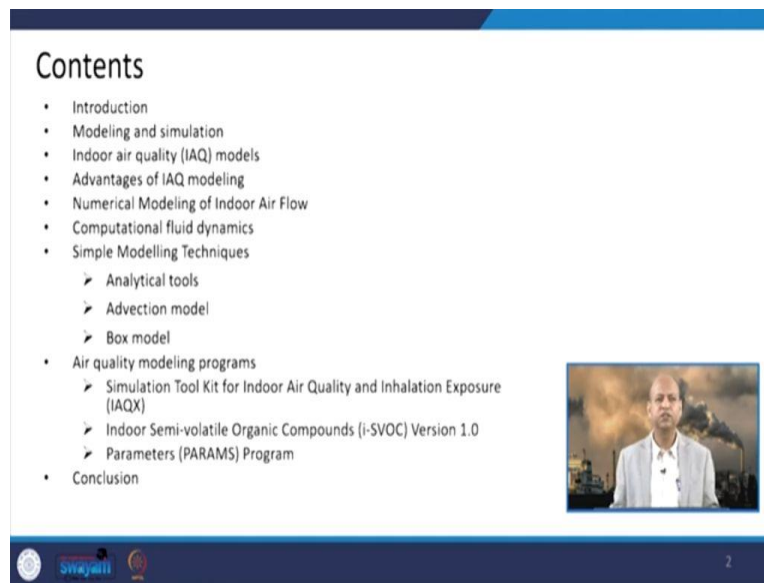


**Air Pollution and Control**  
**Professor Bhola Ram Gurjar**  
**Department of Civil Engineering**  
**Indian Institute of Technology, Roorkee**  
**Lecture – 33**  
**Indoor Air Quality Modeling**

Hello friends, you may recall we discussed at certain point of time about ambient air quality modeling like Gaussian dispersion model and so on. Today we will discuss about indoor air quality modeling, how do we model the indoor air quality? Because, just before this lecture, we have already discussed about various sources of the indoor air pollution; and then exposure assessment through monitoring sampling of the indoor air quality or indoor air pollution. So, today we will discuss how to model or simulate the indoor air quality.

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This will include introductory part, and then what are the modeling and simulation; how do we relate these modeling issues and simulation aspects of mathematical modeling, when we do about the indoor air pollution. Then indoor air quality related models, very simple models those kind of models we will discuss; and advantages of the modeling means with respect to monitoring or sampling. The numerical modeling of air flow indoor air flow we will look into, then computational fluid dynamics related important aspects which are used for indoor air flow or modeling, so, that we will discuss.

Then simple modeling tools or techniques like analytical tools, and advection model or box model, which are quite popular for modeling indoor air quality; so that we will attach. And later we will discuss on air quality modeling programs or tools, which are already developed by USEPA like simulation toolkit for Indoor Air Quality and Inhalation Exposure; that is known as IAQX, Indoor Semi Volatile Organic Compounds i-SVOC Version 1.0 and then third one is parameters or PARAMS program, these three popular tools or easy to handle tools we will discuss, which take care of air quality modeling in indoor environments; and then we will conclude.

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**Introduction**

- Estimation of emissions, fate and transport of indoor air pollutants is an essential part of multi-pathway exposure assessment since most people spend a large portion of their time indoors.
- Indoor air quality modeling plays an important role in indoor air research because laboratory and field testing is costly, time-consuming and technically challenging to appropriately characterize chemicals in a broad range of indoor environments.

Source: Pepper et al., 2009

The slide includes a circular diagram with 'Emitting Sources' on the left and 'Air Quality' on the right, connected by arrows. Below the diagram is a small video inset showing a man speaking. The slide footer contains logos for 'Sri Jayawanti' and a page number '3'.

So, when we talk about introductory part of indoor air pollution modeling, basically whatever sources are there or sinks are there, if we do not consider them to simulate or modal; then it is difficult to find out how much concentration will be at a particular place. And moreover, if you go for sampling like each and every corner in the indoor environment, then it needs lots of resources and a lot of time.


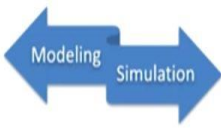
So, better we have optimum number of samples and based on the sample data, we can have certain modeling techniques which can be used for taking these results further, for let us say health risk assessment etc. But before that, we need to do the air quality modeling of the indoor environment; only then we would be able to use that further in health risk assessment, and those sort of activities.

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### Modeling and simulation

- **Modeling** is the art of developing a set of mathematical equations that allow a user to reproduce a cause-effect relation.
- **Statistical models** are based on learning experiments to link inputs to outputs without following all physical and chemical processes.
- **Determinist models** represent the physical and chemical phenomena and then solving the equations to simulate the behavior of real-life systems.
- The process of using the models to analyze the behavior of the real-life system is called **simulation**.

Source: Fangfang Guo, 2017



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When we talk about modeling and simulation, so modeling as you know it is nothing but the set of equations, which represent the reality of whatever thing we want to model. And there may be different modeling techniques like a statistical models which are used based on certain input output relationship, without giving much importance to physio-chemical interactions or processes.



But, there are other modeling techniques like deterministic models, which take care of physical and chemical phenomena; and they solve those physical chemical characteristics related equations, then they get the result. But, they are like resource consuming or time consuming; and it also needs a skilled manpower to handle those kind of models.

And whenever we process using any sort of model, whether it is a statistical model or deterministic model; whenever we are using a model to process the data and we are analyzing the behavior of any real life system, then we call it as a simulation, we are doing a simulation. So, whatever whether it is an ambient air or an indoor air, or any kind of environment we are talking about; and we are trying to use certain model to represent that those processes which are related to that environment, whether of indoor or outdoor. So, we are basically simulating that particular environment of different aspects of that environment.

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### Indoor air quality models

- Indoor-air-quality (IAQ) models are developed to understand and predict indoor air-pollutant concentrations and dosages as functions of;
  - indoor air-pollutant sources and sinks,
  - outdoor air-pollutant concentrations, and
  - indoor-outdoor air-exchange rates.
- Given familiarity with the system to be described and with the purpose of developing and using an indoor air pollution model, the starting point in developing a model is usually a statement of the mass balance concerning the pollutant of interest.



Source: Pepper et al., 2009

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Now, if we talk about indoor air quality models, which have been developed to predict or to estimate indoor air pollutant concentrations. And then after that dosages you can see because dose function is important for exposure assessment and risk assessment. So, basically, three functional parameters are important to model indoor air environment, like indoor air pollutants sources and sinks we should know about. What are the different sources of those indoor air pollutants and water sinks also? Because some portions will be absorbed or adsorbed those kind of sinking related phenomena will also be there. Then, outdoor air pollutant concentration, we should also know.

The reason is because outdoor air pollution also come to the indoor environment through windows, through other doors whenever we open. So, the concentration outside will also influence the indoor environment like this outdoor air can enter into the inside of the house. So, we need to know how much ambient air concentration is there, and also the indoor outdoor air exchange rates; because they will interact indoor environment and outdoor environment. They will interact whenever door is opened, window is opened, or any other system we are using. So, those air exchange rates we should know.


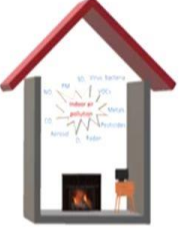
Now, we know this system which is described in the form of developing or using an indoor air quality model or indoor air pollution model. So, we need to begin with certain principles and the mass balance concerning those pollutants which are of our interest in the indoor environment, basically we will look into that. So, you might have heard about mass conservation or energy

conservation. So, from that perspective, mass balance related equations we use in this particularly indoor air quality modeling efforts.

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### Advantages of IAQ modeling

- IAQ models provide a way to **link sources, sinks and building factors** to estimate indoor pollutant concentrations.
- Furthermore, the IAQ models can be used to **investigate many IAQ problems** without the expense of large field experiments.
- They provide **information on the factors** that are important and can help to determine what must be measured in priority.



Source: Pepper et al., 2009  
image: www.mdpi.com/1660-4601/17/8/2927

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And what are the advantages? Why do we do this indoor air quality modeling? Although we have touched upon, because we cannot go for monitoring or sampling each and every corner of the environment, and it needs a lot of resources. So, one advantage is that whenever you have a valid model, so you can run it and get the concentration with respect to different scenarios. So, it provides the way or understanding to link the sources and sinks and the building factors. Building factors which influences the air exchange rate, as I said outdoor environment, indoor environment are interacting through those windows and doors.

So, those factors building factors they influence; so, these kind of parameters or variables are linked through that modeling effort. Then, also it is used for investigating many IAQ or indoor air quality related problems without any additional expenses, which are required for field experiment. So, we can avoid field experiment, we can just create a scenario; and with respect to that scenario, we can get or predict certain concentrations. And we can know that this will be the effect of the changes if you want to make in the indoor environment. Suppose we want to go for some other energy system, like heating system in the indoor environment.


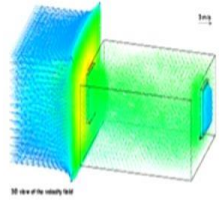
Whether it will influence the air quality or not? Or we are going for another kind of furniture. And furnitures also have certain sources of these VOCs. So, those variables can be there and those

variables can easily be simulated in the modeling technique. They also provide information about the factors which are very important and they determine the indoor environment related issues, whether not only the air quality is the final result, but before that there are many variable factors. So, those variable factors can easily be considered in the indoor environment indoor air quality modeling.

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**Numerical Modeling of Indoor Air Flow**

- In recent years there has been extensive activity in the development and use of **Computational Fluid Dynamics (CFD) software** and special programs for room air movement and contaminant transport applications.
- These investigations range from the prediction of **air jet diffusion, air velocity and temperature distribution** in rooms, spread of contamination in enclosures, to fire and smoke spread inside buildings.



Source: Pepper et al., 2009      image: knopp et al. 2005

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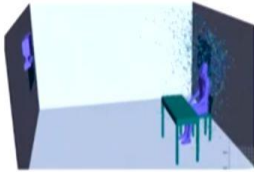
When we talk about numerical modeling of indoor air flow, because there are several techniques; and one of those techniques is numerical modeling. In recent years, extensive activities and research and development have been done through Computational Fluid Dynamics related processes or software CFD. So, these are the special programs for room air flow movement or contaminant transport applications within those indoor environment.

And these investigations they can range from prediction of air jet diffusion, or air velocity, or temperature distribution in the rooms, or humidity related issues or contamination, diffusion, dispersion within those enclosures; or any smoke spread inside the buildings. So, all those kinds of issues can be tackled by CFD techniques.

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## Computational Fluid Dynamics

- Computational fluid dynamics (CFD) is a computational technique/tool that produces quantitative predictions of fluid-flow phenomena based on the conservation laws (conservation of mass, momentum, and energy) governing fluid motion.
- Thus, CFD is a tool for analyzing fluid-flow problems.
- If it is used correctly, it can provide useful information cheaply and quickly.
- It uses methods such as:
  - finite difference method
  - finite volume method
  - finite element method



Source: Howard H. Hu, 2012

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So, the CFD is a computational technique or tool, which produces quantitative predictions of fluid flow through conservation laws; like conservation of mass or momentum, conservation of momentum or conservation of energy. So, those basic principles are used for this particular CFD technique.

So, they govern fluid motion; so, these are the principles which are used. So, CFD is a tool for analyzing air fluid or air flow problems. And it is used, it can provide when it is used correctly; then it can provide useful information very quickly and with minimum resources, just you have computer and you can run that model, and you can get the results. And it can use different methods or procedures, finite difference method or finite volume method or finite element method. Those kinds of popular techniques can be used for CFD models.


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## Simple Modelling Techniques

- The use of **simple modeling tools** can quickly provide great insight and an overall grasp of the problem.
- Such models are useful in **establishing at least an order of magnitude assessment**, and in some instances may be sufficient for determining IAQ values.
- There are a variety of analytical tools and simple model configurations that can be useful to a designer in predetermining **contaminant levels within an interior**.

They are:

- **Analytical tools**
- **Advection model**
- **Box model**



Source: Pepper et al., 2009

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Then, there are other models which are of very simple nature. So, these simple modeling techniques can also be used for indoor air quality modeling, and they can be related to analytical tools or advection model or box model. So, we will those tools.

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## Analytical tools (1/2)

Simple modelling techniques

- There are generally two concepts used when developing simple models for indoor air quality calculations:
  - (1) **well-mixed model**
  - (2) **partially mixed ventilation model**.
- In a **well-mixed model**, the concentration is spatially uniform within the enclosure
- In a **partially mixed model**, the concentration is non-uniform generally due to poor mixing.
- In some situations, it is convenient and relatively safe to assume well-mixed conditions – this type of assumption leads to the use of simple analytical models.



Source: Pepper et al., 2009

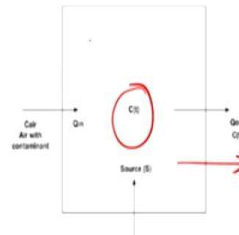
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## Analytical tools (2/2)

### Simple modelling techniques

- Assume an enclosed space exists in which the concentration is considered to be spatially uniform.
- The mass concentration at  $t = 0$  is  $C_0$ .
- A source begins to generate contaminants at a constant rate ( $S$ ).
- Outside air with contaminant  $C_{air}$  is added to the enclosure at a constant volumetric flow rate  $Q$ , contaminated air is removed from the space at the same rate.



Source: Pepper et al., 2009



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## Analytical tools (3/3)

### Simple modelling techniques

- Applying the equation for conservation of mass, the governing equations for the contaminant concentration entering and leaving the enclosure can be written as:

$$\frac{\partial}{\partial t} \int_{cv} C dV + \int_{cs} CV dA + S = 0,$$

- $C$  is the concentration,  $S$  is rate which contaminant is emitted,  $V$  is volume,  $Cv$  denotes the control volume, and  $Cs$  is the control surface.



Source: Pepper et al., 2009



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When we talk about analytical tools basically they are based on two concepts; when we develop the simple models for indoor air quality calculations or estimations. So, one is well-mixed model and another one is partially mixed ventilation model. In a well-mixed model, we assume that concentration is uniformly distributed; because it is mixed very well in that enclosure or in that indoor environment. In partially mixed model, the concentration is non-uniform, it can vary from one point to another, because of poor mixing or ventilation related issues.

But in some situations, there may be kind of mix of the things; and it is relatively safe to assume well-mixed conditions for simplification purpose, for approximation purpose; so that you can quickly calculate the needed parameters. So, these type of assumptions just leads to the use of

simple analytical models or tools. Further, there are certain assumptions. We assume that an enclosure or that indoor environment exists in which the concentration is considered to be especially uniform. As I said, when we assume that it is uniform, then we assume that at each point the concentration is same.

But, the mass concentration at time  $t_0$ , it is  $C_0$ ; then at the point at the time  $t$  it is  $C_t$ . So, maybe  $C$  air which is the air with contaminant outdoor air; if is entering or not only in the outdoor, but within the indoor environment also. If you are assuming certain tubes or certain small enclosures, so from one enclosure to another air movement may be there. So, this  $C_{\text{air}}$  which is with certain contaminant, if it is entering into this particular enclosure; then it can have this volumetric flow rate  $Q_{\text{in}}$ . And the concentration it can have  $C_{\text{in}}$ . Or, at the time  $t_0$ , if we assume  $C_0$ , then at time  $t$  the concentration may be  $C_t$ . And then  $C_t$  can be  $C$  air when it is uniformly distributed in this enclosure.

And that same concentration will go out, because every corner every point has the uniform concentration in that particular space. When we talk about equations, there are several equations. But for the sake of information, I give you this very only one conservation of mass related equation, which is used for estimating the concentrations and solving this these equations.



So, where these parameters are concentration, then this contaminant rate which is being emitted,  $V$  is the velocity; and then this volumetric parameter is there. Then control volumes factor can be there, and control surface related factor can be there. So, these equations are solved by the model and they can estimate the concentrations ultimately.

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### Advection Model (1/3)

Simple modelling techniques

- Many times a **source exists** that is moving within a **confined space**.
- Examples of such situations are **automobiles or trains that are traveling through tunnels**, or a smoker walking from one room to another.
- In this instance, a **simple control volume approach** can be used to establish the governing equation for concentration.
- In many instances, makeup air consisting of fresh air is used to provide local **ventilation**.




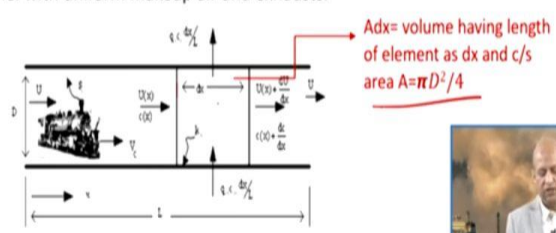
Source: Pepper et al., 2009

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### Advection Model (2/3)

Simple modelling techniques

- A schematic diagram of **air and contaminant transport** from a train traveling within a tunnel is shown in Fig.
- An **elemental volume denoted by  $A dx$**  exists within a tunnel with uniform makeup air and exhausts.



Source: Pepper et al., 2009

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Simple modelling techniques

## Advection Model (3/3)

- The conservation of mass for contaminant transport can be written as:


$$c(x) = \frac{s + q_m c_m}{k + q_m} + \left[ c_0 - \frac{(s + q_m c_m)}{k + q_m} \right] \left[ \frac{U(x)}{U_0} \right]^{-b}$$

$$\frac{U(x)}{U_0} = 1 + \frac{x(q_m - q_e)}{U_0}$$

where

- $s = S/LA$  ( $\mu\text{g}/\text{m}^3 \cdot \text{min}$ ) and
- $k = 4k_d/D$  ( $\text{min}^{-1}$ ),  $q_m = Q_m/LA$  ( $\text{min}^{-1}$ ),  $Q_m$  = flow rate entering ( $\text{m}^3/\text{min}$ ),
- $q_e = Q_e/LA$  ( $\text{min}^{-1}$ ),  $Q_e$  = flow rate at exit ( $\text{m}^3/\text{min}$ ),
- $D$  is the tunnel diameter,
- $c_m$  is the contaminant deposited in tunnel walls,
- $C$  is the concentration of contaminant,
- $S$  is the source ( $\text{mg}/\text{hr}$ ),  $b = (k + q_m)/(q_m - q_e)$
- $k_d$  ( $\text{m}/\text{s}$ ) is the rate at which contaminant is deposited on the tunnel walls.
- $U$ : velocity of air inside the tunnel.
- $C_0$  = initial concentration of contaminant inside tunnel ( $\mu\text{g}/\text{m}^3$ )
- $U_0$  denotes air entering tunnel
- $X$  is distance from starting of tunnel where we are calculating  $c$ .

Source: Pepper et al., 2009



Then, other model is advection model. Advection horizontal movement as convection is vertical movement, advection is horizontal movement. In many times source exist that is moving within a confined space, like in a tunnel train is moving; or within the household activities people are doing, and they are also moving, somebody is smoking and moving in the corridor. So, those kind of moving sources may exist; so it is a horizontal movement. So, advection models are used to simulate or model the effect of those sources; and to know what would be the concentration at the point of interest.

So, we see all those parameters of course volume approach is used, control volume approach is used; and then these ventilation related parameters are also used. You can see in this particular figure, it is shown very nicely that this  $\Delta x$  is volume having length of element as  $dx$ ; this much of slice of the  $dx$ . And area is you can have this area of this tunnel, where this engine or train is moving.  $U$  is the velocity, so you can use those equations; and you can further solve it to get the concentration. Then advection model usage all kind of those equations, but ultimately this is the final equation, which is used for estimating the concentrations; where different parameters are there, like contaminant deposited internal walls  $C_m$ .


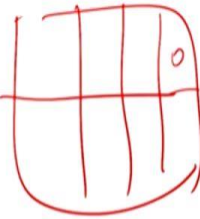
$C$  is the concentration of the contaminant, which is  $c(x)$  at the  $x$  distance,  $L$  is the length of the tunnel; and  $x$  wherever point you are denoting the  $x$  distance; so, that is used in this equation. Then,  $U$  is the velocity of air inside the tunnel,  $U_0$  denotes the air at the entrance of the tunnel basically;  $x$  is the distance from starting of tunnel at the point, where we want to estimate the concentration. So, all these parameters are used to estimate the concentration through the advection model.

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### Box model (1/3)

Simple modelling techniques

- When the concentration within an enclosure is **nonuniformly distributed**, it is inaccurate to assume the enclosure can be treated as a well-mixed region.
- An alternative approach to the analytical tools utilized in the previous section is the **box model**, also sometimes referred to as the **multi-cell well-mixed model**.
- It is the **most commonly used model for indoor environment** because generally, the concentration within the enclosure is non-homogenous.


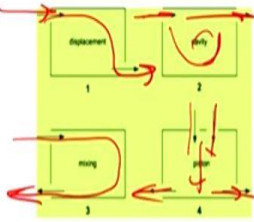


Source: Pepper et al., 2009

### Box model (2/3)

Simple modelling techniques

- There are basically four types of mixing that can occur within an enclosure.
- Displacement:** The incoming air **displaces** the existing air within the enclosure.
- Cavity:** Air flows into and out of the enclosure, much like flow over a cavity (which in turn creates a recirculation).
- Mixing:** Flow enters at the top and exits at the bottom, creating a mixed region within the enclosure.
- Piston:** Air is pumped into a container and then exits out the sides – like the piston and cylinder effect in an automobile.



Source: Pepper et al., 2009

## Box model (3/3)


- The model generally used is as follows:

$$\frac{dCV}{dt} = QA + uC_{in}WH - uCWH$$


where,

- $C$  = concentration of pollutant throughout the box,  $\mu\text{g m}^{-3}$
- $C_{in}$  = pollutant concentration entering the box,  $\mu\text{g m}^{-3}$
- $Q$  = pollutant emission rate from source per unit area,  $\mu\text{g m}^{-2} \text{s}^{-1}$
- $V$  = volume of the box,  $\text{m}^3$ ;  $A$  = horizontal area ( $L \times W$ ),  $\text{m}^2$
- $W$  = box width, m;  $L$  = box length, m;  $H$  = mixing height (mixing height), m
- $u$  = wind speed normal to the box,  $\text{m s}^{-1}$

Simple modelling techniques



Source: Jain et al., 2016


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Next is the box model. And this box model is used when non-uniform conditions are there, when concentration is existing in a non-uniform way, which is a reality basically. Uniform concentration we assume in certain enclosures, but if larger enclosures or indoor environment is there, it is not necessary that uniform concentration will be there of a particular pollutant. So, box model is based on multi-cell well-mixed model; means the small cells are like if this is the box model creating, so it can be divided into several cells. And those cells can have different concentration of uniform level.

So, each cell can be termed as a uniform concentration related phenomena and then integration can be done at later stage. So, basically non-uniform condition is existing, but that non-uniform condition can be divided into several uniform cells. And this box model have four types of mixing, which can occur in those cells which we have divided; for example, displacement. So, let us say if air is entering in that way and it is coming and going outside this way; so, it is displacing basically. So, incoming air displaces the existing air, which is in the enclosure or in the cell, it goes out.

And then cavity formation can be there if short circuit is there; air is coming and it is going directly, so here this is the cavity. So, this cavity can form and concentration may build up rather than forcing it out. In displacement kind of phenomena, the flushing of concentration of pollutants may be there; but in this kind of condition or context, the cavity formation can be there. And concentration buildup can be over the period of time can be there; and recirculation of concentration maybe there. And then there is this mixing, if this air goes and travels a long distance and come back.

So, kind of mixing region or mixed region is produced and uniform concentration you can assume in this particular cell. Then, there maybe another way like piston, where air is coming from this and air is going out of this; so, it is working like a piston, and it is pushing out this air outside. So, several kind of combinations can be there, which can be catered or simulated by box model. And this is the fundamental equation which is used for estimating concentrations based on several parameters, like pollution emission rate. And then the area, this horizontal area length into width; and H is the box height.

So, box height when we are talking about the mixing height within that enclosure; mixing height in ambient air is boundary layer height. But, within the enclosure or within the indoor environment, it can be again the some mixing height.

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The slide is titled "Air quality modeling programs". It contains a text box on the left with a list of tools and a video thumbnail on the right. The text box lists three tools: Simulation Tool Kit for Indoor Air Quality and Inhalation Exposure (IAQX), Indoor Semi-volatile Organic Compounds (i-SVOC), and Parameters (PARAMS) Program Version 1.1 for indoor emission source modeling. It also states that these programs are Microsoft Windows-based and user friendly. The video thumbnail shows a man speaking in front of a background of industrial smokestacks. The slide footer includes a source URL and a page number 19.

**Air quality modeling programs**

Researchers at EPA have developed indoor air modeling programs/tools to assist with understanding indoor air pollution. They include:

- Simulation Tool Kit for Indoor Air Quality and Inhalation Exposure (IAQX)
- Indoor Semi-volatile Organic Compounds (i-SVOC)
- Parameters (PARAMS) Program Version 1.1 for indoor emission source modeling

These programs are Microsoft Windows-based and user friendly.

Source: epa.gov.in, image: <https://depositphotos.com>

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But, fundamental concept in same you we use box modeling in ambient air quality modeling also. Then we come to air quality modeling programs which are readymade tools available, because USEPA Environmental Protection Agency has developed certain tools, which can be used by people to simulate air in different indoor environment. And they can get easily those models are handled or those programs are handled. So, one program is simulation toolkit for Indoor Air Quality and Inhalation Exposure (IAQX). Another one is Indoor Semi-Volatile Organic Compounds (i-SVOC).



Then, third one is parameters or PARAMS Program Version 1.1. It was earlier 1.0 as we had discussed; and this for indoor emission source modeling basically. So, these programs are window based, so user friendly; and anybody who knows simple computer handling they can easily use those tools or models.

(Refer Slide Time: 21:23)

## Indoor Air Quality and Inhalation Exposure (IAQX) (1/2)

IAQX version 1 consists of five stand-alone programs: one is for general-purpose simulation, and four are for special-purpose simulation.

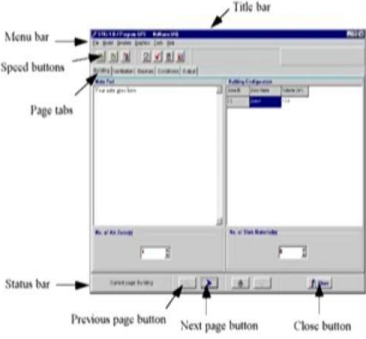
No.	Program	Purpose
1	GPS.EXE	A general-purpose simulation program
2	VBX.EXE	Models for predicting VOC emissions from solvent-based indoor coating materials based on product formulation
3	SPILL.EXE	Models for indoor solvent spills
4	SLAB.EXE	A model for VOC emissions from diffusion-controlled homogeneous slabs such as new carpet backing
5	PM.EXE	A model for indoor particulate matter





Source: epa.gov.in

## Indoor Air Quality and Inhalation Exposure (IAQX) (2/2)

General appearance





Source: epa.gov.in

In Indoor Air Quality and Inhalation Exposure like IAQX model, there are different standalone programs or modules, like five modules are there; one is like GPS. So, this file can be executed or this program, or this module can be executed for the purpose of general purpose simulation program.



When this VBX is related to VOCs, so it models to predict the VOC emissions from solvent based indoor coating materials based on product formulation; this maybe furniture, this maybe from walls etc. Then SPILL, this SPILL related module is there, which simulate or models for indoor solvent SPILLS; where some solvent has been spilled out. Then it can be modeled, because it will give some VOCs; or then this is SLAB.

So, this model gives the VOC emissions from diffusion controlled homogeneous slabs, such as new carpet backing. So, if carpet is there, new carpet is there, lot of fumes may be there. So, this particular model can be used for that particular emission. A model for indoor particulate matter is PM related module.

So, if we want to run a particular module depending upon the requirement, we can run; otherwise we can run five modules, if all these conditions are applicable. You can see this is the general appearance of that particular tool. So, different buttons are there and because it is window based, you can just press the button, you can go through the menu bar; and you can choose whatever possibilities are there.

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Indoor Semi-volatile Organic Compounds (i-SVOC) (1/3)

- i-SVOC Version 1.0 is a general-purpose software application for dynamic modeling of the emission, transport, sorption, and distribution of semi-volatile organic compounds (SVOCs) in indoor environments.

This program:

- Covers the functions of most commonly used models for indoor SVOC.
- Provides the user with more flexibility than the existing models.
- Frees the user from numerical computations.

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## Indoor Semi-volatile Organic Compounds (i-SVOC) (2/3)

### Limitations

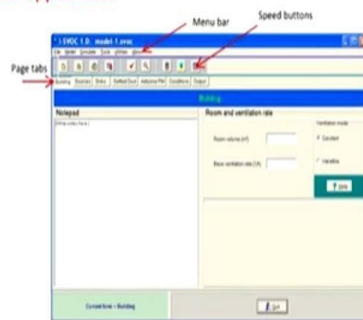
- The current version of program i-SVOC is for a single air zone and a single SVOC.
- The program does not support chemical reactions.
- Program i-SVOC ignores the interactions between the settled dust and the surface which the dust particles are in contact with.
- Many indoor pesticides are SVOCs. This program does not contain any mass transfer models for liquid applications.



Source: epa.gov/in

## Indoor Semi-volatile Organic Compounds (i-SVOC) (3/3)

### General appearance



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So, the next one is Indoor Semi-Volatile Organic Compounds (i-SVOC). So, this is 1.0 i-SVOC version is there; and this model the emissions and its transportation, or absorption or adsorption and distribution or dispersion of semi-volatile organic compounds SVOCs, in the indoor environment.

And this program is capable of covering the functions of most commonly used models for indoor semi-volatile organic compounds. And it can also provide the user with more flexibility than the other existing models; so, that way it is versatile. And it frees the user from numerical computational computations which are quite resource intensive; as well as it needs a lot of skilled manpower. So, that way it is quite easy to handle and it has versatility.

But, there are certain limitations also, like the current version of this program is for a single air zone and a single semi-volatile organic compound. So, it cannot model the mixture of different kinds of VOCs. The program does not support chemical reactions, so that way very simplified assumption is there. This program ignores the interactions between settled dust and the surface, which the dust particles are in contact with. Many indoor pesticides are there which emit as VOCs; so, this program does not contain any mass transfer models for liquid applications, so, these are limitations.

But as you know, even in Gaussian dispersion model when we talked about in ambient air quality modeling, there were several assumptions. So, that because there are so many uncertainties and complex things are there, we cannot handle everything; otherwise the model will be very complex and very difficult to handle. So, it is fine if there are certain limitations, but if it is given good results. But, other in this particular model, we had these five modules. So, that way this is better model if you want to model several kind of VOCs, particulate matters, or spilled over related issues.

But, if you want to concentrate only on semi-volatile organic compounds, then this model is fine; but only limitations are there that because it handles single SVOC at a time. Then, it can be seen this general appearance again similar to other one, window based model it is. So, you can just use these buttons and you can run the model.

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## Parameters (PARAMS) Program Version 1.1 (1/3)

Parameters (PARAMS) 1.1 is a Microsoft Windows-based computer program that can be used to implement methods for estimating the parameters in indoor emissions source models.

These methods fall into seven categories:

1. Properties of indoor air
2. First-order decay rate constants for solvent emissions
3. Gas-phase, liquid-phase, and overall mass transfer coefficients
4. Molar volume ✓
5. Molecular diffusivity in air, liquid, and solid materials.
6. Solid-air partition coefficient
7. Vapor pressure and volatility



Source: epa.gov/in



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## Parameters (PARAMS) Program Version 1.1 (2/3)

Users can benefit from this program in two ways:

- It serves as a handy tool by putting commonly used methods in one place.
- It saves users' time by taking over tedious calculations.

### Limitations

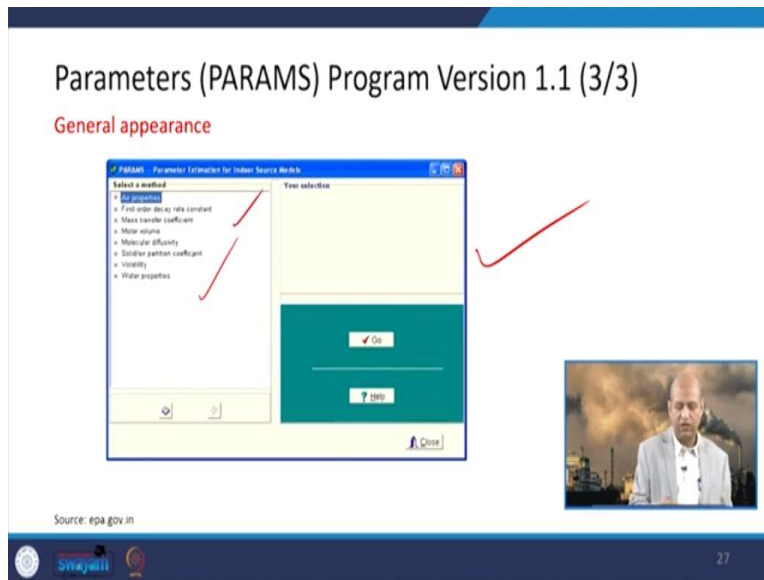
- Users are reminded that the number of parameters that can be estimated with this program is only a fraction of the total number of parameters in the existing indoor source models.
- Methods for particulate matter are not included in the current version.



Source: epa.gov/in



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The third one is parameters PARAMS Program Version, which is of 1.1, i-SVOC was of 1.0 and this is 1.1. So, this particularly program can be used to implement methods for estimating the parameters in indoor emission source models. That is why it is known as parameters PARAM 1.1. And the methods which fall in seven categories which are used in this particular program or tool, are properties of the indoor air. First order decay rate constants for several emissions can easily be handled; then gas-phase, liquid-phase or overall mass transfer these coefficients can also be taken into account.

Molar volume related the parameters, then molecular diffusivity in air, liquid, or solid materials, solid-air partition coefficients, vapor pressure and this volatility; all these things are not taken into account with this software.

Then, users can benefit from this program in this two fundamental ways. This can serve as a handy tool by putting commonly used methods in one place, and it can save a lot of time; because tedious calculations are avoided; this program does all those calculations at the backend. But, there are limitations again like earlier model also had limitations. These users are reminded that the number of parameters that can be estimated with this particular tool is only a fraction of the total number of parameters in the existing indoor source models.


So, not all parameters are being handled, but important parameters are being included. And these methods for particulate matter are not included in the current version; so, that is one limitation. It can have other pollutants, but particulate matter related if you want to model, then go for that

IAQX that is fine. This is the general appearance again, all these selected methods are given. So, anything you can choose as per the requirement and you can run the model.

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## Conclusion

- Indoor air quality (IAQ) models are used to predict the pollutant concentrations both spatially and as a function of time within the building environment.
- They are divided into 3 categories: statistical, mass balance and computational fluid dynamics (CFD) models.
- Simple modelling techniques include analytical tools, advection models and box model.
- The three most popular software used for indoor air quality modeling are IAQX, i-SVOC and PARAMS.
- These software help the user by putting the commonly used modeling techniques at one place and also taking over tedious calculations.



## References

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So, in conclusion, we can say that the indoor air quality models are very important for predicting the pollutant concentrations, in terms of especially from one point to another, or as a function of time. Means over the period of time, how this variation will be there with respect to the sources; and with respect to the variation in different influencing factors like temperature, humidity, etc. And they are divided into three categories: statistical, or mass balance, and computational fluid

dynamics CFD models. Simple modeling techniques are also there, which can include analytical tools, or advection model, or box model as just we have discussed.

And there are three very simple programs which have been developed by USEPA like IAQX, i-SVOC, and PARAMS. These are simple tools which can be used by any computer savvy person. So, this software can help us putting all those commonly used modeling techniques in one place. And we can avoid tedious calculations which are required in other complicated models; so, this is all for today. I hope now you can appreciate why indoor air quality modeling is important, how it is carried out. So, these are the references based on which we have presented this particular lecture. You can go through them at leisure. And thank you, see you in the next lecture. Thanks again.