Executive Summary

Agreement No. CE 27/2007 (EP) Upgrade of a Regional Air Quality Modelling System (PATH) – Feasibility Study

Prepared for:

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Hong Kong

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1. INTRODUCTION

In order to address the complicated air quality issues confronted by Hong Kong, the Environmental Protection Department (EPD) established in 2000 a comprehensive numerical air quality modelling system, known as PATH ("Pollutants in the Atmosphere and their Transport over Hongkong"). The PATH modeling system was based on well-developed computer modelling technologies available in the modelling community at the time it was developed (Agreement No. CE46/95).

Recent studies carried out by EPD have indicated that the present modelling system requires an upgrade in order to better understand and resolve some air quality problems in Hong Kong and the Pearl River Delta Region. The upgrade efforts included updates to the meteorological, emissions and chemical transport models. The objectives of the study include:

- To replace the existing modules of the PATH modelling system with current state-of-the-art open source software for performing the core functions of PATH and providing enriched functionality;
- To determine the computing hardware requirements for supporting the operations of the proposed system including making daily air quality forecasting operation;
- To perform sensitivity model simulations for determining the optimal configurations for each component of the proposed system, and
- To review the performance of the proposed system and provide a development road map to cater for future technology advancement.

The agreement called for the following specific tasks to be undertaken:

- Review the latest development in the science and technology of emission modelling, meteorological modelling and regional air quality modelling;
- Review the state-of-the-art software available to the air quality modelling community;
- Review the current setup and operation of the PATH modelling system;
- Compile transport data for Hong Kong and the Guangdong Province for the estimation of vehicular emissions;
- Propose state-of-the-art open source software to replace the core modules in the PATH modelling system;
- Implement the proposed software into the upgraded PATH modelling system;
- Identify the parameters that have significant impact on the modelling results of the upgraded system;
- Evaluate the performance of the upgraded system;
- Provide training to Government assigned personnel on the setup and operation of the upgraded system; and

- Recommend further development of the modelling system to cater for technology advancement.

2. The Old modelling system and the upgraded modelling system

A numerical modelling system for air pollution must deal with three processes: meteorology, emission and chemical transformation. The development framework used in the current PATH system is schematically represented in **Figure 1**.

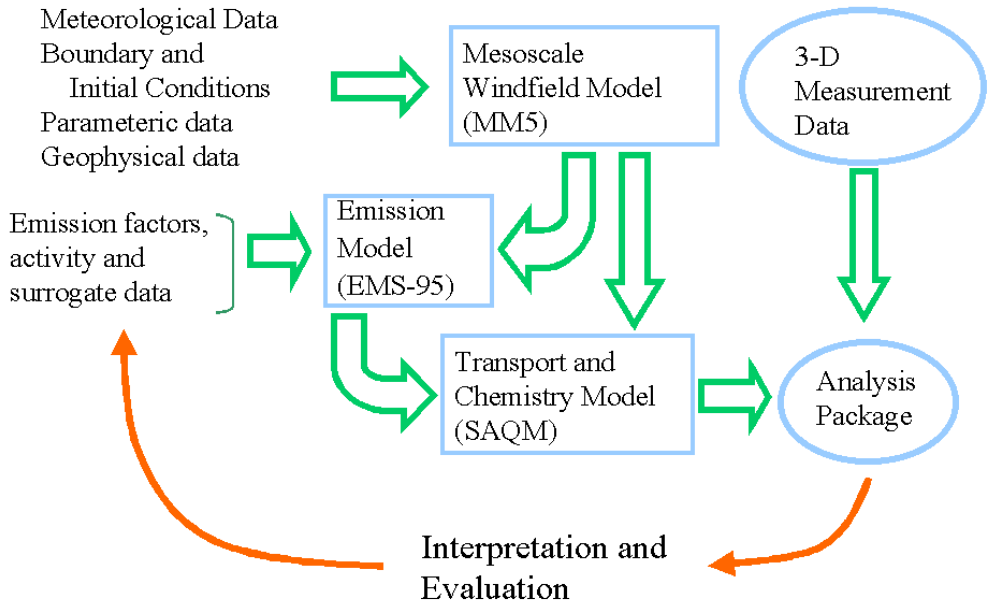

Figure 1: Schematic Diagram showing interaction of the old PATH Components

Three types of atmospheric processes are numerically represented in the old PATH by three distinct simulation modules:

- Mesoscale Model Version 5 (MM5) for meteorological simulation;
- Emission Modelling System (EMS-95) for emission modelling; and
- SARMAP Air Quality Model (SAQM) for transport and chemistry simulation.

The upgraded PATH system consists of a number of separate modules whose execution flow is shown in **Figure 2.** The major components of each system module based on current state-of-the-art software that was selected and used to upgrade the current PATH system are as follows:

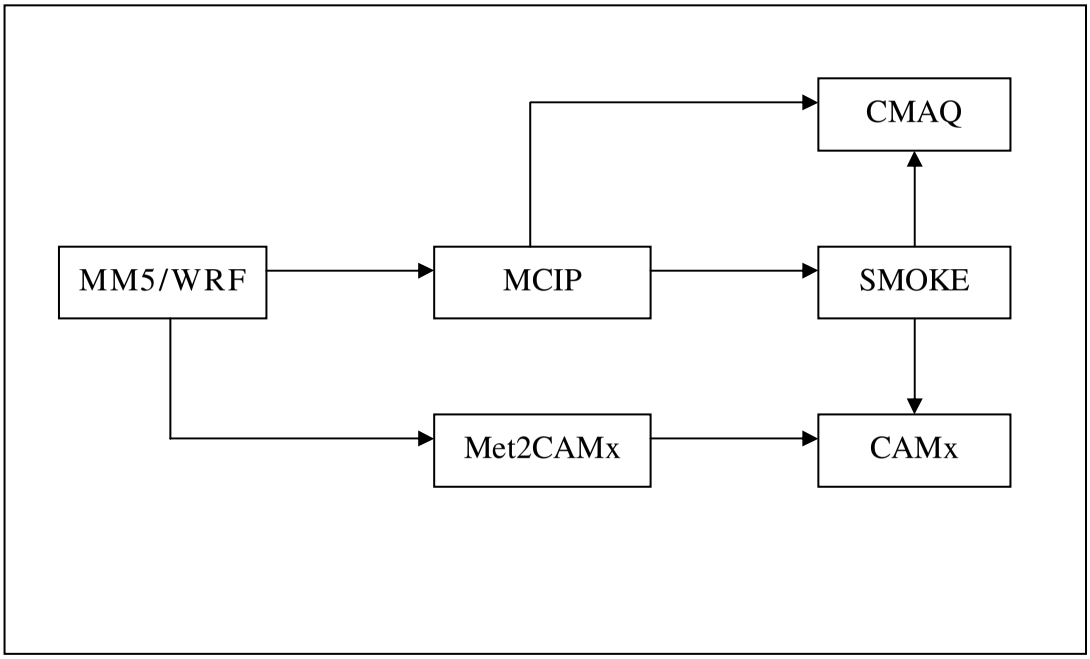

Figure 2. Schematic Diagram showing interaction of the Upgraded PATH Components

- Mesoscale Model version 5 (MM5) and the Weather Research Forecast (WRF) are meteorological model software that requires input data as 1) routine observations with upper air and surface reports, including wind, temperature, relative humidity, sea-level pressure, and sea surface temperature, 2) global model and other regional model's output either as first guess for objective analysis, or as lateral boundary conditions, and 3) topographic and landuse data. The MM5/WRF software generates meteorological output data required by the SMOKE, CMAQ, and CAMx modules.

- MCIP is a data conversion utility to convert MM5/WRF output to be used by CMAQ and SMOKE.

- Met2CAMx is a data conversion utility to convert MM5/WRF output to be used by CAMx

- The Sparse Matrix Operator Kernel Emissions (SMOKE), the Consolidated Community Emissions Processing Tool (CONCEPT), the Model of Emissions of Gases and Aerosols from Nature (MEGAN) and the Biogenic Emission Inventory System (BEIS) were selected as the emission modelling systems for the upgraded PATH.

- Community Multiscale Air Quality (CMAQ) and Comprehensive Air-quality Model with extensions (CAMx) Chemical Transport Models (CTMs) were selected for the upgraded PATH system as transport and chemistry simulation. It requires meteorological data output by the MM5 or WRF module, and pre-generated or real-time generated emissions data output by SMOKE, CONCEPT, MEGAN and/or BEIS modules. The CMAQ and CAMx generate air quality data.

3. Modelling Domains and Grid Structure

The old PATH modeling system used a 40.5/13.5/4.5/1.5/0.5 km grid structure. The modeling domains were developed a decade ago and represented an appropriate trade-off between computational requirements and resolving emissions and air quality in the highly dense Hong Kong area at that time. There are areas for improvement in the grid structure to address the current Hong Kong air quality and air quality related problems for long term applications. By studying the current PATH modeling system domain definitions and taking advantage of the advancement in computing power over the last decade, an alternative expanded grid system has been selected for the upgraded PATH modeling system.

Four nested meshes with grid spacing of 27, 9, 3 and 1 km are used for the modeling domains of the meteorological and emissions/CTM models. The characteristics of these domains are as follows:

D1 -- Grid 1 (27 km): The coarsest outer grid would include almost all of China and Japan as well as Taiwan, Vietnam, Laos, Cambodia, Thailand, etc. This is much larger than the old PATH modelling system outer grid that just covers Southeastern China, Taiwan and North Vietnam.

D2 -- Grid 2 (9 km): The second grid would cover Southeastern China including Guangdong Province, Hong Kong and Macao. This is in contrast to the old PATH model configuration whose second (13.5 km) grid covers the majority of Guangdong Province.

D3 -- Grid 3 (3 km): The third nested grid covers most of Guangdong Province, Hong Kong and Macau. The old PATH system third (4.5 km) grid covers mainly Hong Kong and the PRD.

D4 -- Grid 4 (1 km): The final grid in the alternative domain configuration is focused on the PRD region, as compared to just Hong Kong with the old PATH configuration.

Figures 3 to 6 show the horizontal extents of the four modeling domains. The domains of the Chemical Transport Model (CTM) and emissions models will be slightly smaller and are nested in the meteorological model domain.

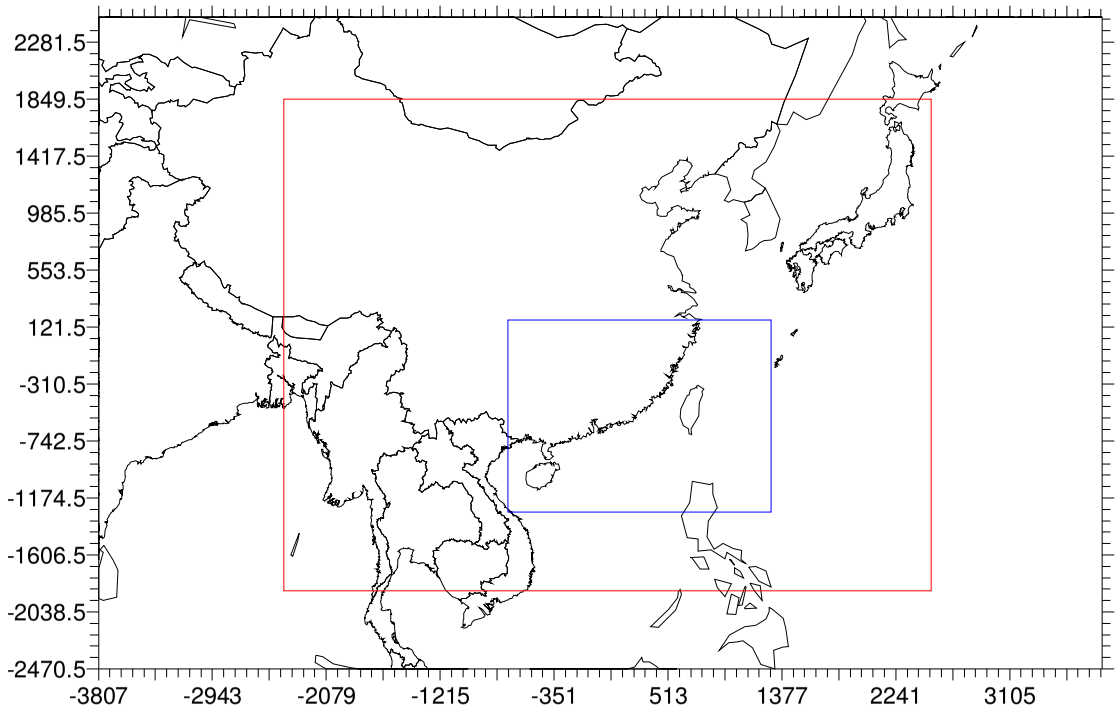

Figure 3. 27-km MM5/WRF meteorological model domain with the 27-km CTM domain (red) and the 9-km MM5 domain (blue).

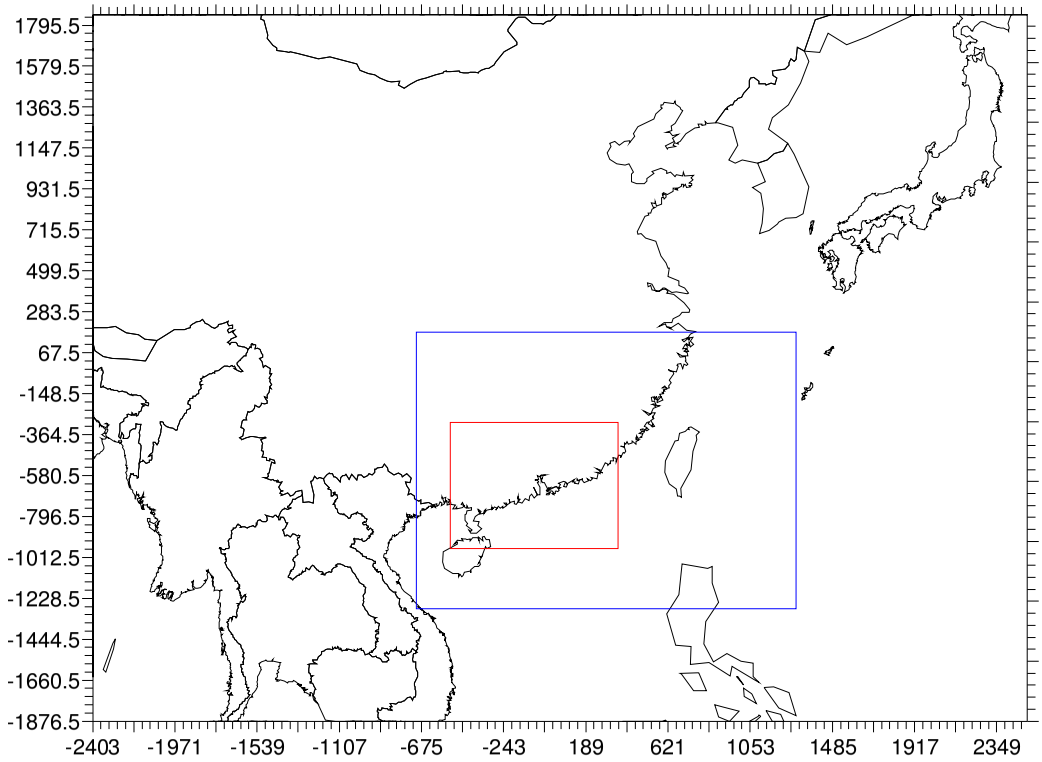

Figure 4. 27-km CTM domain with the 9-km MM5 domain (blue) and the 9-km CTM domain (red).

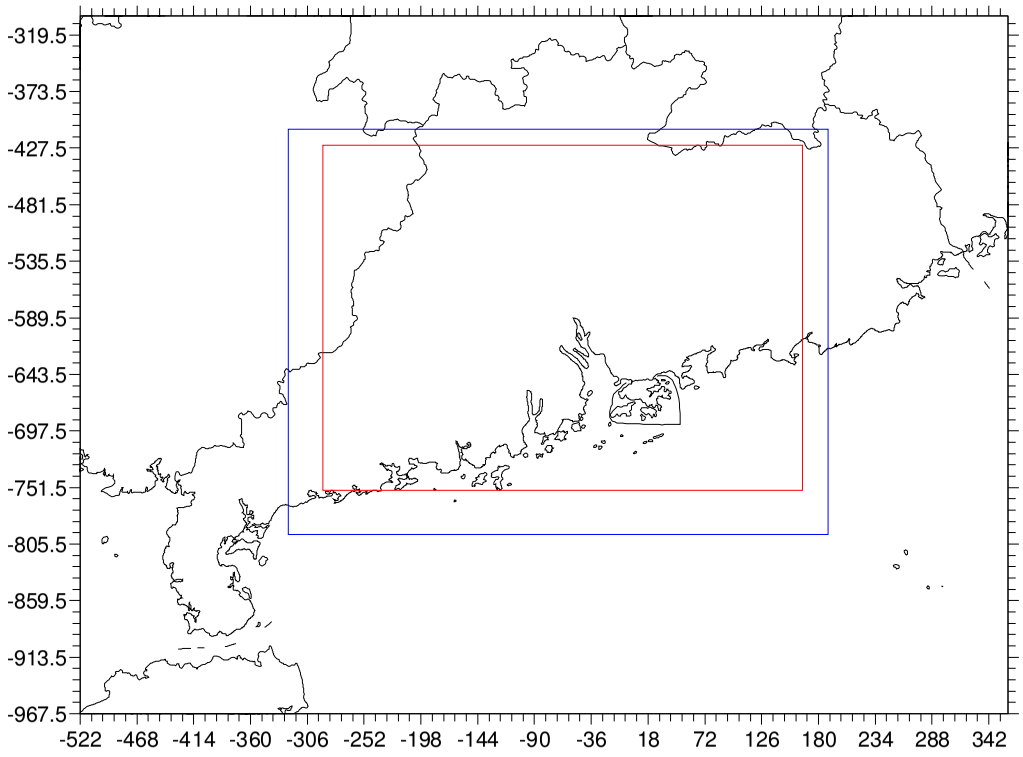

Figure 5. 9-km CTM domain with the 3-km MM5 domain (blue) and the 3-km CTM domain (red).

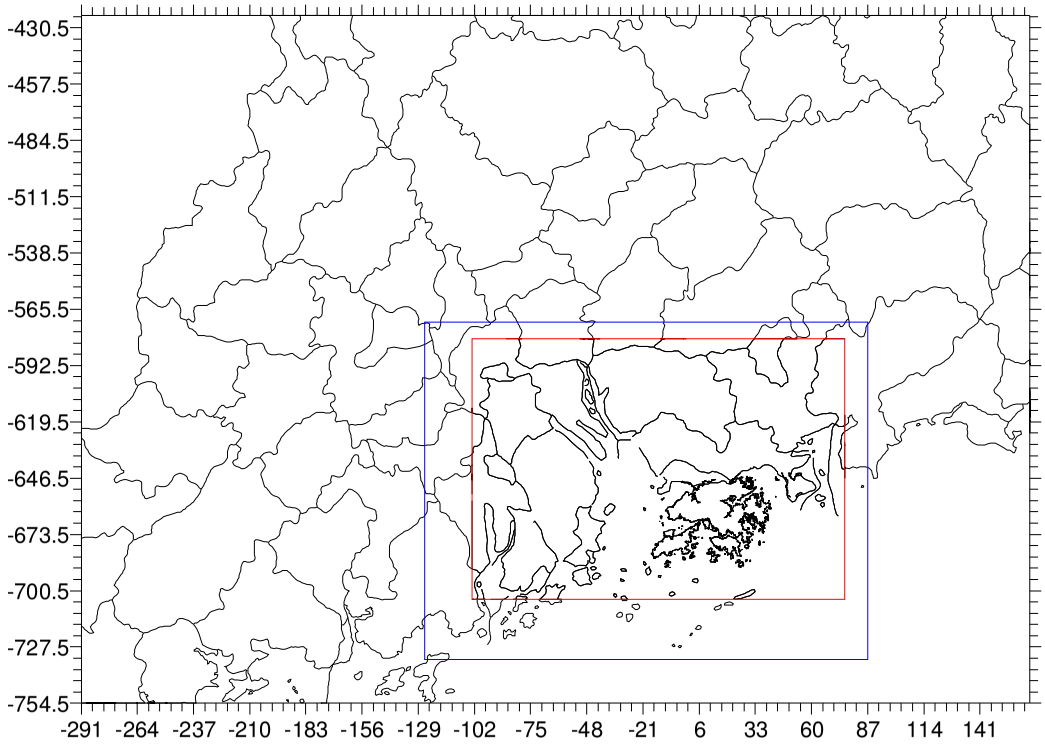

Figure 6. 3-km CTM domain with the 1-km MM5 domain (blue) and the 1-km CTM domain (red)

The CTM vertical structure is primarily defined by the vertical layer definitions used in the MM5/WRF modelling. The MM5/WRF model employed a terrain following coordinate system defined by pressure, using 38 vertical layers that extend from the surface to the 50 mb pressure level (approximately 20 km AGL). A layer averaging scheme was adopted for the CTM that collapsed the 38 layers used in the MM to 26 layers for the CTM to reduce the computational time of the CTM simulations. The CTM vertical layer structure exactly matched the MM model layer structure for the lowest portion of the atmosphere (below approximately 1800 m AGL) within the Planetary Boundary Layer (PBL) where most of the atmospheric processes occur that lead to elevated pollution levels in the HK and PRD regions. Thus, the CTM layer structure will match the MM5 vertical layers with no layer collapsing for the bottom 20 layers in the two models. Above the PBL the CTM will employ layer collapsing of the MM layers to be more computationally efficient.

4. Modelling Episodes

Four historical modelling episodes were selected by the Hong Kong Environmental Protection Department (EPD) for testing and demonstrating the upgraded PATH system. Note that for each episode, ten (10) initialization days were added to the beginning of the episode for the 27 km outer grid with shorter initialization days for the smaller grids as appropriate:

- Episode 1: September 10 through October 12, 2004;
- Episode 2: November 2-3, 2003;
- Episode 3: July 24-25, 2006; and
- Episode 4: March 16-17, 2006.

Figure 7 displays the locations and identifiers for the air quality monitoring sites within the Hong Kong region that were used to characterize each of the modelling episodes and evaluate the CTMs.

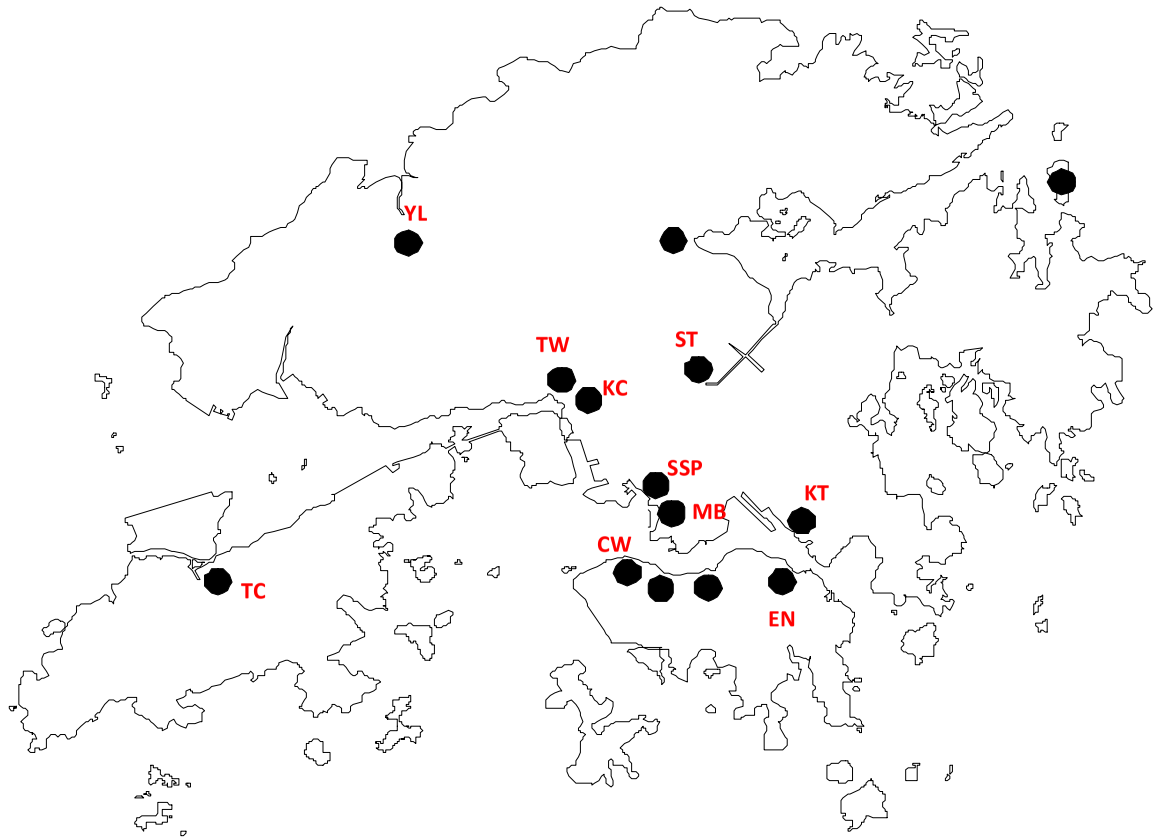

Figure 7. Air Quality monitoring stations in Hong Kong

5. System Components

5.1 Emissions Modelling Software

The Sparse Matrix Operator Kernel Emissions (SMOKE) emissions modelling system was the primary emissions model used in the PATH upgrade study for all sources but biogenic emissions and on-road mobile source emissions within the Hong Kong area. Sensitivity tests were conducted using the Consolidated Community Emissions Processing Tool (ConCEPT) emissions modelling system as an alternative emissions model for processing point, area and mobile source emissions. The CONCEPT emissions model produced similar CTM-ready emissions inputs as SMOKE, but was slower so the SMOKE emissions model was adopted for the final modelling system. The CONCEPT emissions modelling system was also used with link-based vehicle activity data for on-road mobile sources in Hong Kong to produce highly resolved on-road mobile source emissions in Hong Kong. The Model for Emissions of Gas and Aerosol in Nature (MEGAN) was the primary emissions model for biogenic emissions, although sensitivity tests were also conducted using the Biogenic Emissions Information System (BEIS) biogenic emissions modelling system.

SMOKE: The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system is an emissions modeling system that generates hourly gridded speciated emission inputs of mobile, non-road, area, point, fire and biogenic emission sources for photochemical grid models. As with most 'emissions models', SMOKE is principally an emission processing system and not a true emissions modeling system in which emissions estimates are simulated from 'first principles'. This means that, with the exception of mobile and biogenic sources, its purpose is to provide an efficient, modern tool for converting an existing base emissions inventory data into the hourly gridded speciated formatted emission files required by an air quality simulation model. SMOKE was used to prepare emission inputs for non-road mobile, area, point and non-link on-road mobile sources for all modeling domains.

CONCEPT: The Consolidated Community Emissions Processing Tool (ConCEPT) is a new emissions modeling system that was used to generate on-road mobile source emissions covered by the link-based Travel Demand Model (TDM) activity data within Hong Kong. The CONCEPT on-road mobile source component can make full use of linked-based vehicle kilometers traveled (VKT) data including temporal and spatial variations in speeds and fleet distributions.

MEGAN: Biogenic emissions are modeled using the Model of Emissions of Gases and Aerosols from Nature (MEGAN). MEGAN is the latest biogenic emissions model developed by researchers from the National Center for Atmospheric Research (NCAR) incorporates the full range of ozone and PM precursor species. In addition, the latest version of MEGAN includes biogenic species not found in other biogenic emissions model that are used by the latest CAMx secondary organic aerosol (SOA) module. MEGAN is a fairly new biogenic emissions model so biogenic emissions were also generated using the BEIS algorithms that have been used more extensively in the past in a sensitivity test.

BEIS: Biogenic emissions are also modeled using version 3 of the Biogenic Emission Inventory System (BEIS3). BEIS3 was developed in 2001 and is the latest generation in the BEIS family. All BEIS3 versions are designed for use with the Sparse Matrix Operational Kernel Emissions (SMOKE) system. BEIS3.09 is currently the default version in SMOKE. BEIS3.10 was developed for the 2002 release of the Community Multiscale Air Quality (CMAQ) modeling system. BEIS3.10 includes a 1-km vegetation database that resolves forest canopy coverage by tree species; emission factors for 34 chemicals including 14 monoterpenes and methanol; a soil NO algorithm dependent on soil moisture, crop canopy coverage, and fertilizer application; and specification for the CBIV, RADM2, and SAPRC99 chemical mechanisms. The soil NO algorithm in BEIS3.10 has since been revised (BEIS3.11) to better distinguish between agricultural and nonagricultural land,

and to limit adjustments from temperature, precipitation, fertilizer application, and crop canopy to the growing season and to areas of agriculture. A leaf shading algorithm has been added for estimating methanol emissions from non-forested areas. BEIS3.12 was released in November 2003 and is the most recent version of BEIS. It was assembled as a stand-alone module to the Sparse Matrix Operational Kernel Emissions (SMOKE) system for generating gridded, hourly emissions in a format consistent for air quality modeling.

5.2 Meteorological Modeling System

Mesoscale Model version 5 (MM5) the Weather Research Forecast (WRF) are used for the Meteorological Modeling to develop hourly and, three-dimensional, multi-scale meteorological fields to support photochemical modeling to address HKEPD's air quality and air quality related planning activities. The MM5/WRF meteorological models were applied at the various grid resolutions (27 km, 9 km, 3 km and 1 km) and the modelling results (e.g., wind speed, wind direction, temperature, etc.) were compared against available surface meteorological observations in a model performance evaluation.

MM5/WRF: The Fifth-Generation NCAR / Penn State Mesoscale Model Version 3.7 (MM5) and the NCAR Advanced Research Weather Research and Forecasting Model Version 3 (WRF-ARW) were selected as the two meteorological models implemented in the upgraded PATH modeling system. Preprocessor programs of the MM5 modeling system including terrain, REGRID, LITTLE_R, and INTERPF were used to develop model inputs. The current WRF software framework supports two dynamical solvers (dynamic cores): the Advanced Research WRF (ARW) and the nonhydrostatic Mesoscale Model (NMM). Both solvers are fully compressible, Eulerian, nonhydrostatic and conservative for scalar variables. Considering that the WRF-ARW is well supported by the NCAR, the latest released WRF-ARW Version 3 for the WRF modeling system was selected for implementation in the PATH upgrade project. The overall WRF code (Version 3) includes the WRF Software Framework (WSF), the Advanced Research WRF (ARW) dynamic solver, the WRF Preprocessing System (WPS), the WRF Variational Data Assimilation (WRF-Var) system, and numerous physics packages contributed by WRF partners and the research community.

The goal of the MM5/WRF model evaluation was to assess whether and to what extent confidence may be placed in the modeling system to provide three-dimensional wind, temperature and moisture to air quality models. The basis for the assessment is a comparison of the predicted meteorological fields to available surface data collected by the Global Telecommunication System (GTS) and HK Observatory automatic weather stations around HK. This is carried out both graphically and statistically.

5.3 Chemical Transport Modelling Software

The Community Multiscale Air Quality (CMAQ) and Comprehensive Air-quality Model with extensions (CAMx) modeling systems were selected as the two Chemical Transport Models (CTMs) implemented in the upgraded PATH modeling system.

CMAQ: For more than a decade, the United States Environmental Protection Agency (EPA) has been developing the Models-3 Community Multiscale Air Quality (CMAQ) modelling system with the overarching aim of producing a 'One-Atmosphere' air quality modelling system capable of addressing ozone, particulate matter (PM), visibility and acid deposition within a common platform. The most recent editions are CMAQ Version 4.7 (V4.7) publicly released in October 2008 and

Version 4.7.1 released in June 2010, although the current Study started with the CMAQ V4.6 that was released in October 2006 and all three versions were used in the PATH upgrade study.

CMAQ consists of a core Chemical Transport Model (CTM) and several pre-processors including the Meteorological-Chemistry Interface Processor (MCIP), initial and boundary conditions processors (ICON and BCON) and a photolysis rates processor (JPROC). A number of features in CMAQ's theoretical formulation and technical implementation make the model well-suited for ozone and particulate matter (PM) modeling.

The CMAQ Version 4.6 was used initially in the HK/PRD modelling. We updated to the October 2008 version of CMAQ (V4.7) as part of the sensitivity test modelling. In particular, the new October 2008 V4.7 of CMAQ includes many SOA processes that are missing in the standard version of CMAQ, which was initially addressed with the SOAmods enhancement that was used extensively for regional PM and visibility modelling in the U.S. The final system optimisation and demonstration used CMAQ V4.7.1 in the PATH upgrade study.

CAMx: The Comprehensive Air-quality Model with extensions (CAMx) modelling system is a publicly available three-dimensional multi-scale photochemical/aerosol grid modelling system that has been developed and maintained by ENVIRON International Corporation. The most current version of CAMx is Version 5.3 released in December 2010, although the PATH upgrade study started with CAMx Version 4.51 released in May 2008.

The CAMx V4.51 was employed and the model was set up and exercised on the same 27/9/3/1 km grid as CMAQ. However, in the initial configuration CAMx was run using two-way grid nesting on the 27/9 km domains with one-way nesting employed between the 9 km and 3 km and 3 km and 1 km domains (CMAQ does not support two-way grid nesting). The entire 27/9/3/1 km grid structure was too large to model using two-way grid nesting among all four domains using typical computer memory. Most sensitivity tests just verified parameters within the 3 km and 1 km domains so performing one-way grid nesting was more computationally efficient. The basic configuration of CAMx used 26 vertical layers to a 50 mb region top (~20 km AGL) that exactly match those used by CMAQ. The PPM advection solver was used along with the spatially varying (Smagorinsky) horizontal diffusion approach. Vertical diffusion in CAMx was modeled using K-theory. The Met2CAMx processor, which is similar to the CMAQ MCIP3.3 "pass through" option, was used to process the MM5 and WRF data. For the initial configuration, CAMx was exercised with the CB05 gas-phase, RADM aqueous-phase, and CMU/ISORROPIA aerosol chemistry schemes. The updated SOAP secondary organic aerosol scheme was used for the base configuration in CAMx. This version includes updated treatment for SOA from isoprene and sesquiterpenes. The final optimization and demonstration runs used the latest CAMx V5.3 CTM.

5.4 Transport Data Compilation and Modelling

The EPD currently uses the EMFAC-HK vehicle emissions model for air quality planning and related activities. EMFAC-HK is not readily adaptable for use within ConCEPT for emissions processing, a step included in the upgrade of the PATH modeling system. The EMFAC-HK was adapted from the 2002 EMFAC software used in U.S. State of California. The U.S. EPA MOBILE6 model is an on-road emissions model that has been used extensively for regulatory air quality analyses in the U.S. for all states other than California. As required by the Study Brief, the USEPA MOBILE6 was adapted for use in estimating vehicle emissions in Hong Kong and the Study Team developed a version of the MOBILE6 for Hong Kong.

The ConCEPT MV emissions model was used to combine the MOBILE6-HK emission factors with vehicle kilometers travelled (VKT) data, by roadway link, to estimate overall emissions for on-road mobile sources in Hong Kong. The VKT and speeds by roadway link were obtained from a transportation demand model (TDM) developed for use in Hong Kong by MVA Hong Kong Limited. The MVA model was exercised for the 2005 base year. The VKT activity data were projected or backcast to the other years of the study (2003, 2004, and 2006) using forecast/backcast factors developed from analysis of Transport Department annual traffic count data. The MOBILE6-HK emissions model and the link-based VKT data were used in the ConCEPT MV to develop a highly resolved, temporally and spatially, on-road vehicle emission inventory for Hong Kong. The gridded temperature and humidity from the MM5 and WRF meteorological modeling runs were used to implement appropriate adjustments to the MOBILE6-HK emission factors in ConCEPT MV.

5.5 Data Analysis and Visualisation Software

The Study Team implemented data analysis and visualisation software for displaying the results of the meteorological, emissions and chemical transport modelling. The data analysis tools were customized to process the emission modelling, meteorological modelling and chemical transport modelling results to generate scatter plots, time series plots, model performance statistics, spatial maps and other graphical displays of the modeling results. In addition, these tools were customized to display the input and output data from the emissions, meteorological and chemical transport models and provide interactive 2-D and 3-D visualisation functions.

6. System Optimization and Demonstration

The final optimisation and demonstration runs were conducted using the very latest versions of CMAQ (V4.7.1, June 2010 release) and CAMx (V5.3, December 2010 release) CTMs using meteorological inputs based on the MM5 and WRF meteorological models for three of the historical episodes used in the testing, which included the September 2004, July 2006 and March 2006 modelling episodes. Prior to performing the final optimisation and demonstration runs, a final set of sensitivity tests were conducted to address the following two issues.

1. Define the optimal final configuration for the CTMs in the final optimisation and demonstration model runs using the very latest versions of the CMAQ and CAMx CTMs; and

2. Better understanding of the CTM model performance for the July 2006 episode (Episode 3) and in particular why the CTM ozone model performance is much better using meteorological inputs based on the WRF than the MM5 meteorological model.

The latest versions of the CMAQ and CAMx CTMs were successfully applied to three historical episodes to estimate air quality within the Hong Kong area as well as the greater Pearl River Delta (PRD) region. No problems were encountered in applying the two CTMs and demonstration runs were made using meteorological inputs based on both the MM5 and WRF MMs. The final runs demonstrate that the two CTMs are operational and ready for use in assisting the Hong Kong EPD in managing their air quality issues.

7. Post Implementation

Once the upgraded PATH modelling systems was delivered to EPD, installed on their computer system and EPD was trained on its use, EPD set up the modelling system to perform forecasting of meteorological and air quality conditions in the Hong Kong and surrounding areas, a Post Implementation Review was conducted which reviewed and evaluated the EPD forecasting results for the four month period of August through November 2010. An additional analysis of the EPD's MM5/CAMx forecast demonstration run for the entire calendar year was documented in the study's final report.

8. Conclusion

A new meteorological, emissions and air quality modelling system has been developed and setup for the Hong Kong (HK) and Pearl River Delta (PRD) region. The new modelling system was demonstrated using four historical modelling episodes from 2003-2006. The modelling system was delivered to HK Environmental Protection Department (EPD) and EPD was trained on its use. EPD has applied the modelling system to make meteorological and air quality forecasts for the HK/PRD region and the entire 2010 calendar year.

During the course of the development of the new air quality modelling system, the study team has strived to continuously update the modelling system so that it uses the very latest modelling components. To this end, the final optimisation and demonstration runs used the very latest versions of the Community Multiscale Air Quality (CMAQ Version 4.71 released June 2010) and Comprehensive Air Quality Model with extensions (CAMx Version 5.3 released December 2010) Chemical Transport Models (CTMs).

The application of the CTMs for the historical episodes from 2003-2006 and for forecasting for the 2010 calendar year demonstrate the usefulness of the new air quality modelling system for air quality management planning in the HK/PRD region. The modelling system is now fully operational and ready for routine application.