Air Quality Modelling and Forecasting Guidebook for the States of the Gulf Cooperation Council

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PREFACE

Air pollution affects the health and well-being of people and the environment and is considered to be the world's single largest environmental health risk. As in other parts of the world, the countries of the Gulf Cooperation Council (GCC) are also facing the challenge of air pollution. Their geographical location makes them particularly prone to natural air pollution sources such as sand, dust, and sea salt.

Realizing the challenge, the GCC and the United Nations Environment Programme (UNEP) embarked on an ambitious project under the "Green Gulf Initiative: delivering on the environmental dimensions of the SDGs." One of the aims of the initiative was to develop regional guidance for the collection of air quality (AQ) data. Consequently, a set of three guidebooks have been produced: **(1)** Air pollutant Emission Inventory Guidebook for the States of the Gulf Cooperation Council, and Introductory Guidance on Air Emissions Dispersion Modelling; **(2)** Air Quality Modelling and Forecasting Guidebook for the States of the Gulf Cooperation Council; and **(3)** Air Quality Monitoring and Data Management Guidebook for the States of the Gulf Cooperation Council.

The current guidebook presents widely used AQ models employing different modelling approaches for atmospheric and AQ processes, over length scales ranging from the microscale (1 km or less) to the global scale (more than 1000 km). To this end, distinctions are made between operational and experimental models, between dispersion,[1] photochemical,[2] and receptor[3] models, between forecasting[4] and assessment[5] models, and between models adopted and models recommended by regulatory agencies such as the US Environmental Protection Agency (US EPA).[6]

This guidebook also highlights recommendations made by regulatory agencies concerning AQ models, including how to evaluate them, data input and other important requirements. It is essential to point out that there is no single model that is optimal for use over a wide range of situations. This is, in part, because the complexity of meteorological phenomena requires different modelling approaches, depending on numerous conditions.

This implies that AQ model selection is problem-dependent. Ideally, the optimal AQ model for a given situation is the one that most accurately represents atmospheric transport processes, pollutant dispersion, and chemical reactions in the subject domain.

Features and characteristics of widely used dispersion models, photochemical models, chemical forecasting operational models, and integrated operational models (that include dust modelling) are also presented in this guidebook. AQ models used to study pollution in GCC countries are also presented. Statistical AQ models are not covered in this document.

It should be noted that the guidelines in this guidebook are not legally binding but are intended to assist the GCC States in modelling the dispersion of air pollutants. Use of this guidebook will enable the GCC States to understand air pollution sources and make informed decisions for control and prevention.

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[1] Used to estimate the concentration of air pollutants at specific locations near emissions sources.
[2] Used to study the impact of emission sources of both inert and chemically reactive pollutants over large spatial scale.
[3] Used to quantify the source contribution to receptor concentrations.
[4] Used to predict future air quality, starting with a set of initial conditions.
[5] Used to assess time-averaged air quality at locations where observations are insufficient or lacking.
[6] Used in conformity analysis and regulatory decisions concerning source permits and emission control requirements (US EPA, 2017).

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Air pollution is the presence of substances in the atmosphere that are harmful to humans and other living organisms, and damaging to human activities and the environment.

Key pollutants include particulate matter (PM), carbon monoxide (CO), polycyclic aromatic hydrocarbons (PAHs), volatile organic compounds (VOCs), nitrogen oxides (NO_x), ozone (O_3), sulfur dioxide (SO_2), and persistent organic pollutants (POPs) (Omidvarborna et al., 2018a). Air pollution is generated both by human (anthropogenic) activities and natural (or biogenic) processes.

It should be noted that naturally occurring dust (including desert dust), albeit a nuisance, does not have a serious impact on human health (Environmental Protection, UK), unless inhaled at high volumes. However, in the presence of other particulate matter from anthropogenic sources (such as from fossil fuel combustion), desert dust particles are likely to entrap and carry these harmful particles downstream. In other words, the combined effect of natural and anthropogenic particles can be detrimental to human health (EEA, 2012).

1.1 Climate effects of air pollution

Air pollution has short-term regional climate effects (Moore, 2009). By changing the amount of reflected or absorbed sunlight, and by affecting various aspects of cloud formation, some types of air pollution cause the climate to cool (such as sulfates and nitrates), while others have a temporary warming effect that lasts a few days or weeks (such as black carbon). In particular, black carbon (also known as soot, a component of fine particulate matter ($PM_{2.5}$)) is estimated to be responsible for approximately 15 per cent of the current excessive warming of global temperatures (Forster et al., 2007) and is considered the second biggest contributor to global warming after carbon dioxide (CO_2) (Ramanathan and Carmichael, 2008). Hence, these so-called short-lived climate pollutants contribute to climate change (Smith et al., 2020).

On the other hand, climate change can also impact air quality (AQ). In particular, global warming is likely to increase concentrations of ground-level ozone pollution since the rate of ozone formation increases with temperature. Although air pollution and climate change are closely related (Moore, 2009), and although they share common natural and anthropogenic origins, they are usually treated as separate problems due to the large difference in the associated timescales. Hence, climate change is not discussed any further in this guidebook, which is dedicated to AQ assessment and limited to air pollutants causing a degradation of AQ.

1.2 Causes of air pollution

Anthropogenic pollution is caused by human activities. It includes emissions from fossil fuel burning (including in transport and power generation), from oil, gas and chemical industries, construction and agriculture. These industries typical of rapidly growing economies are the primary causes of pollution in Gulf Cooperation Council (GCC) countries (Ebinger et al., 2011). The ensuing degradation in AQ in GCC countries is exacerbated by the hot and arid/semiarid climate, which in the absence of rain promotes the production and transport of aerosols, comprised mainly of dust particles (Al-Ghamdi et al., 2015; Reiche, 2010; Omidvarborna et al., 2018a).

1.3 Air pollution status and challenges in GCC countries

The recent and current status of pollution in the GCC countries can be assessed from a number of sources, including exposure studies. These studies reported significant SO_2 emissions from refineries, power plants and desalination plants (Al-Rashidi et al., 2005; Al-Jahdali and Bisher, 2008). Moreover, measured annual PM_{10} and $PM_{2.5}$ concentrations in the GCC countries were found to significantly exceed World Health Organization (WHO) AQ standards (Lanouar et al., 2016; Brown et al., 2008; Munir et al., 2013; Habeebullah, 2014, 2016; Habeebullah et al., 2015).

The high levels of PM are mainly related to the desert-type climate in GCC countries characterized by high concentrations of natural dust. Although considered a pollutant by the WHO, recent evidence shows that natural dust does not have a serious impact on human health, unless inhaled in large quantities (Environmental Protection, UK). Studies that thoroughly and conclusively report on the combined effect of natural dust and anthropogenic PM on human health are still lacking.

Identification of the emission sources that contribute to the observed pollutant concentrations enables the implementation of emissions controls to mitigate harmful impacts.
Source apportionment studies demonstrate that the major contributors to overall observed air pollution in the GCC countries are sand, dust (natural and anthropogenic), chemical and oil industries, and transportation activities (Omidvarborna et al., 2018a). Emission and dispersion modelling studies conducted by the environmental authorities of Bahrain, Kuwait, and Qatar in 2012-2013 showed that the major emission sources **(i)** for PM_{10} and $PM_{2.5}$ are transport and power plants, **(ii)** for coarse PM (>PM_{10}) are re-suspended dust, and **(iii)** for CO, VOCs, NO_x and SO_2 are oil and gas industries and power plants (Naber, 2015).These studies also revealed that among the challenges facing the GCC countries are insufficient monitoring and lack of common AQ indices and data assimilation platforms.

A major source of $PM_{2.5}$ emissions in the GCC is transported dust from natural sources. In a recent study by Ukhov at al. (2020), it was mentioned that the contribution of the non-dust component to $PM_{2.5}$ is less than 25 per cent in the Middle East, which limits the impact of emission control on AQ. Alolayan et al. (2013) investigated the major sources of $PM_{2.5}$ in the atmosphere of Kuwait and concluded that around 54 per cent of $PM_{2.5}$ was transported sand dust.

1.4 The way forward

In the margins of the 18th United Nations climate change meetingin Doha, Qatar in 2012, a conference was organized to address the environmental challenges in the GCC countries, including air pollution (Klemes et al., 2012). The conference identified as key factors the population growth, rapid urbanization, and transport (state of urban transit systems, traffic congestion, low fuel prices, large number of vehicles) (Elmi and Al-Rifai, 2012). Another challenge is accurately quantifying, especially in the smaller countries, the contributions from local emissions and those from transboundary transport. Therefore, to improve AQ, additional effort is needed to assess AQ at the urban and national scales by improving monitoring, modelling, and building emissions inventories (Omidvarborna et al., 2018a).

1.5 Mitigation and prevention: air quality (AQ) management

Mitigating and preventing the adverse effects of air pollution requires an AQ management framework for the regulation and control of emissions, strong environmental policies (urban planning, siting) and guidelines and early warning systems to reduce people's exposure to pollutants. A viable and successful framework requires pollution monitoring, public awareness-raising, the building of accurate and up-to-date emission inventories, source apportionment, and pollution forecasting over short and long length and timescales. Understanding of the transport processes and the underlying physico-chemical mechanisms, in addition to being able to explore what-if scenarios, are also key ingredients of an AQ management framework.

1.6 AQ modelling

In the absence of air pollution monitoring that sufficiently resolves time and space, AQ modelling emerges as an attractive solution that can predict the spatio-temporal distribution of several pollutants (Omidvarborna et al., 2018a). Nevertheless, validation of AQ modelling results still requires data from representative, high quality AQ monitoring. A diagram presenting the building blocks of an AQ forecasting/modelling system that is commonly deployed within an AQ management framework is shown in **Figure 1**.

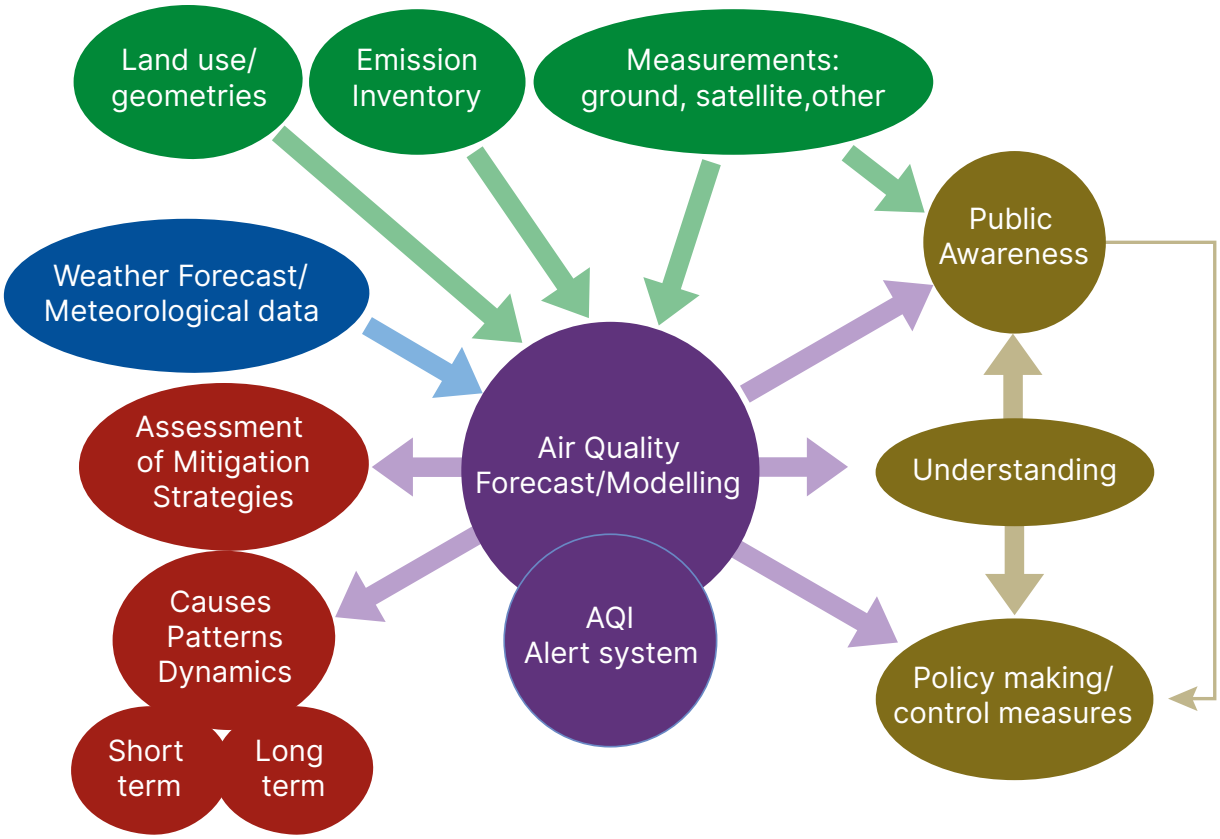

Figure 1 *The building blocks of an aq forecasting/modelling system*[7].

[7] AQI stands for air quality index

2. Introduction to AQ models

A model is a (relatively) simplified mathematical description of a real system that captures key physical and chemical mechanisms at the temporal and length scales that are suitably selected to answer the scientific question raised. AQ models are used to forecast weather and AQ, to assess short- and long-term environmental impacts on domains of size ranging from the microscale (1 km or less) up to the global scale (over 1,000 km), and to identify solutions for the management of environmental problems (Harbawi, 2013). As depicted in **Figure 2**, an AQ model involves coupling the momentum and energy transport governing atmospheric dynamics (the meteorological model) with pollutant species transport (the chemical transport model), which, in addition to advection and mixing, incorporates chemical reactions. Representations of the initial and boundary conditions on the model grid are often enhanced by assimilating measurements. In addition, an AQ model requires input data on emissions, land use, topography, and obstructions. Due to the complexity of the systems being modelled, building accurate and cost-effective AQ models, which are being enabled by advances in computational power and speed, continues to be a challenging endeavor (Baklanov et al., 2013).

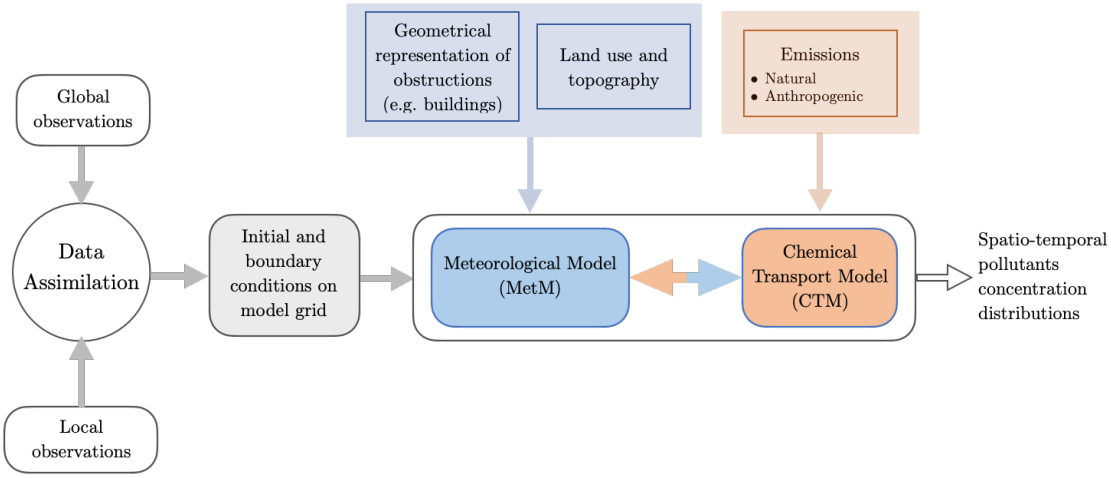

Figure 2. *Elements of an AQ model for assessment and forecasting.*

The coupling of the meteorological and chemical processes dictates an integrated modelling approach that can handle the transport of multiple pollutants over the spatiotemporal scales needed to identify control strategies to improve AQ.

Choice of an AQ model depends on many factors including size of study domain and duration, availability of input data, and whether chemical reactions are relevant. These factors dictate, to a large degree, the type of AQ model to be used. To this end, AQ models are categorized based on chemical components, emission sources, modelling approach, and the time and length scales of the atmospheric and chemical processes involved. These categories are discussed below.

2.1 AQ monitoring vs. AQ modelling

AQ monitoring is the systematic spatio-temporal collection of measurements to determine pollutant concentrations and other related quantities such as human exposure and fluxes to surface (land or water). AQ measurements ought to be continuously collected, in a spatially representative manner, to monitor and characterize criteria pollutant concentrations in the atmosphere. Due to limitations in their spatial coverage, AQ measurements are rarely sufficient to enable acceptable description of the spatial concentration fields, or to assess the impact of emission sources on ambient air-quality (US EPA, 2017). Where/when measurements are not sufficient, models are used to calculate the spatio-temporal distributions of pollutant concentrations levels and deposition fields (Moussiopoulos et al., 1996).

When used complementarily to AQ measurements, AQ models allow more accurate assessment. Measurements should also be used to validate and even tune a model thereby reducing uncertainties that may arise from uncertainties in the input data and/or the model itself. In addition, an AQ model provides a valuable means for interpolating measurements onto locations where no measurements are available.

AQ models can be deterministic,[8] statistical or hybrid. Statistical and hybrid AQ models are not covered in this document.

2.2 General description of deterministic AQ models

Deterministic AQ models simulate pollutant dispersion and reactions in the atmosphere by solving, mostly numerically, the mathematical equations describing the laws governing the associated physical and chemical processes (Gea et al., 2017). As depicted in **Figure 2**, these models take as input the emission sources (such as emission rates and stack heights), a geometrical representation of the domain, in addition to meteorological fields (wind velocity, temperature and pressure). The CTM within estimates the atmospheric levels of primary pollutants and in some cases the levels of secondary pollutants. As such, in contrast to statistical methods, deterministic AQ models describe, quantitatively, the causal relationship between meteorology, atmospheric concentrations, emissions, and deposition, among other factors. Choice of the type of the deterministic AQ model is decided by the field of application, geographical domain, time periods of interest, desired spatial and temporal resolutions, and choice of the level of detail in modelling chemical processes (Moussiopoulos et al., 1996).

2.2.1 AQ assessment vs. AQ forecasting

Deterministic AQ modelling can be broadly divided into two main categories: Air Quality assessment and Air Quality forecasting. AQ assessment entails inferring the time-averaged air quality at locations where observations are insufficient or lacking. Time averaging can be done on a monthly, seasonal or annual basis. In these studies, maps of pollutant concentrations enable the identification of hot zones, and when coupled with population patterns, provide valuable insights about exposure. In addition, some of the modelling tools allow the exploration of what-if scenarios, thus providing an effective framework for mitigation, informing policymakers, and planning. On the other hand, AQ forecasting entails the prediction of future AQ, starting with a set of initial conditions. An accurate and reliable AQ forecast is a key component of an AQ management system that **(i)** provides timely health alerts to vulnerable population groups, **(ii)** supplements traditional emission control programmes, **(iii)** empowers operational planning, and **(iv)** enables more effective emergency response.

[8] The literature often refers to physically based models as deterministic models. While purely statistical models do not rely on any physical modeling, physically based models may be purely deterministic or may have a statistical component. An example is modeling the mixing coefficient using a Gaussian probability distribution.

Both assessment and forecasting models require meteorological data. AQ forecasting requires meteorological forecasts that predict the time-dependent thermo-physical properties of air that drive and characterize the local transport of pollutants. Thus, the accuracy of the AQ forecast depends, in part, on the reliability of the weather forecast. To produce the most accurate weather forecast possible, the output of several forecasting models is typically combined with local experience and knowledge. Thus the most accurate AQ forecast possible is one that follows a similar approach.

2.3 What are deterministic AQ models useful for?

Deterministic AQ models enable atmospheric science and AQ management (see **Figure 1**) by providing a 360-degree description of the AQ problem, including analysis of factors and causes, assessment of the relative importance of relevant processes, identification of patterns, investigation of what-if scenarios, and assessment of proposed mitigation/control strategies, all of which feed into developing policies and strategies for efficient air pollution control (Nguyen, 2014).

Deterministic AQ Models are widely used by agencies, such as the United States Environmental Protection Agency (US EPA), tasked with controlling and regulating air pollution. These models enable these agencies to identify the contributing sources and to design effective mitigation strategies. AQ models are also commonly used during the permitting process to check whether or not pollutants from a new source result in ambient levels in excess of AQ standards. In the absence of any practical alternatives, AQ models are used as predictive tools to assess the effectiveness of (and decide on) new regulatory programmes (e.g. for source permits and emission control requirements) in reducing human and environmental exposure (US EPA, 2017). The applications of deterministic AQ Models are summarized in **Figure 3** (Collett and Oduyemi, 1997).

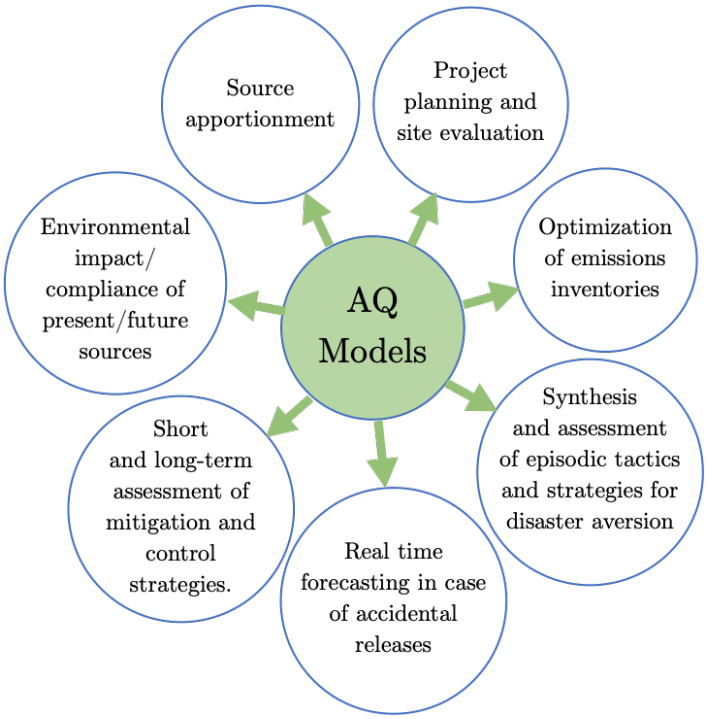

Figure 3. *Applications of deterministic AQ models.*

2.4 Suitability of deterministic AQ models for the assessment of source impacts

The following factors should be considered when assessing the suitability of a deterministic AQ model for assessing source impacts on the ambient air quality (US EPA, 2017).
Terrain and flow-field complexity: AQ models are commonly more accurate for terrains with smoother spatial transitions in topography and land use. These simple terrains translate into more uniform meteorological conditions, which allow simpler AQ models to yield representative predictions. Adequate AQ models for complex environments are available but are more computationally expensive, require in-situ measurements, and in many cases involve adjustment or calibration of the sub-models. Validation of AQ models, especially when used for complex environments, is crucial to building confidence in their predictions.
Accuracy and level of detail of input (meteorological, emissions, and AQ data): availability of the data required for an AQ model is a deciding factor on whether the model can be used. In addition to terrain and meteorological data, detailed spatial and temporal representation of the emission sources enables the model to more accurately assess the source impact.
How atmospheric processes are modeled: AQ models that incorporate complex and diverse atmospheric processes allow testing for a variety of interesting meteorological conditions, which ultimately enables effective evaluation of various control strategies.
Available resources.
Technical competence of the user.

2.5 Preparation phase for model selection

To identify the optimal modelling approach, it is recommended to follow the steps suggested by the European Environment Agency (EEA, 1998, Ch. 5):

1. Define the pollutant, and the output quantity to be modelled (concentration fields, or (spatial maximum) concentrations in streets or near point sources, usually for concentration statistics, for instance annual average, 98 percentile of hourly values ...).
2. Define the time resolution needed (the averaging time for the concentration).
3. Define the "model output area" for which the model calculations should be made (usually a zone or agglomeration) and the spatial resolution needed.
4. Define the accuracy in the output quantity that is required.
5. Determine the model area (this may extend considerably beyond the output area, particularly in case of pollutants with long range transport).
6. Investigate the availability of emission data (in the model area).
7. Investigate the availability meteorological and topographical data (in the model area).
8. Investigate available AQ data (in the model output area).
9. Check available computer resources.
10. Select models that are suitable for the pollutant (taking into account its chemistry and deposition), for the relevant output quantity, with the appropriate resolution in space and time, within the required accuracy, and for the area under consideration (taking into account its topography and meteorological characteristics).
11. Consider the computer requirements of the model(s); if these surpass available computer resources, reconsider model choice.
12. Reconsider the requirements on emission and meteorological data of the model(s) selected and, if necessary, collect more detailed input data (or reconsider the model choice).
13. Prepare input data.
14. Run the model.
15. Compare results to available AQ data and critically evaluate.

03

3. Categories of deterministic AQ models

Deterministic AQ models can be categorized in different ways. We present below categorizations based on **(i)** type of chemical components, **(ii)** type of emission sources, **(iii)** the modeled physics (model type), and **(iv)** the temporal and spatial scales (EEA, 1998).

3.1 Categorization based on type of chemical components

Based on the type of components and chemical reactions involved, deterministic AQ models can be non-reactive or reactive. Non-reactive models are applied to pollutants such as CO and SO_2 since their chemical reactions can be described in a simple way using pollutant half-life or decay parameters (Nguyen, 2014). In contrast, reactive models address complex multispecies reaction mechanisms common to atmospheric photochemistry that involve pollutants such as NO, NO_2, and O_3 (Conti, 2017).

3.2 Categorization based on type of emission sources

Based on the geometric representation of the emission sources, deterministic AQ models can be further divided into three main categories **(Figure 4)** (Harbawi, 2013):

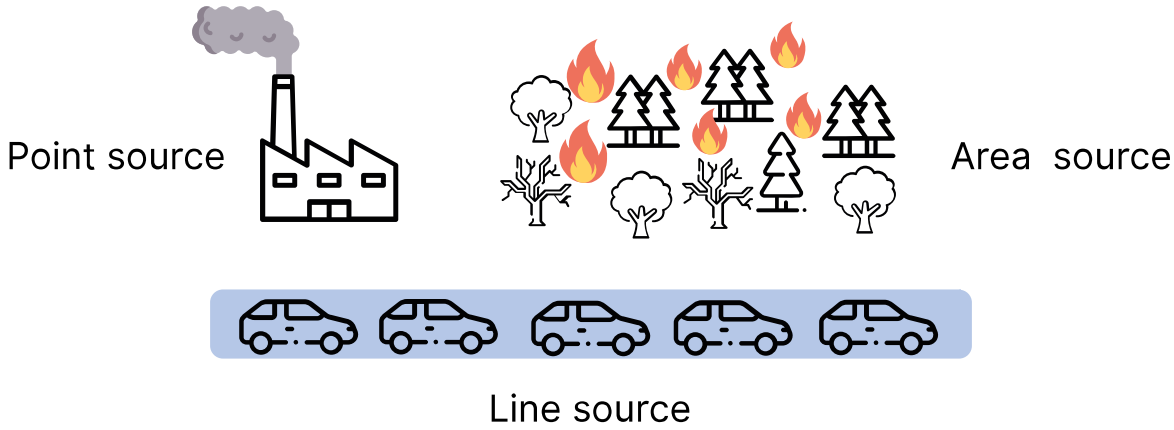

Figure 4. *emission sources used to categorize AQ models.*

- Point source AQ models used for industrial sources
- Line source AQ models used for airport and roadway air dispersion modelling
- Area source AQ models used for forest fires, dust storms, or coarse emission representation of large urban or industrial areas

3.3 Categorization based on modelling approach

The most used AQ models are the box model, Gaussian plume model, Lagrangian models, and Eulerian (grid-based) models **(Figure 5)** (Gea et al., 2017; US EPA, 2017).

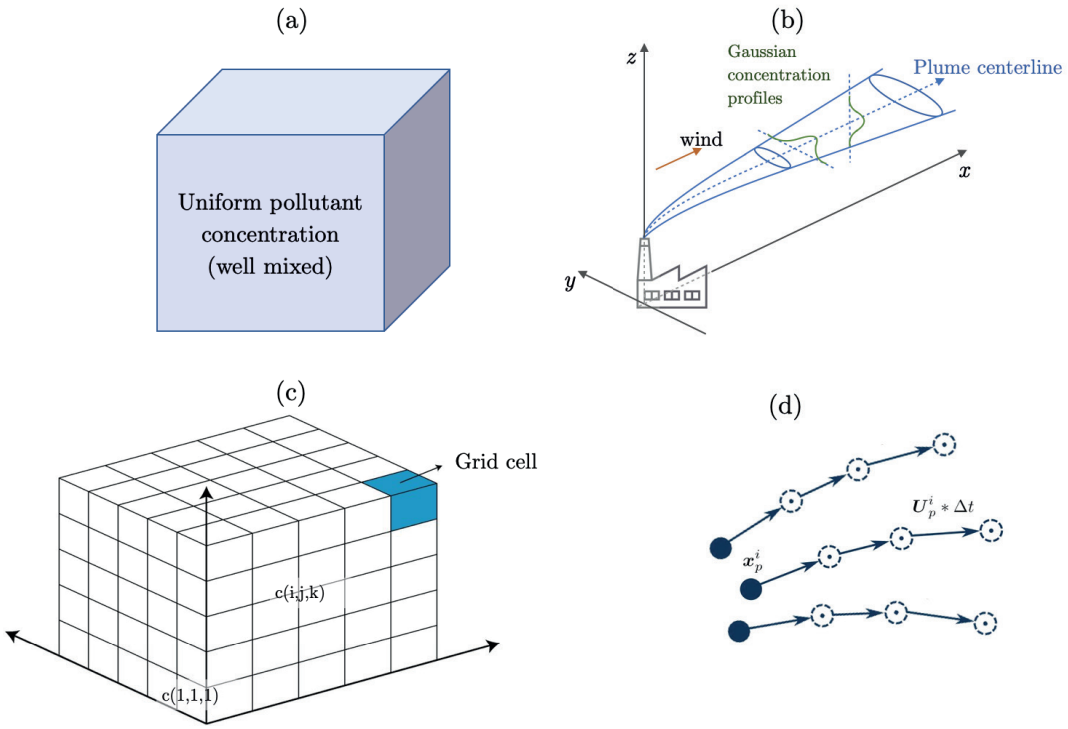

Figure 5. *AQ modelling approaches:* ***(a)*** *box model,* ***(b)*** *gaussian plume model,* ***(c)*** *eulerian model, and* ***(d)*** *lagrangian model.*

3.3.1 Box model

The Box model (Lettau, 1970) is the simplest type of AQ model. It is based on the mass conservation of pollutant inside a fixed box, which generally represents a large area such as a city (Zannetti, 1990). The model assumes that the air pollutants inside the box are homogeneously distributed and uses this assumption to estimate the average pollutant concentrations anywhere within the box. Although useful in some cases, this model is, however, very limited in its ability to accurately predict the dispersion of air pollutants because the assumption of homogeneous pollutant distribution is overly simple and unrealistic (Gea et al., 2017). The box modelling approach is well discussed in Lettau (1970); Derwent et al. (1995); Middleton (1995, 1998); Sportisse (2001); Cheng et al. (2006); Johnson et al. (2011) and Harbawi (2013).

3.3.2 Gaussian plume model

The Gaussian plume model is mostly used for predicting dispersion in the near-field of continuous air pollution plumes originating from ground-level or elevated sources. The Gaussian model is based on the assumption that all model inputs are constant throughout the domain over the model time step, resulting in a plume concentration, at each downwind distance, of independent Gaussian distributions both in the horizontal and in the vertical (Moussiopoulos et al., 1996; US EPA, 2017), as depicted in **Figure 5-(b)**. The species concentration is defined as being proportional to the emission rate of the source, diluted by the wind velocity at the source of emission. The dispersion behavior of a pollutant is determined by the standard deviations associated with the Gaussian distribution function. These standard deviations are typically functions of atmospheric stability, localized turbulence and distance downwind from the source (Collett and Oduyemi, 1997).

The Gaussian plume model is globally used as a standard technique to calculate the stack height required for the granting of permits (Daly and Zannetti, 2007) and is considered as the most accepted computational method to estimate the concentration of a pollutant at a certain point (Harbawi, 2013). The Gaussian plume model still suffers from severe limitations that restrict its applicability and accuracy, and as such, it is inaccurate in real-time response situations (Bluett et al., 2004). These restrictions render the model inaccurate **(i)** at large distance from the source (more than 10 km), **(ii)** for unsteady conditions (emission source and/or meteorological), **(iii)** over complex terrains, and unsuitable for modelling complex events such as inversion breakup fumigation events and stagnation events, and **(iv)** when pollutant deposition and chemical reactions need to be included.

The Gaussian model has been the subject of extensive research aimed at expanding it applicability to complex situations of the real world (Zannetti, 1990).

To handle non-stationary and non-homogeneous conditions, the segmented plume approach (Chan and Tombach, 1978; Chan, 1979) and the puff approach (Lamb, 1969; Roberts et al., 1970) were proposed to handle pseudo steady-state conditions. Both methods break up the plume into a series of independent elements (segments or puffs) that evolve in time as a function of temporally and spatially varying meteorological conditions (Zannetti, 1990).

Moreover, modelers have modified the Gaussian equation to consider total or partial reflection at the surface and at the top of the atmospheric boundary layer. Furthermore, Gaussian models have been modified to account for complex terrain. In addition, a simplified version of the Gaussian model – the Gaussian climatological model – can be used to calculate long-term averages (e.g. annual values) (Moussiopoulos et al., 1996).

3.3.3 Eulerian model

Most current regional photochemical models are Eulerian models, which are arguably the most powerful among the different model types as they involve the least restrictive assumptions. Eulerian models are, however, the most computationally intensive. Eulerian models solve a finite approximation of the equations governing the physics and chemistry of atmospheric processes by dividing the modelling region into a large number of cells (see **Figure 5-(c)**), horizontally and vertically, which interact with each other to simulate the various interactions that affect the evolution of pollutant concentrations, including chemistry, diffusion, advection, sedimentation (for particles), and deposition (both wet and dry).

As depicted in **Figure 5-(c)**, Eulerian dispersion models use a fixed three-dimensional Cartesian grid as a frame of reference. The flow within the domain is typically turbulent (Brown, 1991) and is mathematically described by expressing any dependent variable as the sum of a locally average component and a fluctuating component (Collett and Oduyemi, 1997). Advanced Eulerian models include refined sub-models for the description of turbulence (e.g. second-order closure models and large-eddy simulation models) and other microscale physics.

Input data requirements for Eulerian models include temporally and spatially resolved fields of emissions (resolved by species), meteorology (e.g. wind velocities, temperatures, solar insolation, etc.), topographic features, initial and background pollutant concentrations (for initial and boundary conditions), and domain definition (Russel, 1997).

3.3.4 Lagrangian model

Lagrangian models are used to determine time-dependent near- and far-field impacts from a limited number of sources (US EPA, 2017). In these models, Lagrangian fluid particles (or segments or puffs), periodically injected from emission sources into the domain, are advected by the instantaneous flow field, as depicted in **Figure 5-(d)**. The particles, which serve as a discretization of the pollutant density distributions in the domain, carry their respective shares of the masses of the different pollutants, in addition to other integral quantities such as the internal energy, which enables simulation of the dynamics of the associated physical parameters. Because it is unsteady, the Lagrangian model (sometimes referred as the Lagrangian puff model), in contrast to the Gaussian plume model, allows for time-varying emissions and meteorological conditions.

Particle motion in Lagrangian models can be produced by both deterministic velocities and semi-random pseudo-velocities generated using Monte Carlo techniques. Hence, turbulent transport is accounted for by superimposing a pseudo-random velocity fluctuation on the locally averaged wind velocity (Moussiopoulos et al., 1996). As the centre of mass of a particle is advected by the local wind velocity, diffusion is simulated by an additional random translation corresponding to the atmospheric diffusion rate (Russel, 1997). The Lagrangian model then calculates the air pollution dispersion by computing the statistics of the trajectories of a large number of pollution plume parcels (Gea et al., 2017).

Lagrangian models require spatially and temporally resolved wind fields, mixing-height fields, deposition parameters, and data on the spatial distribution of emissions (Russel, 1997).

Lagrangian modelling possesses several advantages over Eulerian modelling (Pearson 2001; Gertler 2006; Harbawi, 2013). These include the affordable computational cost, seamless numerical modelling of the advection term,[9] and the ability to trace particles back to the source, thus enabling quick evaluation of the effect of emissions inventories on pollutant levels. Lagrangian models, however, still face the grand challenge of handling complex chemistry by accurate modelling of the chemical interactions between different particles.

In particular, secondary pollutant formation requires adequate spatial and temporal representation of involved species in the background atmosphere, such as oxidants and ammonia (US EPA, 2017 and references within). As such, Lagrangian models have experienced very limited recent use in photochemical modelling, and have been predominantly used for relatively inert pollutants, with some capabilities for deposition.

In contrast, the main advantage of the Eulerian models is the well-defined three-dimensional continuous numerical representation of the domain which enables numerical formulation of complex interactions. This advantage rendered Eulerian models as the models of choice for studying air pollution problems on the regional scale. A more detailed explanation of the advantages and disadvantages of various AQ models can be found in Gertler (2006).

A comparison between the Gaussian plume, Lagrangian and Eulerian models is presented in **Table 1**.

Model Category	Gaussian Plume	Lagrangian (puff)	Eulerian (grid-based)
Steady/Unsteady	Steady	Unsteady	Unsteady
Temporal scale	Hours to year	Hours to year	Hours to century
Spatial scale	Local and urban scales	Local to continental scales	Local to global scales
Pollutants deposition	Limited dry deposition	Limited dry and wet deposition	Sophisticated dry and wet deposition
Chemical reactions	Limited reaction, usually accounted for by a decay parameter	Limited reaction within each puff; only first order chemistry	Complex, multispecies reactions; second order and higher chemistry
Most convenient applications	Non-reactive pollutant assessment for regulatory purposes at local scale (<50 Km)	Pollutant transport in complex terrain; back-trajectory analysis to determine the origin of air masses	Long range transport with complex chemical reactions
Major disadvantages	Some difficulty in simulating dispersion at low wind speeds	Difficult to model reactive pollutants	Numerical diffusion; High computational cost

Table 1. *Comparison between gaussian plume, lagrangian puff and eulerian models.*

[9] One of the key challenges in Eulerian methods has been the accurate and stable modeling of the nonlinear term $\vec{u} \cdot \Delta \vec{u}$, where $\vec{u}$ is the velocity vector field.

3.4 Categorization based on temporal and spatial scale

AQ models study pollutant transport in the study domain with spatial and temporal resolutions dictated by the problem statement. The spatial and time scales required to resolve the transport of mass, momentum, and energy, in addition to those governing chemical reactions, are the major deciding factor for what air-quality model to choose. Pollutants are advected according to local wind velocity, which is determined by the physical conservation laws (mass, momentum and energy) governing atmospheric processes. In addition, the spatio-temporal evolution of the pollutant concentration fields is governed by mixing induced by turbulence and chemical reactions.

Presented below is a discussion of the key physical mechanisms that characterize the atmospheric processes at different length scales, and as such deciding the complexity of the underlying model for prediction of the flow field. What follows is a discussion of the chemical reactions characterizing the air-quality processes at different length scales, and as such deciding the complexity of the underlying model for accurate representation at the desired length and time scales.

3.4.1 Scales of atmospheric processes

AQ models are decisively influenced by atmospheric processes, which are commonly classified with regard to their spatial scale. Orlanski (1975) recommends distinguishing between atmospheric processes at the macroscale (more than 1,000 km), mesoscale (between 1 km and 1,000 km) and microscale (less than 1 km) **(Figure 6)**.

3.4.1.1 Macroscale processes

At characteristic length scales exceeding 1,000 km (which is of the order of magnitude of Earth's radius), atmospheric flow is mainly associated with synoptic phenomena, i.e. the geographical distribution of pressure systems. The synoptic flow field that governs macroscale atmospheric processes evolves as a result of the balance between the pressure forces and the Coriolis force. While the pressure is hydrostatic along the radial direction, as can be inferred by scaling of the velocity components, the spatial variation of the pressure in the longitude-latitude plane is dictated by large-scale in-homogeneities of the surface energy balance. Global and the majority of regional-to-continental scale dispersion phenomena are strongly tied to macroscale atmospheric processes (Moussiopoulos et al., 1996).

3.4.1.2 Mesoscale processes

The flow configuration in the mesoscale (characteristic lengths between 1 and 1,000 km) depends on both hydrodynamic effects (e.g. flow channeling, roughness effects) and in-homogeneities of the energy balance. When the synoptic forcing is weak (i.e. in the absence of ventilation), pollutant dispersion is strongly governed by thermal effects.

Mesoscale atmospheric processes affect primarily local-to-regional scale dispersion phenomena, for which urban studies are the most important examples. The description of such phenomena requires, even for practical applications, the utilization of fairly complex modelling tools (Moussiopoulos et al., 1996) since mesoscale meteorological models should be capable of simulating local circulation systems, such as sea and land breezes.

3.4.1.3 Microscale processes

In general, air flow is very complex at the microscale (characteristic length less than 1 km), as it depends strongly on the detailed surface characteristics (e.g. the form of buildings, and their orientation with regard to the wind direction). Although thermal effects may contribute to the generation of these flows, they are mainly determined by hydrodynamic effects (e.g. flow channeling, roughness effects) which have to be described well in an appropriate simulation model. In view of the complex nature of such effects, local scale dispersion phenomena (which are to a large extent associated with microscale atmospheric processes) are mainly described with robust "simple" models in the case of practical applications, such as street canyon models (Moussiopoulos et al., 1996).

3.4.2 Scales of AQ processes

Atmospheric air pollution is a multiscale problem ranging from the microscale (e.g. urban heat islands), to the mesoscale (e.g. regional pollutant transport, dust storms), to the macroscale (e.g. global warming, ozone depletion).

Based on their spatial scale, AQ models can be divided into fourcategories **(Figure 6)**: **(i)** global scale, **(ii)** regional-to-continental scale, **(iii)** local-to-regional scale, and **(iv)** local scale air pollution models (Moussiopoulos et al., 1996). **Table 2** lists the most common model type, meteorological input, and physical/chemical processes used for AQ assessment at various scales.

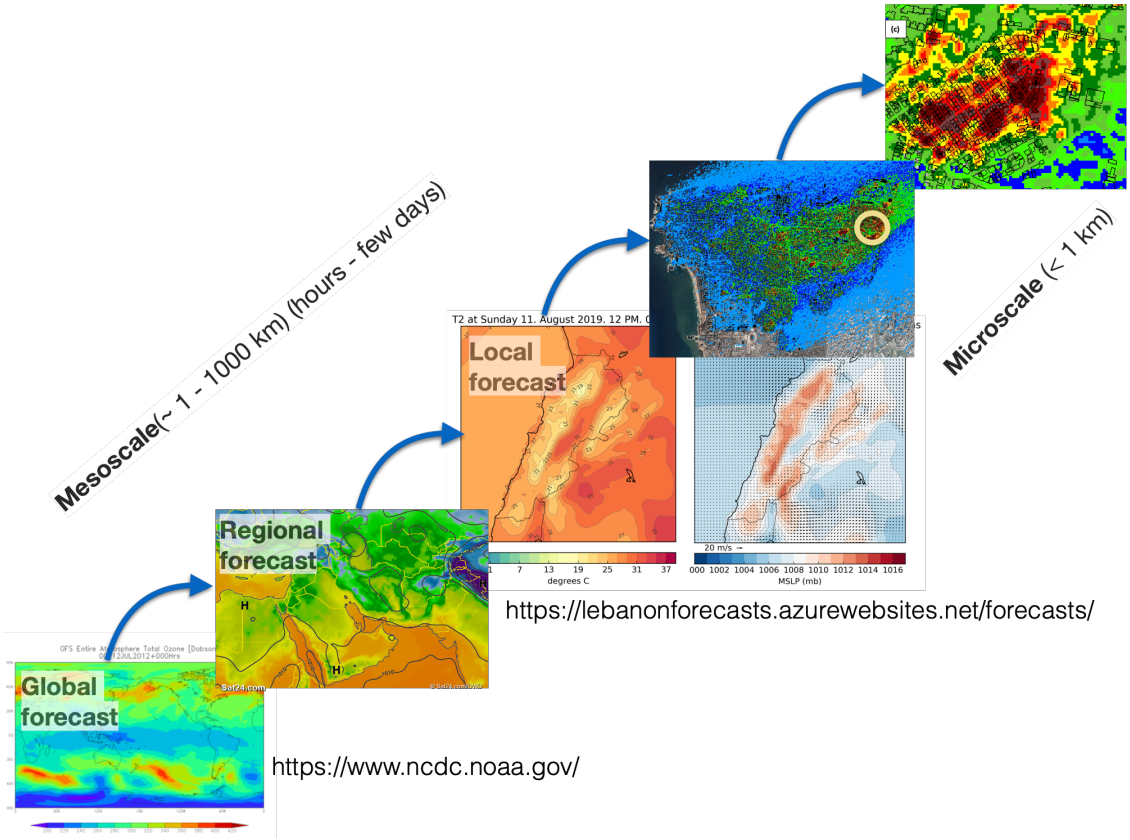

Figure 6. *Scales of AQ processes.*

3.4.2.1 Global-scale air pollution models

Global-scale air pollution models (over 10,000 km) are used to predict, on the global scale, the chemical composition[10] of the troposphere and study its interactions with the overlying stratosphere. In addition, these models are often used in climate studies to assess long-term future impact. Large-scale models also provide smaller-scale models with the required boundary conditions to enable prediction at the smaller scale (Moussiopoulos et al., 1996).

Several three-dimensional global- or hemispheric-scale models have been developed. These include MOCAGE, SILAM, and NAAPS. In these models, physical processes that take place at smaller length scales (such as cloud processes, convective mixing, transport between the boundary layer and the free troposphere, exchange between stratosphere and troposphere) are modeled on a sub-grid scale using parameterizations (Donnell et al., 2001). Meteorological input to these large-scale pollution models is provided by general circulation models (GCMs) or by assimilating observations.

3.4.2.2 Regional-to-continental scale air pollution models

Regional-scale models (250-10,000 km) emerged as essential tools to study the formation, transport and deposition of key pollutants (e.g. ozone, PM, acids) on the regional scale. In addition to aiding understanding of the underlying physico-chemical processes and their impact, these models enable quantification of **(i)** atmospheric pollution levels and their response to emission controls, **(ii)** transboundary fluxes, **(iii)** deposition to ecosystems and **(iv)** the relationship between emissions and depositions (Russel, 1997).

Regional-to-continental models, such as the EMEP Unified, WRF-Chem and the REMSAD models, resolve the spatial domain with grid spacing of 10-150 km, and cover time periods of up to two years. Both Lagrangian (single- and two-layer) and Eulerian dispersion schemes are used (Moussiopoulos et al., 1996). As their input, these models require meteorological fields, emissions data from emissions inventories, land use and topography data from GIS, in addition to concentrations of pollutants at the boundary (boundary conditions). Meteorological fields are usually provided by a meteorological preprocessor, such as Numerical Weather Prediction (NWP) models. Due to the challenges associated with building an accurate and up-to-date emissions inventory, emissions remain among the largest sources of uncertainty in the input.

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[10] Focusing primarily on methane (CH_4), CO, NO_x, non-methane hydrocarbons (NMHC), chlorofluorocarbons (CFC), hydrofluorocarbons (HFC), hydro-chlorofluorocarbons (HCFC) and sulphur compounds (SO_2, aerosols, dimethyl sulphide (DMS), hydrogen sulphide (H_2S)), together with their combined effects on the concentrations of O_3 and the oxidizing capacity of the atmosphere (defined largely by the concentrations of O_3, hydroxyl (OH) and hydrogen peroxide (H_2O_2).

3.4.2.3 Local-to-regional scale air pollution models

At the local-to-regional, or urban, scale (1-300 km), describing the turbulent flow field arising from the complex interactions between the atmospheric boundary layer flow and obstacles (e.g. buildings) poses a challenge to pollution models at this scale (Salim, 2011; Easom, 2000; Lateb et al., 2015). These interactions may lead to poor ventilation in parts of the domain, resulting in entrapment of pollutants, and at the other extreme may lead to strong ventilation resulting in fast removal of the pollutants. For an overview of these interactions in cities, see Deck (2005), Chang and Meroney (2001), Easom (2000) and Lateb et al. (2015).

One approach, albeit an expensive one, to studying pollutant dispersion in an urban environment is to carry out measurements in the whole domain. Alternatively, the Gaussian-based semi-empirical models can be used for simple problems of steady flow over a flat unobstructed terrain.

For more complex flow configurations, Mesoscale AQ models (Lagrangian and Eulerian) that solve the equations governing species transport are used (EEA, 1998). Mesoscale air pollution models require several types of data input including geographic data, meteorological data and emission data. All types of emission sources (point, line, area) are used, where it is common to combine many small sources into a single area source. If the emitted pollutants react over the desired timescale of the study, chemical modules, varying from a simple single reaction (SO_2 into sulfates) to more complex photochemical reactions (ozone and NO_x) are used.

The grid spacing in mesoscale AQ models is typically 4-5 km. Compared to regional-scale models (grid spacing of 18-100 km), this low resolution enables mesoscale models to capture variation in concentrations in regions with intense emissions and to study the formation of secondary pollutants (such as ozone) via nonlinear chemical reactions with reasonable accuracy.

Although this finer mesh is crucial to address non-linear pollutant formation in cities and near sources, coarser mesh is acceptable in rural areas and far from sources and allow great computational savings. This led to the development of a new technique called nested and/or multiscale modelling that enables the use of fine grid resolution inside cities and coarse grid resolution in rural area. Multiscale models (nested models) are considered the current state-of the-science for modelling highly reactive pollutants.

Moreover, they are extensively used to provide boundary conditions to finer resolution models. In this regard, several levels of nesting can be applied **(Figure 7)**.

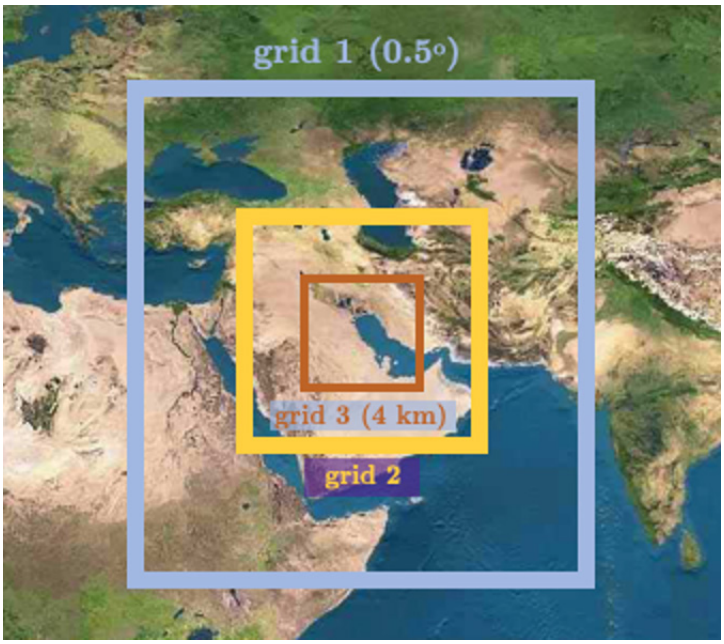

Figure 7. *Nesting involves propagating the solution between a coarse grid* ***(grid 1)*** *and a fine grid* ***(grid 2)****, and between the fine grid* ***(grid 2)*** *and a finer grid* ***(grid 3)****. The coarse grid cell size is similar to the grid size used in synoptic solvers (0.5-1 degree). The grid size in the finer grid can go as low as 3 km.*

Widely known air pollution models to address problems at the local-to-regional scale include HYPACT, UDM-FMI, DISPERSION, EURAD and UAM-V.

3.4.2.4 Local-scale air pollution models

Over scales of 1-1,000 m, atmospheric pollution models are based on the Gaussian distribution. These models, which are widely used for regulatory and planning purposes, evolved to meet increasingly stringent and detailed AQ guidelines. The first local-scale Gaussian models were based on the Pasquill-Gifford classes that categorize atmospheric turbulence into six stability classes. More recently, models based on boundary layer parameterization have been developed. These models use meteorological data (such as wind speed and direction, ambient temperature) and surface characteristics (such as surface roughness, Bowen ratio, and albedo) to calculate some atmospheric boundary layer scaling parameters (such as friction velocity, Monin-Obukhov length, convective velocity scale, temperature scale, both the shear- and convection-driven mixing heights). These scaling parameters are then used to construct the temperature and velocity similarity profiles across the atmospheric boundary layer.

Widely known air pollution models for problems in the local scale include AERMOD, UK-ADMS, OCD, ISC3, CTDMPLUS, CAR-FMI, CAL3QHC, OSPM and GRAL.

Description	Local (1-1,000 m)	Urban/Local to regional (1 – 300 km)[11]	Regional/continental (25–10,000 km)	Global
Model type	Gaussian models; Statistical models; Lagrangian particle models	Gaussian models; Eulerian chemical transport models; Lagrangian particle models	Eulerian chemical transport models; Lagrangian chemical models	Eulerian models
Meteorology	Local meteorological measurements; diagnostic wind field models	Mesoscale meteorological models; localized meteorological measurements; diagnostic wind field models	Synoptic/mesoscale meteorological models	General circulation models
PM_{10}	No chemical processes	Dry and wet deposition; secondary inorganic particle formation	Dry and wet deposition; secondary inorganic and organic particle formation	Same as regional-continental
$PM_{2.5}$	No chemical processes	Dry and wet deposition; secondary inorganic particle formation	Dry and wet deposition; secondary inorganic and organic particle formation	Same as Regional-continental
NO_2	Simple photo-oxidant chemistry	Dry and wet deposition; Limited photo-oxidant chemistry	Dry and wet deposition; Full photo-oxidant chemistry	Same as Regional-continental
O_3	Same as NO_2	Same as NO_2	Same as NO_2	Same as NO_2
SO_2	No chemical processes	Dry and wet deposition; secondary inorganic particle formation	Dry and wet deposition; secondary inorganic particle formation; full photo-oxidant chemistry	Same as Regional-continental

Table 2. *Model type, meteorological input, and physical/chemical processes for AQ assessment at various scales.*

[11] Some models (e.g., CMAQ) can also treat $PM_{2.5}$, NO_2, O_3, SO_2, and secondary organic components with full photo-chemical reactions at this scale.

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4. Deterministic AQ models

Worldwide, a number of AQ models have been developed and applied in the fields of AQ management and atmospheric science research. These models mainly fall into three categories (Nguyen, 2014):

- Dispersion models, typically used to estimate the concentration of air pollutants at specific locations (receptors or targets) near emissions sources
- Photochemical models, typically used to study the impact of emission sources by estimating pollutant concentrations and deposition of both inert and chemically reactive pollutants over large spatial scales
- Receptor models, observational techniques which use the physico-chemical characteristics of gases and particles measured at source and receptor to quantify the source contribution to receptor concentrations (source apportionment)

4.1 Dispersion models

4.1.1 What are dispersion models?

Dispersion modelling numerically solves the mathematical equations that describe atmospheric processes to simulate the dispersion of air pollutants originating from different emission sources (line, point, and area sources) at both local and regional scales (Nguyen, 2014; Irwin, 2014; Pan et al., 2014; Batterman et al., 2010), yielding accurate quantification of the sources' impact on the distribution of spatio-temporal concentrations of pollutants (Gea et al., 2017).

4.1.2 What are dispersion models used for?

Based on emissions and meteorological inputs, a dispersion model can be used to predict concentrations of pollutants at selected downwind receptor locations. As such, dispersion models can be used to determine compliance with national ambient air quality standards. Dispersion models are widely used in the risk assessment of hazardous effects of air pollution on humans and the environment (Van Leuken et al., 2016) and the appraisal of potential mitigation and control strategies. Other applications of dispersion modelling include:

- Assessment of emission compliance with guidelines, criteria, and standards for clean air
- Evaluation of the environmental impact of new plants
- Determination of appropriate chimney heights
- Management of existing emissions
- Planning of air monitoring networks
- Identification of main sources of air pollution

4.1.3 Types of dispersion models

As discussed in **Chapter 3**, there are different types of dispersion model with specific requirements for different spatial scales and deficiencies with respect to particle dispersion and aerosol dynamics within those scales. The most used dispersion models, presented in **3.3**, are Box, Gaussian plume, Gaussian puff, and the more detailed Eulerian and Lagrangian models, which can be applied for simulation of air pollutant concentrations from different emission sources (line, point, and area sources) at both local and regional scales.

4.1.4 Input data requirements

The required inputs of data in dispersion models include (Turner, 1970; Harbawi, 2013):

- Meteorological data such as wind speed and direction, atmospheric stability, ambient air temperature, and mixing height
- Source-emissions parameters including source location, height and diameter of the stack, exit velocity, exit temperature, and pollutant emission rate
- Land use and terrain elevations at the receptor location
- Location, height, and width of any obstructions in the path of the emitted gases plume
- Ambient or background concentrations of pollutants

4.1.5 How dispersion models are used

In many cases, a screening model is first employed to provide conservative estimates of the AQ impact of a specific source (or source category) assuming preset worst-case meteorological conditions, as depicted in the flowchart in **Figure 8**. This simple model can indicate whether more detailed modelling is needed based on whether the contribution of the sources to ambient concentrations is in excess of relevant AQ standards or allowable concentration increments. Detailed dispersion modelling involves numerically solving the laws that govern the physical and chemical atmospheric processes in a higher level of detail. Refined dispersion models also require more detailed and precise input data. As a result, they provide a more refined and, at least theoretically, more accurate estimate of source impact and the effectiveness of control strategies (Nguyen, 2014).

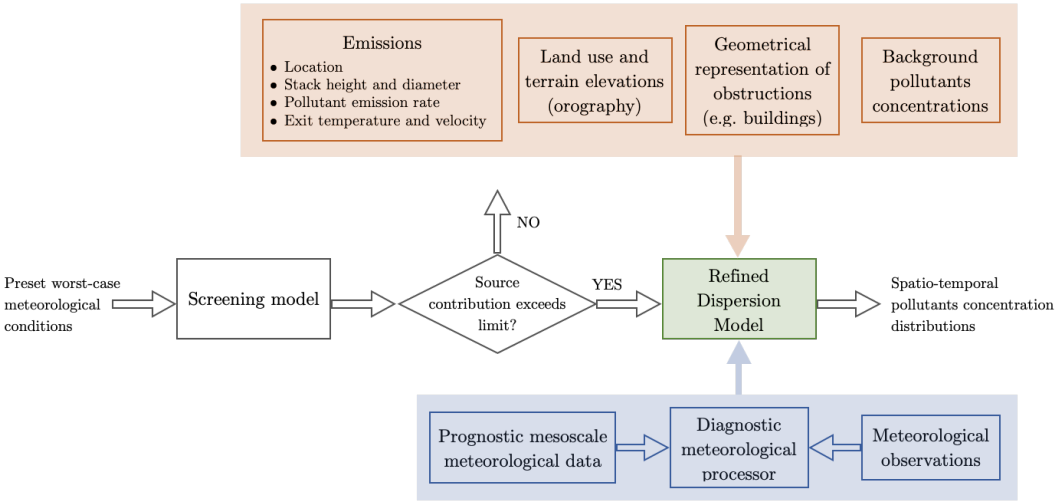

Figure 8. *A screening model is commonly used to decide whether a refined dispersion model is needed.*

When the application involves using unsteady dispersion models for long-range transport assessments or assessments where the transport winds are complex, use of the output from prognostic mesoscale meteorological models is encouraged. Some diagnostic meteorological processors are designed to appropriately blend available comparable meteorological observations, local site-specific meteorological observations, and prognostic mesoscale meteorological data, using empirical relationships, to diagnostically adjust the wind field for mesoscale and local-scale effects. These diagnostic adjustments can sometimes be improved using strategically placed site-specific meteorological observations (Nguyen, 2014). The meteorological data used as input to a dispersion model should be selected on the basis of spatial and temporal representativeness. For a more detailed discussion, refer to Gea et al. (2017).

4.1.6 How to choose a dispersion model

To choose the most suitable dispersion model for a given application/question, the following considerations should be considered (Bluett et al., 2004; Harbawi, 2013):

- The complexity of dispersion (e.g. terrain and meteorology effects)
- The potential scale and significance of potential effects, including the sensitivity of the receiving environment (e.g. human health versus amenity effects)
- Type of pollutant (e.g. gaseous, particulate, reactive)

Many air dispersion models have been discussed or applied, and their heterogeneity makes it difficult to select one approach above the others. A comparison of widely used dispersion models is presented in **Table 3** below.

Name	Full Name	Application	Steady/ Unsteady	Model Type	Range	Important Features	Developer/last update
ADMS	Atmospheric Dispersion Modeling System	Regulatory purposes and compliance for small towns, rural road networks, airports and industrial sources	Steady	Advanced Gaussian model	Near-field dispersion (few hundred meters or a few km)	Most frequently used model in the UK; accounts for downwash effects of nearby buildings; Include the effects of complex terrain	Cambridge Environmental Research Consultants (2020)
AERMOD	American Meteorological Society/Environmental Protection Agency Regulatory Model	Near-field impacts from a variety of industrial source types and mobile sources	Steady	Gaussian plume model	Short-range (up to 50 km)	EPA preferred dispersion model for many regulatory applications; handles pollutant impacts in both flat and complex terrain within the same modeling framework; treats "plume lofting" tracks any plume mass that penetrates into the elevated stable layer; includes dry or wet deposition	American Meteorological Society/Environmental Protection Agency Regulatory Model Improvement Committee (2021)

Table 3. *Features and characteristics of widely used dispersion models.*

CTDMPL US	Improved Complex Terrain Dispersion Model	Dispersion of pollutants in all stability conditions for complex terrain in rural or urban area for elevated point sources	Steady	Gaussian plume model	Short-range; transport distances less than 50 km	US EPA preferred model; includes a screening version (CTSCREEN); uses critical dividing streamline height to separate flow in the vicinity of a hill into two layers	US EPA (1993)
DISPERSION 21	Local Scale Atmospheric Dispersion Model	Evaluate effects on AQ from existing or planned sources including traffic and industrial sources	Steady	Gaussian model	Short-range; horizontal Domain dimension up to 20 km	Widely used in Sweden; Includes plume rise and building wake effects. also accounts for plume penetration	Swedish Meteorological and Hydrological Institute
HGSYSTEM	Dispersion models for ideal gases and hydrogen fluoride	Assessing accidental chemical releases with an emphasis on denser-than-air (dense gas) behavior	Steady/ Unsteady	Gaussian plume/ Gaussian puff	Near-field (AEROPLUME, HFPLUME, HEGABOX) and far-field (HEGADAS, PGPLUME) description of the dispersion process	Includes state-of the art dispersion algorithms for dense gases and treats the chemistry and thermodynamics of hydrogen fluoride (HF)	Shell Research Ltd. (1994)
ISC3	Industrial Source Complex	Pollutant concentrations from a wide variety of sources associated with an industrial complex for regulatory purposes	Steady	Gaussian plume model	Local scale, short term (ISCST3) or long term (ISCLT3)	Account for the following: complex and simple terrain, buoyancy-induced dispersion, plume rise as a function of downwind distance; separation of point sources, exponential decay and limited terrain adjustment the models contain algorithms for modeling the effects of aerodynamic downwash	US EPA (2002)

Table 3. *Features and characteristics of widely used dispersion models.*

OCD	Offshore and Coastal Dispersion model	Impact of offshore and onshore emissions from point, area, or line sources on the AQ of coastal regions	Steady	Gaussian model	Short range (up to few km)	EPA preferred model; incorporates overwater plume transport; accounts for building downwash and plume rise; treats plume dispersion over complex terrain; incorporates plume reflection from elevated terrain; accounts for pollutant removal	US EPA (2000)
OSPM	Operational Street Pollution Model	Simulation of air pollution from traffic in urban streets	Steady state	Combined plume and box model	Local scale (up to 30 km)	The model can be used for streets with irregular buildings; speed-dependent expressions for vehicle-specific emission factors are supplied with the model.	National Environmental Research Institute, Denmark
UDM-FMI	Urban Dispersion Modelling System - Finnish Meteorological Institute	Near-field impacts from a variety of industrial source types; impact of a network of line sources (road pollution)	Steady state	Gaussian model	Local scale; domain dimension up to 50x50 km	Includes a treatment of chemical transformation (for NO_2), wet and dry deposition (for SO_2), plume rise, downwash phenomena and dispersion of inert particles	Finnish Meteorological Institute;
CALPUFF	California Puff Model	Near-field impacts in complex flow (complex terrain, overwater transport and coastal conditions, light wind speed and calm wind conditions)	Unsteady	Lagrangian puff dispersion model	Scales of tens to hundreds of km	Includes algorithms for sub-grid scale effects as well as, longer-range effects; contains modules for near-source effects, building downwash, transitional plume rise, complex terrain effects, over-water transport, and coastal interaction effects	Sigma Research Corporation/TRC Environmental Corporation (2020)

Table 3. *Features and characteristics of widely used dispersion models.*

FLEXPART	The flexible particle dispersion model	Long-range and mesoscale dispersion of air pollutants from point, line, area or volume sources	Unsteady	Lagrangian model	Local to global; it can be used at scales from dozens of metres to several hundred km	Large international user community; includes below-cloud scavenging and in-cloud scavenging; account for chemical reactions with the hydroxyl radical (OH); a dust mobilization routine has been included	International team (2019)[12]
HYPACT	Hybrid Particle and Concentration Transport Package	Modelling highly sheared flows, recirculating coastal and mountain/valley wind systems, urban heat islands, plume fumigation and bifurcation	Unsteady	Combination of a Lagrangian particle model and a Eulerian concentration transport model	Local to regional scale; domain extend from few metres to hundreds of km	Offers great advantages near a source region for tracers when the source is small and irresolvable on the Eulerian grid; plume rise parameterizations and a dry deposition scheme have recently been added	Colorado State University and ASTER Division, Mission Research Corporation (2009)
HYROAD	The Hybrid Roadway Model	Traffic emissions and dispersion; operations in congested conditions	Steady	Lagrangian puff dispersion module	Short range (within 500 m of an intersection)	Listed as EPA alternative models; has features that enhance traffic emissions modelling; capable of functioning as both a screening and a refined model for analyzing CO dispersion	US EPA (2002)
HYSPLIT	Hybrid Single-Particle Lagrangian Integrated Trajectory model	Back-trajectory analysis to determine the origin of air masses; tracking and forecasting the release of radioactive material, wildfire smoke, wind-blown dust, pollutants	Unsteady	Hybrid between the Lagrangian approach and the Eulerian methodology	Local to global scales	One of the most extensively used atmospheric transport and dispersion models; includes wet and dry deposition and radioactive decay; integrates dust storm emission algorithm; incorporates nonlinear chemical transformation modules to simulate O_3	National Oceanic and Atmospheric Administration (NOAA) (2021)

Table 3. *Features and characteristics of widely used dispersion models.*

SCIPUFF	Second-order closure integrated PUFF model	Modeling power plant plume dispersion; assessing radiological impacts associated with nuclear reactor accidents	Unsteady	Gaussian puff model	Urban scale: Ranges up to 1,000s of km	SCIPUFF is the atmospheric dispersion modeling component of two US Department of Defense hazard prediction systems; uses adaptive time steps and spatial grids	Titan Corporation, ARAP Group (2020)
Caline3	California Line Source Model	Predict air pollutant concentrations at receptor locations downwind of highways located in relatively uncomplicated terrain	Steady	Gaussian plume model	Within 500 m of roadways	US EPA alternative model; requires relatively few inputs; flexibility in terms of user input complexity; short computational time	California Department of Transportation (CALTRANS) (1989)
CAL3QHC	California Line Source Model with added capabilities	Model emissions from vehicles queuing at intersections; estimation of total CO concentrations from both moving and idling vehicles	Steady state	Gaussian model	Near field dispersion (within a few hundred metres)	Recommended by the US-EPA; certified by both the California Air Resources Board and the EPA for modeling CO or other inert pollutant concentrations from motor vehicles at roadway intersections; includes a traffic algorithm for estimating the number of vehicles queued at an intersection	California Department of Transportation (CALTRANS) (2013)
CAR-FMI	Contaminants in the Air from a Road, Finnish Meteorological Institute	Evaluation of atmospheric dispersion and chemical transformation from a network of line sources in local scale	Steady state	Gaussian model	Local-scale model; domain dimension of up to 10 km	Includes an emission model, a dispersion model, statistical analysis of the computed time series of concentrations and a graphical Windows-based user interface; dry deposition is included in the treatment of particulate matter; extensively tested against results from urban measurement networks	Finnish Meteorological Institute (FMI)

Table 3. *Features and characteristics of widely used dispersion models.*

4.2 Photochemical models

4.2.1 What are photochemical models?

Photochemical models are large-scale AQ models that simulate the changes of pollutant concentrations in the atmosphere using a set of mathematical equations characterizing the chemical and physical processes in the atmosphere. These models are applied at multiple spatial scales, including the local, regional, national, and global scales (US EPA, 2017) (Nguyen, 2014). Examples of photochemical AQ models include CMAQ, CAMx, REMSAD, UAM, and RADM (Kukkonen et al., 2012).

4.2.2 What are photochemical models used for?

Photochemical AQ models are widely used for regulatory analysis and attainment demonstrations[13] by evaluating the efficacy of control strategies.

The major application of photochemical models has been in assessing the relative importance of VOC (Chen et al., 2010) and NO_x controls in reducing ozone[14] levels and to model acid deposition and its relation to SO_2 emissions, over scales ranging from urban to regional (Gea et al., 2017).

4.2.3 Types of photochemical models

There are two types of photochemical AQ models commonly used in AQ assessments: the Lagrangian model and the Eulerian model. Their general characteristics are similar to their dispersion counterparts.

The Lagrangian model follows the trajectories of parcels (or columns) as they are advected by the local wind velocity and undergo diffusion and chemical reactions (Gea et al., 2017). Because it is computationally efficient, early studies used the Lagrangian approach to simulate pollutant formation (US EPA, 2017). As discussed in section **3.3.3**, Lagrangian methods face difficulty in accurately modelling some physical and chemical atmospheric processes.

For this reason, most current operational photochemical AQ models use the 3D Eulerian grid approach due to its ability to accurately and fully account for these processes and thus predict pollutant concentration fields over the entire study domain. The Eulerian grid model numerically models the transport processes on a fixed three-dimensional grid that represents the study domain, and all chemical reactions are simulated in each cell at each time step.

[13] An attainment demonstration shows that a standard has been achieved as expeditiously as practicable in a given area before the attainment date specified for its classification.
[14] O_3 is not directly emitted but is formed by nonlinear reactions of NO_x and VOCs

4.2.4 Photochemical model components and processes

Under its hood, a photochemical model must incorporate key processes (as presented in **Figure 9**) that contribute to the spatial and temporal distributions of pollutant concentrations (Kukkonen et al., 2012).

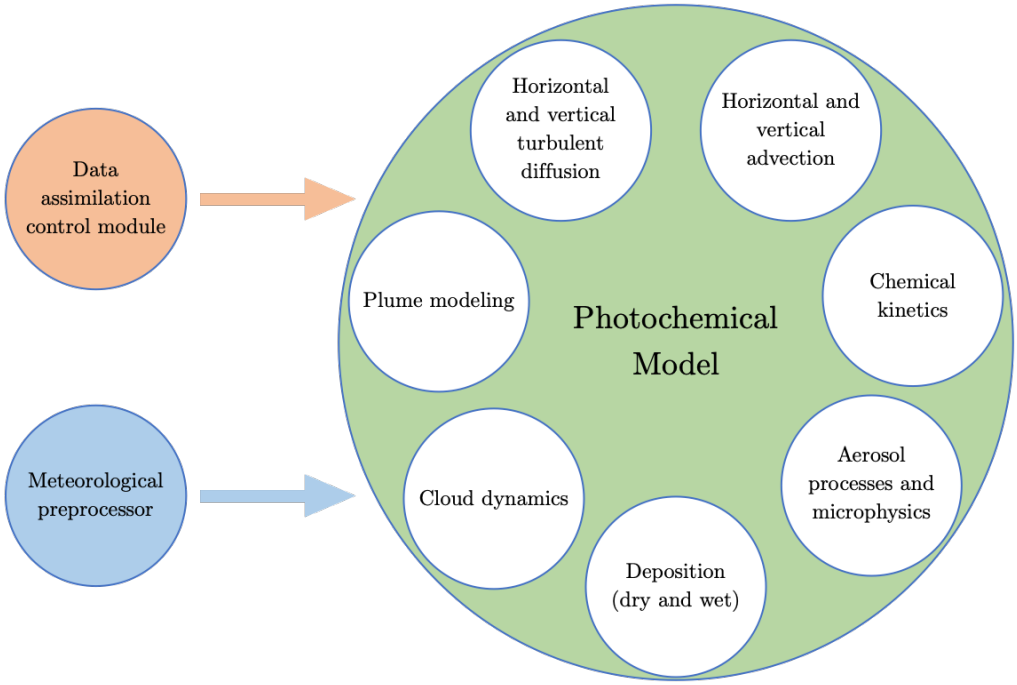

Figure 9. *Key processes in a photochemical model.*

4.2.4.1 Horizontal and vertical advection

Advection refers to the movement of pollutant species by the mean wind velocity field, whereas diffusion involves sub-grid-scale turbulent mixing of pollutants, which effectively lowers pollutant concentrations due to dilution. Some of the key requirements for the advection schemes include local and global mass conservation, minimal numerical viscosity, high stability, and high numerical efficiency (Kukkonen et al., 2012). Among these requirements, mass conservation is particularly crucial in photochemical models. When the input meteorological data and the numerical advection scheme are not mass consistent, a mass conservation scheme must be used. In such a scheme, the vertical velocity component at each grid is calculated by solving the continuity equation using the meteorological horizontal velocities and air density inputs.

The choice of the numerical advection algorithms is critical to the speed and accuracy of the photochemical model, especially for long-term simulations (Chock and Winkler, 1994). As such, these algorithms should be tested under various conditions (Russel and Dennis, 2000).

4.2.4.2 Horizontal and vertical turbulent diffusion

Turbulent transport in atmospheric applications is determined by complex interactions between meteorological conditions and topography (mechanical turbulence) and by the local daytime heating of the ground resulting in upward and downward vertical currents (convective turbulence). To supplement gross topographical features, surface "roughness" scales have been devised to parameterize surface characteristics according to land-use categories. Very small values are assigned to smooth water or ice, and increasingly higher values to grasslands, croplands, residential areas, and urban/industrial centres. In general, the rougher the surface, the greater the local turbulence (Russel, 1997). For convective turbulence, updraft and downdraft currents are characterized by incoming solar fluxes and surface properties such as albedo. During sunny days, convective turbulence dominates, and the atmospheric boundary layer is characterized by strong vertical mixing.

The mixing processes in turbulent flows are characterized by a wide range of mixing lengths associated with the cascading breaking down of eddies. To directly resolve all the length scales in the domain of interest, numerical solution of the Navier-Stokes equations requires a mesh so fine that the cost is prohibitive, especially for atmospheric flows. To reduce the cost, turbulence models are employed to numerically simulate flows on grids of affordable size. (Russel and Dennis, 2000). Turbulence interactions that are resolved by the grid are called grid-scale and those that are act at smaller scales are called sub-grid-scale. A popular method to describe sub-grid-scale interactions is the so-called turbulent closure used to solve the turbulence equations (Boussinesq, 1877). In particular, the first-order closure approximates any sub-grid turbulent quantity (scalar or vector) by using only the mean values of the dependent and independent variables.

First-order closure can be applied locally (as in K-theory and mixing-length theory) or non-locally (as in transilient turbulence theory). In the K-theory approach, the turbulent flux of any variable is proportional to the gradient of the associated mean variable, where the proportionality constant is the eddy diffusivity. In this approach, the eddy diffusivity tensor (for vector quantities) is determined as a function of atmospheric stability class and mixing height following some parameterizations. However, K-theory is valid only over short distances, and cannot simulate counter-gradient transport, which can be important in highly convective mixed layers. Non-local closure methods such as transilient matrix theory and asymmetrical convective models, have been implemented in some photochemical modelling applications to better capture the enhanced mixing from convective clouds.

Smagorinsky (1963) suggested a useful formula for eddy viscosity in numerical models based on local derivatives of the wind speed and the model resolution. It is still used by many atmospheric dynamics models to model horizontal diffusion (Kukkonen et al., 2012) including ALADIN-CAMx, SKIRON/Dust, FARM, CAMx-AMWFG and MM5-CAMx. In contrast, MM5-CHIMERE and MM5-CAMx use the Medium-Range Forecast Planetary Boundary Layer (MRF PBL) scheme. Horizontal diffusion in the CMAQ model is based on a grid size-dependent algorithm that combines Smagorinsky's approach with a term to minimize numerical diffusion (Byun and Schere, 2006).
For vertical diffusion, the K-diffusion scheme is widely used (Kukkonen et al., 2012).

4.2.4.3 Cloud dynamics

A key challenge facing AQ photochemical models is accounting for clouds, whose presence significantly affects the dynamics of pollutant transport, especially at the regional level.
The prediction of cloud formation and dynamics continues to be challenge, even using advanced prognostic meteorological models that assimilate observations. In a photochemical AQ model, the clouds module commonly estimates the vertical water distribution, precipitation, and vertical motion in convective clouds (Russel, 1997).

4.2.4.4 Chemical kinetics

Atmospheric chemistry is a key component of any photochemical model. The number of chemical compounds and reactions is too large to be incorporated in a model. As such, simplifications that include key compounds and processes are essential for a computationally affordable AQ model. The choice of a chemical scheme is based on a trade-off between complexity, cost, and the questions to be answered (Kukkonen et al., 2012).

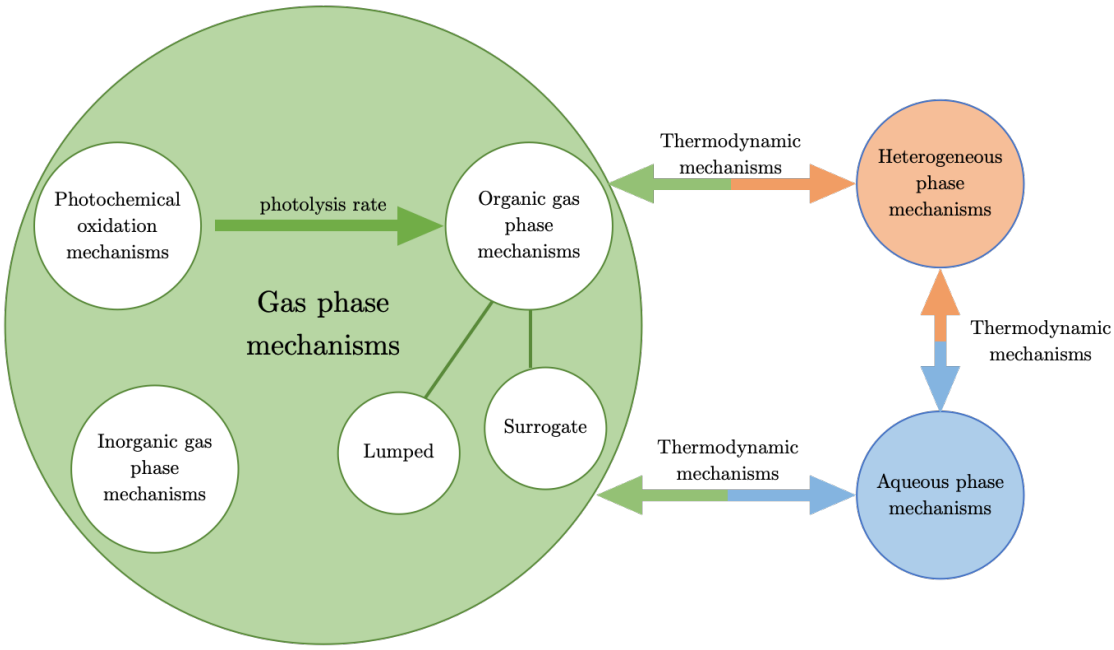

Figure 10. *Chemical mechanisms.*

Chemical mechanisms may be categorized based on the phases involved: homogeneous gas phase mechanisms, liquid phase (aqueous) mechanisms, and heterogeneous phase mechanisms (Russel, 1997) (see **Figure 10**). Homogeneous gas phase mechanisms include both organic and inorganic chemistry. Inorganic gas phase models are well established and are included in all photochemical models. Simplified organic gas phase mechanisms were developed primarily to study the formation of O_3 and NO_2 in photochemical smog and for acid deposition.

Most photochemical AQ models (e.g. SAPRC-90, RADM/RACM) use an organic gas phase mechanism that lumps together most of the organic species based on molecular type (i.e. those with similar structure and reactivity) (Russel, 1997). AQ models that aim to predict ozone concentration must incorporate one of the photochemical oxidation mechanisms of VOCs in order to evaluate the photolysis rates. These oxidation mechanisms are available with different levels of detail and parametrizations (Kukkonen et al., 2012). In addition to homogeneous gas phase chemistry, heterogeneous chemistry can be important, particularly for acid deposition and aerosol formation (Kukkonen et al., 2012).

AQ models (e.g., ADOM, RADM, and STEM-II) that aim to model the evolution of aerosols and/or acid deposition or acidification/eutrophication, especially in situations where fog and/or clouds are present, implement aqueous phase chemical mechanisms. These mechanisms could include up to 100 species and 200 reactions. However, large numbers of species and reactions are rately incorporated into an AQ model due to the prohibitive computational cost (Nguyen, 2014).

AQ models that simultaneously consider multiple phases must incorporate a thermodynamic mechanism in order to account for mass transfer between the phases (Russel, 1997).
The ISORROPIA thermodynamic equilibrium scheme is used in most of the chemical mechanisms.

Recent AQ photochemical models are equipped with a mechanism compiler that enables switching between mechanisms. **Table 4** lists the various chemical sub-models (Kukkonen et al., 2012) used by leading chemical weather prediction models.

Chemical sub-model	Photochemical Model	Comments
CBM-IV	CAMx, CMAQ, Enviro-HIRLAM, LOTOS-EUROS, OPANA, RCG, SILAM	33 compounds; 81 reactions
RADM2	CAMx, CHEM, CMAQ, Enviro-HIRLAM, EURAD, OPANA, WRF-Chem	36 compounds; 156 reactions
RACM	Enviro-HIRLAM, EURAD, MOCAGE	77 compounds; 214 reactions
MELCHIOR	CHIMERE	80 compounds; 320 reactions (can be used with reduced mechanism)
SAPRC-99	CAMx, CMAQ, FARM, OPANA	80 compounds; 214 reactions
NWP-Chem	Enviro-HIRLAM	17 compounds; 27 gas phase reactions
UNI-OZONE	EMEP model, MATCH (EMEP-MSC-W)	71 compounds; 123 reactions

Table 4. *Chemical sub-models used in AQ photochemical models.*

4.2.4.5 Aerosol processes and microphysics

Aerosol dynamics differ from gaseous pollutant dynamics since they involve different physical processes that affect the aerosol size distribution. These processes include nucleation, condensation, evaporation, coagulation, and deposition. Hence aerosols require special treatment in photochemical models. Aerosol processes and microphysics are discussed in more detail in **Section 6.1.**

4.2.4.6 Deposition

Deposition is the process through which pollutants are removed from the atmosphere and deposited on soil and vegetation (causing, for example, acidification) or in water bodies (causing for example, eutrophication). Inaccurate accounting for deposition can results in significant over-prediction of atmospheric pollution levels (Kukkonen et al., 2012; Wesely and Hicks, 2000) in addition to under-prediction of ground level pollution forecasts. Dry and wet deposition are commonly key components of long-term environmental studies or assessment programmes (e.g. EMEP).

4.2.4.6.1 Dry deposition

Dry deposition is a two-step process. The first step is the mechanical process by which the pollutant is transported to the earth's surface. The second step is the chemical interaction between the pollutant and the surface. In a photochemical model, dry deposition is generally characterized by the dry deposition velocity (as reviewed by Wesely and Hicks (2000), defined such that its product with the reference concentration (at a reference height) matches the flux of species to the ground. The dry deposition velocity is a function of three transport resistances: the aerodynamic resistance in the turbulent layer (essentially species-independent), the resistance in the laminar fluid sublayer close to the surface (depends on gas diffusivity), and the surface resistance (a function of surface affinity to diffusing species).

4.2.4.6.2 Wet deposition and rain, fog, and cloud processing

Wet deposition is process by which aerosol particles are scavenged by falling rain droplets and/or snow particles (precipitation scavenging) or scavenged into cloud droplets or cloud ice crystals (in-cloud scavenging). Rain, fog and cloud droplets can absorb gases, capture or be formed on pollutant particles, and promote chemical reactions. As such, wet deposition is an effective means of cleansing the atmosphere of pollutants.

Accurate modelling of the wet deposition process requires accurate representation of the size distribution of water droplets and ice crystals in the clouds, in addition to accurate modelling of transport processes through which the particles interact with the clouds. This information is commonly provided by meteorological models, which are improving with time in terms of the certainty of their predictions (Nguyen, 2014).

4.2.4.7 Plume modelling

A powerful technique to resolve fine-scale features (e.g. in urban areas) without incurring high computational cost is to use nesting. In AQ modelling, nested grids in Eulerian grid-based approaches allows the use of a relatively coarse grid to resolve pollutant concentration in regions (such as rural regions) where such concentrations do not exhibit large spatial variations, while using a finer grid to resolve regions (such as urban areas) where these variations are large. There remains, however, the challenge of accurately modelling pollution from concentrated sources, such as power plants, in the region covered by the coarse grid (Russel and Dennis, 2000). An effective way to tackle this challenge is to embed a plume model into the Eulerian grid model (usually called plume-in-grid or PiG models), which allows the resolution of the physico-chemical processes at the appropriate scales near the pollutant source. After the plume is sufficiently diluted, the pollutants are then mixed into the appropriate grids (Russel and Dennis, 2000). A few plume models have been developed and used in photochemical models. One of the first was the PARIS model that was used in the Urban Airshed Model (UAM).

4.2.5 Input data requirements

Regional photochemical AQ models commonly require the following categories of input: **(i)** meteorology, **(ii)** emissions, **(iii)** topography, **(iv)** observed atmospheric compounds concentrations, and **(v)** grid structure (Russel, 1997) **(Figure 11)**.

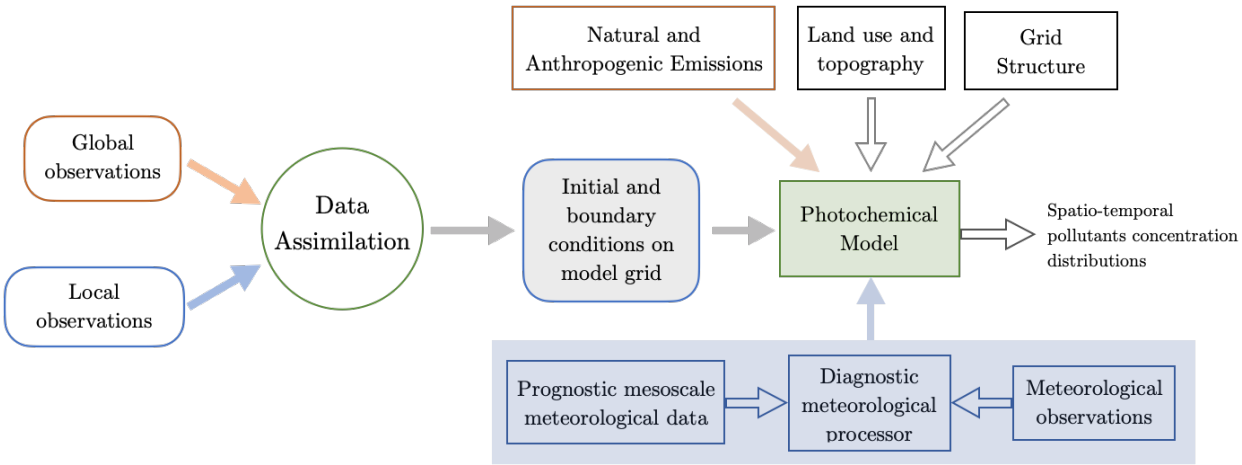

Figure 11. *Input data to AQ photochemical models.*

4.2.5.1 Meteorological input

Meteorological inputs into photochemical models, consisting of hourly velocity, temperature, humidity, mixing depth, and solar insulation fields, govern pollutant transport, chemical reaction rates and deposition fluxes (Nguyen, 2014). These and other inputs that may be required by the photochemical AQ model, such as cloud data (liquid water content, droplet size, etc.) and vertical diffusivities, are typically provided by non-hydrostatic diagnostic meteorological models coupled with four-dimensional data assimilation (Russel 2003).

4.2.5.2 Emissions input

Accurately describing the emissions input to a photochemical AQ model is necessary for the model to accurately predict the response of pollutant concentration distributions. The emissions input must be (Nguyen, 2014) compatible with the chemical reactions used in the model, sufficiently resolved in time and space, and adequately represented on the grid.

There are two categories of emissions that generally need to be characterized for input into AQ models: natural emissions and anthropogenic emissions. Pollutants such as PM, non-methane volatile organic compounds, NO_x, ammonia, CH_4, SO_2, and CO are emitted from natural sources such as windblown dust, sea-salt particles, soil, animals, vegetation and forests. Anthropogenic emissions are those produced by human activity including factories, traffic, and household sources. Accurate description of anthropogenic emissions is key to assessing the human impact on AQ and the environment, especially in domains containing populated areas (Russell and Dennis, 2000; Kukkonen et al., 2012). While anthropogenic emissions from utilities and major industrial activities are typically well described, other natural and anthropogenic, mainly organic, emissions are coarsely represented due to the inherent difficulty in collecting their data. As such, emissions remain one of the major sources of uncertainties in the input to AQ models.

Emission inventories, by virtue of the way they are built, contain data that represent the domain of interest with a varying degree of detail, both spatially and temporally. To be used as input compatible with the AQ model, an emission processor is used to map the emission inventory to the AQ model grid. A widely used processor that integrates high-performance computing sparse matrix algorithms is the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System. The SMOKE system, which can be used for both urban and regional applications, enables AQ forecasting and serves as an important tool for decision-making on air emission controls (Nguyen, 2014; Gea et al., 2017).

Natural emissions, mainly dust and sea-salt particles, are mostly calculated from emission models such as MEGAN (Model of Emissions of Gases and Aerosols from Nature) (Kukkonen et al., 2012). Dust emission mechanisms and models are discussed in **Chapter 6**.

4.2.5.3 Initial and lateral boundary conditions

Observed compound concentrations are needed to specify the initial and boundary conditions for photochemical AQ model simulations.

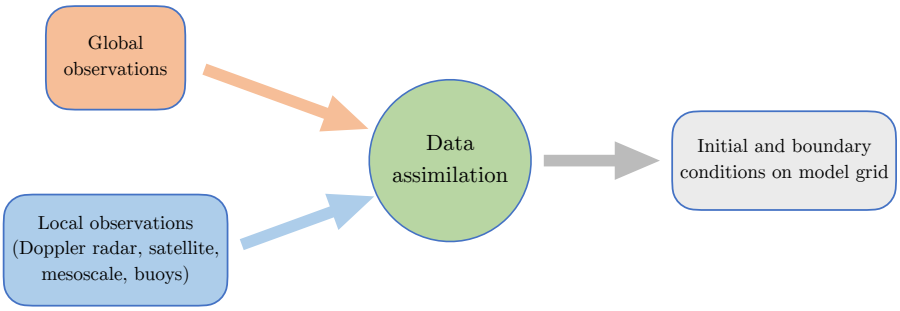

Figure 12. *Data assimilation is used to convert observations from different sources to initial and boundary conditions.*

To arrive at the initial field distributions of the dependent variables, globally and locally collected observations are interpolated onto the grid in a physically consistent and balanced manner using data assimilation approaches (Kukkonen et al., 2012), such as the Kalman filter methods and three-dimensional (3DVAR) and four-dimensional (4DVAR) variational methods (Kalnay, 2003) **(Figure 12)**. Data assimilation is now commonly used in regional AQ operational forecasting models and assessment models.

In addition to initial conditions, boundary conditions are required for AQ photochemical models in bounded domains. The data on the boundaries are usually interpolated in time from output of a larger-scale model, such as a global model, available every 3 or 6 hours.

4.2.5.4 Topography

Topography data are key for accurate modelling of near-ground pollution as it influences both pollutant transport and deposition.

4.2.5.5 Grid structure

Selection of the grid structure and the vertical extent of the study domains is decided by the particular application and the level of detail needed to adequately answer the questions, such as the desired spatial and temporal resolutions, the chemical compounds followed and the associated chemical reactions. Typically, smaller domains require smaller grid size horizontally (approximately 1-20 km) but do not extend into the stratosphere. Regional-or continental-scale domains employ a larger grid size horizontally (10-50 km) but may extend vertically all the way up to the lower stratosphere (Kukkonen et al., 2012).

4.2.6 Assessment of the performance of photochemical models

Many procedures and statistical metrics can be used to assess photochemical model performance across different applications, scales, and inputs. The main goal of these procedures and metrics is to inform regulators on model robustness and reliability, and to identify and address model weaknesses (Emery et al, 2017).

US EPA proposed a four-tiered approach to evaluating the performance of photochemical models (Dennis et al, 2010): **(1) "operational,"** in which model results are quantitatively compared to measured data using a variety of statistical metrics; **(2) "dynamic,"** in which the model output is analyzed for various perturbations to key inputs; **(3) "diagnostic,"** in which each process within the model is analyzed separately; and **(4) "probabilistic,"** in which the overall model confidence is assessed within an ensemble[15] system.

Photochemical models are usually accompanied by quantitative operational model performance evaluation using different statistical metrics. The model performance evaluation statistical metrics used across 69 published North American photochemical modelling studies is presented in Simon et al. (2012). The most used metrics are the normalized mean bias (signed error), normalized mean error (unsigned) and correlation coefficient. Emery et al. (2017) developed ozone and $PM_{2.5}$ benchmarks for these three statistical metrics for different spatial and temporal scales. These benchmarks can be used to identify where the results fall in the spectrum of past published results and hence to assess the performance of photochemical model for some applications.

4.2.7 How to choose a photochemical model

Photochemical AQ models, which predict pollutant spatio-temporal concentrations distributions by solving the conservation laws governing their transport, share many commonalities. To assist in choosing the appropriate photochemical AQ model for a given application, **Table 5** lists the most commonly used models along with their characteristics and features.

[15] The ensemble approach integrates modeling results from different AQ models. Generally, it displays better performance than the individual model products.

Name	Application	Model Type	Range	Important Features	Developer
CAMx	Source attribution, sensitivity, and process analyses; ozone abatement emission control strategies	Multiscale, 3D Eulerian grid model; two-way nesting grid	Multi-scale; Urban to regional; grid size from 1 to 1,000s of km	Four gas-phase mechanisms: CB05, CB6r2h, CB6r4 and SAPRC07TC; includes several "probing tools" for diagnostic and sensitivity studies; 16 aerosol chemical species	ENVIRON International Corporation
CMAQ	Simulates ozone, PM, toxic airborne pollutants, visibility, and acidic and nutrient pollutant species throughout the troposphere	3D Eulerian model with nesting capabilities	Multiscale: urban to hemispheric	Gas-phase chemistry can be simulated with the CB05, SAPRC-99 or RADM2 photochemical mechanisms; advanced users can modify the existing photochemical mechanisms, or even add new ones; PM is represented using three lognormal sub-distributions, or modes; includes a process analysis (PA) module that tracks mass throughout all individual processes (reactions, advection, diffusion, etc.)	US-EPA
UAM-V	Air quality studies focusing on ozone; evaluating the air-quality changes from emission control scenarios	3D multilayer, Eulerian model with multiple two-way grid nesting	Urban to regional scales; grid sizes range from 4-50 km	CB-IV-TOX: an extension of version IV of the Carbon Bond Mechanism (CB-IV) for solving chemical kinetics; An aerosol mass distribution over eight bins is automatically set when the model is initialized (Sectional approach); Include a process analysis extensions and integrated reaction rates	Systems Applications International (SAI)
REMSAD	Simulates the chemistry, transport and deposition of airborne pollutants with emphasis on particulate matter (PM)	3D Eulerian model with two-way nesting capability	Regional to continental scales; grid size of 10-80 km	Two photochemical mecha-nisms: CB-V and "micro-CB" (reduced-form version of CB-V); detailed secondary organic aerosol (SOA) treatment and improved performance under stagnant meteorological conditions	Systems Applications International (SAI)

Table 5. *Features and characteristics of widely used photochemical models.*

Name	Application	Model Type	Range	Important Features	Developer
Enviro-HIRLAM	Chemical weather forecasting; climate change modelling; contamination from volcanic eruptions, sand and dust storms and nuclear explosions	3D hydrostatic, online integrated Eulerian model with nesting capabilities	Multiscale; regional to urban scales; optimal resolution 2.5 km	Four mechanisms for gas-phase chemistry: NWP-Chem, RADM2, RACM and CBMZ; four aerosol dynamics modules: Modal CAC, MADE, Sectional MOSAIC and SALSA; accounts for all aerosol microphysics	Danish Meteorological Institute (DMI) in collaboration with several European universities
EURAD	Prediction of air pollution episodes and trends; study of emission reduction scenarios	3D multilayer Eulerian model with nesting capabilities	Urban to regional model; horizontal grid size typically of 2-80 km²	Three mechanisms for gas-phase chemistry: RADM2, RACM and Euro-RADM; two options for aerosol dynamics models: MADE and SORGAM	Institut fuer Geophysik und Meteorologie
FARM	Episodes analysis and investigation of pollutant formation and accumulation processes; analysis of scenarios and of the effects of regional emission control policies; pollution forecast in complex situations	3D Eulerian grid model	Urban to regional scales; grid size typically between 500 m and 50 km	Two mechanisms for gas-phase chemistry: an updated version of the chemical mechanism EMEP-acid or SAPRC-99; two options for aerosol dynamics: aero3 or aero0; ISORROPIA and SORGAM models to include aerosol thermodynamics	ARIANET
LOTOS-EUROS	Modelling of pollutants (photo-oxidants, aerosols, heavy metals)-over Europe; AQ forecasting	3D Eulerian model	Regional to continental scales; standard horizontal resolution of 0.5 x 0.25 degree (lon-lat)	Two chemical mechanisms: the TNO CBM-IV scheme and the CBM-IV by Adelman; bulk scheme with several non-interacting size ranges for aerosol representation; the model is equipped with a data assimilation package with the ensemble Kalman filter technique	TNO, RIVM and KNMI Institutes; PBL Netherlands Environmental Assessment Agency

Table 5. *Features and characteristics of widely used photochemical models.*

Name	Application	Model Type	Range	Important Features	Developer
MATCH	Studies of tropospheric chemistry and ground level ozone; studies of sulphur deposition over continental scales; detailed deposition assessments with higher horizontal resolution (5 km) in regions	Multiscale three-dimensional offline Eulerian model	Urban to continental horizontal scales; horizontal resolutions of 1-50 km	Extended EMEP MSC-W model chemistry; bulk scheme with several non-interacting size ranges for aerosol representation; equilibrium between particle and gas phase is included	Swedish Meteorological and Hydrological Institute (SMHI)
CHIMERE	Daily forecasts of ozone, aerosols and other pollutants; long-term simulations for emission control scenarios	3D Multi-scale off-line Eulerian model	Urban to regional scales; horizontal domains of 50-5,000 km; horizontal resolution of 1-100 km	Two gas phase chemical mechanisms can be included: MELCHIOR1 and MELCHIOR2; sectional aerosol scheme with six size bins (each bin internally mixed); all microphysical processes included; secondary organic aerosol formation is considered	IPSL/LISA/ INERIS
MOCAGE	Chemical weather forecasting; tracking and back-tracking of accidental point-source releases; trans-boundary pollution assessment	3D multi-scale semi-lagrangian model	Regional to global scales; typical global grid resolution of 2 × 2 degrees and regional grid resolution of 0.5 × 0.5 degrees	The chemical scheme used is RACMOBUS; aerosols are described using a bulk approach with size bins (typically 5 to 20 bins per species)	Meteo-France

Table 5. *Features and characteristics of widely used photochemical models.*

Name	Application	Model Type	Range	Important Features	Developer
OPANA	AQ impact assessment studies to obtain government permission to install combined cycle power plants and incinerators; real-time forecasting systems over cities and regions; sensitivity study of dry deposition fluxes	3D non-hydrostatic, prognostic mesoscale model;	Urban to regional scales; domain dimensions of 10-500 km; horizontal resolution of 1-10,000 m	CBM-IV chemical mechanism in short and long; RADM model and SAPRC-99 chemical scheme are also included; modal scheme with three modes and all microphysics	Environmental Software and Modelling Group, Computer Science School, Technical University of Madrid (Spain)
SILAM	Simulating episodes or long-term periods, for operational forecasting and for studying emission scenarios; computes probabilities in the "inverse" mode of the model	Hybrid Eulerian and Lagrangian model	Global, regional- (several thousand kilometers) and mesoscale (50-200 Km) simulations; grid spacing down to 1 km	The main gas-phase chemical mechanism is CBM-4; bulk and ADB (Aerosol Dynamics Basic research mode only) schemes; both schemes use the user-defined set of bins	Finnish Meteorological Institute (FMI)
WRF-Chem	Modeling emission, transport, mixing, and chemical transformation of trace gases and aerosols simultaneously with the meteorology; chemical weather forecasting	3D online integrated Eulerian model with nesting capabilities	Mesoscale model; routinely run at high resolution of 1–4-km grid spacing	Several choices for gas-phase chemical mechanisms including RADM2, RACM, CB-05 and CBM-Z; give choices for aerosol models are three modal models (MADE/SORGAM, MADE/VBS, MAM), one sectional model aerosol (MOSAIC) and a bulk aerosol module from GOCART	NOAA/ESRL
EMEP Unified Model	Modelling transboundary acidification, eutrophication, ground-level ozone and particulate matter ($PM_{2.5}$, PM_{10}); modelling short-term episodic ozone and long-term (growing season) ozone	Three dimensional Eulerian model	Regional to continental scales; horizontal resolution: 50x50 km	Two standard chemistries, UNI-ACID and UNI-OZO; EMEP aerosol model (UNI-AERO) describes emissions, chemical transformation, dynamics, transport, and dry and wet deposition of atmospheric aerosols	Norwegian Meteorological Institute

Table 5. *Features and characteristics of widely used photochemical models.*

4.3 Receptor models

Unlike dispersion models, receptor models[16] identify and quantify the contributions from different pollution sources (source apportionment) by analyzing the physico-chemical characteristics of observations at receptor locations (Watson et al., 2002). The receptors can be fixed (indoor or outdoor) or follows human activities. Because they are sensitive to measurements, receptor models require measurements at several receptor locations and over a representative time period. These models are also very sensitive to the distance between source and receptor, given that the role of atmospheric processes is bigger for larger distances (Nguyen, 2014).

Receptor models employ statistical tools to relate emissions to observations, albeit they abide by mass balance. The most widely used receptor models are Chemical Mass Balance (EPA-CMB), EPA-Unmix, and the Positive Matrix Factorization (PMF) (Gea et al., 2017). Key features of these three receptor models can be found in Nguyen (2014).

Notable studies that use receptor models include Liu et al.'s (2015a, 2015b) investigation of the sources and contributions of PAHs, which subsequently enabled quantification of the cancer risks for each source by incorporating incremental lifetime cancer risk (ILCR) values. Another study used PMF models to assess ILCR associated with sources of $PM_{2.5}$-bound PAHs (Callén et al., 2014). Heo et al. (2014) employed the PMF receptor model to assess the relationship between $PM_{2.5}$ and mortality in Seoul, Korea (Gea et al., 2017).

Recent promising trends in research on source apportionment include mixing dispersion and receptor modelling.

[16] Dispersion "source" models and "receptor" models are complementary rather than competitive (Nguyen, 2014).

5. Chemical weather forecasting

Chemical weather forecasting (CWF) entails predicting the chemical composition of the atmosphere over a short term (less than two weeks). A chemical weather forecast is the outcome of coupling a Meteorological model (MetM), which estimates the distributions of thermo-physical properties (such as velocity, temperature, pressure, humidity), with an atmospheric chemical transport model (CTM) that accounts for the evolution of the pollutants from emission sources as they undergo convection, mixing, chemical reactions, and deposition (Kukonnen et al., 2012).

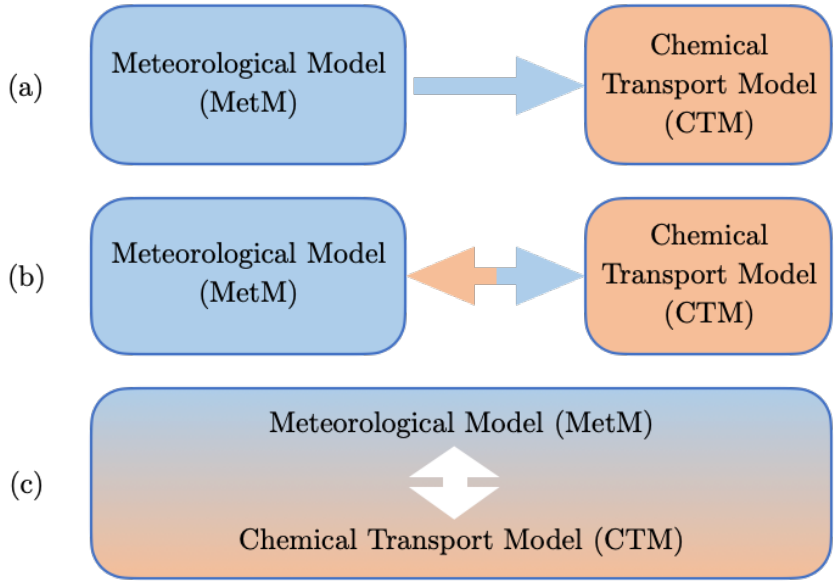

Figure 13. (A) *offline model,* ***(B)*** *online access model, and* ***(C)*** *online integrated model.*

The coupling between a MetM and a CTM can be either offline or online (Baklanov et al., 2013), as depicted in **Figure 13**. In offline modelling, the coupling is one way, where metrological data from the meteorological pre-processor is used as input to the CTM. The meteorological data could in the form of measurements and/or the outcome of a diagnostic model or an operational numerical weather prediction (NWP) model (Baklanov et al., 2013). In contrast to offline models, the coupling in an online model between the MetM and CTM models is two-way. There are two types of online CWF models: online integrated models and online access models. In an online access model, the coupling between MetM and CTM is a two-way exchange via a model interface on a regular and frequent basis. All other model aspects, such as the grid and time step, are not shared between the two models (Mathur et al., 2010). On the other hand, online integrated models compute the meteorological and chemical property fields by simultaneously solving, on the save grid and using the same global time step, the system of coupled equations governing the associated physical and chemical laws (Baklanov et al., 2013). In addition to advantages offered by the consistency in numerical representation in space and time, integrated models are more suitable for modelling feedback mechanisms such as aerosols and gas forcing on atmospheric processes.

On the other hand, offline coupling of meteorological and AQ models is more flexible, has a lower computational cost, and is more suitable for a variety of studies (e.g. ensembles and operational activities, inverse modelling, emission scenarios analysis, and AQ management) (Korsholm, 2007).

As mentioned above, an NWP model is not only important for providing periodic weather forecasts, but also serves as a key component of AQ models, including those used for CWF. Most currently used NWP models are prognostic, non-hydrostatic,[17] employ a horizontal grid spacing of less than 10 km, and use as the vertical coordinate the pressure coordinate or a terrain-following coordinate. While diagnostic models estimate the meteorological fields by interpolating, subject to some conservation constraints, available measurements, prognostic models predict these fields by solving the system of coupled equations governing the physical conservation laws. NWP models use microphysical parametrizations to account for physical processes that occur at the sub-grid scale, such as cloud and precipitation processes, boundary layers, and convection processes (on coarse grids) (Baklanov et al., 2013). Handling of initial and boundary conditions in NWP models is done in a similar manner to that in AQ models, as discussed in section **4.2.5.3.**

A plethora of online and offline operational CWF weather forecast models have been developed and maintained by institutions around the world in order to produce daily short-term AQ forecasts. Some of these models have been fully operational for more than 20 years. Table 6 introduces some of the most commonly used weather forecast systems along with their online/offline coupled meteorological and chemical transport models. The countries in which these models are operated and maintained are also presented.

Model Name	MetM	CTM/Photochemical model	Coupling	Country
ALADIN-CAMx	ALADIN	CAMx	Offline	Austria
Enviro-HIRLAM	HIRLAM	Enviro	Online integrated	Denmark
MATCH	ECMWF or HIRLAM	MATCH	Offline	Sweden
MM5-CAMx	MM5	CAMx	Offline	Greece
MM5-CHIMERE	MM5	CHIMERE	Offline	Greece
MM5/WRF-CMAQ	MM5/WRF	CMAQ	Offline	Spain
SKIRON/Dust	ETA	SKIRON	Online	Greece
WRF-Chem	WRF	CHEM	Online integrated	United states (also used in Germany, UK, Spain, Austria, Slovenia, Italy, etc.)
NMMB/BSC-CTM (BSC-CNS)	NMMB	BSC-mineral dust scheme	Online access	Spain

Table 6. *Features and characteristics of widely used chemical weather forecasting operational models.*

[17] Hydrostatic models, which are less computationally expensive, restrict the vertical acceleration to be small compared to gravity, which leads, according to Newton's second law, to a vertical balance between the pressure force and gravity.

06

6. Dust models and assimilation products

6.1 Atmospheric aerosol particles

Atmospheric aerosol particles, or particulate matter (PM),[18] are a mixture of microscopic solid or liquid particles with a diameter of 1 nm to 100 µm (e.g. sea salt, sulfates, black carbon, organic matter, and mineral dust) suspended in the air (Ukhov et al., 2020). $PM_{2.5}$ and PM_{10} refer to particulate matter with a diameter of less than 2.5 µm and 10 µm respectively.

6.1.1 Impact on climate

Atmospheric aerosols play an important role in the global climate system by interacting with Earth's energy budget. Aerosols[19] directly interact with the energy budget by modifying the radiation balance through the absorption and scattering of incoming solar radiation, resulting respectively in warming and cooling of the surface. In addition, by acting as condensation nuclei for clouds, aerosols not only modify cloud properties (optical depth and albedo) but also regulate their formation. Hence aerosols indirectly affect Earth's energy budget by virtue of the interaction of the clouds (both size and composition) with incoming solar radiation (Kim et al., 2008).

6.1.2 Impact on the environment and human life

Aerosol particle pollution is responsible for millions of premature deaths annually (WHO, 2018). Extended PM exposure may cause a variety of serious diseases including cardiovascular and respiratory diseases and lung cancer (Lelieveld et al., 2015; Ukhov et al., 2020). Aerosols, in the presence of SO_2 and NO_2, are responsible for acid rain, which erodes soil and degrades water quality.

6.1.3 Types and formation

Atmospheric aerosol particles originating directly from natural and anthropogenic sources are called primary aerosols **(Figure 14)**. Primary aerosols from natural sources contribute most to the global aerosol budget, with wind-blown mineral dust as the largest contributor and sea salt from sea spray as the second largest. In contrast, secondary aerosols are produced by gas to particle conversion through oxidation of the precursor, which could be anthropogenic (NO_x from fossil fuels, sulfates), natural (sulfates, VOC). Note that organic aerosols can be primary or secondary (POA and SOA in **Figure 14**) (Poschl, 2005).

About 10 per cent of total atmospheric aerosols is from anthropogenic sources. **Figure 15** shows the average aerosol composition at two locations over a 10-year period (2001-2010). Mineral dust dominates due to the proximity of the two locations to the Desert.

[18] Also known as particulates, atmospheric aerosol particles, atmospheric particulate matter, or suspended particulate matter (SPM)
[19] Especially those of particles size diameter in the wavelength range of incoming solar radiation (i.e. 400–700 nm).

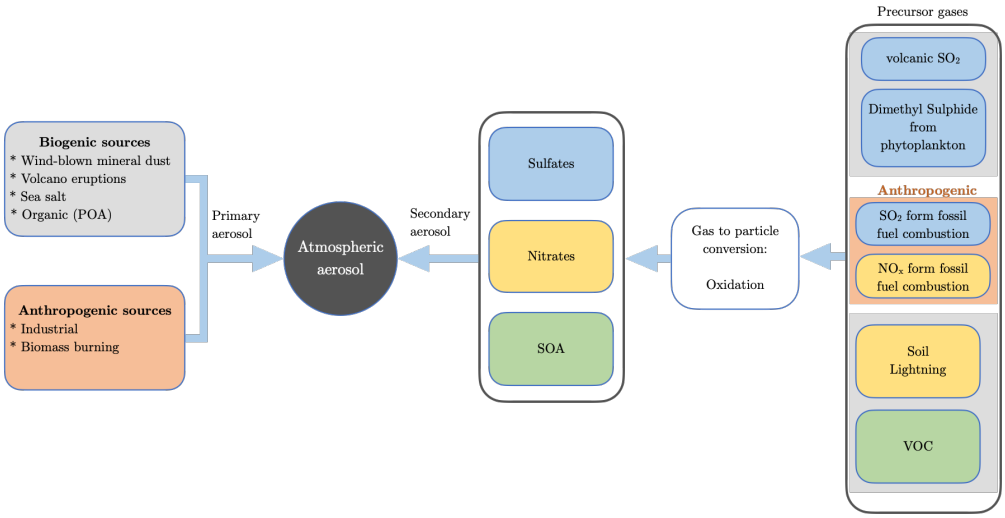

Figure 14. *Primary and secondary atmospheric aerosols.*

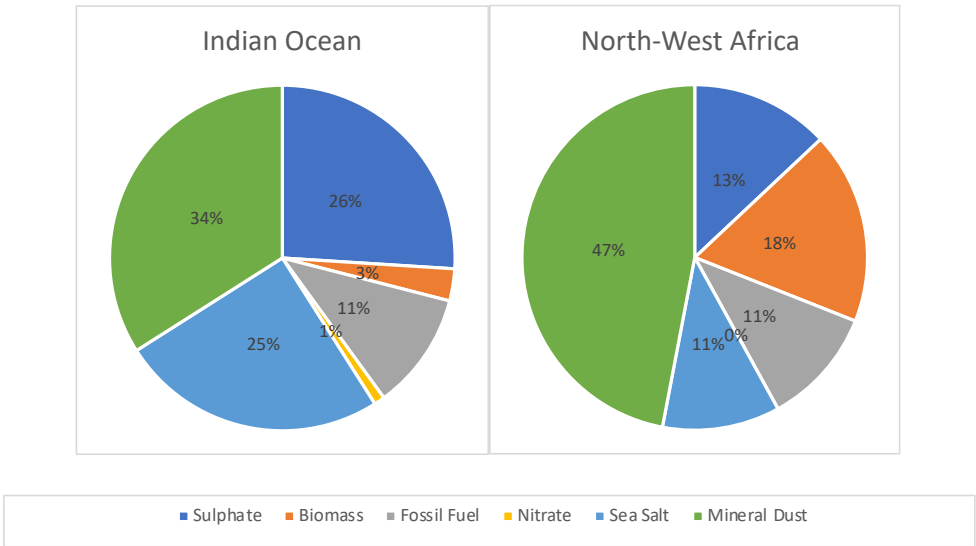

Figure 15. *Pie charts showing the aerosol composition at two locations:* ***Indian Ocean*** *and* ***West Africa*** *(Senegal, Gambia, Guinea-Bissau). Biomass and fossil fuel show contribution of organic carbon and solid black carbon (myhre et al., 2009).*

6.1.4 Particle size distribution

In addition to concentration and composition, particle size is one of the key parameters that defines the role of aerosols in Earth's energy budget, climate, atmospheric processes, and the impact on human health and the environment. Aerosols are typically polydisperse, i.e. the particles do not have the same size. Representing the particle size distribution is commonly done either discretely through binning or using a continuous mathematical function (log-normal distribution) (Mann et al., 2012).

Three different schemes are typically used to represent the aerosol size distribution, namely: bulk schemes, modal schemes and sectional schemes (Kukkonen at al., 2012). In bulk schemes, aerosol size distribution is represented by a small number of non-interacting bins (mainly one or two bins such as TSP, $PM_{2.5}$ and PM_{10}). In contrast, aerosol size distribution in sectional schemes (Jacobson, 2005) is represented by a large number of small interacting bins each having its own physical and chemical properties. Furthermore, the aerosol size distribution in modal schemes (Whitby and McMurry, 1997) is characterized by a small number of modes where each mode is represented by a continuous mathematical function (log-normal distribution). Among these three schemes, the sectional scheme is the most expensive and also the most flexible.

The atmospheric particle size distribution can change as a result of one or more physicochemical process: diffusion, gravitational settling, electrical migration, nucleation, evaporation, chemical reaction, and coagulation. Nucleation can occur by condensation of a gas precursor onto the surface of existing aerosol particles (heterogeneous nucleation) or by condensation under super-saturation conditions (homogeneous nucleation).

Heterogeneous nucleation and coagulation processes cause the size distribution to shift towards larger sizes. In contrast, homogenous nucleation and evaporation processes shift the size distribution towards smaller values. The evolution of the number density of particles in an aerosol due the aforementioned processes is mathematically described by the general dynamic equation for aerosols (Gelbard and Seinfeld, 1979).

6.2 Dust assessment in GCC countries

Noting that mineral dust constitutes approximately 75-95 per cent of total suspended particles (TSP) (Ukhov et al., 2020), the problem of regional and global transport of large quantities of airborne dust originating from deserts is of paramount importance. Half of global dust emissions are from the MENA (Middle East and North Africa) region (Prospero et al., 2002). In terms of dust generation, the Arabian Desert (the east and southern parts of the Arabian Peninsula and Oman desert) ranks third globally after the Sahara and the East Asian deserts (Cahill et al., 2017; Banks et al., 2017; Prakash et al., 2016; Farahat, 2016; Kalenderski and Stenchikov, 2016; Munir et al., 2013; Alghamdi et al., 2015; Lihavainen et al., 2016; Anisimov et al., 2017; Osipov and Stenchikov, 2018). Dust transport from these regions impacts regional climates over scales reaching thousands of kilometers (Fountoukis et al., 2020, Shao et al., 2011).

6.2.1 The impacts of dust on climate, environment and human life

The impacts of dust aerosols on the climate and environment include **(i)** radiative forcing, which affects the global thermal balance and subsequently all dependent physico-chemical and biological processes, **(ii)** altering cloud formation, **(iii)** marine primary productivity through ocean fertilization, **(iv)** changing the PM composition, and **(iv)** biogeochemical and hydrological cycles. Even though natural dust might not have direct negative effect on human health, it can indirectly affect the transport and formation of some pollutants by altering the atmospheric temperature distribution. It can also carry a large number of bacteria and fungi. Moreover, dust severely impacts on human resources including land and air, solar resources for renewable energy, telecommunication and other infrastructures, in addition to damaging crops (Fountoukis et al., 2018b; Ahmadi Dadashi Roudbari, 2017, Li et al., 2017; Almasi et al., 2014; Goudie, 2014; Ginoux et al., 2012; Basart et al., 2012; Goudie, 2009; Goudie and Middleton, 2002).

6.2.2 Aerosol pollution in GCC countries

Local sources of aerosols in GCC countries, in addition to natural dust, include SO_2 from anthropogenic sources (such as power generation, oil processing, and water desalination), which is photochemically converted into sulfate aerosols (Karagulian et al., 2015; Al-Taani et al., 2019; Alharbi et al., 2015; Khodeir et al., 2012; Al-Jahdali and Bisher, 2008). A recent study using the WRF-Chem model showed high SO2 surface concentrations along the east and west coasts of the Arabian Peninsula (Ukhov et al., 2002). The contributions of other aerosols (such as black carbon) to PM in GCC countries were found to be of secondary importance (Randles et al., 2017). Dust events in the Arabian Peninsula are frequent and cause elevated $PM_{2.5}$ and PM_{10} levels that exceed AQ limits in the Kingdom of Saudi Arabia (Ukhov et al., 2020).

Over the past two decades, various studies have investigated dust transport and its impact on AQ. **Table 7** lists studies of dust events in subdomains of the MENA region and GCC countries. The integrated study conducted by Fountoukis et al. (2020) demonstrated that an integrated approach that uses the WRF-Chem model in addition to observations (AERONET, satellite and surface measurements) can capture the spatio-temporal evolution of a dust storm and the corresponding variations in aerosol optical properties.

Study	Period covered	Model	Domain	Comments
Kalenderski et al. (2013)	January 2009	WRF-Chem	Red Sea	Found that dust aerosols significantly changed balance of energy and nutrients
Prakash et al. (2015)	4 days in March 2012	WRF-Chem + AERONET AOD observations	Arabian Peninusla +Red Sea	Impact on terrestrial and ocean environments
Fountoukis et al. (2016)	Summer 2015	WRF-Chem	Middle East including GCC	PM_{10} predictions
Anisimov et al. (2017)	2009-2011	CLM4 (1km res)	Narrow Arabian Red Sea coastal plain	Estimate of fine-scale spatial and temporal distribution of dust emissions
Kontos et al. (2018)	April–June 2015	Natural Emission MOdel (NEMO),driven by the Weather Research and Forecasting (WRF) model, (6 km resolution)	Central Middle East	Assessing the sensitivity of dust modules in various components of the relevant dust parameterization in NEMO
Basart et al., 2012	2004	BSC-DREAM8b	MENA and Mediterranean	Evaluating BSC-DREAM8b model in terms of aerosol optical depth (AOD) using hourly data from AERONET stations and averaged satellite observations
Fountoukis et al., 2020	March-April 2015	WRF-Chem + Satellite data + PM surface measurements + AERONET AOD observations	Arabian Peninsula	Studied impact on optical properties and surface radiation

Table 7. *Studies of dust events in GCC countries.*

6.3 Integrated dust models

Dust transport is a complex process encompassing the lifting mechanism, in addition to the meteorological mechanisms of its transport, over long distances, through the planetary boundary layer- into the troposphere, and its eventual deposition on the land and ocean (Liu et al., 2003). This process necessitated the development of equally complex integrated dust models (Shao and Dong, 2006) in order to be able to:

- understand and quantify dust transport processes on various time and length scales, including global dust cycles and reconstruction of past climates
- predict dust storms and issue early warnings
- carry out assessments

Integrated dust models are based on coupling monitoring form various sources with modelling of atmospheric and dust transport processes, in a data assimilation environment, as depicted in **Figure 16** (Shao and Dong, 2006). The building blocks of the integrated framework are briefly described below.

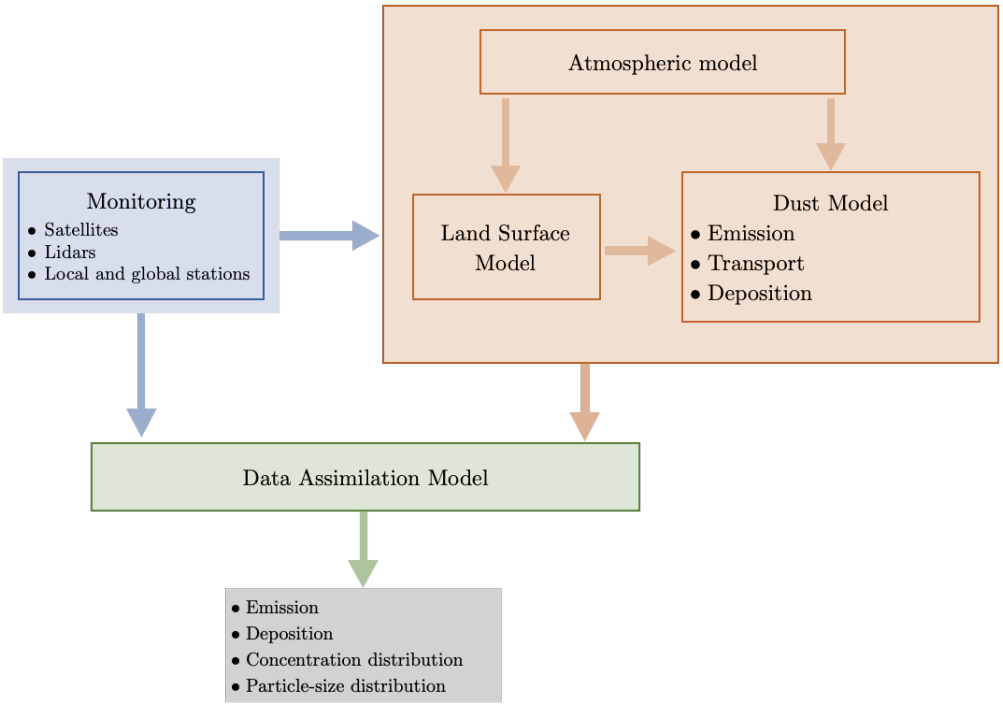

Figure 16. *Framework of an integrated system for dust monitoring, modelling and prediction.*

6.3.1 Dust monitoring

Observations from various dust monitors include **(i)** AOD data from satellites (e.g. Terra and Aqua satellites) equipped with MODIS (Moderate Resolution Imaging Spectrometer) and from ground-based networks (e.g. AERONET), **(ii)** aerosol volume size distribution (AVSD) (from AERONET) and **(iii)** in-situ surface $PM_{2.5}$ and PM_{10} concentration measurements.

The Aerosol Robotic Network (AERONET) is a global network of more than 1,000 ground-based sky radiometers and sun photometers used to provide column integrated aerosol optical properties including AOD and column-integrated AVSD data (Holben et al., 1998; Fountoukis et al., 2020; Dubovik and King, 2000). Currently, there are around 30 AERONET stations in the Arabian Peninsula.

6.3.2 Emission models

Dust emission is the outcome of complex nonlinear interaction between land surfaces and the adjacent meteorology (Darmenova et al., 2009). As such, spatio-temporal characterization of both meteorological and land surface properties is key to a consequential dust emission model. Many of these properties, such as hydrological processes, vegetation dynamics, and energy balance, are readily provided by atmospheric models. What makes dust emission modelling particularly challenging is that it also requires accurate characterization of the properties of the uppermost layer of the soil (top 2 cm), including soil moisture and the "undisturbed" soil particle distribution.

Many dust emission schemes have been proposed. All proposed schemes suffer from the inability to account for spatio-temporal variations of scheme parameters (Shao and Dong, 2006)

In simple emission schemes, the emission rate is a function of surface wind speed, while all other properties are fixed (Darmenova et al., 2009; Darmenova and Sokolik, 2007; Shao and Dong, 2006). Intermediate schemes, used in global dust modelling, incorporate satellite observations to tune the scheme parameters (Shao and Dong, 2006; Ginoux et al., 2001; Woodward, 2001). Complex dust emission schemes are based on spectral modelling of the dust emission mechanisms (aerodynamic entrainment, saltation bombardment and aggregates disintegration) in wind-erosion physics (Shao, 2004; Shao and Dong, 2006). These schemes, however, require soil and land surface data that is often unavailable.

Two widely used emission models, developed by Marticorena and Bergametti (1995) and by Shao et al. (1996), and implemented within the WRF framework, are described in depth in Darmenova et al. (2009).

6.3.3 Data assimilation

Aerosol data assimilation products enables estimation of AOD and near-surface PM concentrations in regions where observations are not available. They do so by assimilating available AOD and in-situ PM measurements (Ukhov et al., 2020).

The most widely used integrated models that assimilate atmospheric PM are MERRA-2[20] (Randles et al., 2017; Buchard et al., 2017) and CAMS-OA[21] (Inness et al., 2019; Flemming et al., 2015; Inness et al., 2015). These two global-scale models use emission inventories of anthropogenic pollutants, and as such, their accuracy deteriorates when these inventories are outdated and/or incomplete, as is the case in the Middle East region (Ukhov et al., 2020; McLinden et al., 2016).

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[20] Modern-Era Retrospective analysis for Research and Applications, Version 2, implemented by the National Aeronautics and Space Administration, Goddard Space Flight Center (NASA-GSFC).
[21] Copernicus Atmosphere Monitoring Service Operational Analysis, implemented by the European Centre for Medium-Range Weather Forecasts (ECMWF).

6.3.4 Integrated operational models

All integrated operational dust models have similar structure to the one presented in **Figure 16**. The most widely used integrated operational models are **(1) COAMPS** (Coupled Ocean/Atmosphere Mesoscale Prediction System), **(2) NAAPS** (Navy Aerosol Analysis and Prediction System), **(3) NMMB/MONARCH** (Non-hydrostatic Multiscale Model/Multiscale Online Non-hydrostatic Atmosphere Chemistry Model), **(4) WRF-Chem**, **(5)** MOCAGE (Modele de Chimie Atmospherique a Grande Echelle), and **(6) ECMWF-IFS** (European Centre for Medium-Range Weather Forecasts Integrated Forecasting System).

A description of these models and their characteristics is presented in **Table 8**

Name	Description	Scale	Observation	Operational	Developer
COAMPS	Non-hydrostatic compressible mesoscale weather prediction system with nesting capabilities	Mesoscale limited area model; typically grid point mesh with about 30 km grid spacing	NAVDAS: 3D variational data assimilation that assimilates a variety of observations including radiosonde data, surface observations from land and sea, radiances or temperature profiles, surface wind speed and satellite-derived quantities (AOD)	Operational by the U.S. Navy for short-term numerical weather prediction	Marine Meteorology Division (MMD) of the U.S. Naval Research Laboratory (NRL)
NAAPS	Global three-dimensional aerosol model producing 144-hour forecasts of dust, smoke, sea salt,and anthropogenic/ biogenic fine mode particles	Global scale; 1080 × 540 grid with 1/3 degree spatial resolution and 42 vertical levels	Two-dimensional variational (2D-Var) data assimilation system (NAVDAS-AOD) which incorporates AOT retrievals from MODIS to forecast initial conditions every 6 h	Operational at the U.S. Naval Research Laboratory (NRL) since 1998	Marine Meteorology Division (MMD) of the U.S. Naval Research Laboratory (NRL)
NMMB/ MONARCH	Fully online multiscale chemical weather prediction system for regional and global-scale applications	Multiscale: global to regional (up to 1 km) scales allowed	Assimilation of MODIS Dark Target and Deep Blue observations in the dust aerosol component of NMMB-MONARCH using an ensemble-based Kalman filter technique	Provides operational regional mineral dust forecasts for the World Meteorological Organization (WHO), and participates in the WMO Sand and Dust Storm Warning Advisory and Assessment System for Northern Africa-Middle East-Europe	Barcelona Supercoputing Center (BSC-CNS) in collaboration with the NOAA's National Centers for Environmental Prediction (NCEP)

Table 8. *Integrated operational AQ frameworks that include dust models.*

WRF-Chem	3D online integrated Eulerian model with nesting capabilities typically used to model emission, transport, mixing, and chemical transformation of trace gases and aerosols simultaneously with the meteorology	Mesoscale model; routinely run at high resolution 1-4 km grid spacing	The three-dimensional variational method (3D-Var) and the Hybrid RTFDDA-3DVAR assimilate surface observations and satellite data (AOD from MODIS) to the WRF-Chem model and provide improved initial conditions for the forecasting system	Fully operational in many countries around the word to produce daily (72 hours) online AQ forecasts with a horizontal resolution of 4 km (e.g. in USA, Austria, Germany, UK, Spain, Slovenia, Italy)	NOAA/ESRL
MOCAGE	3D multiscale semi-Lagrangian model used in chemical weather forecasting, tracking and back-tracking of accidental point-source releases and trans-boundary pollution assessment	Regional to global scales; typical global grid with horizontal resolution of 2 × 2 degrees and a regional grid resolution of 0.5 × 0.5 degrees	A variety of variational methods (3DVAR, 3DFGAT or 4DVAR) can be used to assimilate profiles, columns or surface measurements of key atmospheric pollutants	Operational since 2001; provides 72-hour forecasts including ozone, precursors and aerosols over the globe, Europe and France	Meteo-France
ECM-WF-IFS (C-IFS)	Global numerical weather prediction system including modules for atmospheric composition (aerosol and gas phase)	Can be run at varying vertical and horizontal resolutions; highest horizontal resolution is 9 km	3D-Var and 4D-Var was implemented in ECMWF operations to assimilate a wide variety of observation including surface measurement of wind speed, temperature, species concentration, and satellite derived AOD	ECMWF and Météo-France both use IFS to make operational weather forecasts but using different configurations and resolutions	European Centre for Medium-Range Weather Forecasts (ECMWF)

Table 8. *Integrated operational AQ frameworks that include dust models.*

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7. AQ models for GCC countries

The climate in the GCC region is characterized by significant spatial and temporal variations, due to its large-scale atmospheric circulation, diverse topography, and chemical and radiative processes taking place in the atmosphere (Patlakas et al., 2019). Overall, the region is mainly characterized by a desert-type climate with extreme heat, particularly during daytime, and low and infrequent rainfall, and therefore experiences some of the harshest climatological conditions on Earth (Farahat, 2016). In addition, the region is considered among the most important centres of production and emission of dust in the world (Prijith et al., 2013). In particular, the Arabian Desert is the third-largest source of global dust emissions after the Sahara and the East Asian deserts (Ukhov et al, 2020). Hence, desert dust is found in high concentrations in the atmosphere throughout the year, leading to diverse impacts on Earth's energy balance. Furthermore, dust from the Sahara, the world's largest source, can be transported over thousands of kilometers, affecting AQ in GCC countries (Fountoukis et al, 2020). Moreover, most of the region is surrounded by ocean, which is a source of sea salt aerosols. All these features have an important role in the formation of the regional climate.

GCC countries are experiencing some of the fastest growth rates in economic activity and energy consumption in the world due to rapidly increasing population, industrial development and motorization. This rapid growth is accompanied by the emission of huge quantities of air pollutants of different types into the atmosphere, with damaging effects on ambient AQ. Each pollutant type has different characteristics and physical properties. This highlights the necessity of modelling the transport of these air pollutants to provide governments with information that enables them to take preventive measures, draft policies and plan for the future. This is particularly important in the presence of desert dust, whose which can trap and transport particulate matter from anthropogenic sources in the downstream wind direction, resulting in pollutant concentrations that are potentially harmful to humans and the environment (EEA, 1998).

Due to the diversity of the climate, topography and pollutant characteristics in the GCC region, there is no single model that can answer all relevant questions. A considerable number of studies have been conducted to explore various aspects of pollution in the GCC countries. These aspects include different types of pollutants, applications and special scales.

It should be noted that there is some evidence that combustion-related $PM_{2.5}$ may be more harmful to human health than $PM_{2.5}$ from natural sources, such as dust storms (Cooke et al., 2007; Laden et al., 2000). Thus, the impacts of emissions from anthropogenic sources on public health could be greater than their contributions to total $PM_{2.5}$ mass (Farahat, 2016). Since over half of the measured $PM_{2.5}$ levels appears to be due to crustal material from natural sources (Alolayan et al., 2013), there is growing interest in GCC countries in using AQ models that can assess the contributions of individual sources to overall chemical concentrations. As such, **Table 9** highlights some AQ models that possess such a capability.

Table 9 presents AQ models that have been used to answer a multitude of research questions on pollution transport in GCC countries. The Table also lists descriptions of the different applications of each model in the GCC countries as reported in previous studies in the literature.

Model Name	Typical Application in GCC	Advantages/previous related studies in GCC
AERMOD	Studying the impact of non-reactive pollutants (SO_2) and the locations of maximum concentration around the vicinity of a source (power plant, refinery); evaluation of vehicular pollution levels; assessment of hydrogen sulfide emissions; dispersion and deposition estimation of fugitive iron particles	Require reasonable input data and computer resources; results can be exported to Google Earth **Previous studies:** Al-Baroud et al., 2012; Amoatey et al., 2020; Baawain et al., 2017; Omidvarborna et al., 2018b; Al-Jeelani, 2013; Abu-Eishah et al., 2014; AL-Haddad et al., 2012; Yassin et al., 2010; Deb et al., 2014
ISCST3	Calculating maximum non-reactive pollutant (SO_2) values and their locations around the vicinity of a source (power plant, refinery); assessing the impacts of methane and non-methane hydrocarbon emissions from flaring activities; quantifying the impact on SO_2 release when changing fuel sulphur content; investigating the efficiency of existing monitoring sites	Account for complex and simple terrain, buoyancy-induced dispersion, plume rise and building downwash **Previous studies:** Al-Rashidi et al, 2005; Abdul-Wahab et al, 2002, 2003, 2004, 2006, 2011a, 2009; Al-Rashidi et al, 2005; AL-Azmi et al, 2009; Ramadan et al, 2008; Deb et al, 2014
ADMS-Urban	Study Vehicular emissions dispersion	Able to assess the contributions of individual sources to overall chemical concentrations; can be coupled to the regional mesoscale model WRF **Previous studies:** Munir et al., 2018
ENVIMAN: (combination of AERMOD and OSPM)	Assessment of air pollutant emissions from distillation plants	**Previous studies:** Alkatheeri et al., 2012
CALPUFF	Predicting concentrations of CO, NO_x, and CO_2 released from line source traffic; assessing the impact of some pollutants emitted from industrial plants; assessing the impact of the monsoon season on the dispersion of some pollutants; modelling and analysis of hydrogen fluoride and non-methane organic compound (NMOC) dispersion	Contains modules for near-source effects, building downwash, transitional plume rise, complex terrain effects, over-water transport, coastal interaction effects; can be coupled with WRF **Previous studies:** Abdul-Wahab et al., 2011a, 2011b, 2012, 2016, 2017, 2018, 2019, 2020; Abdul-Wahab and Fadlallah, 2014; Al-Naimi et al., 2015; Charabi et al., 2018; Al-Rawas et al., 2018; Deb et al., 2014

Table 9. *AQ models used to study pollution in GCC countries.*[22]

[22] For further information on these models, please refer to **Table 3** and **Table 5**.

CAL3QHC	Predicting CO concentrations from motor vehicles near a roadway intersection; modelling the effect of fuel change on air quality	Recommended by US EPA; includes a traffic algorithm for estimating the number of vehicles queued at an intersection **Previous studies:** Abdul-Wahab, 2004a; Al Adwani et al., 2004
CALINE4	Assess the CO pollution level form a line source emission	US EPA alternative model; requires relatively few inputs **Previous studies:** Albassam et al., 2009
OpenAir	Assessment of air pollutant emissions from traffic	**Previous studies:** Hamoda et al, 2020
WRF-Chem	Assessing the impact of African dust; modelling typical dust events; modelling haboob dust storms; modelling dust emission; modelling seasonal variations and distributions of aerosol pollutants; assessing the sensitivity of dust schemes; modelling of surface ozone at regional scale	Perfectly suited for examining meteorology-chemistry feedbacks on local to global scales; five choices for aerosol models; several choices for gas-phase chemical mechanisms including RADM2, RACM, CB-05 and CBM-Z chemical mechanisms; three choices for dust emissions (generated during the actual run, no need for an emission inventory) **Previous studies:** Kalenderskti and Stenchikov, 2016; Anisimov et al., 2018; Parajuli et al., 2019; Fountoukis et al., 2018; Prakash et al., 2015; Shahid et al., 2021; Fountoukis et al., 2016; Karagulian et al., 2019; Kontos et al., 2018; Kalenderski et al., 2013;
HYSPLIT	Back-trajectory analysis to determine the origin of air masses (dust storms); estimating PM_{10} air concentrations from dust storms; clarifying the seasonal distributions of atmospheric pollutant concentrations	One of the most extensively used atmospheric transport and dispersion models in the atmospheric sciences community; surface roughness in the emission model has been correlated with the soil properties of Kuwait, Iraq, Syria, Saudi Arabia, Oman and UAE **Previous studies:** Yassin et al., 2018; Dasari et al., 2020; Ozdemir et al., 2018; Othman et al., 2021; Draxler et al., 2001

Table 9. *AQ models used to study pollution in GCC countries.*

CHIMERE	Investigating the predictability of dust events; modelling of surface ozone at regional scale	Outputs from the model simulations have been validated against meteorological and AQ data collected from monitoring stations in Qatar and showed globally acceptable agreement **Previous studies:** Beegum et al., 2018; Mulla et al., 2009
NMMB/ BSC-Dust	Assessing the impact of model resolution in dust propagation in a region with complex terrain	Fully online multiscale chemical weather prediction system for regional and global-scale applications; dust model is fully embedded; accounts for feedbacks among gases, aerosol particles and meteorology **Previous studies:** Basart et al., 2016
Bsc–Dream8b	Examining the meteorological conditions causing a dust storm	**Previous studies:** Ozdemir et al., 2018
MERRA-2	Assimilation of AOD	**Previous studies:** Parajuli et al., 2019; Roshan et al., 2019; Shahid et al., 2021
Chemical Mass Balance (CMB)	Determine main contributor of PM_{10} and gaseous pollutants	**Previous studies:** Al-Salem, 2008
Positive matrix factorization (PMF)	Identify $PM_{2.5}$ sources and apportion their contributions;	**Previous studies:** Alolayan et al., 2013; Alahmad et al., 2021; Alghamdi et al., 2015
Comprehensive Air quality Model with extensions (CAMx);	Simulate AQ over many geographic scales; conduct source attribution, sensitivity, and process analyses	Includes several "probing tools" for diagnostic and sensitivity studies in a single model: 1. Source Apportionment Tool (SAT) to track attribution of ozone and PM to emissions by category and region 2. Decoupled Direct Method tools (DDM, HDDM) to track chemical sensitivity to emissions and other parameters by category and region

Table 9. *AQ models used to study pollution in GCC countries.*

Community Multiscale Air Quality (CMAQ)	Simulating ozone, PM, toxic airborne pollutants, visibility, and acidic and nutrient pollutant species throughout the troposphere; addressing the complex couplings among several AQ issues simultaneously across spatial scales ranging from urban to hemispheric (multiscale)	Includes a process analysis (PA) module that tracks mass throughout all individual processes (chemistry, advection, diffusion, etc.) and provides quantitative information about how each process affected the predicted hourly species concentrations
Urban Airshed Model Variable Grid (UAM-V)	AQ studies focusing on ozone; evaluating air quality changes from emission control scenarios	Includes PA extensions and integrated reaction rates; information can be saved on pollutant concentrations from each mechanism (advection, diffusion, deposition, emissions, and chemistry, on chosen grid areas) for each time step, allowing for an unprecedented level of detail in understanding simulated episodes
Regional Modeling System for Aerosols and Deposition (REMSAD)	Simulates the chemistry, transport (over regional scales), and deposition of airborne pollutants (both inert and chemically reactive) with emphasis on PM	The Particle and Precursor Tagging Methodology (PPTM) allows users to tag and track the release, transport, chemical transformation, and deposition of precursor species and toxics (sulfur, nitrogen, mercury, cadmium, dioxin, and lead) from emissions sources, source categories, or source regions throughout the REMSAD modelling domain

Table 9. *AQ models used to study pollution in GCC countries.*

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