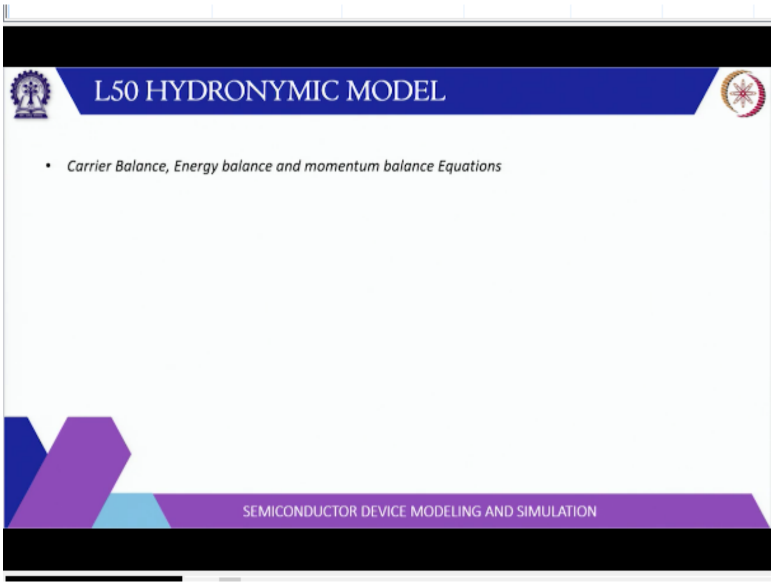
Semiconductor Device Modelling and Simulation
Prof. Vivek Dixit
Department of Electronics and Electrical Communication Engineering
Indian Institute of Technology-Kharagpur

Lecture-50
Hydrodynamic Model (Contd.,)

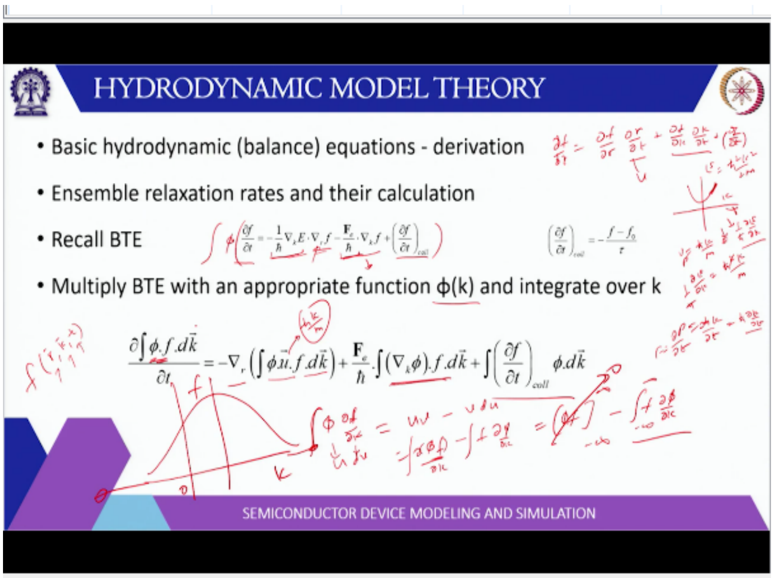
Hello welcome to lecture number 50; we will continue our discussion on hydrodynamic model.

(Refer Slide Time: 00:32)



So, in this lecture we will drive the governing equations for carrier balance, energy balance and the momentum balance equations.

(Refer Slide Time: 00:41)



We will drive them from the Boltzmann transport equation. So, let us consider let us recall the Boltzmann transport equation where f is the distribution function. So, that means it tells you the number of electron or carriers with position r movement wave vector k at k 1 time t. So, it tells you the probability of finding electron at position r wave vector k at k 1 time t and of course if you integrate this distribution function you will get the number of carriers.

So, if you integrate it over k space then you will get the density at given position at a given time and then da by dt is basically you can take partial derivative with respect to all the three variables. So, del f by del r dela f by del k and del f by del t and then of course you can write del f by del r times del r by del t and del r by del t is basically your velocity. So, force del f by del t total derivative is equal to del f by del r del r by del t plus del f by del k del k by del t plus t l f by del t.

So, del f by del r is this term, this is of course in 3D and del r by del t is a velocity. Now this velocity we get from the energy band diagram. So, if you recall this is the E-K diagram. So, if you look at E-K diagram, for parabolic band E = h bar square k square by 2 m and you can get the velocity from here. So, velocity is h bar k by m, because h bar k is a momentum. So, this is also called the phase velocity, but for parabolic band this is same as the group velocity and that you can find del E by del k h bar square k by m.

So, if you divide by h bar you get h bar k by m. So, this is your velocity. So, 1 over h bar del E by del k. Of course when you do in 3D then becomes gradient. So, 1 by h bar del E by del k. So, this is the group velocity. So, this is actually called group velocity and this is the phase velocity and they are equal for parabolic band structure. Then other part is del f by del k times del k by del t.

So, del k by del t you can say that momentum is h bar k. So, del p by del t is del by del t of h bar k. So, this is h bar del k by del t and this is your force. So, this is force by h bar is now force is basically minus q times E. So, for electron plus times E for whole, so you can add f by h bar times del f by del k and this del f by del t is due to the collisions. So, this is your equation. Now what we do to drive the hydrodynamic model?

We multiply this Boltzmann transport function with an appropriate function phi and integrated over k space. So, if you integrate this one you multiply by phi and integrate. So, multiply by phi everything is multiplied by phi integrate. Now here if you see phi is a function of k, so if you see this del f by del t that means this derivative can be taken out. So, this derivative and the integral kind of interchange.

So, instead of operating del f by del t on f we are integrating over the product of phi and f. That basically tells you the del by del t of phi f integral d k. So, we just extend the integral and the differentiation because phi is function of k only not t. Similarly here del E by del k del f by del r times phi d k. So, this is basically you can write u the group velocity. So, del E by del k by h bar, so phi u f dk and this del by del r is taken outside.

So, this derivative is taken outside because phi is a function of k and u is a function of velocity basically. So, you can take this del by del r outside, because you can use h bar k or something. So, it is a function of k. So, you can take it inside. So, this del by del r can be taken out. Similarly, del by del k of f then it is F e by h bar. So, force due to electric field is a constant, can be taken out. So, this is del f by del k times phi.

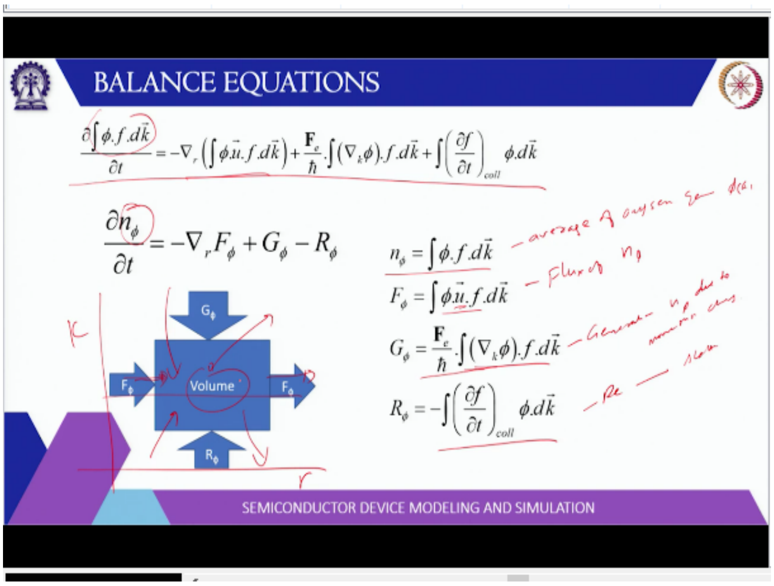
Now here there is some change here. So, what we are doing here for the third term? This term here phi times del f by del k and we are integrating it. Now we can say this is u dv. So, we can use this mathematical law where there is a integral of u dv can be written as uv - v du. So, this is u, this is dv. So, this can be written as phi times f - f times d phi by dk. So, you can write like this. So, this is del by del k.

Now if you integrate this one this is phi f. So, this will be simply integral phi f - integral f del phi by del k. So, this will be limit will be basically you can say minus infinity and if you look at the phi and f, phi is basically function of k, f is basically something like this because distribution function is like this, f versus k and if it is displaced Maxwell n or some field is applied then origin may be here and it looks but in any case at plus infinity and minus infinity it goes to 0 phi.

So, phi f because f is finite, so it will also go to 0. So, this term will always be 0. So, this can be written as integral f d phi by dk. So, this is written integral f d phi by dk and of course the sign is changed here. So, from minus it becomes plus here and this is basically del f by del t due to collision. So, we can do phi dk. Now we can calculate all the three equations the carrier balance, momentum balance and energy balance.

If you see here if phi is 1 then it will be simply f dk. So, that will tell you that dn by dt. If phi is k then k times f dk will give you some type of current because k is basically related to the velocity, phi is related to n. So, it will be current density. So, this will be the current density balance, so you can say the momentum balance and if you take f is some proportional of k square then it is related to energy. So, this will be energy balance equation.

(Refer Slide Time: 08:47)



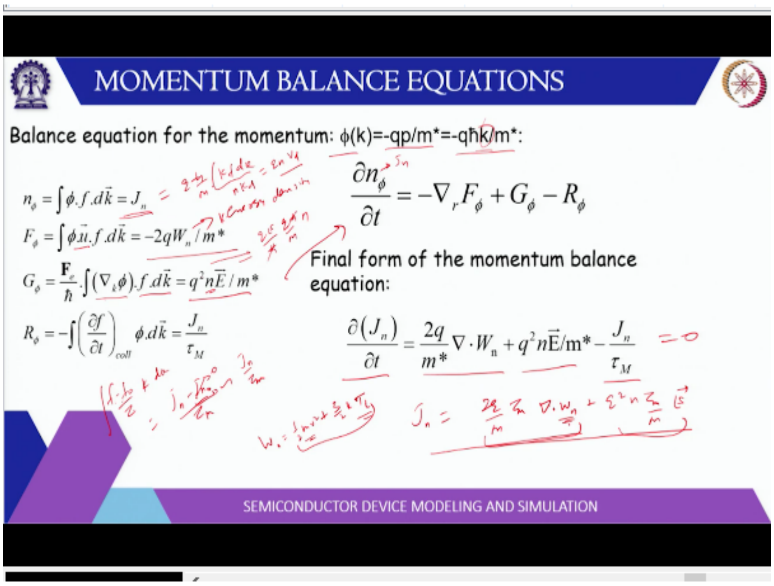
So, let us go one by one. So, this is your equation Boltzmann transport equation multiplied with phi and integrated. So, this term integral phi f dk, you can say it is n phi. Now n phi is basically you can say this is the average of any general quantity phi which is function of k. So, this is the n phi. So, this is basically the left side is telling the time evolution of this quantity. Then second is phi u f dk. So, this basically tells you there is a velocity here. So, this is some kind of flux.

So, this is basically you can say it is a flux of n phi the first quantity. So, the increase in the quantity n phi is proportional to the negative gradient of the flux of n phi plus due to the force this f is basically changing. So, this distribution function the carriers are moving from one k space to another k space. So, their k vectors are changing. So, this basically tells you a generation.

It is not carrier generation as such, but is the generation of n phi due to momentum change, this is due to momentum change. Similarly due to collision they are scattered, so you can say this is a recombination due to scattering. So, if you look at this equation it is very similar to the content equation. So, the content equation it tells you that n phi the rate of evolution of n phi is the negative greatness of flux plus generation minus recombination due to the momentum change and the scattering. So, if you consider a space here, so there is a k space, there is a position here. So, this carries scattered, so from one volume there can be a scattering.

So, it goes like this scattering then there may be an entrance into this k space. So, there may be due to the field, so in this volume this quantity n phi is basically increasing. Then of course there is negative gradient of flux that basically tells you that there are more plugs or the entering quantity is more than the leaving quantity. So, entering flux is more, leaving flux is less? So, there will be negative gradient of flux which will give rise to increase in the quantity n phi.

(Refer Slide Time: 12:14)



Now if we assume that phi is 1 then this n phi f phi G phi and r phi, this term simplify. So, this becomes integral f dk which is basically carrier consultation. So, left term becomes d n by d t. Then flux vacancy u f dk. Now u is the velocity f dk. So, f dk you can set is d n. So, it is like u dn. So, that will give you n times the average velocity or the drift velocity and which is basically related to the current density because j = q n v d.

So, if electron charge then you can say – q. So, it will be j n by q. So, that means if n phi quantity is the carrier concentration then the flux will be current density by q. So, the flux of these carriers give rise to the current density. The generation will be del phi by del k. Now because k is 1, phi is 1. So, del phi by del k will be 0. So, there is no generation as such. So, this generation term is 0.

Then similarly that recombination term del f by del t times phi dk. So, this you can write f - f not y tau integral f dk. So, you have phi f dk and phi f naught dk. So, phi f will be n and phi f naught will be naught. So, n - n naught by tau. So, this is basically some kind of this is tau is a collision relaxation time and it is n – n naught by tau. So, if you substitute these values in the equation what you get dn by dt is del J n by q because it is del f.

And then g term is 0. So, r is dn by dt. So, if you see here this is exactly the carrier conduit equation and of course for equilibrium transport where there is no change in n. So, you can say dn by dt is 0 so, because there is no change in the carrier concentration due to the collision. So, n is same as n naught. So, then you can say dn by dt is the flux of current derivative of the current density special value divided by q.

So, that tells you that dn by dt and of course here you can add a term electron hole pair generation minus recombination due to maybe some optical source or whatever reason that generation term can be there. So, please find the difference this G phi and r phi are different then this optical generation recombination. Now similarly you can get the momentum balance equation by substituting phi is equal to q p by m or you can substitute p or simply k.

These options are there only the scaling factor will change. So, you can write q h bar k by m. The purpose of choosing this is basically you get J, if you choose just k then you will get J by q h bar by m those things. So, the main factor here is the k. So, when phi is proportional to k you have term related to the current density. So, now n phi becomes J n because you see here it will be q h bar by m integral k f dk.

So, this will give you n times k d, k d is the mean position of the wave vector due to the field. So, h bar k d by m becomes v d that the drift velocity. So, it becomes q n by v d. So, this is your J basically and you can use - q for electron. Now the flux of this electron becomes phi f phi u f dk. So, phi sk u sk. So, it becomes k square. So, k square means is energy term. So, with this scaling factor it goes -2q W by m.

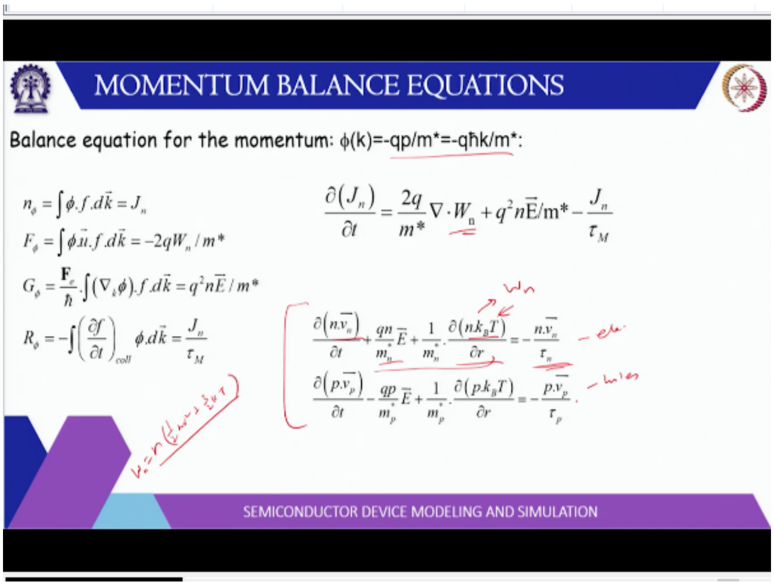
So, W is a kinetic energy density. So, if kinetic energy is increasing as a function of position that means this n phi is now J n. So, J n basically increasing. Similarly the generation term f by h terms del f by del k f dk now because phi is proportional to k. So, del phi by del k will be constant. So, this constant will be q h bar by m. So, it becomes F e q H bar by m times f dk. So, it will be simply n here and f is q times E.

So, it is basically if you see here this f is q times E by h bar and del F by del k becomes q h bar by m times f dk which is n. So, 1 h bar will cancel out. So, q square E by m times n. So, this is your generation term basically. So, that means the selective field give rise to the current density. Electric field generates the current density then similarly recombination term. So, it is f - f naught by tau integral phi dk. So, it is also proportional to k and dk.

So, f k becomes your J n - J n naught by tau. So, this tau will be average time, moment of the accession time. So, now you see here if there is for equilibrium case J n naught will be 0. So, this will be basically 0. So, you can write J n by tau m here. So, if you substitute this in the equation you will get d J by dt is equal to the gradient of the kinetic energy plus electric field times q square n by m - J m by tau. Now if you consider a stead state case that means d J by dt 0.

So, that tells you that J n is 2q by m tau, m times del dot W n + q square n tau m by m times electric field. So, you get exactly his is a drift term due to the electric field and this is due to the gradient of energy density. Now energy density you can write some k t half mv square + 3 by 2 k T L or you can write k T E also. So, the gradient of these things will give you the gradient of the temperature and so this will give you a diffusion term due to the temperature gradient.

(Refer Slide Time: 19:21)

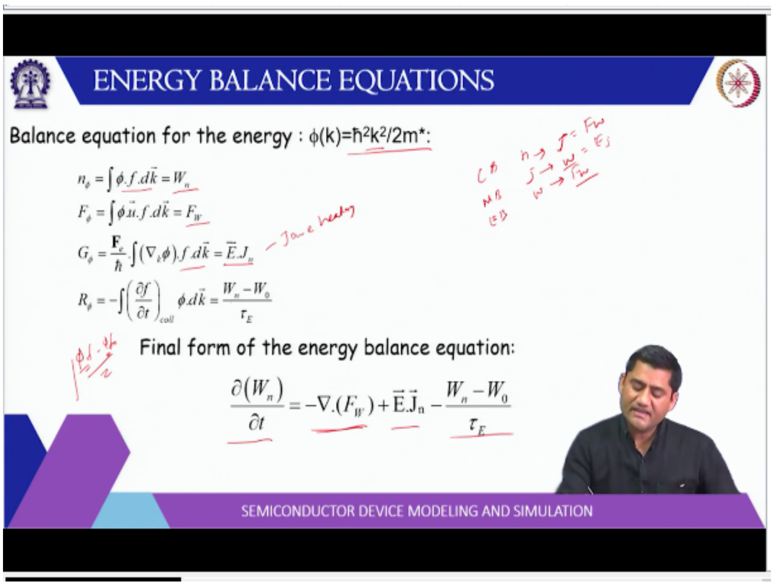


Now so if you substitute this phi, here we are substituting only qh bar k by m. So, if you take out the charge term here, if you just integrate with respect to h bar k you get d by dt of n v t + qn by E + n k T. So, this is the energy term. So, del I del r. So, the energy density is n k T because for single electron is half m v square + 3 by 2 k T and for n electron is multiplied by n.

So, W n is basically the total of these n electrons. So, you get the derivative of n as well as T. So, the derivative of n will give you the concentration gradient and derivative of T will give you the temperature gradient. So, then the thermal candidate will come into the picture and then you can write these two equations for both electrons and holes. So, d by dt is the electric field term then the diffusion term, temperature gradient term and so on.

So, this is total dn by dt basically. So, what we have done? We have basically rearranged it basically. So, from right side we move to the left side and right side is basically remaining n v by tau and n p v by tau for holes.

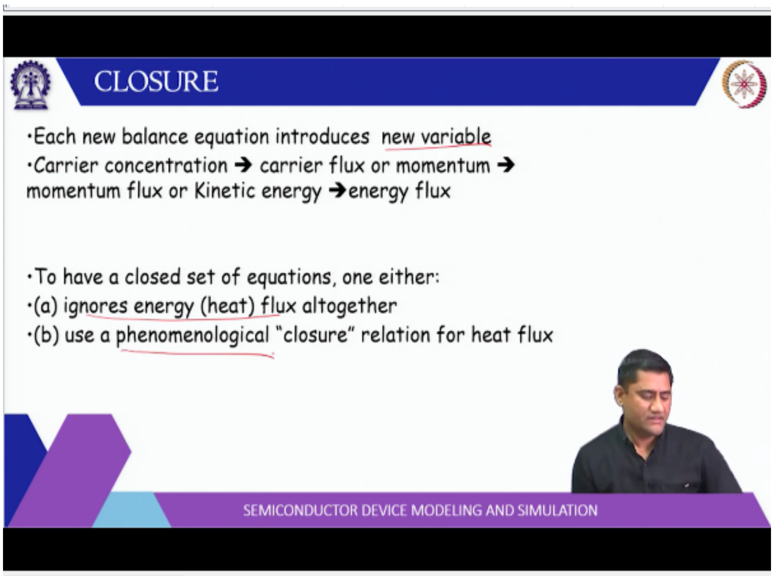
(Refer Slide Time: 20:48)



Now similarly we can draw the balance equation for energy by substituting phi equal to h bar k square by 2m. So, now n phi becomes h bar k square by 2m times f dk. So, that gives the energy density and the flux of the energy density is phi times u. So, it becomes k q basically and then generation is derivative. So, it becomes only instead of k square it becomes k. So, k f dk becomes J. So, f E times J is basically electric field times J and that you can say this kind of joule heating.

And then recombination term del phi by del t is f - f naught by tau times phi dk. So, for f into phi into f - phi into f naught by tau. So, that becomes energy density and equilibrium energy density. So, W n - W 0 by tau E and then of course you substitute you get d W by dt is minus derivative of flux plus joule heating minus W n - W n by tau E.

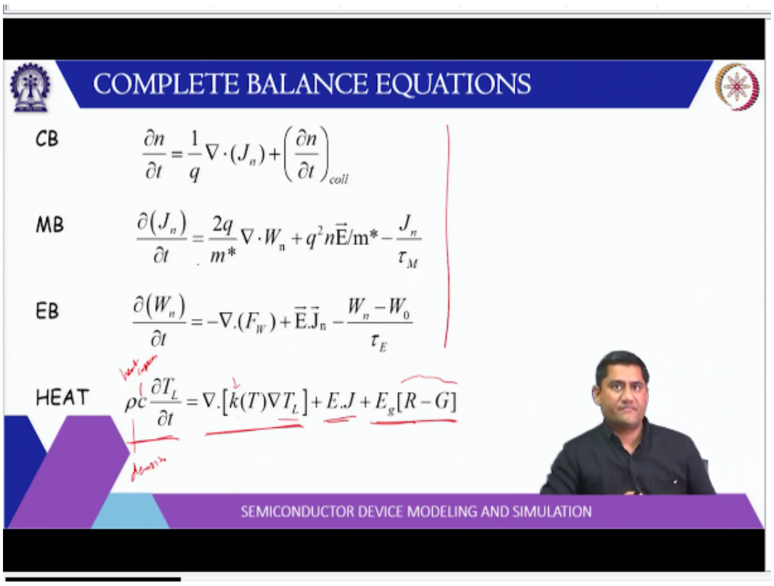
(Refer Slide Time: 21:57)



So, that means if you see all these three equations the equation for the carrier introduce J. So, in equation for carrier balance equation then we have the momentum balance equation. So, J it enters the W, then we have energy balance equation W which introduce the derivative of this F, the flux of energy density. So, the flux of carrier is current density, flux of current densities energy density and flux of energy and so on.

So, that means each equation is introducing a new variable. So, that way we can go on. So, we can infinite number of such equations basically. So, we have to close it somewhere. So, generally these three equations are considered carrier balance, momentum balance and energy balance. To close it basically what we can do we can either ignore the last heat flux term all together or we can use a phenomenological relation for the heat flux.

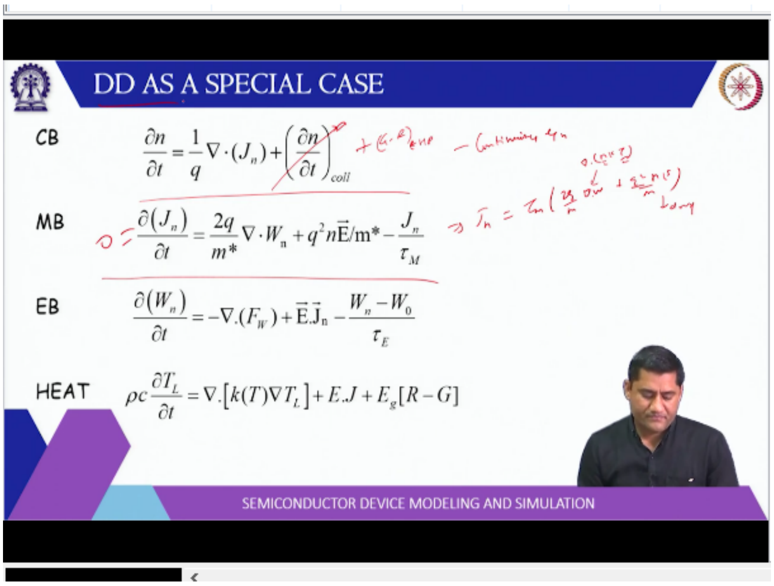
(Refer Slide Time: 23:10)



So, heat flux we can use phenomenological model. So, where you can say that the lattice temperature gradient del T L by del t is basically the heat flux plus joule heating plus the energy absorbed due to the recombination process. So, in the recombination this electron will combine and give energy equal to the band gap energy. So, E g times R and of course there is generation then this energy is taken away. So, we have R - G. So, this is electron voltage generation recombination.

Then the joule heating and then plus the heat flux basically. So, the heat flux is basically the gradient of heat conductivity times the temperature gradient and this basically increases the temperature of the material. So, that is given by rho c times dT by dt. So, rho is basically here, this is the density of the material, c is the heat capacity and k is a thermal conductivity and so on. And these are the relationships which are carrier balance, momentum balance and energy balance.

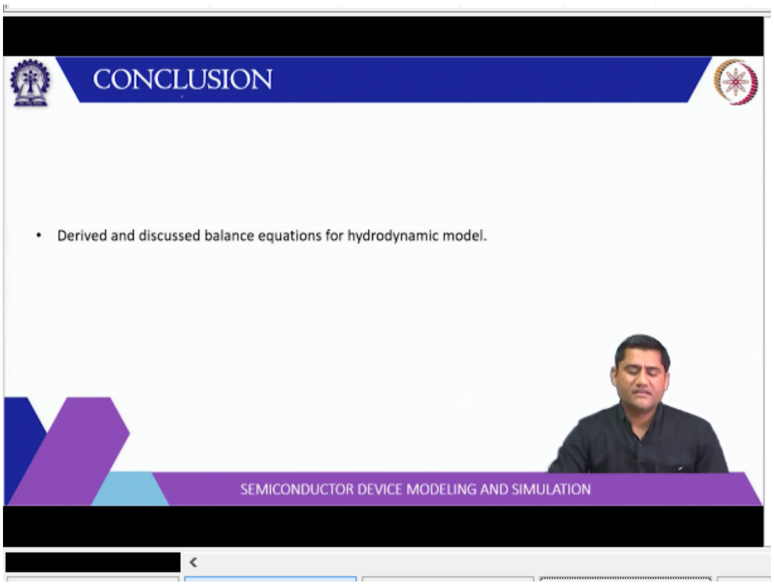
(Refer Slide Time: 24:34)



Now we can understand that drip division is a special case of this carrier valence and the momentum balance. So, the carrier balance if you recall if it is equilibrium dn by dt 0 plus you have generation term like electron hole pair generation. So, G - R due to electron generation mechanism. So, this is your basically carrier balance give you the continuity equation, it is a carrier continuity equation.

Then the momentum balance in equilibrium, this is 0. So, this gives the equation for J n = tau m times 2q by m del dot W + q square and E by n. So, this gives you and then this del dot W is basically your n k T, that is a energy density derivative. So, this is a drift term, then derivative of n is a diffusion term, derivative of temperature is temperature gradient term. So, these two equations give you the drift diffusion model. So, drift diffusion model is a special case of generalized thermodynamic model.

(Refer Slide Time: 25:48)



So, in conclusion we have derived and discussed the three balance equations for the hydrodynamic model and in next lecture we will consider how to solve these equations or how to discretize time domain and later on we will take up some problems. Thank you very much.