Integrated Programme for Better Air Quality (IBAQ Programme)

CITY SOLUTIONS TOOLKIT :

AIR QUALITY MODELING TOOLS

BACKGROUND

Air quality modeling is a component of air quality management (AQM) that offers an alternate, computational approach in determining the concentration of pollutants in the atmosphere. Models help in simplifying situations by integrating actual data with assumptions that reflect the context of the domain under study. In the same way a picture is a representation of the subject, air quality modeling is a representation of what is happening to the air quality of an area. Although modeling requires very specific technical expertise, the process can provide air quality data without intensive air quality monitoring that can be very expensive (please refer to module on Air Quality Modeling Concepts and Process for more elaborate discussion of principles and its advantages).

With developments in technology and computational tools, air quality modeling has also gone through significant changes in terms of capacity and usability. Models can now cover more pollutants, integrate more factors, and provide more robust data. The initial steps in performing air quality modeling, especially for cities who have not done it before, is expected to be challenging. However, once everything has been set up, all succeeding model runs would be a lot easier since only the input data will be periodically changed (refer to module on Air Quality Modeling Data Needs and Operational Guidelines for more information). Assuming that infrastructure and technical capacity is already in place, modeling can be less costly compared to air pollutant monitoring.

The key in preparing well for performing air quality modeling is to understand the tools that can make the process much easier. In this toolkit, description of some of the most common air quality models are discussed. This will help the reader become more familiar with the features of different air quality modeling tools which will best fit the available resources and AQM objectives of the city. Time, effort, and cost can go down if proper models are used and implemented by experts in the field. Ultimately, the validated outcomes can be used to shape decisions of policymakers (refer to module on Air Quality Modeling Application to Policymaking), which can lead to improved air quality.

COMMON AIR QUALITY MODELING TOOLS

One of the main classifications of air quality modeling tools is how meteorological data are incorporated. Described below are the description of steady and non-steady state models (Clean Air Asia and UN Environment, 2019; US EPA, 2017a).

Steady-state models assume that there are constant meteorological conditions within the space-time area of the application. In this case, meteorological data can be collected only at one point near the pollution source and is assumed to be representative of the whole area. This can only be applied in locations where topographic parameters such as surface roughness, ground cover, presence or absence of water bodies, mountains, urban structures has little to no effect on the overall meteorological conditions in the area. These models are usually applied for dispersion modeling focused on single stack sources, where the focus is on the metrological conditions at the release height of the pollutants.

Non-steady state models on the other hand, take into account the three-dimensional meteorological conditions based on measurements at surface and upper air (anything above the height of a tower) sites. Meteorological models are used to extrapolate supplementary data which cannot be provided by weather station data alone. There are two types of meteorological models with outputs that can be used as input for air quality models:

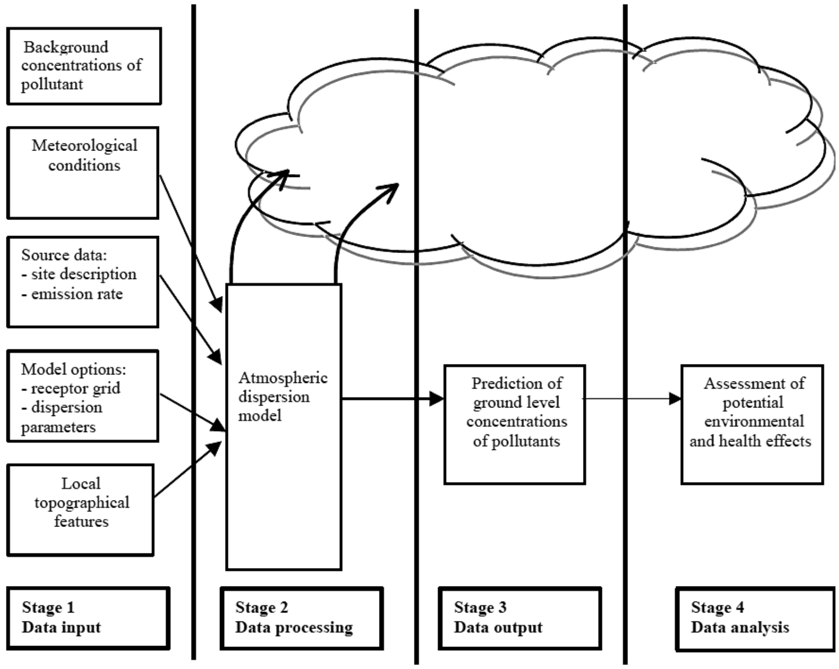
- Diagnostic meteorological models – interpolate and extrapolate meteorological variables throughout a three-dimensional grid; non-predictive
    - Example: CALMET
        - reconstructs the three-dimensional wind and temperature fields from meteorological measurements, orography and land use data

- Prognostic meteorological models – calculates and simulates meteorological parameters such as the change of winds and temperature in time; can be predictive
    - Example: MM5
        - provides realistic dynamical and physical meteorological fields even in data-sparse areas, suitable for simulations in a complex environment (PSU/NCAR, 2015)

<u>Common Tools Available for Dispersion Modeling</u>:

Most air pollutant dispersion models are computer programs that use information on (MOE, 2004):

- contaminant emission rate;
- characteristics of the emission sources;
- local topography;
- meteorology of the area; and
- ambient or background concentrations of pollutants.



Input and output in the air pollutant dispersion modeling process. (Source: MOE, 2004)

Here are some air quality dispersion tools that the US EPA recommends. For more information, visit the links in the table.

Model name	Model type	Preprocessor for meteorological data	Preprocessor for terrain data	Processor for downwash effects	Scale	Visualization/ Postprocessor	Remarks
AERMOD	Steady-state	AERMET	AERMAP	PRIME	meso	Tables, plots,	may be inappropriate for some near-field modelling in cases where the wind field is very complex due to terrain or a nearby shoreline https://www.epa.gov/scram/air-quality-dispersion-modeling-preferred-and-recommended-models
CALPUFF	Non-steady-state	CALMET	GIS landuse	MTIP	meso	CALPOST	complex and data inputs and interrogation of model outputs can result in errors: http://www.src.com/

'Screening' air dispersion models check if more detailed modeling requires contaminant emission rate. It can also determine stack height and is usually used for rapid assessments of environmental impacts. Screening models can thus also be used in emergency planning (CERC, 2018). Below are some of the common Screening models.

Model name	Screening version of	Source Types	Source releases	Source locations	Visualization

AERSCREEN	AERMOD	Point, area volume	surface, near surface, elevated	urban, rural	Tables, plots
ADMS-Screen	Atmospheric Dispersion Modeling System (ADMS3)	Industrial single stack	surface, near surface, elevated	Large urban areas, cities, towns	Printout listings
Complex Terrain SCREENing model (CTSCREEN)	Complex Terrain Dispersion Model (CTDMPLUS)	Point	elevated	urban	Tables, contours

Common Tools Available for Source Apportionment, Receptor Modeling and Photochemical Modeling:

Source-oriented air quality models use data input from emissions inventories and dispersion models, through chemical transport models (CTMs). CTMs estimate the contribution of each source at a specific location or receptor site. An example of a CTM is CAMx which integrates assessment of gaseous and particulate air pollution.

Receptor-oriented models, on the other hand, statistically computes for the presence and fraction of source contributions, in specific sources and receptors. It determines the best-fit linear combination of emission source chemical composition profiles needed to reconstruct the measured chemical composition of ambient samples (US EPA, 2017b). Examples of such models are Chemical Mass Balance (CMB) models and factor analyses (e.g. Positive Matrix Factorization (PMF) technique).

Some of the most common photochemical models are summarized in the table below.

Model name	Application area	Meteorology	Photolysis	Postprocessors (Outputs)	Pollutants
Community Multi-scale Air Quality model (CMAQ)	urban, regional, continental, hemispheric	MM5, MCIP			O_3, $PM_{2.5}$, toxic pollutants, acidic compounds https://www.epa.gov/cmaq
Comprehensive Air quality model with Extensions (CAMx)	urban, regional, continental, hemispheric	WRF, MM5, RAMS	O3MAP, TUV	AVGDIF, CAMxPOST, EPASTAT, MATS	O_3, inorganic and organic $PM_{2.5}$/PM_{10}, mercury, other toxic pollutants www.camx.com
REgional Modeling System for Aerosols and Deposition (REMSAD)	regional, continental, hemispheric	MM5	no	Plots, GIS	PM, other, acidic compounds, toxic pollutants

Urban Airshed Model with Variable grid (UAM-V)	Regional, continental	CALRAMS, CALMET	inbuilt	Plots, tables	Inert & chemically reactive pollutants

CONSIDERATIONS FOR AIR QUALITY MODELING

Here are considerations to be maintained to achieve credible modeling:

1) Choice of Model: It is important that the user selects the model that fits the demands of the task. There are three levels of assessment in this regard:

- Screening assessment - when one needs to determine a specific event or the likelihood of a specific event.
- Refined assessment - higher resolution modeling where it more closely estimates actual air quality impacts.
- Advanced assessment - treats specific dispersion processes in greater detail. It potentially gives more accurate results but requires more input data. This is more difficult to use since the model must also be specific for the situation or context it's trying to model.

2) Input Data: Models will require data to run. This data depends on the needs of the modeler and can be broken down into:

- Emissions – pollutants that are generated by the source or sources being studied
- Geophysical data – data about surface parameters, topography and vegetation type
- Meteorology – the weather parameters such as wind, rain and stability of the air
- Initial and Boundary Conditions – initial chemical concentrations for a number of the major species in the model

Refer to the module on Air Quality Modeling Data Needs and Operational Guidelines for a more detailed discussion on data inputs required for air quality modeling. Take note that the scope of the analysis, which is defined by the 'domain' or geographical location scope of the model, should be taken into account. Some air quality models would only work in smaller or finer resolution grids, and the use of larger grids can dilute the accuracy of the model output. Models must be checked if it runs on global scales or local scales.

3) Resources: Most of the models are easy to get since most of them are open sourced and can be freely downloaded. However, guidance from an experienced modeler might be needed in the installation of the programs. Computer resources will not be too challenging because most individuals and groups are able to run the models using standard computers or a network of computers. For more complex models which run country-level or huge global datasets, supercomputers may be needed.

4) Practitioners: The need for skilled practitioners to run models should be a priority. Since many models are now freely available, there is a danger that the models can produce misleading results in the hands of

an inexperienced user. Capacity building through sustained training of new generation of modelers is therefore seen as a very important component of modeling.

UNCERTAINTIES IN MODELING

The approach presented in this document and in any process in modeling ultimately leads to a discussion on reliability and validity of the results. One must understand the concept and extent of uncertainty for any decision making based on a model. In this discussion, there are three main general sources of error and uncertainty in dispersion modeling:

- Inaccurate input data – make sure the data inputted is correct and appropriate for the model, otherwise the output would also be inaccurate.

- Inappropriate use of the model (or expecting too much from it) - specific models can only provide a specific level of detail and accuracy. The model employed mut be understood so that limitations are levelled-off and the advantages are maximized.

- Poor performance of the model itself – maintain use of models that have been extensively used and acknowledged by agencies and experts. There are many researches on the efficacy of air quality models and can be found online.

In summary, the tool will only be as good as the user. No matter how sophisticated the tool is, the output will not be good if the user lacks understanding on how to use it properly. Understanding the concepts in this module and in the other related modules in this toolkit prepares the users in undertaking air quality modeling, in the context of improving the quality of air in the city.

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