k}^{\prime}\right)}$	(266)
	$\alpha_{T} = \frac{\int_{T_{ref}}^{T} C_{p} dT}{-\sum \Delta h_{f,k}^{0} W_{k} \left(\nu_{k}^{\prime\prime} - \nu_{k}^{\prime}\right)}$	(267)
Using the above in the Schvab-Zeldovich equations		
	$\mathcal{L}(\alpha) = \omega$	(268)
where $\alpha = \alpha_k$, Schvab-Zeldovich gives species equations and $\alpha = \alpha_T$, Schvab-Zeldovich gives energy equation. where		
	$\mathcal{L}(\alpha) = \nabla . \left[\rho \vec{v} \alpha - \rho \mathcal{D} \nabla \alpha \right]$	(269)
NPTEL	$\mathcal{L}(\alpha) = \nabla [\rho \vec{v} \alpha - \rho \mathcal{D} \nabla \alpha] = \omega$	(270)

So it is possible for us to now subtract $L(\alpha)$ from the other and right hand side is the same for all these equations, therefore you should get a 0 there right. So notice $L(\alpha)$ is a linear operator okay. So the non-linear chemical source term can be eliminated in all, but one equation by subtracting that equation from all other equations right. Then we have we have $L(\alpha) = 0$ okay. Where $\beta = \alpha t - \alpha 1$, so let us call this beta T and β can also be equal to $\alpha K - \alpha 1$ let us call this $\beta k k = 2$ to n right.

Schvab-Zeldovich Formulation • Since \mathcal{L} is a linear operator and hence non-linear source term can be eliminated in all but one equation by subtracting that equation from all other equations. $\mathcal{L}(\alpha_1) = \omega \qquad (271)$ $\mathcal{L}(\beta) = 0 \qquad (272)$ where $\beta = \alpha_T - \alpha_1 = \beta_T$ and $\beta = \alpha_k - \alpha_1$, k= 2 to N.

So the β is then or what is called as a coupling terms right. So you now have linear homogeneous n minus, wherever this is this is one equation, this is actually again n - 1 + 1 originally we had n + 1 equations, and species equations and one energy equation right. And if you now subtract all equations one equation from all other equations and keep this one equation you should still have n + 1 equations.

But n of those equations is now have now have become homogeneous right, it is only one equation that continues to have the homogeneity. Therefore, now change to your system of equations into n linear homogeneous equations and one linear inhomogeneous equation all right. So that is what you achieve by doing the Schvab-Zeldovich formulation, this is a good point to stop, we will start thinking about what to do with the formulation as we proceed.

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