Air Pollution and Control
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Lecture – 15
Introduction to Air Quality Modelling

Hello friends, today we will discuss about introduction to air quality modelling. Before that you might recall like air quality monitoring we have discussed and then air quality index also we have discussed. So, what is the importance of air quality modelling? Where it is used? As you know because in monitoring we cannot do extensive monitoring, because it requires a lot of resources. And each and every nook and corner we cannot install instruments to monitor air quality.

So, basically air quality modelling helps us to estimate ambient air concentrations at various points of our desired destination or of our interest.

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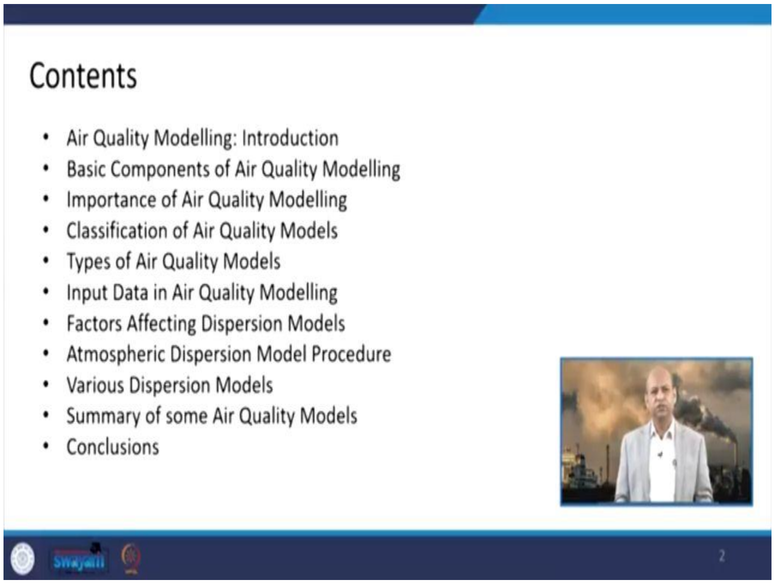

So, in this particular lecture we will consider like brief introduction about air quality modelling. What is the air quality modelling? Why it is used? And then the basic components of AQM that is the Air Quality Modelling and its importance. Then, classification on various ways we can classify them depending upon different kind of viewpoint. Then types of air quality models and the input data which are required for running the air quality model, and the factors that affect the dispersion models basically, because, modelling is a rough estimation or rough representation of reality in terms of mathematical equations.

So, some assumptions are there, some influencing factors are there, so that we will discuss. Then what is the atmosphere dispersion modelling procedure, how it is really like input parameters, how it is incorporated into the model, how it is processed, how output is taken and all those kinds of things. Then different kinds of dispersion models we will discuss, and we will summarize some air quality models. Because there are a lot of variety of air quality models, but we will discuss very few of them, and later on we will conclude.

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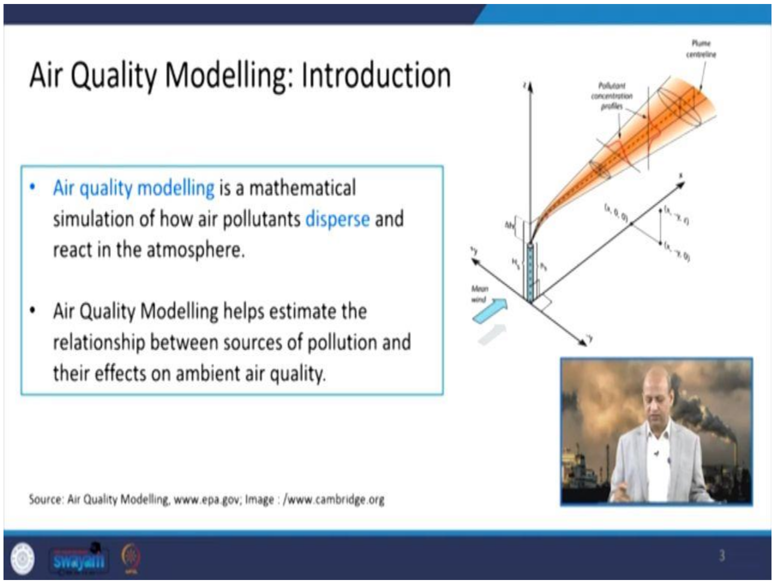

So, if we talk about air quality modelling, basically it is nothing but as I said mathematical representation or expression or simulation of how air pollution disperses and react in the atmosphere. Because it will move, it will change its face; so that kind of transformation as well as transportation. But, in simple dispersion models we sometimes assume that the gases and the pollutants are inert or they are not reactive. So, whatever they are being emitted in the form, they will transport in that way only.

Although it is very simplified assumption in reality does not happen; but for the sake of simplification, we do it quite often. Air quality modelling it also helps us in estimating the relationship between the sources of pollution and their effects on ambient air quality, or the receptor, on the environment, on human health, all those kinds of things. So, you can see here like at from the stack, some plume is coming out and it is dispersing. So, in x-direction, y-direction, z-direction, and it is diluting the pollution is being diluted.

Because, when it goes into the downwind direction, it disperses from the central line, left, right, and above, and below of the central line; so the dilution happens. And maybe at the point of our interest, dilution is so much that the air quality is not impacted or influenced by the concentration, which is being released due to emissions of the air pollutants from this point source.

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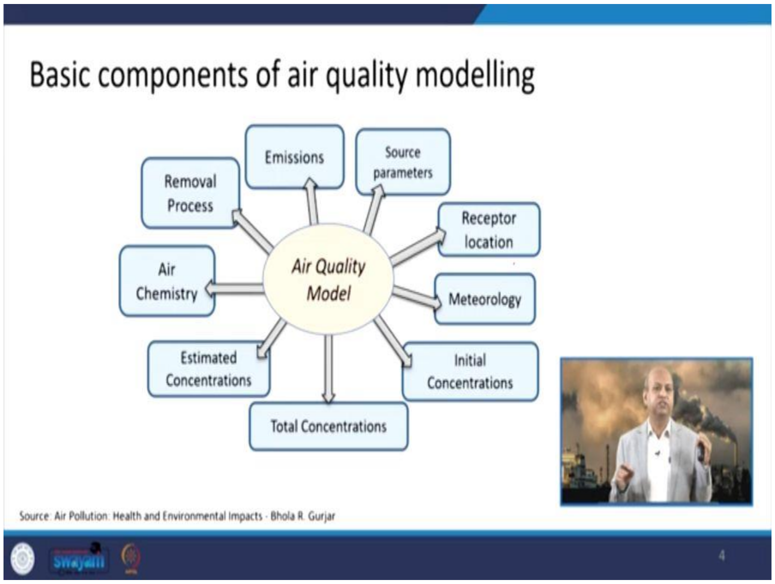

Now, if we talk about like basic components of air quality modelling, what are different components which really help us to build or form the complete model? So, we have to have like mission data, how much pollution is coming out of a particular source that we should be knowing, and then the source parameters. For example, if the stack is there, then what is the stack height? What is the diameter of the stack all those? Sources at the ground level or at certain height, whether it is a mobile source or an area source? So those kind of source parameters we need to know; then the receptor location.

What is the point of interest, where we want to calculate the concentration; because that is the point of interest? For example, from industrial area to a village we want to see how much dilution happens; and what is the impact of air quality of that particular village. Suppose some industrial area is coming up, it is planned. So, you want to know whether the emissions which will be from this industrial area that will influence the quality of that particular habitation, whether it is a city, or town, or a village. And how much air quality will be deteriorated or it will be insignificant?

So, you need to know the concentration because of those emissions like. So, the location of receptor is important because for that you have to calculate. So, X-direction that is the downwind direction; how many kilometers away that receptor point is. Then the meteorology; metrological parameter as you know, like wind velocity, its direction and temperature, humidity, all those kinds of things we should know. And the stability classification, A B C D; whether it is unstable or stable, or inversion happens quite often or not, all those kinds of things we need to know.

Then, the initial concentrations, because the point of interest, where we want to calculate the concentration because of additional emission source, which is coming up. So, what is the background concentration? Because in background concentration that additional concentration will be added; then we will compare with the National Ambient Air Quality Standards, whether those being exceeded or not.

If it is being exceeded, then we have to do something to reduce the emissions from that additional source or to sift the distance something like that. We have to or some technological intervention means you capture the pollutants before it is being released in the atmosphere so that the air quality of that particular point or the receptor, it is not deteriorated from the with respect to the air quality standards.

Then, the total concentration as I said that is the thing that the background concentration, the additional concentration, because of the additional source and the how much total concentration is there. So, the estimated concentrations maybe compared with the NAAQS; air chemistry also plays role sometimes, because if you want to estimate like Ozone products and or secondary aerosols, those kinds of things.

Then air chemistry plays a very significant role. Otherwise, if you are just considering criteria air pollutants like SO_X, NO_X, Particulate Matters etc. You can fairly assume that they are inert; although they are not. They are not inert; they participate in some atmospheric chemistry like sulfur dioxide gets converted into SO_3 or some sulphate. Similarly, ammonia, nitrate, ammonium sulphate all those kinds of things happen. But we for the sake of assumption or simplification, we assume that they are not reactive; so, that is another thing. In that case we can ignore the air chemistry.

But, in certain cases we do not want to ignore the air chemistry like ozone products and secondary aerosols etc. So, there we have to include the atmospheric chemistry into the modelling equations. Then, the removal processes because dry deposition is happening, sometimes where deposition happens because of rain etc. So, that is also to be taken into account if we want to estimate fairly of good quality; and all these things are there part of the complete air quality modelling effort.

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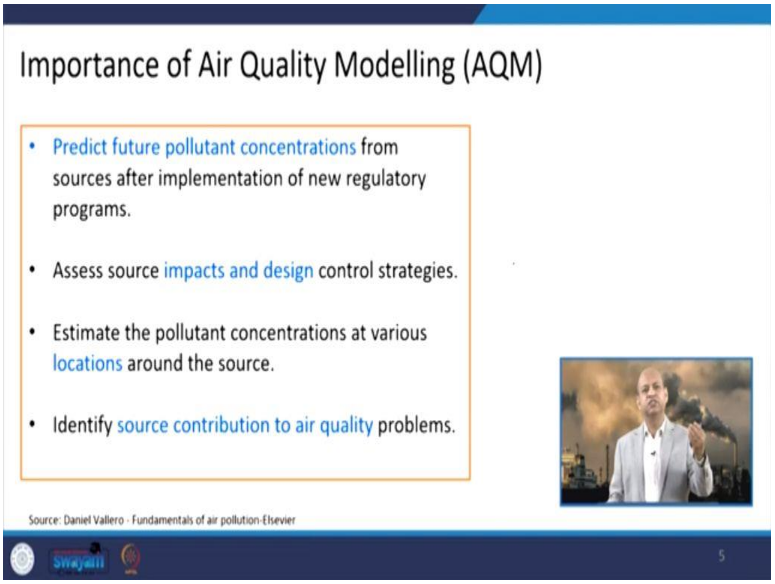

So, the importance of the modelling as I said, if you want to come up with some industrial area, whether it is at a good location or not, whether it will be influence the in downwind direction, some receptor that can be this village or town or it can be some sensitive area in the sense ecologically sensitive area, maybe there some river maybe there or some forest area maybe there, which is like century, which you do not do not want to influence its air quality.

Because, then the whole ecosystem can be negatively influenced. So, all those kinds of things are there and that is done by virtue of predicting the future concentrations from sources after implementing a new regulatory programs, or some new industrial area or something like that. In regulatory program assessment can be done like some, suppose you are going from BS IV to BS VI. So, emissions will be reduced, but quantities of vehicular or vehicles are growing.

So, what will be the impact of that? How much air quality improvement will be there if emissions are being reduced? Those kinds of things can be done by this air quality modelling also. There are other ways also, but that is the more important way. Then, assessing the source impacts as I said, designing control strategies, because if you come to know that because of some industrial area or some additional source, air quality of a particular destination or receptor is being deteriorated beyond the acceptable limits.

Then you will suggest some controlling strategies like some good fuel, less emitting less polluting fuel, or some technological interventions which can capture the emissions before it is being released in the atmosphere. It can also be used for estimating the pollutant concentration at various locations around the source, so that you can just give the information to the stakeholders.

See, this is happening like if your calculations are quite of a good confidence level; you can always argue that look at this, even if this industry is coming up, your air quality concentration will remain within the limits prescribed limits that is kind of thing. If it is coming, then you can also suggest that look at this, we have implemented, we have suggested this particular technological intervention or clean fuel kind of thing; so that the air quality will be not influenced in negative manner or affected in a negative manner.

Then, it also helps in identifying source contribution to air quality problems whatever episodes happen. So, what is the contribution of that source? if something like in a in a particular city for example, you are going to convert the whole fleet in a particular few CNG was implemented in Delhi. So, what is the impact of that? You can do by air quality modelling kind of efforts; you can know what what would be the positive impact on some pollutants, concentration now also. So, how does it work? So, you can see this, pictorial representation.

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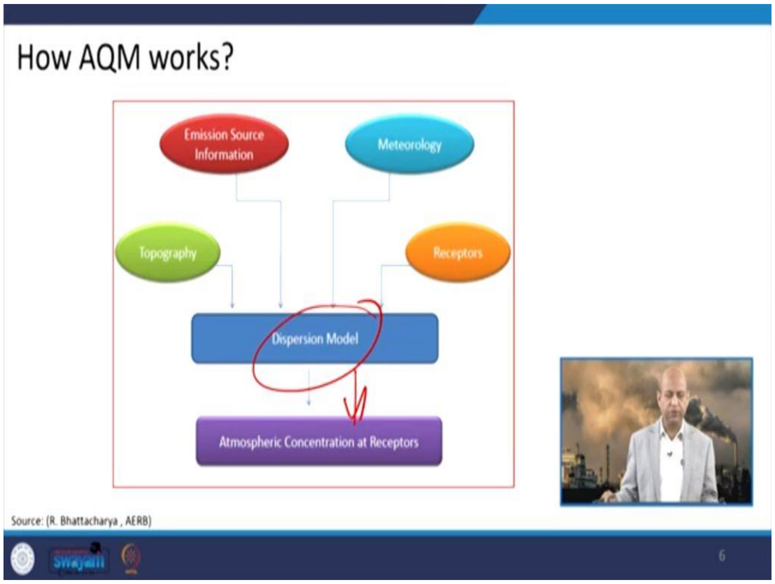

So, emission source information must be there, as we discussed that how much emission is coming, which pollutants are there; then, meteorological parameters as we discussed like temperature, wind, velocity etc. Receptors related for example, if it is a very sensitive eco-zone, or maybe at a particular location like some school is there, kids and those kinds of hospitals are there, those kinds of things.

Then, the topography is also very important, like it is a smooth terrain, or undulated and rough terrain, accordingly dispersion phenomena changes. So, that particular information should also be there. So, all these are the input parameters in dispersion model. And then it gives us the atmospheric (concern) concentration of air pollutants at the receptors location. So, this is the way it really works, very simple way.

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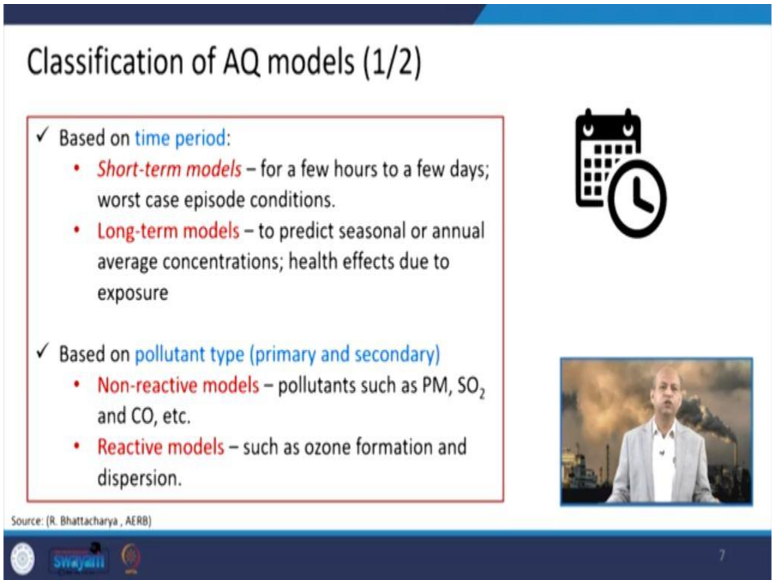

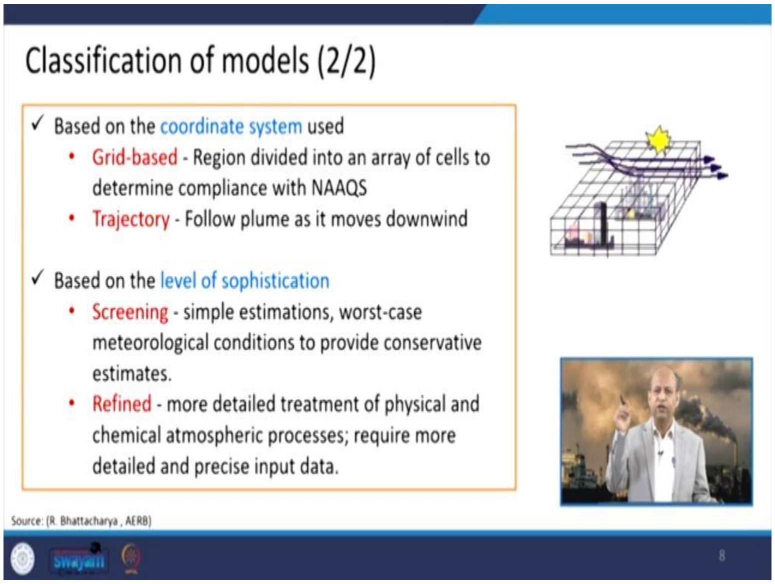

Then, if we want to classify to understand the air quality models, it can be classified in various ways. For example, in respect to the time period, the models can be short term models; that is for a few hours to a few days, it can estimate the concentration. And the like worst case episodes, episode conditions because of accidental release of some air pollutants or something like that, it can be modeled.

The long term models to predict seasonal or annual average concentrations, or health effects due to exposure, continuous exposure, like chronic exposure you can say, short term models acute exposure. Acute exposure means shorter duration, very high concentration. Chronic exposure, lower concentration, but longer term exposure for several months or years.

Based on pollutant type, primary or secondary, it can also be divided or classified like non-reactive models. That is the pollutants for example, Particulate Matter, SO_X, CO etc, which are assumed as non-reactive. Although in reality it is not like that as I said earlier also, but we assume for the sake of simplification; because in air quality models, estimated values are not needed 100 percent nearer to the actual value.

It can be around 40 to 50 percent away; even then, we feel that it is fine for assessing the boundary conditions or background concentrations comparing; and those kinds of things can be done by this very simplified view of modelling. Reactive models as I said, in case of like ozone formation, or some secondary aerosol formation etc. So, what is the dispersion of those particular pollutants? So, we do use the reactive models.

Then, there may be other classifications based on coordinate systems; grid based system like region divided into an array of different cells, which can determine the compliance with National Ambient Air Quality System or standards. The trajectory, which follows some plume as it moves the down in the downwind direction.

So, in grid we can divide the whole urban area in certain grids, even at regional scale, even at global air pollution modelling like general circulation models. They divide the whole earth in different grids, so you can divide into different grids, and you can estimate emissions for those grids. Those are the input values for air quality modelling techniques, and then you can estimate the concentrations into different grids. Then you can compare with the NAAQS or National Ambient Air Quality Standards.

Then based on the level of sophistication, like you want to use quick estimation, and you do some screening exercise. So, some simple estimations like worst case meteorological conditions to provide conservative estimates, okay; so, those are quick calculations. For worst case scenario, you assume like you may assume what will happen when inversion is there, or something like that. So, for a screening purpose, so that you can have some sense whether it is very problematic or not, after that you can go in detail.

Then the refined version is there, which requires detailed treatment of physical and chemical atmospheric processes. It requires more detailed and precise input data; whereas, in case of screening, it does not require so much very precise or robust data. You can just do like back of the envelope calculation kind of thing and you can come up with certain values.

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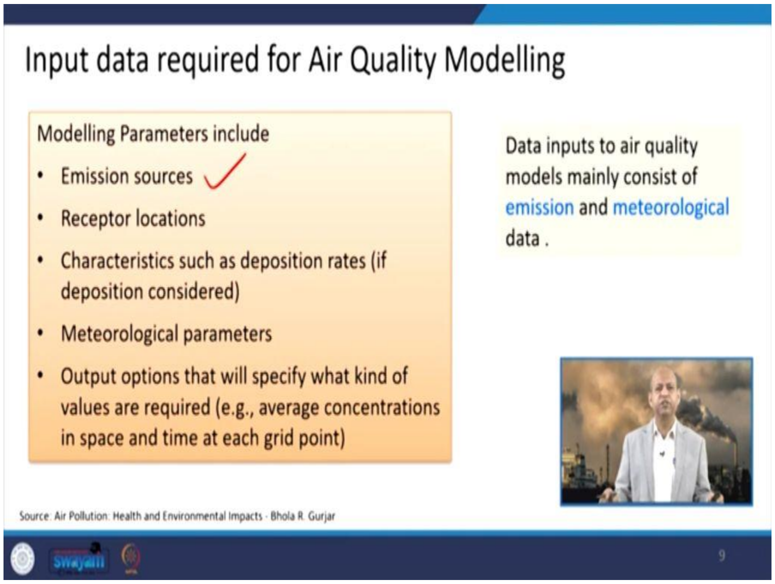

Now, we discuss about what are important input data, which are required for air quality modelling. So, you see here like we discussed earlier also emission sources; so, how much pollutant is being released. And what kind of pollutants are there all those, and whether it is a point source or line source, those kinds of things. If it is a point source like a stack, what is the diameter all those things, we have to see the emission source related data; then, the receptor location. As I said where we want to see the impact means downwind direction like 10 kilometers away, 20 kilometers away, what is the point of interest that we need to know?

Then the characteristics such as deposition rates, dry deposition or wet deposition whatever happening. At what rate it is happening? Because, it will be reducing the total amount of the pollutant which is being dispersed in the downwind direction. Then meteorological parameters which just now we discussed like stability, classification, temperature, moisture, wind velocity, all those things.

And then the output options like what kind of output we need, whether we need like average concentration in space and time in a grid point, or we need what is the unit we need like microgram, or some other kind of unit we need. Those kind of output parameters we need to fix; accordingly we will get the output from the air quality model.

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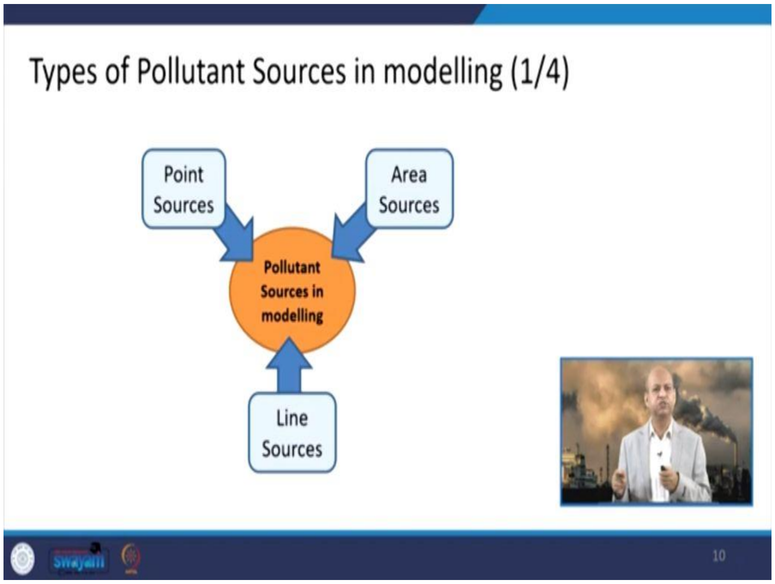

So, if we discuss about major types of pollutant sources in this air quality modelling, then basically three sources we consider like point source, line source and area Source. Somewhere you may also come across like volume source; but that is nothing but another extension of these kinds of sources. Otherwise, some model developers also say that basic thing is the point source model; otherwise, line source is nothing but several points in a line.

Area source means many lines in area. So, if you know how to model the point source atmospheric dispersion modelling, then you can easily extend that particular technique to derive line source modelling or area source modelling. Although, there are some empirical formulas also for line source, area source etc we will see what are those different techniques?

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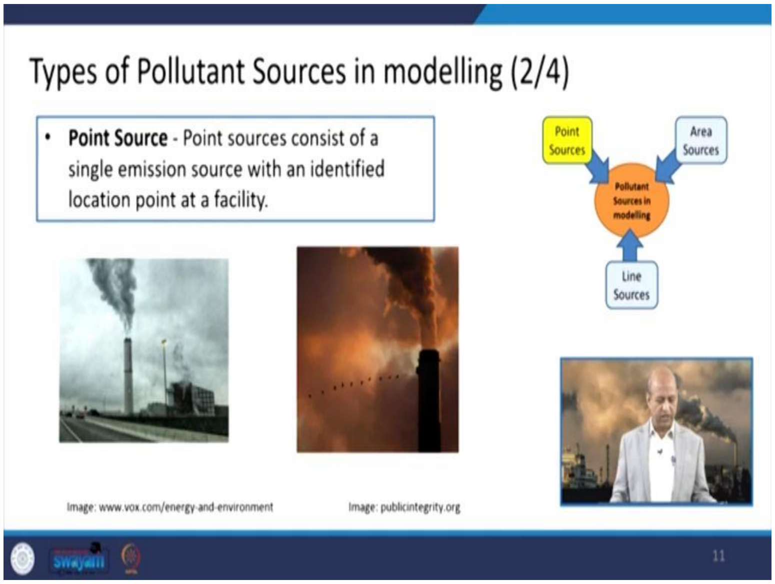

So, now you can see like point source. As I said, if it is a stack, so emission will come out, some exhaust gases will come out of the stack; so, you need to know the stack height etc. And this is the single emission source basically from a particular stack as a thermal power plant, or an industry, or somewhere like that. So, it can be identified as a point source. If there are several point source in a line, then you can call it a line source.

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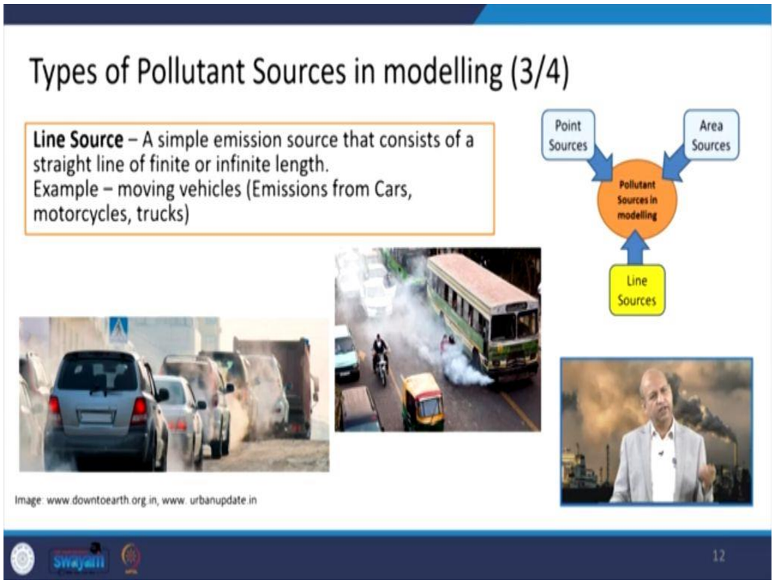

And like mobile sources also like vehicle is moving on the road that can also be considered as line source. So, vehicular emissions can be considered as line source.

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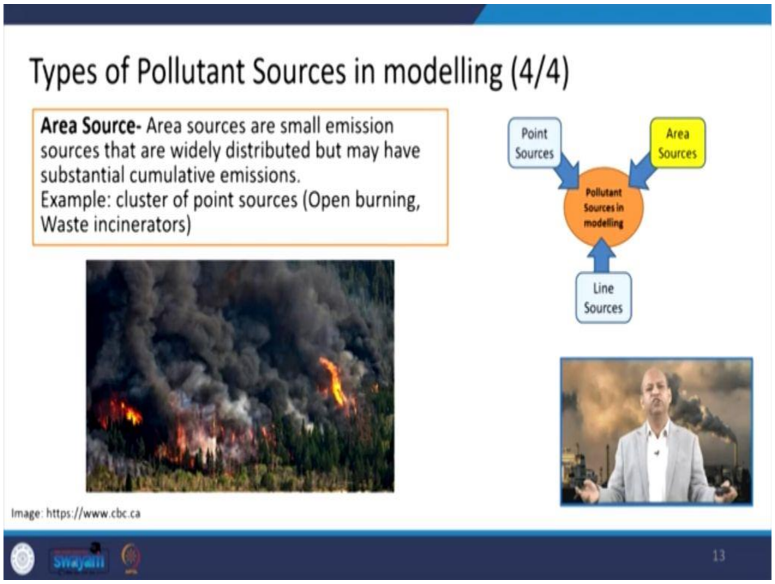

Similarly, in area source, whether it is big industrial area we have so many points sources are there, then you can consider it as an area source. Or, emissions are coming out of like forest fire, or in a landfill site, lot of emission is coming from several square kilometers that kind of area or several 100 square meters something like that; then you can consider it as an area source also.

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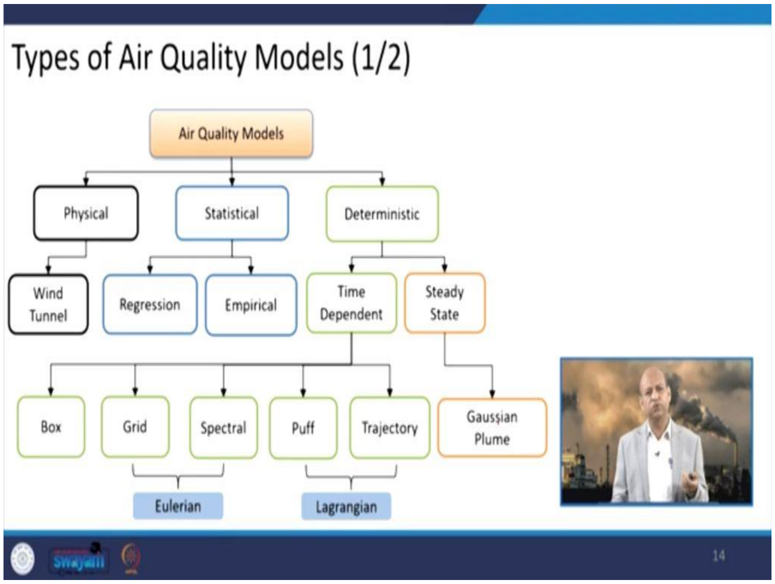

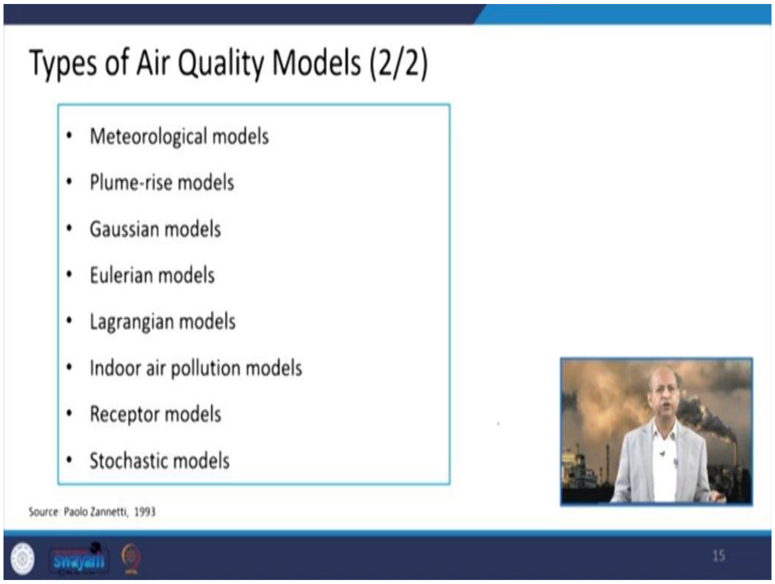

Now, if we talk about different types of air quality models, so it can be classified or categorized in different ways. For example, in general we call like physical models. In physical models, we have to do some structure kind of of that reality like in wind tunnel. You have small cubes etc that represent the buildings. How the pollutant will disperse? So, some kind of inert pollutant or tracers you can use for having the reading set different points. If you want to see the impact on multi storey buildings, those kinds of small structures you can fit in the wind tunnel; and accordingly you can model physical modelling.

But, then mathematical modelling can be there, which could be like a statistical model or deterministic model. In a statistical, it can be regressive or empirical, all those kinds of things. In deterministic, it can be time dependent or a steady state; means after certain time, a steady state means that concentration will be kind of uniform.

So, then Gaussian plume, it may be or in time dependent, it could be like box model, or grid, or spectral, or puff or trajectory related. Then different techniques could be like Eulerian or Lagrangian all those kinds of techniques are there; so, accordingly you can have those air quality models.

There maybe you might have heard about Artificial Neural Network (ANN) or fuzzy logic; those kinds of things are also being used nowadays. So, there are various kinds of modelling techniques you will come across. We are just discussing some kind of those popular modelling techniques, which are people are using extensively.

And even among those, we will discuss only few of them. Meteorological models can be there, because meteorological parameters you cannot have for each point in a city or in a region. So, again you have to estimate wind velocity or temperature at certain locations. So, the meteorological models help you to estimate those physical entities of meteorology like wind, velocity, temperature etc, with the help of some monitor data; so that you can validate those models.

Always these observed values help us in validating the mathematical models. Then we need to have plume rise models, because if we are modelling single point or point source model, so we need to have the effective stack height. So, effective stack height like this is the stack. But, the emission plume is coming out of it; and it rises. Then it is start dispersion. So, how much it will rise? That is Δh, which is known as the plume rise.

So, that Δh has to be added into this physical stack height; and then this will be the effective stack height. So, the plume rise models are also there, how much Δh will be there. There are several techniques for estimating those plume-rise models are also important. Then the Gaussian dispersion models from the stack, or from a particular source; so, that modelling technique is there.

Then Eulerian and Lagrangian we will see what those mean. Indoor air pollution models can be there, because in a room or in a building how those pollutants will disperse? Or they will defuse how much concentration will be in different corners of the building or in the office? So, those kinds of things are to be done at the micro scale. So, micro environment related air pollution modelling techniques are also there CFD etc.

Then, receptor models may be there; what will be the impact at the particular location, where the pollution is being received. Stochastic models maybe there statistical or so, those kind of modelling techniques can also be used.

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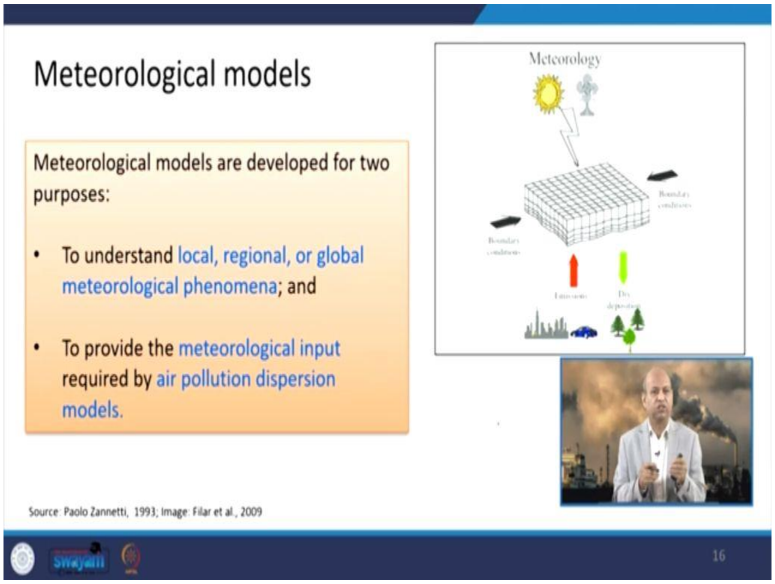

When we talk about meteorological models, so, as I said, it helps us in understanding local, regional or global meteorological phenomena. So that because as I said meteorological observations are at certain points; but, you might need those values for other points, where measurements are not there. So, these meteorological models will help you to get values of that particular at that particular point of interest.

So, to provide the meteorological input required for air pollution dispersion models, these metrological models, output will be input for the air quality dispersion model. You got my point, because meteorological models will give us certain values of temperature, or wind, velocity, or those kinds of things. So, that will be the output of these meteorological models. But, this will be the input for the air quality models, where we are aiming to estimate the concentrations by using these input values.

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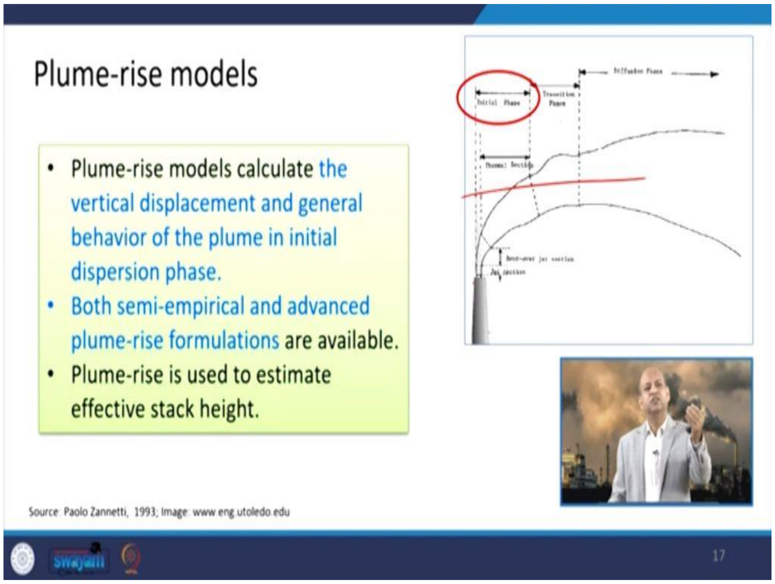

When we talk, as I said like this plume rise, plume rise could be because of buoyancy; because temperature difference is there, atmospheric temperature is less, and the exhaust gases are coming with very high temperature. So, the buoyancy is there because of this temperature difference, it goes out, it comes up. Then momentum is also there, because it is coming out with a speed.

So, the momentum and this buoyancy, though both these things these phenomena, they help in the plume rising up from this particular stack point to certain height. So, that we will measure how much this plume rise is there and those plume rise estimations are done by plume rise models. So, they really helped us in calculating the vertical displacement and general behavior of the plume in initial dispersion phase. Afterwards, Gaussian dispersion will consider it and it will be estimated accordingly.

Both semi-empirical and advanced plume rise formulations are available nowadays. And the plume rise is used for estimating the effective stack height as I said; because in dispersion models, you use the effective stack height, not the physical stack height. Physical stack height plus the plume rise; then that is the effective stack height. So, for that estimating, we need plume-rise estimations and those plume-rise estimations are done by plume-rise models.

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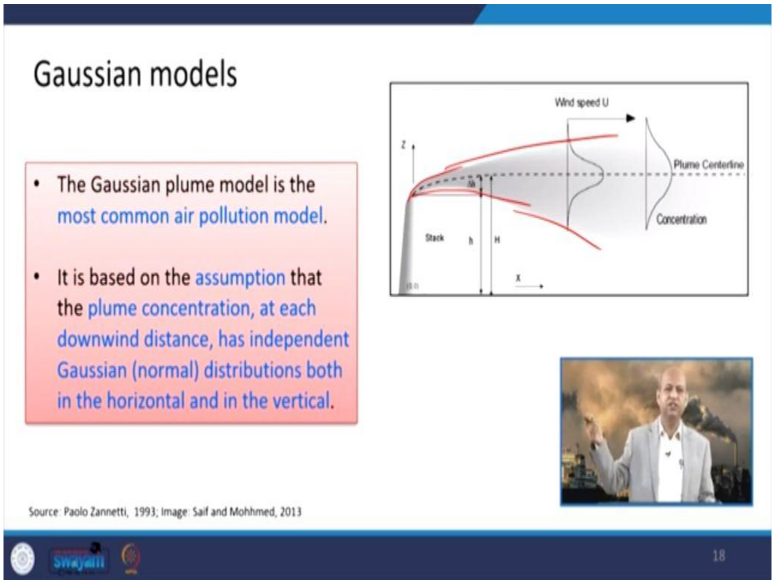

The Gaussian model, dispersion model very simple. So, this is the stack, the pollution is coming out; and it is dispersing in conical form. So, normal dispersion we assume, as it goes from the center line in y-direction, from the center and in z-direction also. So, it funnel kind of thing happens; so that thing known as the normal distribution, you can have these the concentration maximum at the central line; when it goes away, the concentration decreases, dilution happens. That is why this kind of normal distribution curve is there, and that is the reason we call it Gaussian models.

And you can see here Δh is there is smallest, small h is the physical stack guide, capital H is nothing but is small h that is the physical stack guide plus Δh; that is the plume rise. And then, you can use the Gaussian models for knowing the concentration at downwind distances of your interest.

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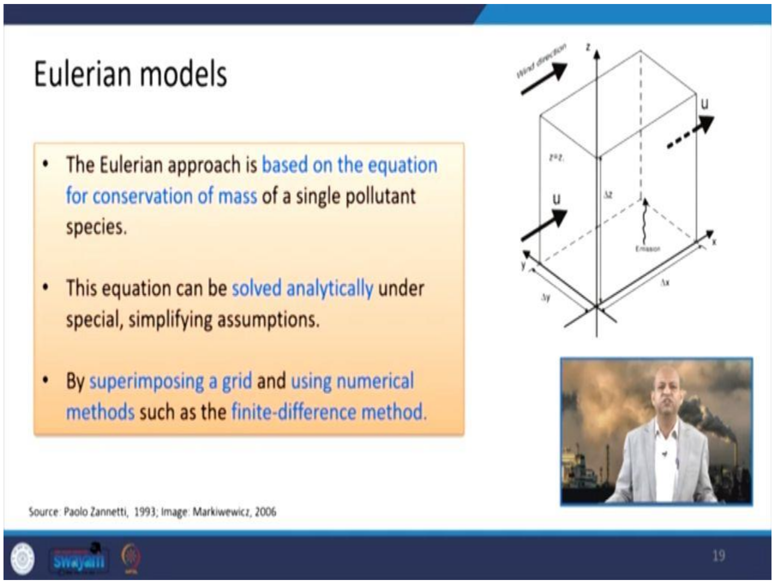

You see these Eulerian models; these are nothing but new techniques which are using equations for conservation of mass of a single pollutant disperses, and then they are integrated. So, this equation can be solved analytically under special and simplifying assumptions. And by superimposing a grid and using numerical methods such as the finite different methods; this particular Eulerian technique is used for estimating the concentrations.

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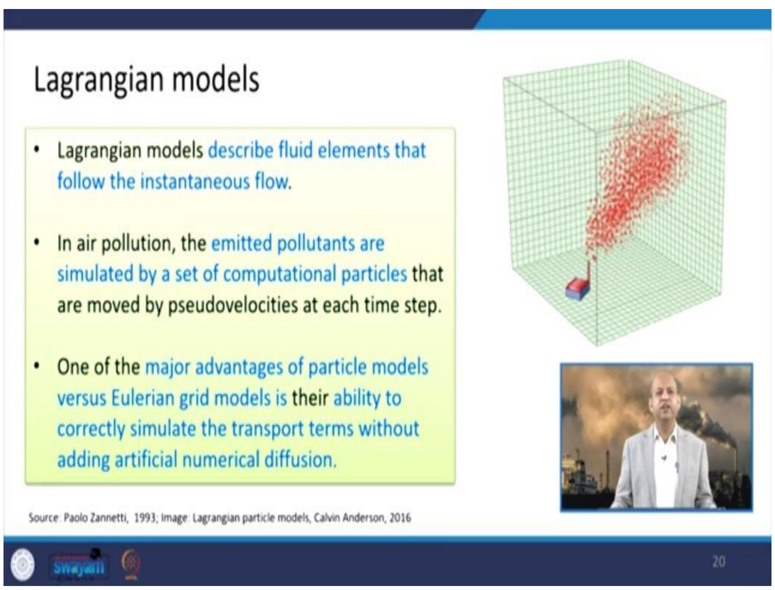

Then there is another technique which is known as Lagrangian models. Those are like fluid elements that follow the instantaneous flow. So, in air pollution and the emitted pollutants are simulated by a set of computational particles that are moving by pseudo velocities, following those pseudo velocities at each time step.

And one of the major advantage of this particular particle models versus Eulerian grid models is their ability to correctly simulate the transport terms, without adding artificial numerical diffusion. So, these two techniques Eulerian and Lagrangian they are very important in that particular sense.

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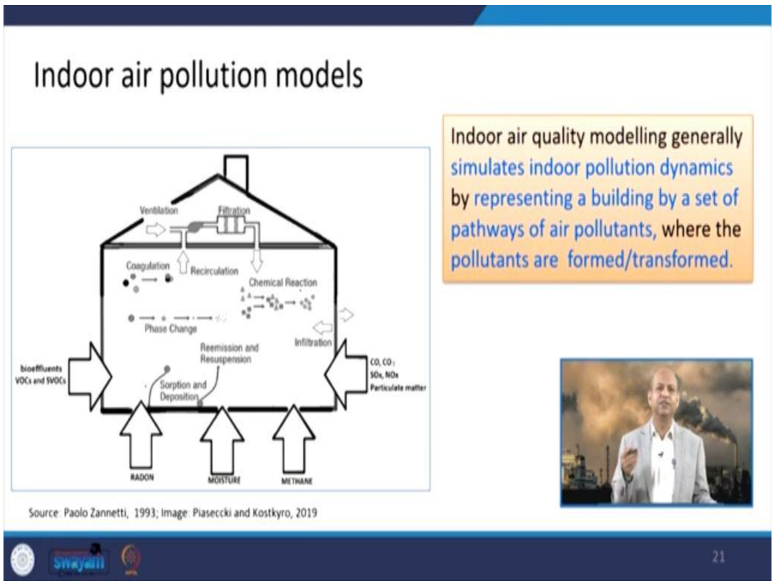

When we talk about indoor air pollution models, so, we need to consider several indoor sources; and also some pollutants are coming from external side also, like through windows, or through doors. Some pollution will from ambient air will enter into the house; so, that that is also to be considered. And the inner sources from kitchen or in office, it may be from computers or, say photocopying machine; in houses it can be from even washing machine, dryers. Pollution maybe in kitchen, all those sources can be there; and the paint, all those kinds of things are there.

And then the ventilation effect, filtration effect, then coagulation maybe small particles, then flocculation all those kind of recirculation because of this air conditioning ducts; so, the pollution may build up. That is why nowadays, many people are using these clarifiers or cleaners on those filters in the in the in house buildings.

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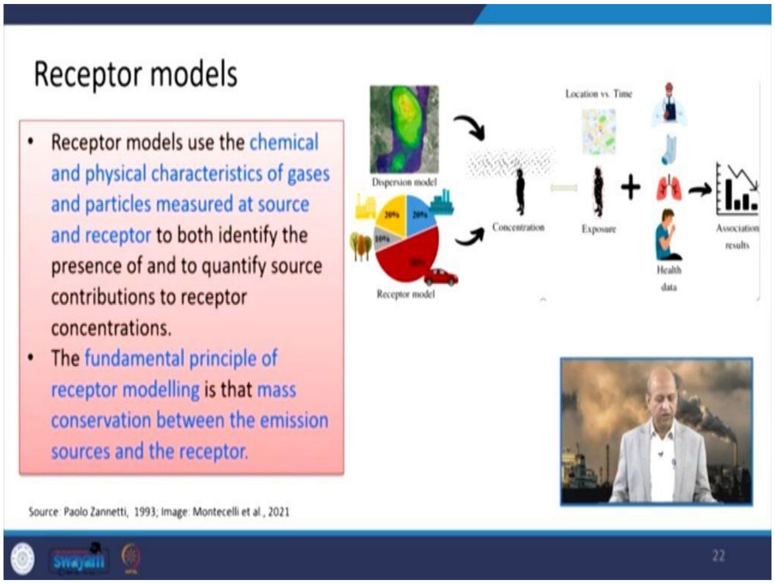

When we talk about receptor models that is used for chemical and physical characteristics of gases and particles, which are measured at source and receptor to both identify the presence of, and to quantify the source contribution to receptor concentration. So, like how much is coming from thermal power plants, how much pollutant is coming from transport sector; so, those kinds of source apportionment can be done by with the help of these models.

The fundamental principle of receptor modeling is basically the mass conservation between the emission source and the receptor. So, there are various techniques to identify those concentration and then the exposure, then its health effect all those kinds of things can be done by using these receptor models.

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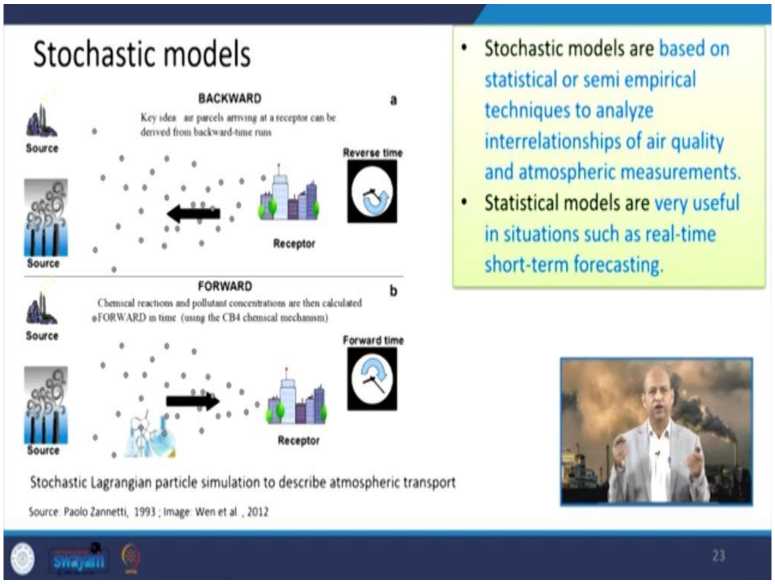

The stochastic models are various types. And the key idea is like air parcels arriving at a receptor can be derived from backward time runs or reverse technique. So, if you know the concentration at a particular place, you can do inverse calculation. You can know how much pollution is being emitted from a particular source. Forward can be chemical reactions and pollutant concentrations are then calculated by the forward in time using this CB4 chemical mechanism.

So, stochastic Lagrangian particle simulation to describe the atmospheric transport is shown in this pictorial representation. And these models are based on statistical or semi empirical techniques to analyze. It is not chemical interaction or those kinds of things, which we are, we use in chemical transport Models.

But, they are simple statistical relationships, semi-empirical techniques to analyze the interrelationship of air quality and atmospheric measurements. So, you develop some sort of relationship. These statistical models are very useful in simulations such as real-time short term forecasting, those kinds of; because they are quick and very easy. Otherwise, like atmospheric chemistry related equations, they are quite complex.

And if you want to know what is happening physico chemical reactions in the atmosphere; if you want to develop equations in that form, then it is quite complex. And it know, it needs very highly specialized knowledge of atmospheric chemistry. But in a statistical you know the only relationships are needed; so, that can be done with the help of the air quality concentration measured and the predicted by the model. So, you can train the model according to a particular situation.

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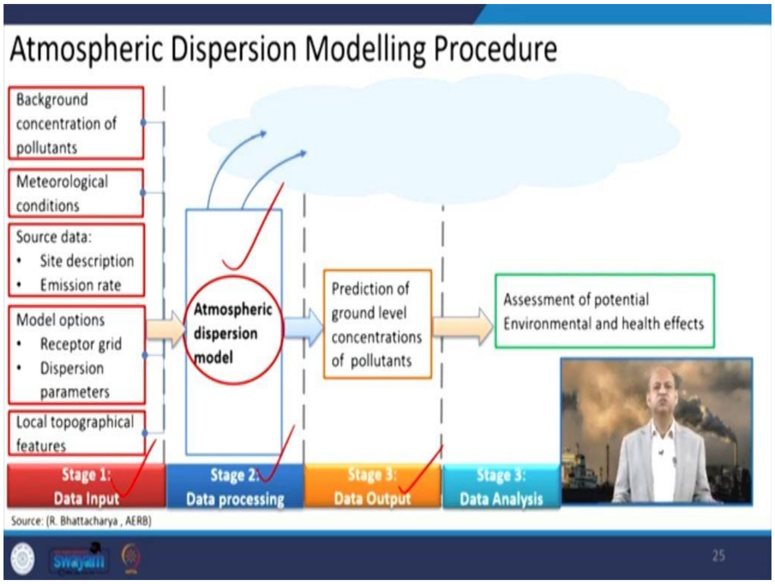

The factors, which affect the dispersion of pollutants in the atmosphere. Earlier also, we have discussed like source characteristics are there, some parameters of the source are there, which will influence the concentration or dispersion of the pollutants and the meteorological conditions. So, emission rate of the pollutant, what is the stack height, what is the plume rise? What is the exit velocity and the exit temperature of the gas? What is the stack diameter from metrological point of view what is the wind velocity, how what is the direction in which direction it is moving.

Then ambient temperature, atmospheric stability class like A B C D; whether it is very unstable or moderately stable or extremely stable or inversion all those kinds of things we need to know.

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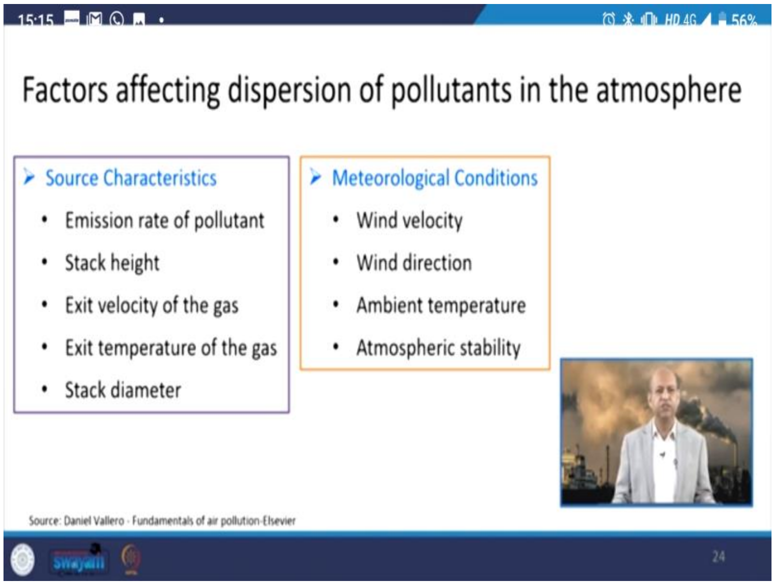

So, the atmospheric dispersion modeling procedure can be seen in simple way with this flowchart kind of thing, like background concentration of air pollutant we should know. So, that we can learn that after dispersion at a particular point, the concentration will be up or it will not be affected.

Then meteorological conditions we should have source data like site description, emission rate, then the model options like receptor grid related model is to be used or dispersion parameters. Then atmospheric dispersion model use all these kind of input values and it runs; so, the prediction of ground level concentration of pollutant is done as the output. And that is compared with the some guideline concentration like National Ambient Air Quality Standards, those kinds of things; so, that we can assess the potential environmental and health effects.

So, the stage 1, the data input, input data we should collect; then the data processing in the model, and the data output is there. And those data output are analyzed in comparison to certain values; so, that we can know whether it is fine or not.

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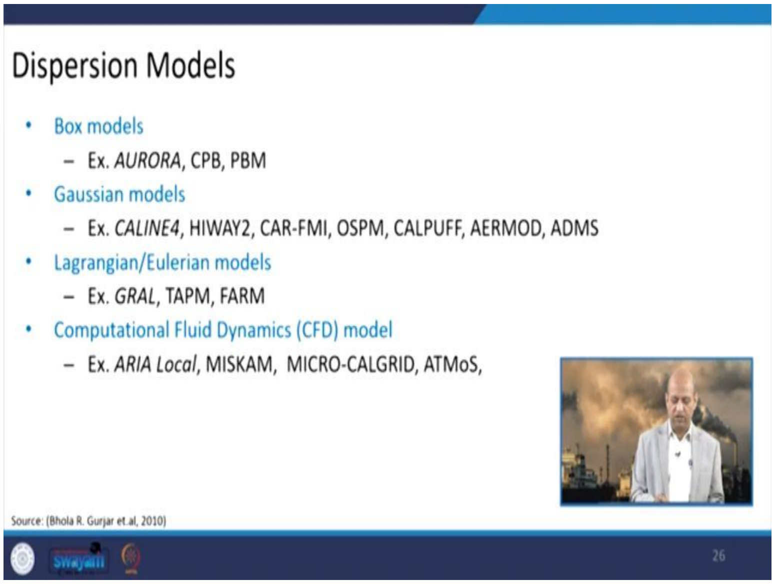

The dispersion models can be categorized in different ways like box models, and according to the developers they have been given different names like AURORA, CPB. Gaussian models can be there like CALINEE4, or HIWAY2, CAR-MFI those kinds of things; even air more which is quite popular, Lagrangian, Eulerian models. GRAL and then FARM; computational fluid dynamics CFD models maybe there, ARIA Local or MICRO-CALGRID, ATMoS those kinds of things models are available.

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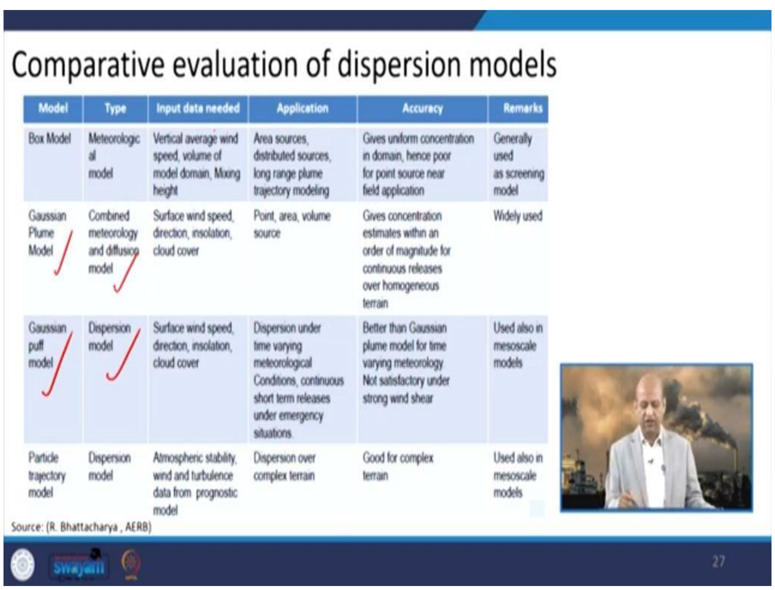
Comparative evaluation of dispersion models

Model	Type	Input data needed	Application	Accuracy	Remarks
Box Model	Meteorological model	Vertical average wind speed, volume of model domain, Mixing height	Area sources, distributed sources, long range plume trajectory modeling	Gives uniform concentration in domain, hence poor for point source near field application	Generally used as screening model
Gaussian Plume Model	Combined meteorology and diffusion model	Surface wind speed, direction, insolation, cloud cover	Point, area, volume source	Gives concentration estimates within an order of magnitude for continuous releases over homogeneous terrain	Widely used
Gaussian puff model	Dispersion model	Surface wind speed, direction, insolation, cloud cover	Dispersion under time varying meteorological Conditions, continuous short term releases under emergency situations	Better than Gaussian plume model for time varying meteorology Not satisfactory under strong wind shear	Used also in mesoscale models
Particle trajectory model	Dispersion model	Atmospheric stability, wind and turbulence data from prognostic model	Dispersion over complex terrain	Good for complex terrain	Used also in mesoscale models

Source: (R. Bhattacharya , AERB)

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So, if you do the comparative evaluation of dispersion models, we have listed different means we have gathered the data from different sources. And in this table we can see the box model, then the Gaussian plum model, Gaussian puff model. So, their type like they are meteorological model or combined meteorological and diffusion model or dispersion model; that is listed in different columns, you can go through that.

Then input data needed, what kind of input data needed in a particular model type; so, that is also listed here. Then application what kind of for point source, area source, or volume source; then accuracy whether it is very accurate or it is rough estimation kind of thing. Then remarks are given like widely used or specialized kind of thing. So, you can go through these models comparisons; so, that you can learn which model is used in what way.

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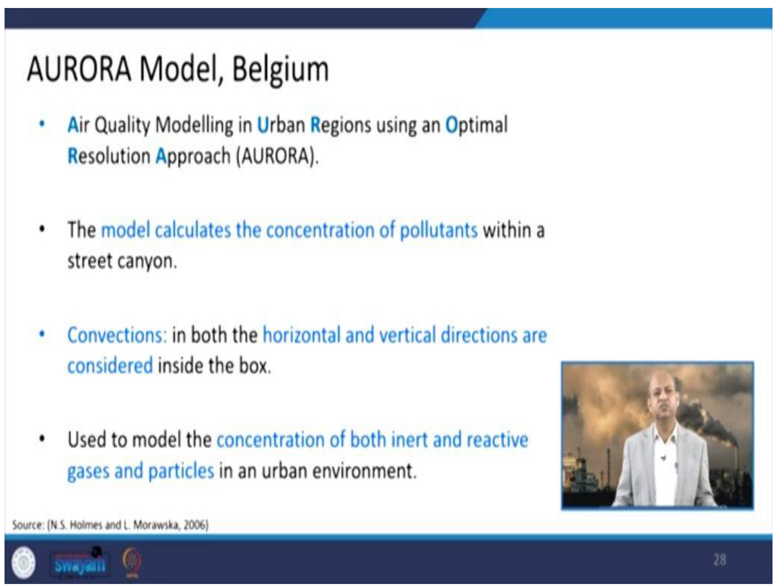

Now, if we go through with brief information of these models like AURORA model, which was developed in Belgium; so, this is nothing but the air quality modeling urban region using an optimal resolution approach. So, the in short it is known as AURORA. And the model calculates the concentration of pollutants within a street canyon; so that in a urban streets and those kinds of things city centers.

And the convections in both the horizontal and vertical directions are considered inside the box; so, that you can know the diffusion and disperse in both the direction. And it is used to model the concentration of both inert and reactive gases and particles in an urban environment. So, it is a kind of versatile model in that sense.

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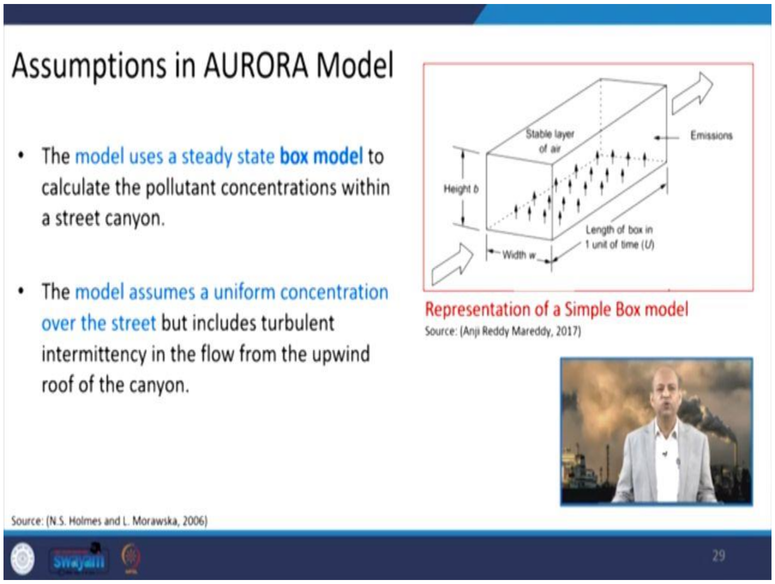

Certain assumptions are there for this particular model. Like it is used as a steady state box model, where uniform concentration is achieved at a certain point; and then it will be the particular model. In this box model, this whole city is like length, width and height boundary layer. So, in that everywhere the uniform concentration is assumed, which may be not so true; but for the sake of simplification as I said, it is assumed. So, in whole street canyon that uniform concentration happens.

The model assumes a uniform concentration over the street, but includes turbulent intermittency in the flow from the wind route of the canyon; so that is also one aspect important aspect of this model.

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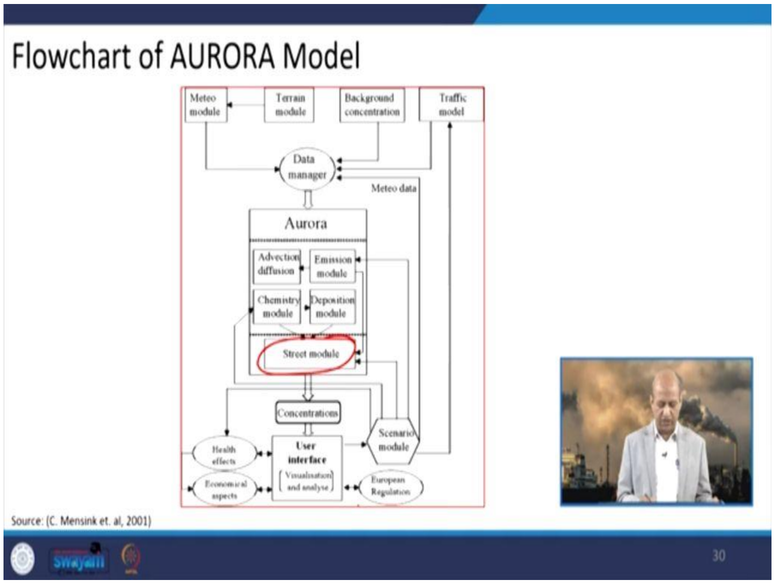

This is the flowchart of the AURORA model. So, this meteorological module is there, then Terrain module like soft; this is smooth terrain is kind of rough terrain is there, background concentration, traffic model, all these are combined. And the data manager takes all these data and put in this model. Then, the advection diffusion kind of module, emission module, chemistry module, deposition module, all these modules work.

And then they model this particular street canyon and the concentration is estimated. And then we can see according to the need, whether we want to use for health effects, or economical aspects or, some scenario based interpretation; all those things can be done by comparing with those kind of standard guidelines.

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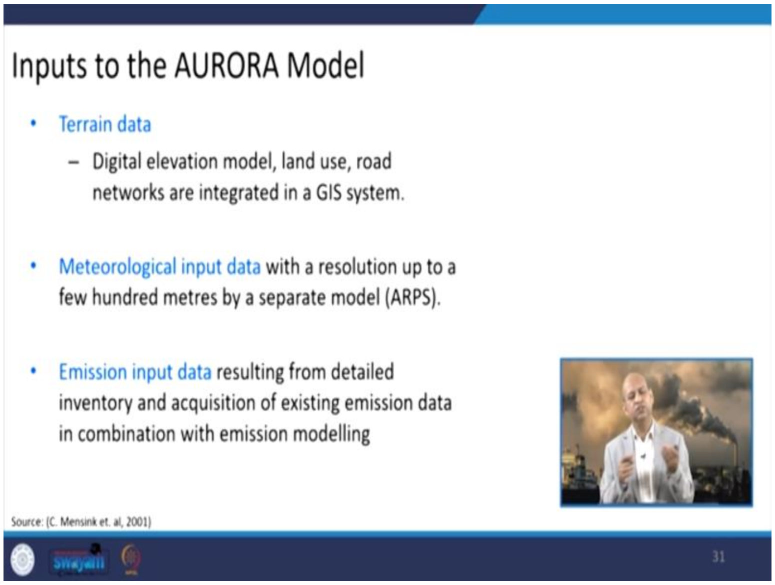

And the input values as I said, the terrain data is to be taken from that particular module, which gives the classification of different land uses, road networks in a GIS system integrated. And meteorological input data with the resolution up to a few 100 meters by a separate module is included in this particular model. And emission input data resulting from detailed inventory and acquisition of existing emission data in combination with emission modeling. So, whether grid pattern or the whole area city that can be defined; and that emission inventory is used as input data for this particular model.

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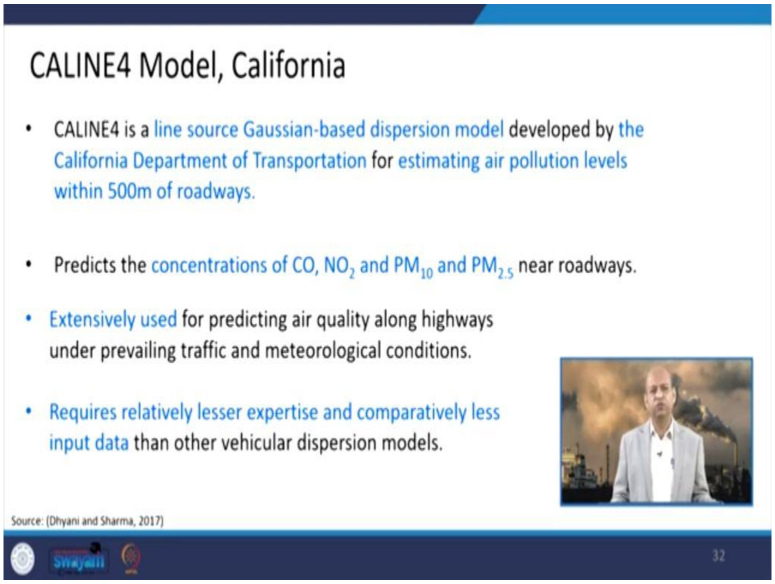

Then, another model like CALINE4 model of California, which is a line source Gaussian based dispersion model, which was developed by the California Department of Transportation. And the aim was for estimating air pollution levels within the 500 meter of the roadways. And it predicts the concentration of carbon monoxide NO_2, PM_{10}, $PM_{2.5}$ near the roadways, extensively used for predicting air quality along highways under prevailing traffic and meteorological conditions. It is quite popular model basically; and it requires relatively less expertise and comparatively less input data, than other regular dispersion models.

That is why it is quite popular in developing countries also. Because, as you know in developing countries, we do not have much data; otherwise in developed countries, they have so much data as per their system. But we do not have much input data and in that case, these kind of simple models are very useful.

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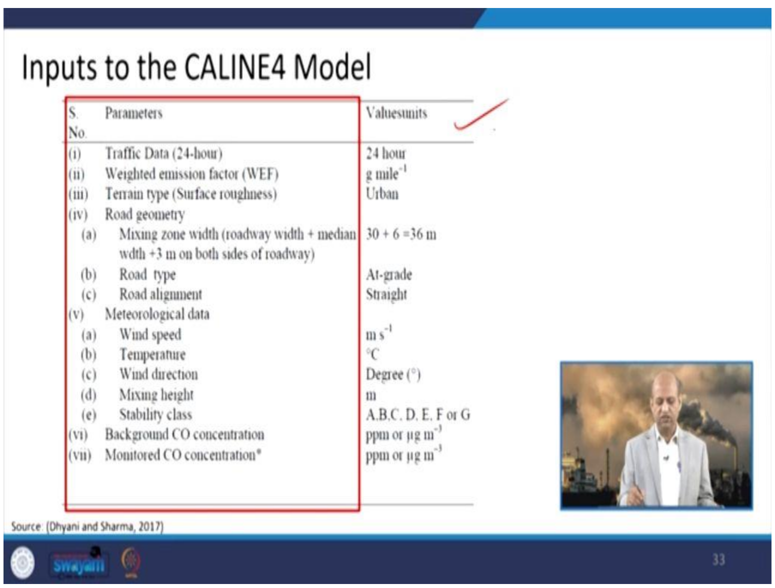

The input input values or parameters for CALINE4 models are given like traffic data for 24-hours; then weighted emission factors. And the terrain type surface roughness related factors can be there; then the road geometry, road type, road alignment, straight or curvilinear all those kinds of things.

Meteorological data as we always say like wind speed, temperature, mixing height, boundary layer height, and the stability class A, B, C, D, E, background CO concentration, monitored CO concentration, whatever. Means whether NO_2, whatever the pollutant you want to estimate; so, those kinds of concentrations and these units are given in that way. They are they should be therefore input values for CALINE4 model.

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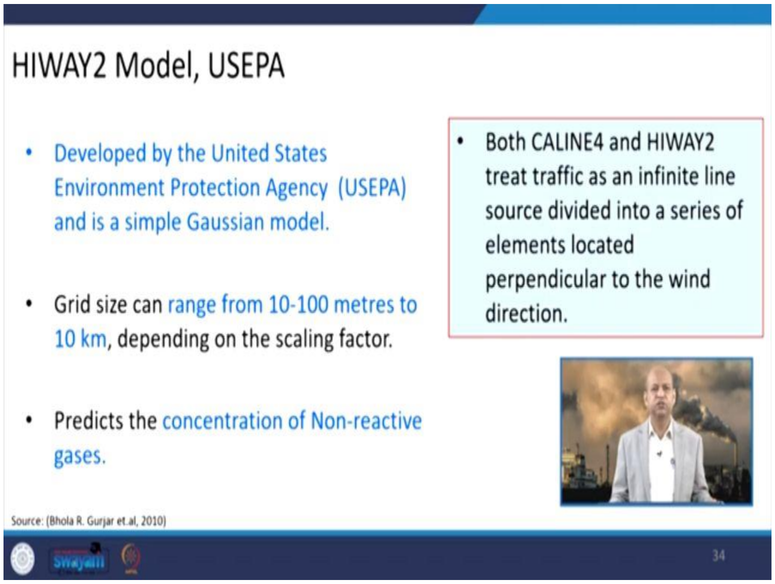

Next is HIWAY2 model, this is developed by United States Environmental Protection Agency. And this is grid size can range for this model from 10 to 100 meter to 10 kilometers; so quite versatile in that sense. Good possibilities there for a small that area to quite large area, depending upon the scaling factor basically; and it predicted the concentration of non reactive gases. So, that is the limitation you can say for reactive it is not being used; but for non reactive gases, it can give a good estimations.

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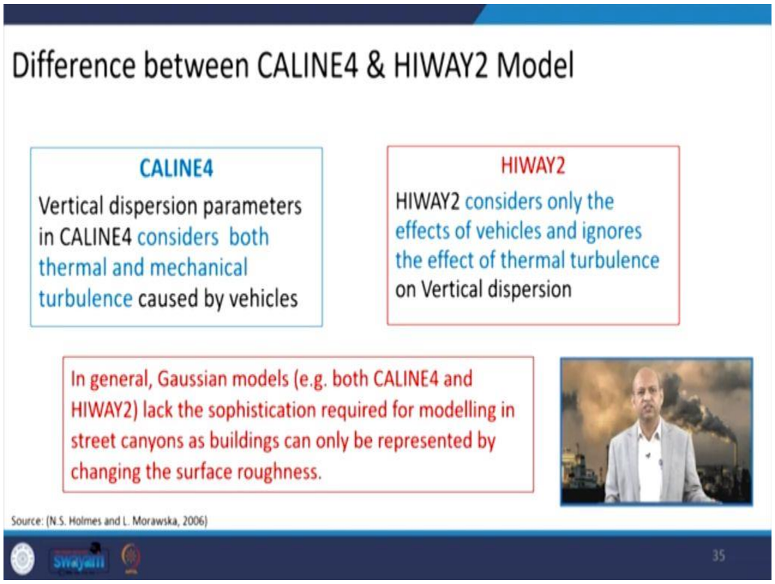

Then the difference between if you want to see CALINE4 and HIWAY2, because they are similar model. They are estimating the impact of highway emissions or line source emissions to the perpendicular direction of the highway in the 500 distance, or so how much effect is there, how much impact is there.

So, if you compare, then you can see that in case of CALINE4, the vertical dispersion parameters are considered both thermal in in the way of thermal and mechanical turbulence caused by the vehicle. So, that is the part or mechanism of CALINE4. Whereas, in this case of HIWAY2, it considers only the effect of vehicles; and ignores the effect of thermal turbulence on vertical dispersion.

So, in general you can see Gaussian models like both CALINE4 and the HIWAY2 lack the sophistication, which is required for modeling in street canyons as buildings can only be represented by changing the surface roughness. So, those kinds of limitations are there, but difference is clear in that sense that CALINE4 is like it is having the inclusion of mechanical turbulence also.

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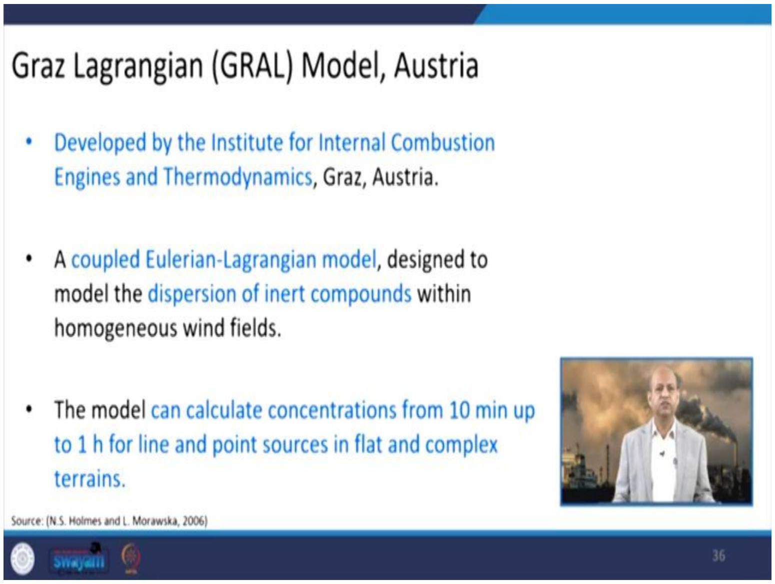

Then you can see this GRAL model, it is Graz Lagrangian. So, this was developed by the Institute for Internal Combustion Engines and Thermodynamics, Graz in Austria. And the coupled Eulerian and Lagrangian model it is designed to model the dispersion of inert compounds within the homogeneous wind fields.

And this model can calculate concentrations from 10 minutes to 1 hour; line and point sources in a flat and complex terrain. So that is one strength of this model that for time is scale of 10 minutes to 1 hour. It can really calculate, which may not be possible in case of those approximations which are used in bigger dispersion models of Gaussian nature.

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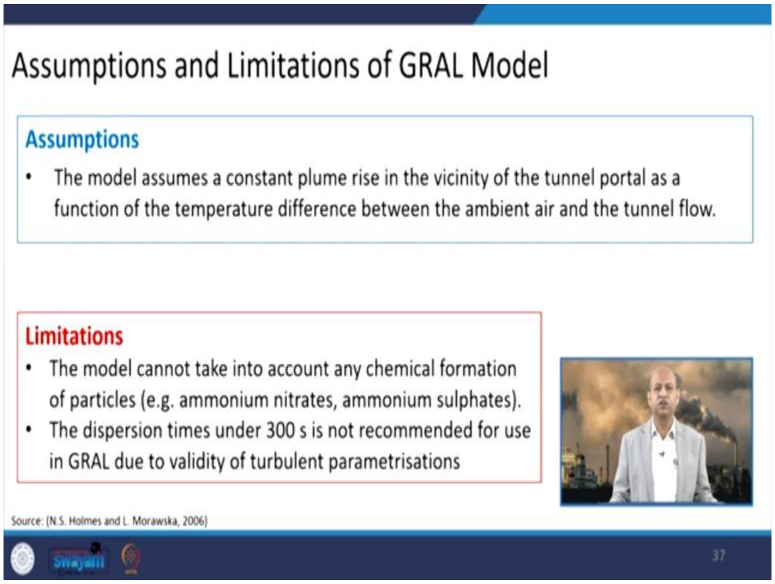

The assumptions and limitations of this particular GRAL model are also there. It assumes the model assumes a constant plume rise in the vicinity of the tunnel portal, and as a function of the temperature difference between the ambient air and the tunnel flow. So, that is the basic assumption, which may not be so true.

And then limitations are there like this model cannot take into account any chemical formation of particles; because it is taking only non reactive gases as I said. So, the reactive reaction related things is not part of this model. So, the ammonium nitrate formation, ammonium sulphate those kind of secondary aerosol formation is not the part of this model. The dispersion times under like 300 second is not recommended for use in this particular model, due to validity of turbulent parameterization; so, that is one more limitation in that case.

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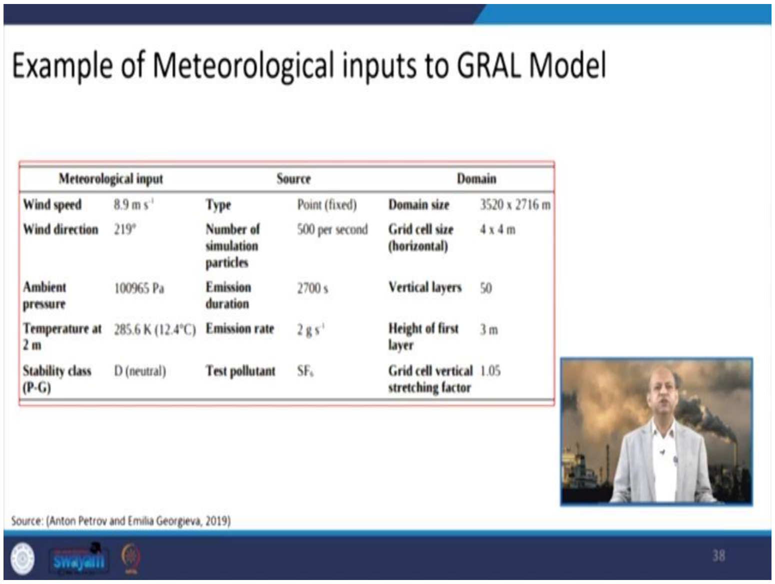

The examples the typical example of meteorological input in this particular model is given in this table. You can see how much wind speed, wind direction. And then, the type like point source or something domain size, grid cell size, vertical layers; all those things are given here, which are typical input parameters for this GRAL model.

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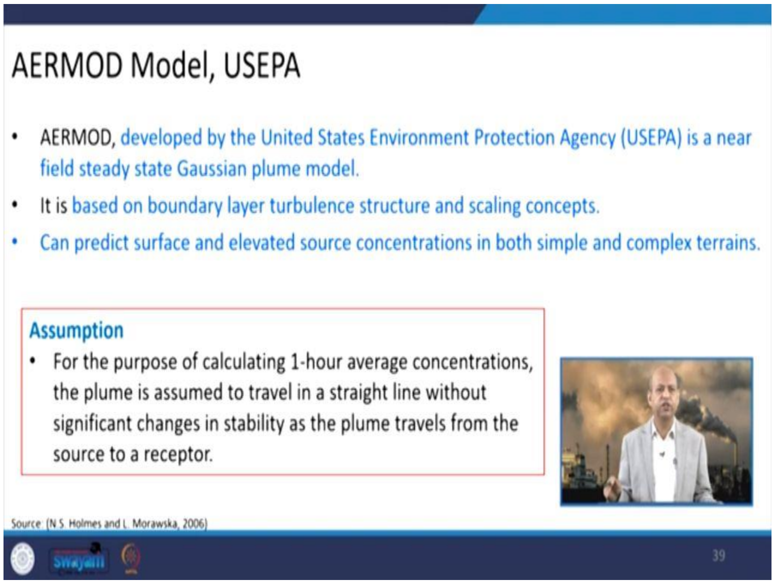

When we talk about AERMOD model, which is quite popular; and it is developed by United States Environmental Protection Agency and American Meteorological Department or Association. So, this is very popular model in the sense it can consider boundary layer turbulence structure and its scaling concepts also. And it can predict surface as well as elevated source concentration in both simple and complex terrains.

So, that is the versatility of this particular model; again, CALINE4 it is also very popular in developing countries. And assumptions are there for the purpose of calculating one hour average concentrations, the plume is assumed to travel in a straight line; wherever it may not be true, because wind changes quite frequently, wind direction.

But we assume in a straight line without significant changes in the stability as the plume travels from source to the receptor. So that is very simple assumption, which, which may not hold true in the real life. But as I said, these kinds of models use these kinds of assumptions; otherwise it is difficult to incorporate all those kind of very complex mechanisms, which are there in the atmosphere.

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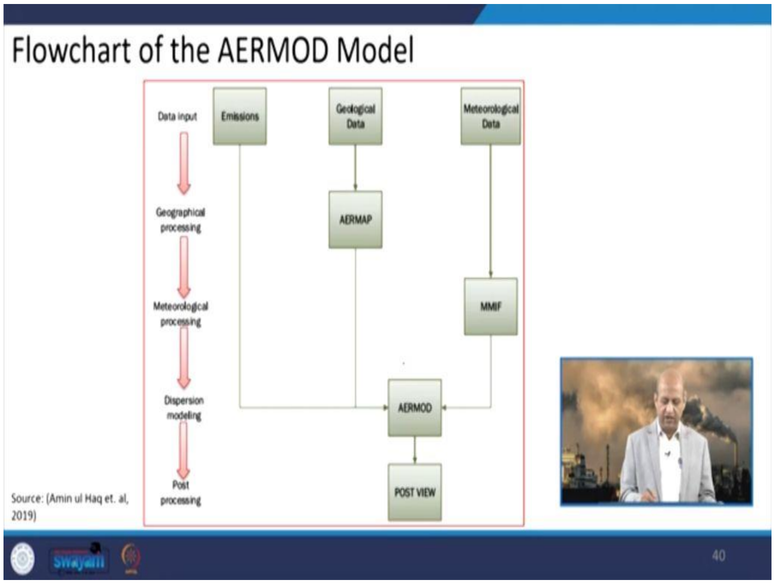

The flowchart which is being shown for the AERMOD model, so data input there like emissions, then geological data related surface terrain, meteorological data, wind, temperature, etc. Then you can see these geographical processing, meteorological processing, and dispersion model. And then the post processing that means, we analyze the data of the estimated values of concentration.

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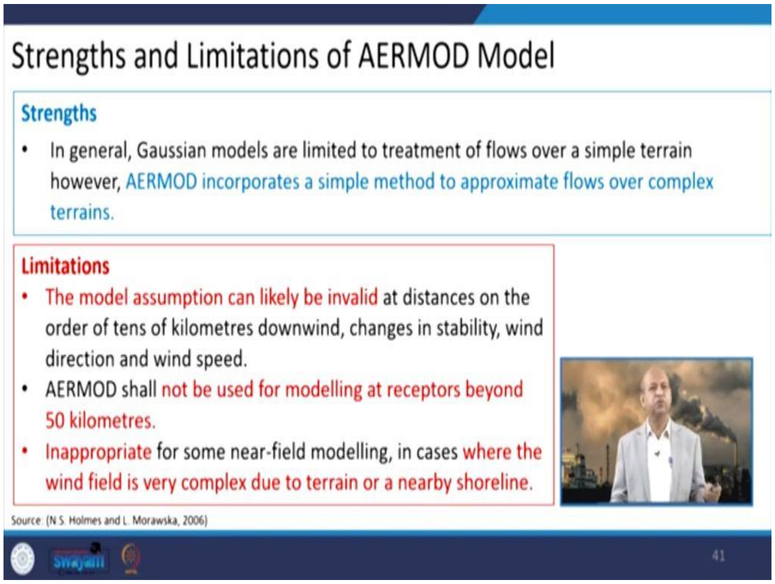

There are certain strengths and limitations of this AERMOD model. So, in case of strengths as I said, it is treatment of flows over a simple terrain; and it incorporates a simple method to approximate flows over complex terrain. So, in that simplified way it is quick to learn and it can quickly process those estimated values.

But, limitations are there like it assumes some invalid kind of thing, like assumptions can be invalid at a distance on the order of tens of kilometers downwind, which can change the stability wind direction and wind speed. So, that is why this is not very suitable for modeling the receptors beyond 50 kilometer; so, that is the limitation of the, how much distance in the downwind direction or for that particular grid, you can.

So, if there are mega cities which are spread over beyond 50 kilometers, then this model is not so good in that sense. Then you have to run it in different modules or ways for different distances. It is inappropriate for some near field modeling in case where the wind field is very complex due to terrain, or a nearby shoreline or so. So, in that case those complex models or CFD etc, they are useful for for that purpose material; but AERMOD model is not good in that particular sense also.

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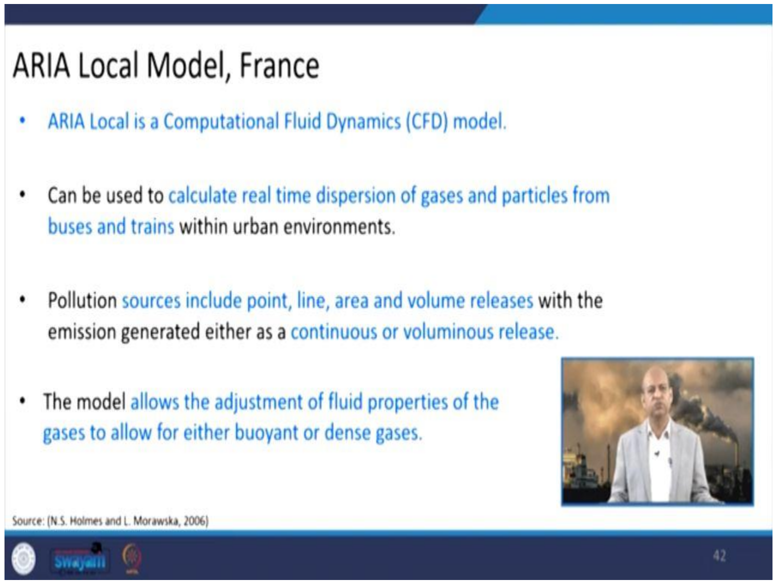

There is another model ARIA model, ARIA local model of the France, which is CFD model; basically, computational fluid dynamics model. And it can be used for calculating real time dispersion of gases and particles from the buses and trains within the urban environment. So, mobile sources, it can be estimating the concentrations from the emissions from mobile sources.

Then the pollution sources include point source or line source, area source, volume; so it is versatile in that sense, and those emissions which are either a continuous or intermittent those kinds of things. Then the model allows the adjustment of a fluid properties of the gases, which can further allowed to either buoyancy kind of characteristics, or the dense gases which comes down. So, both ways it is having that capacity; so that is a wonderful thing in that sense.

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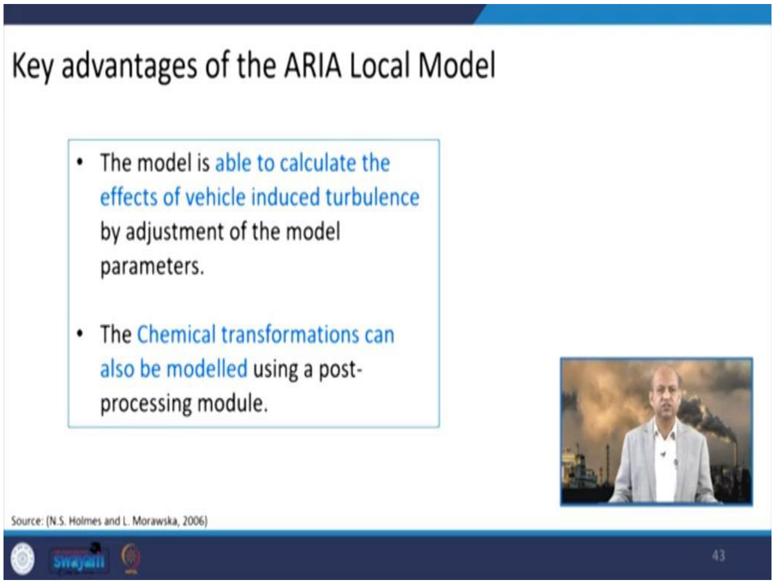

Some advantages are there like it can calculate the effects of vehicle induced turbulence, by adjustment of the model parameters. And the chemical transformations can also be modeled using a post processing modules. So, so it is not necessary that you have to assume inert gases, non reactive gases, non reactive pollutants; it can also, we used for secondary aerosols or those kinds of things. So, that way it is very good model for estimating the concentrations in different ways, using different modules.

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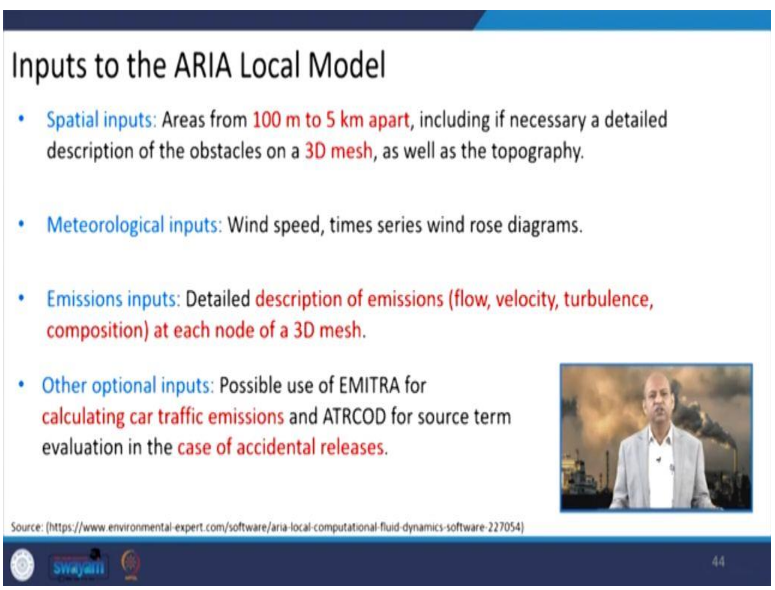

Input parameters, like special inputs are needed. 100 meter to 5 kilometer apart areas, including the necessary a detailed description of the obstacles on a 3D mesh, as well as the topography. So, means high rise buildings, how much stories are there, or the terrain is undulated or smooth; all those kinds of things can be used in this. Meteorological inputs are the same like wind speed, time series, wind rose diagrams; so, that can be incorporated or integrated in this model.

Emission inputs like detailed description of emissions, flow velocity, turbulence, and composition in each node of a 3D mesh. So that is a 3D model basically; it is very sophisticated model in that sense. Other optional inputs are you can use EMITRA for calculating car traffic emissions, and then another module is there for source term evaluation, like accidental releases maybe there. So, different modules can be integrated in that. So that is again, one more good thing about these models.

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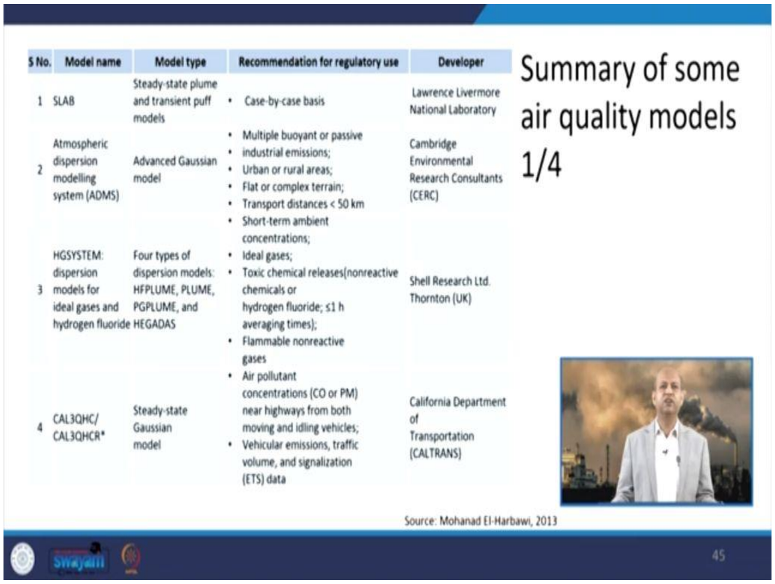


S No.	Model name	Model type	Recommendation for regulatory use	Developer
1	SLAB	Steady-state plume and transient puff models	• Case-by-case basis	Lawrence Livermore National Laboratory
2	Atmospheric dispersion modelling system (ADMS)	Advanced Gaussian model	• Multiple buoyant or passive • industrial emissions; • Urban or rural areas; • Flat or complex terrain; • Transport distances < 50 km	Cambridge Environmental Research Consultants (CERC)
3	HGSYSTEM: dispersion models for ideal gases and hydrogen fluoride	Four types of dispersion models: HFPLUME, PLUME, PGPLUME, and HEGADAS	• Short-term ambient concentrations; • Ideal gases; • Toxic chemical releases(nonreactive chemicals or hydrogen fluoride; ≤1 h averaging times); • Flammable nonreactive gases	Shell Research Ltd. Thornton (UK)
4	CAL3QHC/ CAL3QHCR*	Steady-state Gaussian model	• Air pollutant concentrations (CO or PM) near highways from both moving and idling vehicles; • Vehicular emissions, traffic volume, and signalization (ETS) data	California Department of Transportation (CALTRANS)

S No.	Model name	Model type	Recommendation for regulatory use	Developer
5	Comprehensive air quality model with extensions (CAMx)	Multiscale, 3D Eulerian photochemical grid model	• O_3, CO, and PM concentrations from the urban to regional scale; • Estimates the mean O3, CO, and PM concentrations at longer than hourly time scales: 8 h, daily, monthly, seasonal, and annual	ENVIRON International Corporation
6	Open burn/open detonation dispersion model (OBODM)	Gaussian puff model for open burns and a square-wave quasi-continuous Gaussian plume model for open burns	• Buoyant rise and dispersion of emissions from instantaneous and shortterm quasi-continuous open burn releases	US Army Dugway Proving Ground, Dugway, UT
7	Second-order closure integrated PUFF model (SCIPUFF)	Gaussian puff model	• Short- and long-range (>50 km) transport; • Steady- or nonsteady-state emissions of primary pollutants (gases or particles); • Buoyant or neutral sources	Titan Corporation, Titan Research & Technology Division
8	Hybrid roadway intersection model (HYROAD)	Traffic microscopic simulation module and Gaussian puff dispersion module	• Traffic emissions and dispersion; • Operations in congested conditions	US-EPA

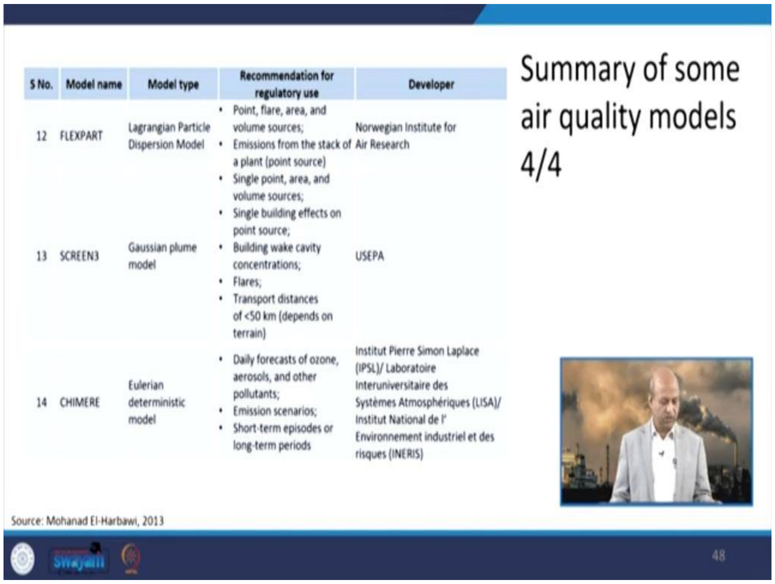
Summary of some air quality models 2/4

Source: Mohanad El-Harbawi, 2013

Summary of some air quality models 3/4

S No.	Model name	Model type	Recommendation for regulatory use	Developer
9	Community multiscale air quality (CMAQ)	Eulerian grid model	• Case-by-case basis	US-EPA
10	California puff model (CALPUFF)	Non-steady-state Lagrangian puff dispersion model	• Long-range transport (source–receptor distances of 50 to 100 kilometres) of emissions from point, volume, area, and line sources; • Forest fire impacts; • Visibility assessments; • Long-range transport studies; • Case-by-case basis	Sigma Research Corporation/ TRC Environmental Corporation
11	AERMOD	Steady-state Gaussian plume model	• Point, volume, and area sources; • Surface, near-surface, and elevated releases; • Rural or urban areas; • Simple and complex terrain; • Continuous toxic air emissions	American Meteorological Society (AMS) and US-EPA

Source: Mohanad El-Harbawi, 2013



When we talk about like summary of different air quality models to compare them according to their strengths or limitations. So again, we have compiled or taken this from a particular source, different kinds of models and their types; then recommended regulatory use and who developed it. Like SLAB model is there, which is the steady state plume and transient model; and case by case basis, it can be used. And Lawrence, this Livermore National Laboratory that has developed this model. So, that way you can see different kinds of models are there which we have not discussed, but they are listed here.

And those we have discussed, they are also listed some of them; so you can go through them in at leisure, like AERMOD is also there, a steady state Gaussian plume model is there; rural urban areas it can be used for. And this American meteorological society and US-EPA are the developers of this very popular model. Then, you can have this SCREEN3 Gaussian plume model, US-EPA developed; so for different situations, for different context, different kind of model techniques are developed by developers or organizations. And they are used by scientists, researchers and practicing engineers.

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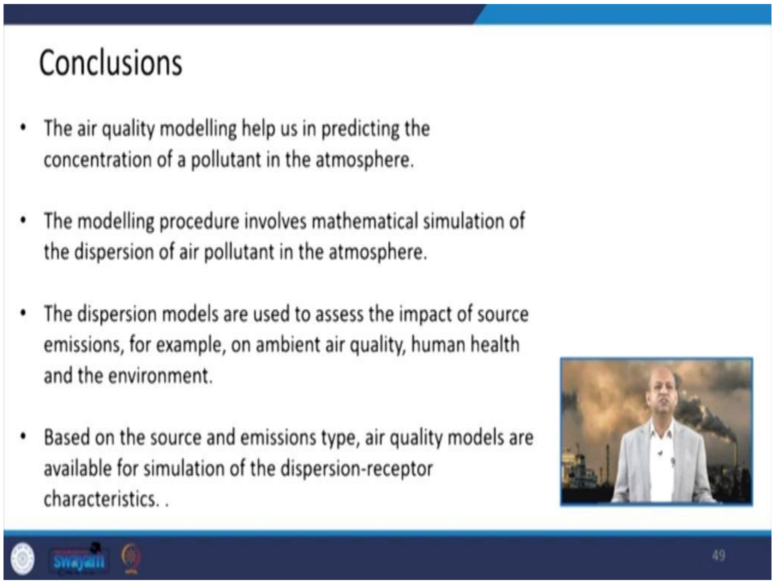

In conclusion, we can say that the air quality modeling really helped us in predicting the concentrations of a pollutant or different kinds of pollutants in the atmosphere for a particular point. The modeling procedure involves mathematical simulations of the dispersion of air pollutants in the atmosphere, which can physical/chemical processes maybe there. The dispersion models are used to assess the impact of source emissions; for example, on ambient air quality at a receptor point, or human health, or the environment. Then the based on the source and emissions type, air quality models are available for simulation of the dispersion receptor characteristics.

So, that way they are very useful for impact assessment or health risk assessment, and to compare the concentrations with the guidelines, those standards. Or, to know whether some new establishment of industrial area will be good or bad for the population, which is living in the downwind direction. So, those kinds of studies can be carried out by these air quality models. So, this is all for today.

I hope you have got a good picture of air quality models, different aspects and parameters their input data requirement, how do they process different techniques. And what are the output values and what they are used for. So, this is all, thank you for your kind attention. These are the references for additional information, you can go at leisure. And see you in the next lecture. Thanks again.