



3D Photochemical Dispersion Models for Secondary Air Pollutant Study: from Input Data Preparation to Model Performance Evaluation

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Abstract

Secondary air pollutants are formed through series of complex reactions occurred in the atmosphere under favorable meteorological conditions. Commonly known species are ozone and secondary aerosols, secondary inorganic and organic aerosols. Through its complexity, varieties of three dimensional (3D) photochemical dispersion models have been developed globally to simulate formations and dispersions of the secondary as well as the primary pollutants in the atmosphere. CMAQ and CAMx are the state of the science models under “one atmospheric approach”, noncommercial and open-source software. These characteristics are attracted and challenged for future air quality management via model simulations. Applications of CMAQ and CAMx are normally based on several steps: preparation of emission input, modeling set-up and model performance evaluation. This article presents the systematic procedures involved with the use of 3D photochemical models starting from theoretical principles for formation of secondary air pollutants, types of photochemical models and its associated physical and chemical modules, input data preparation including reviews on available emission inventories and lastly statistical methods for model performance evaluation.

Keywords: *3D photochemical model, secondary air pollutants, emission input, model performance evaluation*

1. Introduction

Study on the formation and distribution of secondary air pollutants (SAP), e.g. ozone and secondary aerosols, using modeling tools is intensively interesting at present and future perspectives towards better air quality management [1,2]. Among the available numbers of chemical/transport

models for air quality assessment, a 3D-Eulerian photochemical dispersion model is one of the frequently applied models for regional as well as urban scales for SAP formation and distribution [3-5].

Simulation of SAP includes the emission input, dispersion behavior, chemical reaction and pollutant wet and dry removals by using the set of mathematical

equations developed based on continuity principle on a 3D grid network [4]. Hence, simulation of ozone and secondary aerosol using photochemical dispersion model requires extensive input data to address photochemical reactions, emission rates,

initial and boundary conditions, surface characteristics and a large range of meteorological data over the setting-up modeling domain. Simplified framework describing the model simulation is indicated in Figure 1.

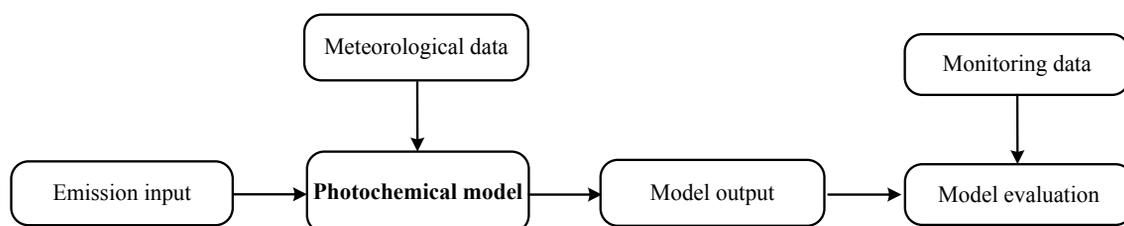


Figure 1. Simplified schematic diagram of a 3D photochemical model application

The reliability of the model output largely depends on the evaluation methods. The traditional method is to compare the model output such as ozone (O_3), particulate matter (PM) with the aerodynamic diameter less than or equal to 2.5 and 10 micrometers ($PM_{2.5}$, PM_{10}), and secondary aerosols with the available observations. Note that in most of Asian developing cities, monitoring networks provided only ozone and PM_{10} , while other mentioned above were fragmented available through some international research projects (i.e. AIRPET, APN and ABC-UNEP/AIT) [6].

In this review article, the stepwise discussion on the procedures of 3D photochemical dispersion model application was addressed. Review of SAP formations was the foremost step, followed by emission inventory (EI) and input data preparation, and model performance evaluation.

2. Formations of secondary air pollutants

SAP are those pollutants that are not directly emitted from the emission sources, but in fact they are formed through complex and nonlinear chemical reactions under the favorable meteorological conditions, i.e. intensity of solar radiation, temperature, relative humidity and atmospheric mixing condition, and importantly sufficient amount of precursors [3,7]. Types of commonly known SAP are ozone and secondary aerosols.

2.1. Ozone

Ozone is produced through series of complex chemical reactions depending on meteorological conditions and concentrations of precursors, mainly nitrogen oxides (NO_x) and volatile organic compounds (VOCs). The chemical formation processes of ozone have been well documented available with sufficient scientific evidences. Simplified schematic diagram for ozone formation is shown in Figure 2.

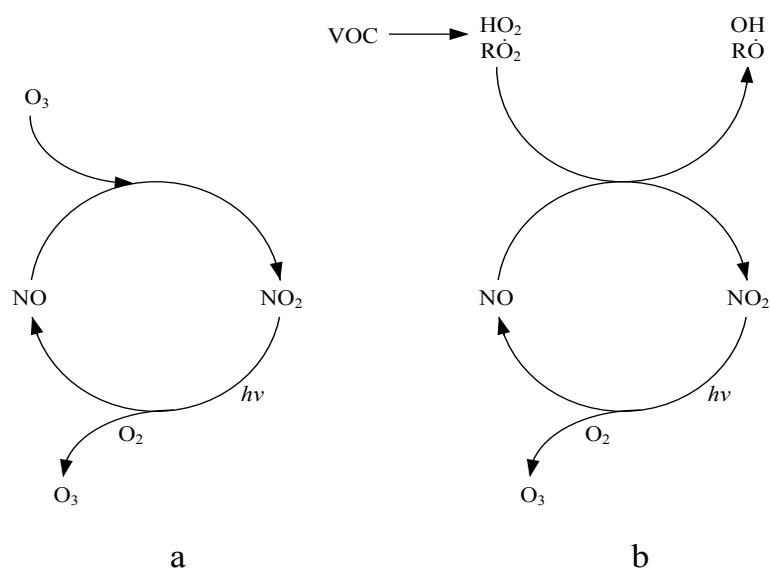
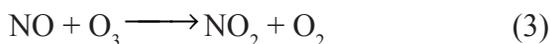
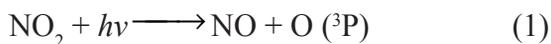


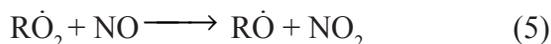
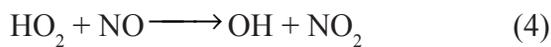
Figure 2. Formations of ozone through NO-NO₂-O₃ the absence (a) and presence (b) of VOC [8]

Tropospheric O₃ is generated via the photochemical reaction initiated by the photolysis of NO₂ which further creates the ground-state oxygen atoms, O (³P). It reacts with O₂ to form O₃ as indicated in reaction (1) and reaction (2), respectively. However, the reaction between NO and O₃ indicated in reaction (3) is the photochemical equilibrium of NO, NO₂ and O₃ [8]. The latter reaction (3) is generally known as titration process or O₃ sink process in the troposphere.



The presence of VOCs with high reactivity leads to the formation of intermediate radicals, such as RO₂ and HO₂. The radicals react with NO enhancing the conversion of NO to NO₂ that further stimulates O₃ formation as indicated in

reaction (4) and reaction (5).



2.2. Secondary aerosols

Secondary aerosols are product of gas-to-particle conversion, the formation of products of low volatility or high solubility, from the oxidation processes. Since these processes are driven by photochemical reaction, the resulting aerosols generally classify as the SAP category which is mainly secondary inorganic aerosol (SIA) and secondary organic aerosol (SOA). The chemistry for SIA is relatively well quantified [9]. However, the chemical formation processes of the organic portion are not well identified [10] and, hence, a number of researches mainly focused on the science of SOA formations [10,11].

The complex physical/chemical reactions of the atmospheric gas, particle and droplet phases are presented in Figure 3. OH-HO₂ cycling system drives

tropospheric O_3 and hydrogen peroxide (H_2O_2), which are major oxidants of soluble SO_2 . Hydroxyl (OH) levels define the oxidation rates of SO_2 and NO_2 to H_2SO_4 and HNO_3 , respectively that in turn are precursors of SIA formation, particulate sulfate (PSO_4) and particulate nitrate (PNO_3). OH and O_3 hit on the reactive

organic gases (ROGs) or VOC to generate semi-volatile SOA.

Discussion of the photochemical reactions involving in the formation of the secondary products is presented in the following subsection.

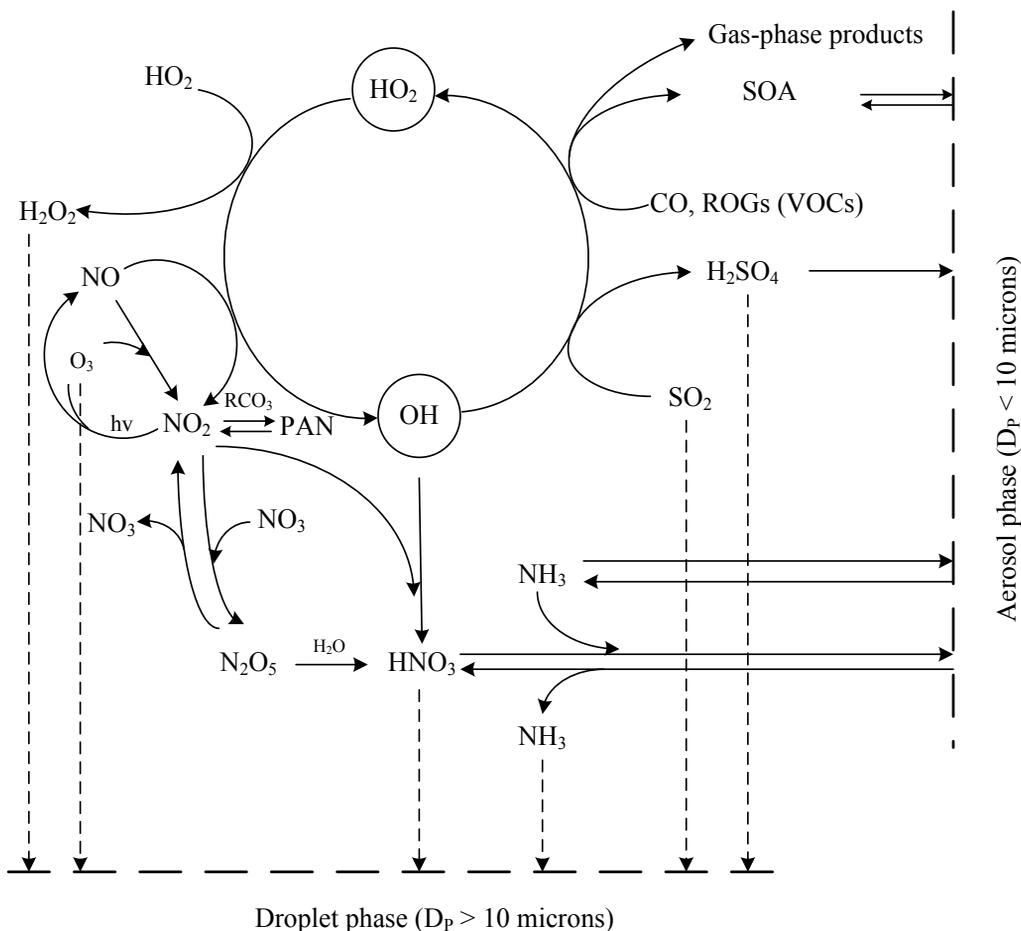


Figure 3. Chemical coupling in the atmospheric gas, particle and droplet phases [14]

2.2.1. Secondary inorganic aerosol

The inorganic components of atmospheric aerosols particularly compose of various ionic species, i.e. ammonium (NH_4^+), sodium (Na^+), calcium (Ca^{2+}), sulfate (SO_4^{2-}), nitrate (NO_3^-),

chloride (Cl^-) and carbonate (CO_3^{2-}). At a certain temperature (T) and relative humidity (RH), the phase of such mixed compounds tends to be thermodynamically stable with the gas phase. Hygroscopic growth during low T and high RH plays the

important role in the SIA formation [12]. SIA generally consists of about 25-50% of the fine PM fraction [13]. The major components of SIA in the atmosphere are NO_3^- and SO_4^{2-} particles [12].

(a) Formation of particulate nitrate

NO_x , the term defined as the combination of NO and NO_2 , plays the substantial role in the tropospheric O_3 formation through the complex varieties of photochemical reactions with the reactive VOCs (see also Figure 2). NO_x is mainly emitted from the anthropogenic sources. Important sources of anthropogenic NO_x emissions are fossil fuel combustion processes in transport and industrial sectors. NH_3 and other nitrogen substances emitted also play the role in formation of particulate nitrate (PNO_3). As indicated in reaction (6), NO_2 reacts with the hydroxyl radical ($\dot{\text{O}}\text{H}$) to create HNO_3 . NH_3 , a basic gas in the atmosphere, reacts further with HNO_3 to form the PNO_3 , i.e. ammonium nitrate (NH_4NO_3) as indicated in reaction (7).



(b) Formation of particulate sulfate

Particulate sulfate (PSO_4) is commonly generated within the atmosphere by oxidation reaction of SO_2 which is directly released from combustion processes of sulfur content in fossil fuel and volcanoes, or produced within the atmosphere by oxidation reaction of reduced oceanic dimethyl sulfide (DMS). Gas-phase conversion of SO_2 to aerosol PSO_4 indicated in reaction (8) to reaction (10) determines by the reaction between SO_2 and $\dot{\text{O}}\text{H}$. It is noted that H_2SO_4 can be immediately converted to particulate phase by coating on other aerosol surfaces [7].



2.2.2. Secondary organic aerosol

Formation processes of SOA are still unclear and not well quantified [10]. SOA formation can be simplified as shown in Figure 3. VOCs precursors in the atmosphere are oxidized primarily by O_3 , NO_3 and $\dot{\text{O}}\text{H}$. The oxidation reaction process introduces functional groups to VOCs molecules to produce semi-volatile organic compounds (SVOCs) and therefore reduces their volatility. However, some part of SVOCs can remain volatilization and does not form the aerosols in the atmosphere. Another part of SVOCs can be condensed to contribute in aerosol formation which depends on the favorable meteorological conditions [14].

3. 3D photochemical dispersion model

Three dimension (3D) photochemical dispersion models based on Eulerian continuity equation have been widely used for assessing the effectiveness of air quality control strategies, development of air pollution regulations and investigation of physical/chemical processes for SAP formation [3,5]. Photochemical smog models simulate the changes and formations of pollutant concentrations in the atmosphere determining by the chemical and physical processes, emission input and wet and dry removals. These models can be applied at wide ranges of geographical scales from local to continental levels [3]. There are a number of photochemical dispersion models that have been developed, i.e. the Urban Airshed Model (UAM-V),

Community Multi-scale Air Quality (CMAQ), the Comprehensive Air Quality Model with extension (CAMx), A Unified Regional Air-quality Modeling System (AURAMS), the Regional Modeling System for Aerosols and Deposition and Weather Research and Forecasting model coupling with Chemistry (WRF-Chem). Details of available photochemical models used and its development can be found in Kim Oanh and Permadi [3] and Kukkonen *et al.* [4]. In this article, only the 3D photochemical models developed under the approach of “one atmosphere”, noncommercial and active open-source models are considered. Models such as CMAQ and CAMx are among of the most widely use for local and regional air quality studies [4,5,15,16].

CMAQ or Models-3/CMAQ is the third-generation of air quality modeling and

assessment tools developed by the United State Environmental Protection Agency (USEPA) with the cooperation with UNC-Chapel Hill to address tropospheric ozone, acid deposition, particulate matter and toxics [17]. CMAQ source code is freely available for download from the website <http://www.cmascenter.org>. CAMx simulates air quality over many geographic scales. It handles variety of inert and chemically active pollutants, including ozone, particulate matter, inorganic and organic PM_{2.5}/PM₁₀ and mercury, and other toxics [18]. CAMx modules and its user’s manual can be obtained from <http://www.camx.com/>. CMAQ and CAMX modeling systems utilize the similar physical and chemical modules to describe diffusion, deposition and chemistry of SAP formations (see Table 1).

Table 1. Characterizations of the physical and chemical components of CMAQ [17] and CAMx [18]

Model	Mechanism	Description
CMAQ	Advection and convection	Eulerian continuity equation
	Diffusion	Horizontal diffusion: single eddy diffusion algorithm based on local wind deformation; Vertical diffusion: Asymmetric Convective Method (ACM).
	Dry deposition	Separate resistance models for gases and aerosols; Bidirectional modules for ammonia and mercury simulate two-way exchange between the atmosphere and the surface for these species; MOSAIC is a configuration that outputs land use specific deposition velocities and fluxes.
	Wet deposition	Separate scavenging models for gases and aerosols; Uptake as a function of rainfall rate, cloud water content, gas solubility and diffusivity, PM size.
	Gas-phase chemistry	CB05: Replaced existing toluene chemistry in CB05 with updated toluene chemistry; SAPRC07: Fully updated organic and inorganic reactions.

Table 1. Characterizations of the physical and chemical components of CMAQ [17] and CAMx [18] (continued)

Model	Mechanism	Description
	Aerosol-phase chemistry	AERO6: Updated secondary organic aerosol yield parameterization; ISORROPIAv2.1: instantaneous thermodynamic equilibrium between the gas and fine-particle modes.
CAMx	Advection and convection	Eulerian continuity equation.
	Diffusion	Horizontal diffusion: K-theory 1st order closure; Vertical diffusion: K-theory 1st order closure and Non-local mixing.
	Dry deposition	Separate resistance models for gases and aerosols; Gases: (1) deposition of gases as surface boundary condition; and (2) additional newer dry deposition scheme by using “leaf area index” to scale pollutant uptake into biota; Aerosols: (1) deposition of particles via diffusion, impaction, and/or gravitational settling; and (2) updating a simple parameterization of particle dry deposition as a function of aerosol size and land use.
	Wet deposition	Separate scavenging models for gases and aerosols; Gases: (1) direct diffusive uptake of ambient gases into falling precipitation; and (2) accretion of cloud droplets that contain dissolved gases; Aerosols: (1) impaction of ambient particles into falling precipitation with an efficiency that is dependent upon particle size; and (2) accretion of cloud droplets that contain particle mass.
	Gas-phase chemistry	CB05: 156 reactions and up to 89 species; CB06: 218 reactions and up to 114 species; SAPRC99: 217 reactions and up to 114 species; Inorganic/organic aerosol precursors.
	Aerosol-phase chemistry	RADM: Aqueous sulfate and nitrate formation; SOAP: Partitioning of condensable organic gases to secondary organic aerosols; ISORROPIA: Partitioning of inorganic aerosol constituents between the gas and aerosol phases.

Remarks: CB is Chemical Bond Mechanisms; SAPRC is the chemical mechanism developed at the Statewide Air Pollution Research Center in Riverside, California; RADM is Regional Acid Deposition Model; SOAP is a semi-volatile equilibrium scheme for partitioning of condensable organic gases to secondary organic aerosols; ISORROPIA is a thermodynamic equilibrium aerosol module designed for the calculation of equilibrium concentrations of semi-volatile inorganic species.

4. Emission input preparation

Emission input data are substantially required for the 3D photochemical modeling study. A number of emission species required can vary depending on the output of SAP, i.e. studying of ozone formation involves at least NO_x and VOCs species while that for secondary aerosols involves additional species, i.e. NO_x , SO_x , NH_3 and VOCs. In some cases of total PM study, additional speciation of PM such as elemental carbon (EC), organic carbon (OC), $\text{PM}_{2.5}$ and $\text{PM}_{10-2.5}$ would be required. However, modeling of the atmospheric reactions involved complex chemical reactions. Acquiring as much as possible emission species could be more appropriate for the study of SAP formations. This section describes the procedures to obtain the emission input data by mean of individual preparation of EI and secondary data assimilation as well as the way forward to map emission species into the study domain.

4.1. Emission inventory (EI)

EI for different sources of air pollutants is basically calculated using equation (11) where i is type of pollutant; Em_i is emission of pollutant i (mass per time); AR_i is activity rate of data related emission of pollutant i (activity unit per time); EF_i is emission factor for pollutant i (mass per activity unit) [19]. Types of pollutants covered by the emission estimation are commonly PM and its speciation (EC, OC, $\text{PM}_{2.5}$ and PM_{10}), SO_2 , CO , CO_2 , NO_x , NH_3 , CH_4 and VOCs.

$$\text{Em}_i = \Sigma (\text{AR}_i \times \text{EF}_i) \quad (11)$$

Generally, emission estimation for different types of pollutants is classified based emission sources: point sources, mobile sources, area sources and biogenic sources [19,20]. The first three sources are collectively known as anthropogenic sources. Point sources refer to the stationary large point sources, i.e. power plants, waste incinerators and major industrial sources. Area sources are for the emissions produced by residential, gas stations, biomass open burning, livestock and fertilizer in agricultural area. Please note that small industries can be simply included in the area sources. Mobile sources can be classified into on-road vehicles and non-road machines. For biogenic sources, they are known as the emissions from natural sources, i.e. vegetation emission of biogenic VOCs (BVOCs) and soil NH_3 and CH_4 emissions due to microorganism activities.

Individual preparation of EI may pose the challenges in information attainment for both emission factors and activity rate of data for a number of emission sources. Local or national data are encouraged to obtain the more accurate emission estimate values and to reduce the associated uncertainties. At the presence, there are a number of EI guidebooks or manuals, i.e. AP-42 (USEPA), EMEP/EEA, GAPF (SEI), IPCC, ABC EIM (UNEP) which are designed for specific purposes (Table 2).

Table 2. Summary of available EI manuals

EI manuals	Specific purposes	Pollutant coverage
AP-42 (USEPA) ^a	Multipurpose including ambient dispersion modeling and analysis, control strategy development, and in screening sources for compliance investigations.	PM ₁₀ , PM _{2.5} , BC, OC, SO ₂ , NO _x , NH ₃ , CO and VOC
EMEP/EEA ^b	Making quantitative assessments of the source contributions to air quality in Europe and the wider UNECE, and developing and implementing associated effective policies.	SO ₂ , NO _x , NMVOC, NH ₃ , CO, CH ₄ , N ₂ O and CO ₂
GAPF ^c	Providing a simplified and user-friendly framework with a training tool for emission inventory preparation that is suitable for use in developing and industrializing countries.	SO ₂ , NO _x , NH ₃ , NMVOC, CO, TSP, PM ₁₀ , PM _{2.5}
IPCC ^d	Producing high quality national estimates of emissions and removals of greenhouse gases for developing and developed countries.	GHGs species (CO ₂ , CH ₄ , N ₂ O, HFCs, PFCs, SF ₆ , NF ₃ , SF ₅ CF ₃ , halogenated ethers and other halocarbons)
ABC EIM ^e	Providing a framework for atmospheric brown cloud (ABCs) emissions inventory that is suitable for use in different countries especially in Asia and presenting methods for temporal and spatial distribution of emissions.	PM ₁₀ , PM _{2.5} , BC, OC, SO ₂ , CO ₂ , NO _x , NH ₃ , CO, NMVOC and CH ₄ and N ₂ O

Remark:

^a <http://www.epa.gov/ttn/chief/ap42/>

^b <http://www.eea.europa.eu/publications/emep-eea-emission-inventory-guidebook-2009>

^c <http://www.sei-international.org/gapforum/tools.php>

^d <http://www.ipcc-nggip.iges.or.jp/public/2006gl/index>.

^e http://www.unep.org/delc/Portals/119/atmospheric/ABC_EIM.pdf

There are several data sources available for EI which are published widely in the internet (see Table 3), i.e. the Center for Global and Regional Environmental Research (CGRER), Emission Database for Global Atmospheric Research (EDGAR), Model of Emissions of Gases and Aerosols from Nature (MEGAN), Regional Emission inventory in

ASia (REAS) and Vongmahadlek *et al.* [20]. The grid resolution of the EI data ranged from coarse (0.5° x 0.5°) to fine (1 km x 1 km). These data are mostly accessible online through their particular website, except for the country specific EI data, i.e. Vongmahadlek *et al.* [20]; users may be requested to contact directly the authors.

Table 3. Sources of EI data and examples of its coverage

Emission source coverage	Global		Asia	Thailand	
	EDGAR ^a	CGRER ^b	MEGAN ^c	REAS ^d	Vongmahadlek [20] ^e
1. Large point source					
1.1 Power plants	X	X		X	X
1.2 Industries	X	X		X	X
2. Mobile sources					
2.1 On-road	X	X		X	X
2.2 Non-road	X				X
3. Area sources					
3.1 Residential	X	X		X	X
3.2 Gasoline stations	X			X	X
3.3 Biomass burning	X	X			X
3.4 Livestock				X	X
3.5 Fertilizer				X	X
4. Biogenic sources					
4.1 Vegetation			X		X
4.2 Soil				X	X

Remark:

^a <http://edgar.jrc.ec.europa.eu/overview.php?v=42>; base year is between 1970 and 2008

^b http://www.cgrer.uiowa.edu/EMISSION_DATA_new/index_16.html; base year is 2006

^c http://eccad.sedoo.fr/eccad_extract_interface/JSF/page_species.jsf; base year is between 1980 and 2010

^d http://www.jamstec.go.jp/frsgc/research/d4/reas_c.html; base year is 1995 and 2000

^e Base year is 2005

4.2. Emission input allocation

4.2.1. Spatial emission allocation

Photochemical dispersion model requires grid-based emission input which depends on the grid resolution. Generally, EI is disaggregated based on the sub-nation levels, i.e. province and district [19]. EI data must be then assigned into the grid box by averaging values over the grid area or following the relevant or surrogate data for particular emission sources. For example, if the EI data for VOCs from transportation are obtained from CGRER for grid

resolution of 0.5° x 0.5°, EI data can be assigned into the grid based on, for example, road network and then averaged into the grid [21]. Spatial emission allocation for modeling study is shown in Figure 4 for example. Figure 4 shows the VOCs emission distribution over fine domain (4 km x 4 km) for Bangkok Metropolitan Region (BMR) and coarse domain (12 km x 12 km) for the Central Thailand [21]. To obtain the respectable model performance, spatial emission distribution should be realistic and up to date [15,21,22].

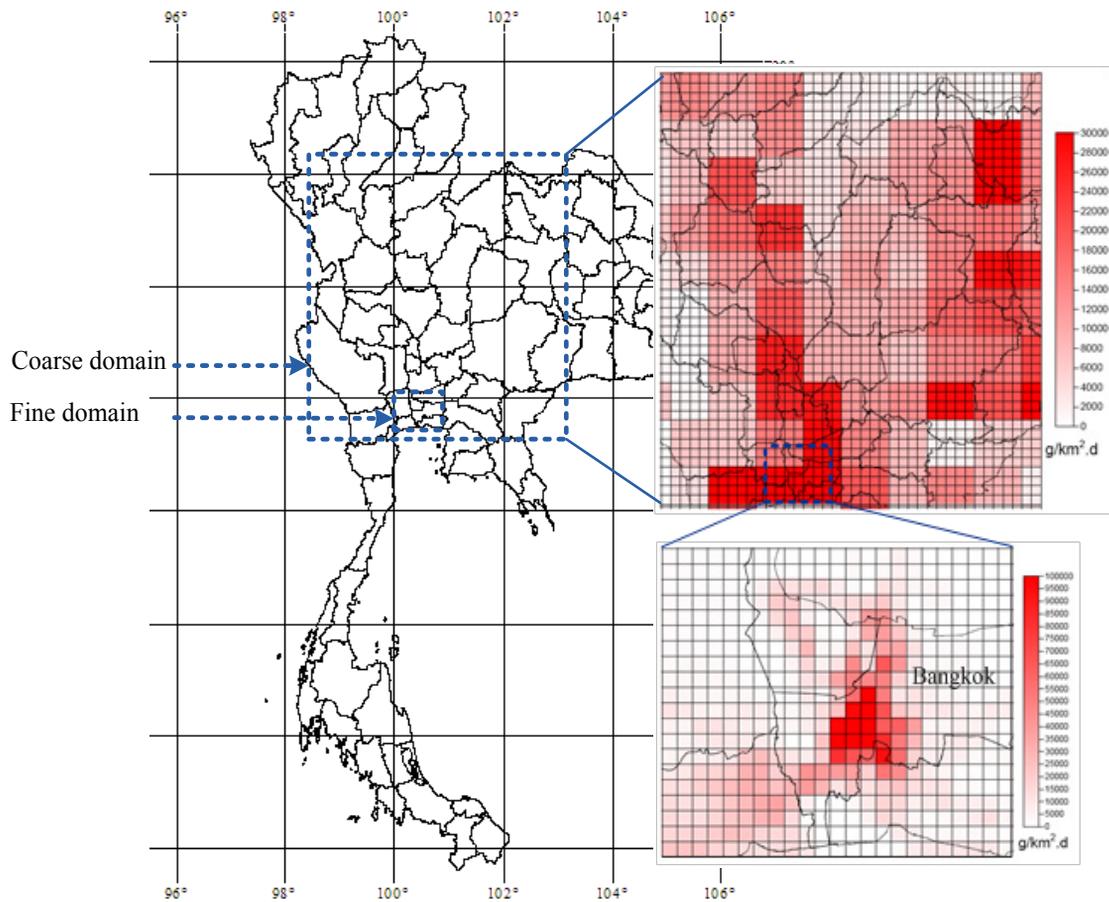


Figure 4. Example of spatial emission allocation of VOCs for fine and coarse domains [21]

4.2.2. Temporal emission allocation

Besides emission over the grid area, temporal emission allocation at least up to hourly variation is also important for photochemical model study because both ozone and secondary aerosol concentrations vary hourly in a day. The example of temporal emission profile for monthly and hourly crop residue field

burning is shown in Figure 5. Particularly, hourly profile information is as high important for investigating ozone and secondary aerosol formations. For instance, the highest hourly emission rate occurred around noon when intensive insolation presents would enhance ozone formation from its precursors (NO_x and VOCs) in urban areas surrounded by agricultural fields such as Bangkok [21].

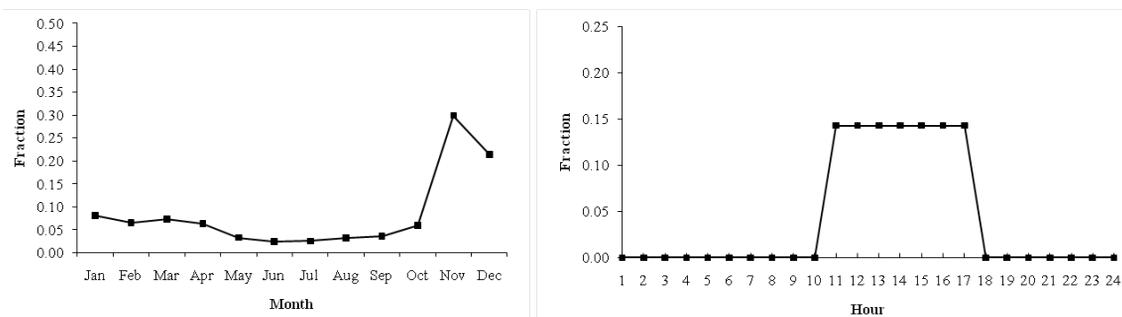


Figure 5. Example of monthly and hourly profiles for crop residue field burning emissions in Thailand [23]

5. Model performance evaluation

The ground-level SAP simulation results are normally evaluated by comparing with the measured values from the ground monitoring stations to assess the model performance. Main parameters for photochemical model evaluation are O_3 and PM and its speciation (EC, OC, PNO_3 , PSO_4 , SOA). Model performance criteria for O_3 were suggested by USEPA [24] while, in contrast, no systematic guidance for PM and its speciation has been established by the agency. Unlike O_3 formation which has been well understood for many decades [24], PM formation is more complex and consists of many components [25]. Mean normalized bias (MNB) and mean normalized error (MNE) were recommended by USEPA [24] for O_3 model performance evaluation, normally with a cut-off (minimum) observation threshold/background, i.e. 60 ppb [25] or 40 ppb [15]. Excluding lower O_3 concentration from performance statistics

is acceptable since the National Ambient Air Quality Standards (NAAQS) for O_3 target the peak concentrations or 8-hour average concentrations.

PM NAAQS are concerned with 24-hour or annual average concentrations making difficulty to set the reasonable cut-off threshold. Very large normalized biases and errors from MNB and MNE can result when observations are close to zero [25]. Mean fractional bias (MFB) and mean fractional error (MFE) are symmetric, i.e. they give equal weight, on a relative basis, to concentrations simulated higher than observations as those simulated lower than observations [25]. MFB is a useful indicator because it produces equal weight between the positive and negative bias estimates [25,26]. MFE is similar to MFB, except the absolute value of the difference is used. Hence, the error is always positive [27]. Table 4 summarizes statistical measures and suggested criteria for O_3 and PM evaluation.

Table 4. Statistical measures for model performance evaluation

Statistical measure	Equation	Suggested performance	
		Goals	Criteria
<i>Ozone</i> [24]			
Mean normalized bias (MNB)	$\frac{1}{N} \sum_{i=1}^N \frac{M_i - O_i}{O_i} \times 100$	-	±15%
Mean normalized error (MNE)	$\frac{1}{N} \sum_{i=1}^N \frac{ M_i - O_i }{O_i} \times 100$	-	≤35%
<i>PM and its speciation</i> [25,27]			
Mean fractional bias (MFB)	$\frac{2}{N} \sum_{i=1}^N \frac{M_i - O_i}{M_i + O_i} \times 100$	±30%	±60%
Mean fractional error (MFE)	$\frac{2}{N} \sum_{i=1}^N \frac{ M_i - O_i }{M_i + O_i} \times 100$	<50%	<75%

Remark: M_i = model prediction value; O_i = observation value; N = total number of data

Note that performance “goals” are defined as the level of accuracy that is considered to be close to the best result a model can be expected to achieve in that application. Performance “criteria” are defined as the level of accuracy that is considered to be acceptable for standard modeling applications [25].

Photochemical dispersion model, CAMx has been used to simulate PM and its associated species in Bangkok, Thailand during February 2007 (the cool dry season) with intensive crop residue field burning surrounding the area [21]. Lack of PM composition data including SIA and SOA in the area, only total simulated PM as PM_{10} was used to compare with the monitoring [21]. Temporal distributions between

modeling results and monitoring data were plotted for 10T-National Housing Authority for example (see Figure 6). Overall, model results overestimated PM_{10} levels. However, the performance statistic evaluation showed that MFB was 33% and MFE was 71%, respectively which were met the performance criteria specified in Table 4. Hence, it was accepted for standard applications and further scenarios study although the temporal variation of the model simulation tended to overestimate the monitored data. There have been a number of reasons for discrepancies between modeled and monitored data, particularly emission input preparation and spatial and temporal emission allocations [28].

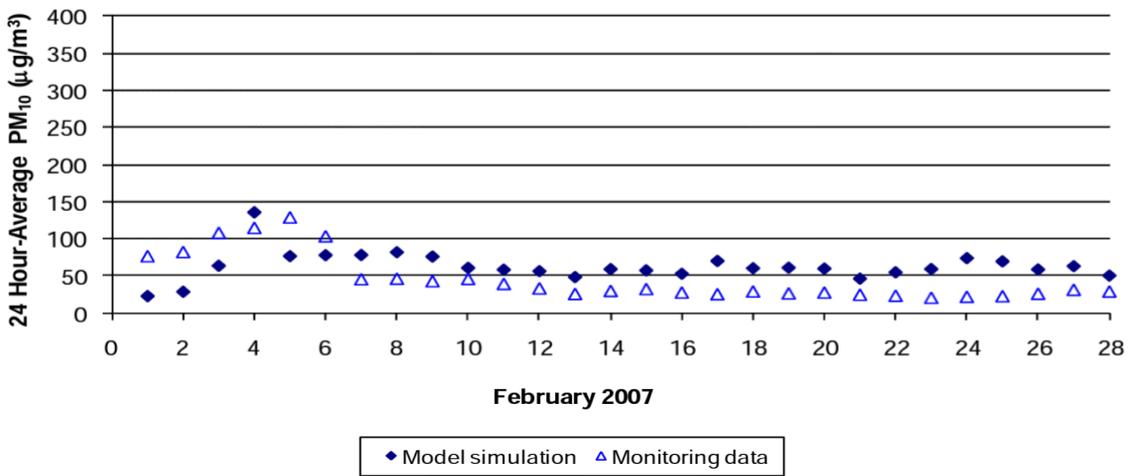


Figure 6. 24 hour-average modeled vs monitored PM₁₀ at selected monitoring station (10T) in Bangkok [21]

6. Conclusions

There are three main steps for photochemical dispersion model simulation: emission input preparation, model set-up and model performance evaluation.

- Emission input data can be prepared through either individual preparation of emission data or collecting the data through available sources, i.e. CGRER and EDGAR for global emission database and REAS for Asia. Emission data should be disaggregated to the desirable grid size (ranging from fine grid, i.e. 1 km x 1 km to course grid, i.e. 1° x 1°) and allocated for temporal variations (hourly profile) before applying to model simulations. Various proxies information can be used to construct the gridded spatial and temporal emissions, such as sub-national levels and the surrogate data.

- A number of 3D photochemical dispersion models have been developed to address the formation and distribution of

SAP in the atmosphere. CMAQ and CAMx are widely used for ozone, fine particles and regional haze pollutions. CMAQ and CAMx are attractive due to, beyond physical and chemical modules, its noncommercial and open-source software.

- Model performance evaluation is of important step to see how close of the simulation to the real situation. Performance criteria have been specified through the statistical measures for ozone (i.e. MNB and MNE) and particulate species (i.e. MFB and MFE). Model results are recommended to achieve at least the performance criteria prior to future applications, i.e. scenarios and impact assessment study.

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