LOWER FRASER VALLEY
PHOTOCHEMICAL MODELLING GUIDELINE

British Columbia Ministry of Environment & Climate Change Strategy
Environmental Protection Division
Environmental Standards Branch
Clean Air

Victoria, British Columbia, Canada

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ACRONYMS AND ABBREVIATIONS

2-D	Two-dimensional
3-D	Three-dimensional
ACM2	Asymmetric Convective Model, version 2
AGL	Above ground level
AMET	Atmospheric Model Evaluation Tool
APEI	Canadian Air Pollutant Emission Inventory
AST	Anemometer starting threshold
ARW	Advanced Research WRF core
AVHRR	Advanced Very High-Resolution Radiometer
BC	British Columbia
BEIS	Biogenic Emission Inventory System
BELD	Biogenic Emission Landuse Database
CAC	Criteria air contaminants
CAM-Chem	Community Atmosphere Model with Chemistry
CAMx	Comprehensive Air quality Model with extensions
CMAQ	Community Multiscale Air Quality model
CMAS	Community Modeling and Analysis System
CMC	Canadian Meteorological Centre
CO	Carbon monoxide
DDM	Direct Decoupled Method of sensitivity analysis
ECCC	Environment and Climate Change Canada
ECMWF	European Centre for Medium-Range Weather Forecasts
ENV	British Columbia Ministry of Environment and Climate Change Strategy
ERA5	ECMWF Reanalysis
FASTJ	CMAQ internal photolysis rate calculator
FDDA	Four-Dimensional Data Assimilation
FINN	Fire INventory from NCAR
FNMOC	Fleet Numerical Meteorology and Oceanography Center
FVRD	Fraser Valley Regional District
g/kg	gram per kilogram
GEM	Global Environmental Multiscale Model
GF	Grell-Freitas cumulus scheme
GUI	Graphical user interface
h	hour
HNO_3	Nitric acid
HONO	Nitrous acid
I/O	Input/output
K	Kelvin
km	Kilometre
km/h	Kilometre per hour
JPROC	CMAQ external photolysis rate calculator
LFV	Lower Fraser Valley
LSM	Land surface model
m	metre
m/s	metre per second
mb	millibar
MCIP	CMAQ Meteorology-Chemistry Interface Processor

MDA8	Maximum daily 8-hour average
MM5	Mesoscale Model, version 5
MMIF	Meteorological Model InterFace
MODIS	Moderate Resolution Imaging Spectroradiometer
MPI	Message Passing Interface parallelization
MSC	Meteorological Service of Canada
MSKF	Multi-Scale Kain Fritsch cumulus scheme
MVRD	Metro Vancouver Regional District
N	Nitrogen
N_2O_5	Dinitrogen pentoxide
NAM	North American Mesoscale model
NAPS	Canadian National Air Pollution Surveillance Program
NARR	North American Regional Reanalysis
NCAR	National Center for Atmospheric Research
NDBC	National Data Buoy Center
NEI	US National Emission Inventory
NH_3	Ammonia
NH_4	Ammonium
NMB	Normalized mean bias
NME	Normalized mean error
NMOC	Non-methane organic compounds
NO	Nitrogen oxide
NO_2	Nitrogen dioxide
NOAA	National Oceanic and Atmospheric Administration
NO_X	Nitrogen oxides (NO + NO_2 + HONO)
NO_Y	Total oxidized nitrogen (NO_X + NO_Z)
NO_Z	Oxidized NO_X
NPRI	Canadian National Pollutant Release Inventory
NSIDC	National Snow and Ice Data Center
NWP	Numerical Weather Prediction
O3MAP	CAMx total atmospheric ozone column preprocessor
OMP	Open Multi-Processor parallelization
PBL	Planetary boundary layer
PCIC	Pacific Climate Impact Consortium
PEC	Particulate elemental carbon
PGM	Photochemical grid model
$PM_{2.5}$	Particulate matter less than 2.5 microns aerodynamic diameter
PM_{10}	Particulate matter less than 10 microns aerodynamic diameter
POA	Particulate organic aerosol (carbon + other constituents)
POC	Particulate organic carbon
ppb	parts per billion by volume
ppm	parts per million by volume
QA/QC	Quality assurance/quality control
RMSE	Root mean square error
R	Correlation coefficient for linear regression
RAMS	Regional Atmospheric Modeling System
ROG	Reactive organic gas
RRTMG	Rapid Radiative Transfer Model for global climate models
s^{-1}	Inverse seconds

SCICHEM	Second-order Closure Integrated Puff model with Chemistry
SCIPUFF	Second-order Closure Integrated Puff model
SMOKE	Sparse Matrix Operator Kernel Emission processing system
SNODAS	Snow Data Assimilation System
S	Sulphur
SO_2	Sulphur dioxide
SO_3	Sulphur trioxide
SO_4	Sulphate
SOA	Secondary organic aerosol (carbon + other constituents)
SO_X	Sulphur oxides
TOG	Total organic gas
TUV	Tropospheric Ultraviolet and Visible radiative transfer model
US EPA	United States Environmental Protection Agency
VBS	Volatility Basis Set organic aerosol chemistry scheme
VOC	Volatile organic compounds
WRF	Weather Research and Forecasting model
WRFCAMx	WRF to CAMx interface program
WSM6	WRF Single-Moment 6-Class cloud microphysics scheme
YSU	Yonsei University boundary layer scheme
$\mu g/m^3$	microgram per cubic metre

ACKNOWLEDGEMENTS

The Metro Vancouver Regional District, Fraser Valley Regional District, and British Columbia Ministry of Environment and Climate Change Strategy, working cooperatively as Partner Agencies, have commissioned this Guideline with in-kind contributions from Environment and Climate Change Canada.

PREFACE – A GUIDE TO THE GUIDELINE

The document provides key guidance on:

- Model selection;
- Sources of model input data;
- Application of models for regulatory purposes in the Lower Fraser Valley; and
- Best modelling practices.

The document is written for modelling practitioners who have a working knowledge of photochemical air quality models and supporting meteorological model and emission processing systems.

1. INTRODUCTION

1.1 PURPOSE OF GUIDELINE

The Metro Vancouver Regional District (MVRD), Fraser Valley Regional District (FVRD), and British Columbia Ministry of Environment and Climate Change Strategy (ENV), working cooperatively as Partner Agencies, have commissioned this Guideline to help ensure that air quality assessments for the Lower Fraser Valley (LFV) that make use of photochemical modelling are: appropriate for the needs of the application, appropriately and consistently applied, and used to reliably inform air quality management decisions. Please be sure to complete a Photochemical Modelling Plan before commencing modelling work (see Appendix A for a template).

Any deviation from the core modelling methodology outlined herein should be presented to the reviewing agency prior to submission of the modelling report.

This Guideline:

- Is not a regulation or policy and thus there is no legal obligation to follow the recommendations included here;
- Recognizes the importance of professional judgment and allows departures from, or additions to, Guideline practice as long as variations are detailed in the Photochemical Modelling Plan; and
- Will be updated as modelling practice changes (as driven by advances in science and user experience with the Guideline).

1.2 SCIENTIFIC AND REGULATORY CONTEXT

Photochemical models are considered refined or advanced models used for “Level 3 Assessments”, as described in the British Columbia Air Quality Dispersion Modelling Guideline (ENV, 2022).

The selection of a specific type of air quality model and its application are driven primarily by two needs: scientific and regulatory. From a scientific perspective, sources that emit “precursor” compounds that can form secondary pollutants downwind, such as ozone and certain components of fine particulate matter ($PM_{2.5}$), must be addressed using advanced, chemically comprehensive modelling techniques that include complex, nonlinear chemical production pathways. From a regulatory perspective, ambient concentrations of secondary pollutants without the Project in question (i.e., “Baseline” conditions) include contributions from global, extra-regional (outside the LFV), and regional (within the LFV) sources. Thus, the Project’s incremental contribution relative to the Baseline and to ambient air quality standards and objectives needs to be assessed. These factors require advanced modelling that can properly produce spatial concentration distributions and the location and frequency of exceedances of air quality standards and objectives.

The following are some technical considerations that need to be considered before undertaking an assessment using a photochemical model:

- The spatial scale of the analysis will need to cover areas where ozone and/or secondary particulate matter formation are of critical importance – this is likely be on the regional scale (up to 100’s of km);
- The temporal scale of the analysis will need to include periods when the pollutant(s) of concern and emission impacts from Project sources are expected to be elevated while addressing a range of

meteorological conditions – this includes the selection of a representative, but suitably conservative timeframe, such as a whole summer season for ozone or an entire year for $PM_{2.5}$ assessments, consistent with the forms of the air quality objectives and standards;

- The modelling will require comprehensive emissions inventories that include a complete characterization of source sectors, their spatial distribution, and chemical speciation profiles;
- The modelling will require the availability of, or ability to develop, meteorological fields from a mesoscale numerical weather prediction (NWP) model;
- The modelling will require sufficient ambient measurement data or other larger-scale modelling products that can provide regional boundary conditions or other background air quality characterization; and
- The modelling will require sufficient ambient measurement data from which to assess model performance in replicating the chosen historical period to be assessed.

1.3 PHOTOCHEMICAL MODEL TYPES

1.3.1 EULERIAN OR GRID MODELS

Photochemical grid models (PGM) are Eulerian models; they employ a fixed frame of reference that is anchored to the Earth's surface and divide the modelling domain into a three-dimensional (3-D) array of grid cells. Examples include the US Environmental Protection Agency's (US EPA) Community Multiscale Air Quality (CMAQ) model (US EPA, 2022a) and the Comprehensive Air quality Model with extensions (CAMx; Ramboll, 2022a). PGMs simulate emissions, transport, diffusion, chemical evolution and removal of multiple chemically linked pollutant compounds. PGMs must incorporate emissions from all sources within and upwind of the assessment region in order to properly perform nonlinear photochemical simulations for ozone and secondary $PM_{2.5}$. PGMs require a set of high temporal resolution (e.g., hourly or more frequent), spatially gridded, mass and energy consistent meteorological inputs derived from NWP models. As limited-area models, they require specification of spatially and temporally varying boundary conditions for all relevant chemical species that realistically define the inflow of pollutants from outside the modelling domain. A schematic of PGM data flow is shown in Figure 1-1.

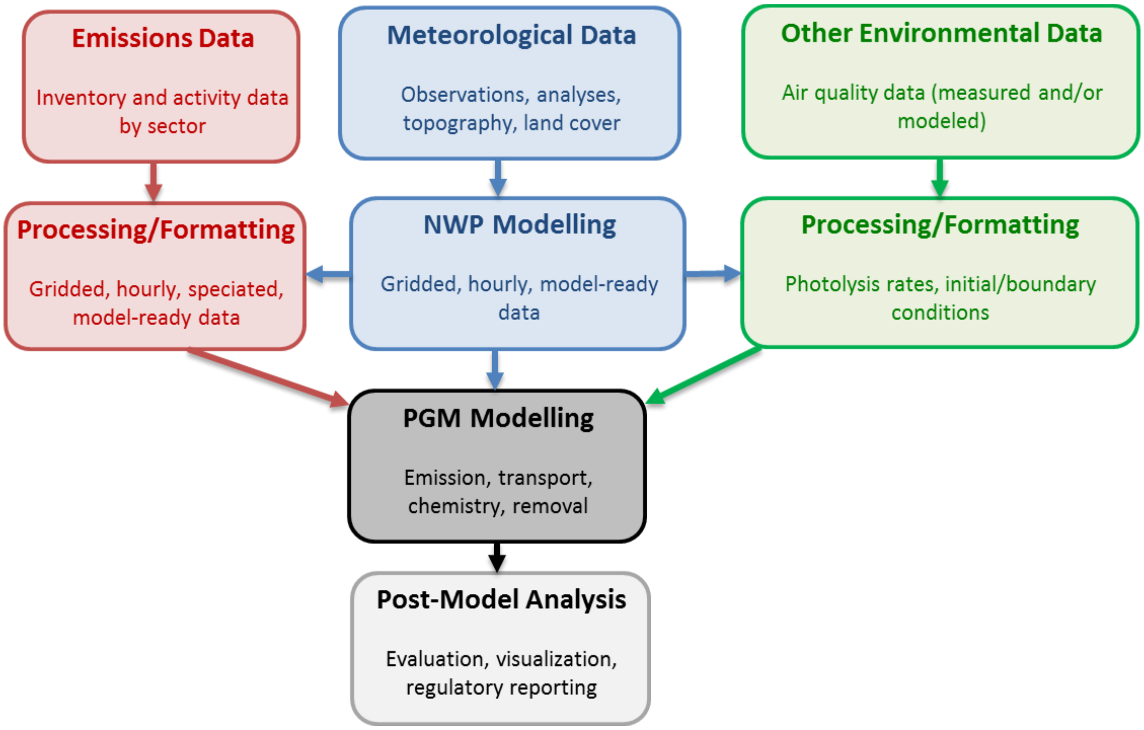

Figure 1-1. A general schematic of photochemical grid model data flow showing preprocessing steps to develop emissions, meteorology, and other environmental inputs, and post-model analysis.

Project impacts can be obtained from the difference between two PGM simulations with and without the new or modified Project source(s), or by using instrumented tools such as source apportionment and/or source sensitivity that are built into the PGMs. The first and most straightforward approach, often referred to as “brute force”, involves running the model twice: (1) for the “Baseline” scenario without the Project source(s), and (2) for the “Project scenario” that adds the Project source(s) to the Baseline. Section 3.2 describes this approach in more detail. Results from these two runs are differenced in a manner that pairs them spatially and temporally. When considering collective impacts from a small set of sources, brute force is the easiest way to apply PGMs and the easiest to understand.

However, brute force quickly becomes computationally burdensome when the model must be run repeatedly to quantify individual impacts from many sources, especially for long term (seasonal-annual) PGM applications that may take on the order of a week of run time on high performance computing systems. “Instrumented” methods or “Probing Tools” are available in PGMs that can estimate contributions and sensitivity for multiple sources in a single model run. However, output from these tools can be voluminous in cases where many sources are tracked simultaneously. Proper interpretation of results from this tool requires some familiarization and experience.

1.3.2 LAGRANGIAN OR PUFF MODELS

The Second-order Closure Integrated Chemistry model (SCICHEM; EPRI, 2021) is a Lagrangian photochemical model that simulates ozone and secondary $PM_{2.5}$ using chemical mechanisms comparable to CMAQ and CAMx. Lagrangian models like SCICHEM employ a moving frame of reference that travels with parcels of air (referred to as “puffs”) containing emissions from sources that are specifically tracked in the simulation. Lagrangian models are inherently well suited to simulating impacts from single sources because they follow the downwind transport, dispersion and chemistry of those specific emissions as a sequence of puffs. The impacts of emissions from the Project plume can be simulated without having to include emissions from all other sources. However, because SCICHEM does not explicitly simulate the air quality impacts from all other sources that may chemically interact with the Project plume, it is critically important when using this modelling framework to provide a time/space varying, representative background chemical environment for all photochemically relevant compounds. SCICHEM allows background concentrations to be specified from ambient monitored data or generated from a PGM, and it accepts meteorological inputs from NWP models or from local meteorological observational data. A schematic of SCICHEM data flow is shown in Figure 1-2.

1.4 PHOTOCHEMICAL MODELLING PROTOCOL

The following are recommended steps to follow for every photochemical modelling application. The steps help determine the pollutants and related objectives to be addressed, data sources, modelling and performance assessment approach, and help ensure the model output addresses the needs of the regulatory agencies.

Step 1: Set the Context. Define objectives and scope of the study. Examine current/past air quality levels with respect to relevant air quality objectives and standards.

Step 2: Characterize Sources and Pollutants. Gather information on Project sources, relevant pollutants, and their emission rates to be simulated. Identify any other major projects under consideration.

Step 3: Characterize Physical and Meteorological Setting. Define the modelling domain, select the period to model, and review geophysical characteristics and atmospheric behaviour of the area.

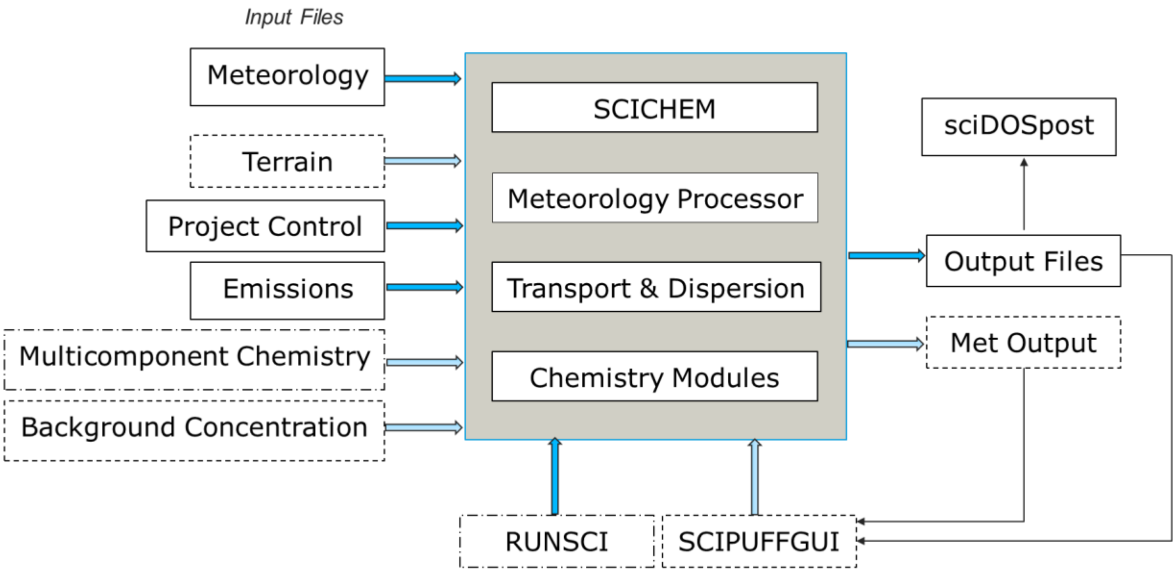

Figure 1-2. A schematic of SCICHEM data flow. Solid boxes and dark filled arrows represent required inputs/processes while dashed boxes and light filled arrows represent optional inputs/processes. For example, multicomponent chemistry and background concentrations are needed for secondary pollutants like ozone and $PM_{2.5}$. Terrain is not needed for flat terrain applications. The use of the graphical user interface (GUI) can be used to view results. Outputting diagnostic meteorological fields (when using meteorological observations) is optional.

Step 4: Select Models. Select models by reviewing their technical capabilities and their recommended use.

Step 5: Determine Model Inputs. Define the meteorological and regional emission inventory needs and data availability based on the model and period selected.

Step 6: Determine Baseline Air Quality. Identify, collect and utilize ambient monitoring data available for the area and characterize Baseline air quality patterns for the pollutants of concern.

Step 7: Develop a Photochemical Modelling Plan. A Photochemical Modelling Plan is required (Appendix A). The plan is a tool to facilitate communication between the different parties to avoid misunderstandings and delays. The final approved plan will require consultations between interested parties.

Step 8: Prepare Input Files, Execute the Models. Prepare meteorological, emissions and air quality input datasets, and then execute the necessary meteorological, emissions, and photochemical modelling systems.

Step 9: Perform Quality Assurance and Quality Control (QA/QC) Review. Exercise QA/QC procedures to confirm accuracy of emission inputs and to assess performance and behaviour of meteorological and photochemical models in replicating observed Baseline meteorological and pollutant patterns.

Step 10: Document Model Application and Results. Document the modelling process and QA/QC results and provide modelling system input/output files to the reviewing agencies for review of the air quality assessment. Provide assessment of Project impacts as determined from the modelling (and as agreed upon in the Photochemical Modelling Plan).

2. RECOMMENDED MODELS AND THEIR APPLICATION

This section presents three well vetted and publicly available photochemical models that are commonly used throughout North America (two Eulerian and one Lagrangian) in the assessment of Project-specific air quality impacts:

- **Recommendation**: The Community Multiscale Air Quality (CMAQ) model (US EPA, 2022a);
- **Recommendation**: The Comprehensive Air quality Model with extensions (CAMx; Ramboll, 2022a); or
- **Recommendation**: The Second-order Closure Integrated Chemistry model (SCICHEM; EPRI, 2021).

Both Eulerian photochemical models recommended in this document (CMAQ and CAMx) have been used extensively in similar impact assessment work, with both providing similar levels of accuracy. The choice to adopt either model is usually based on ease-of-use considerations, flexibility, and special capabilities.

2.1 CMAQ

CMAQ (CMAS, 2022a; US EPA, 2022a,b) is an open source, comprehensive multipollutant PGM that addresses ozone, $PM_{2.5}$ and other hazardous air pollutants (toxics) simultaneously across spatial scales ranging from local to hemispheric. It interfaces directly with the Weather Research and Forecasting (WRF; NCAR, 2022a) model as its source of meteorological data, and directly uses gridded and point emissions generated by the Sparse Matrix Operator Kernel Emission (SMOKE; CMAS, 2022b) processing system. It possesses state-of-the-science gas and aerosol chemistry mechanisms and photolysis calculations, and direct coupling between WRF and the dry deposition and the boundary layer mixing treatments. Numerous other capabilities are available to support special applications, including process and sensitivity analysis and source apportionment. US EPA and the Community Modeling and Analysis System (CMAS) distributes new CMAQ versions regularly.

Advantages of CMAQ include:

- Employs modern and comprehensive treatments for gas and particulate chemistry and deposition;
- Interfaces directly with WRF and SMOKE;
- Internally generates certain natural emissions as it runs, including biogenic, sea salt, windblown dust, and nitrogen oxide (NO_X) from lightning;
- Includes ability to treat bidirectional ammonia fluxes to/from the surface, which is important for areas with large burdens of secondary inorganic $PM_{2.5}$ (sulphate and nitrate); and
- Employs Message Passing Interface (MPI) parallelization on multicore computer systems to shorten runtimes for large and/or long-term applications.

Disadvantages of CMAQ include:

- Requires nested grid applications to be run sequentially, first for the outer grid, then consecutively for any inner nested grids, which negatively impacts runtime efficiency;
- Cannot be run on a subset of WRF model layers (a process referred to as “layer collapsing”), which negatively impacts runtime efficiency; and

- Presents a more complex option; many model configuration options are set during the compilation process so that only needed portions of the CMAQ model are built into the executable. These factors contribute to a relatively complicated build process.

2.2 CAMx

CAMx (Ramboll, 2022a,b) is a state-of-the-science photochemical grid model that also comprises a "one-atmosphere" treatment of tropospheric air pollution (ozone, particulates, air toxics) over spatial scales ranging from neighborhoods to continents. It is an open source system that is computationally efficient and flexible. It possesses state-of-the-science gas and aerosol chemistry mechanisms, photolysis calculations, and dry and wet deposition processes. CAMx input/output (I/O) files are configured similarly to CMAQ file structures, which allows the use of consistent file manipulation tools. CAMx includes interface processors that allow the model to ingest meteorological fields from WRF and emissions from SMOKE. Numerous other capabilities are available to support special applications, including a plume-in-grid algorithm, process and sensitivity analysis and source apportionment. Ramboll distributes new CAMx versions regularly.

Advantages of CAMx include:

- Includes modern and comprehensive treatments for gas and particulate chemistry and deposition;
- Includes ability to treat bidirectional ammonia fluxes to/from the surface, which is important for areas with large burdens of secondary inorganic $PM_{2.5}$ (sulphate and nitrate);
- Allows all nested grids to be run together in a single simulation, maximizing efficiency;
- Offers two options for parallelization: Open Multi-Processor (OMP) parallelization and MPI. OMP and MPI can be used independently or together to optimize CAMx run times;
- Allows for layer collapsing of the WRF vertical grid structure to further enhance CAMx speed; and
- Designed to be somewhat easier to build, use, and runs faster than CMAQ when applied for the same application (chemistry options, modelling grid definition) with equivalent parallelization.

Disadvantages of CAMx include:

- Does not include in line natural emission estimates as the model runs (i.e., biogenic, sea salt, windblown dust, lightning NO_X), except for ocean borne iodine used for ozone chemistry. These emission components must be separately developed using external preprocessors, all of which are distributed with CAMx except for the biogenic model.

2.3 SCICHEM

Until recently, predicting ozone and secondary $PM_{2.5}$ has been the exclusive domain of PGMs. SCICHEM (EPRI, 2021) is an open source, well vetted and peer reviewed Lagrangian photochemical puff model that treats emissions, chemical transformation, transport, and deposition using time and space varying meteorology. SCICHEM simulates primary emitted species as well as secondary pollutants, such as ozone and secondary $PM_{2.5}$, making it suitable for both short range and long-range impact assessments. The model includes state-of-the-science gas-phase and aerosol chemistry, and dry and wet deposition schemes. The dispersion component of SCICHEM is based on the state-of-the-science puff model, SCIPUFF (Second-order Closure Integrated Puff) to represent an arbitrarily complex, 3-D, time-dependent plume from one or more sources. Ramboll and EPRI develop new SCICHEM versions less frequently than the PGMs.

SCICHEM accounts for chemical interactions among puffs that overlap each other, a major technical necessity to properly address nonlinear chemistry. An important benefit of explicitly treating puff overlap is that co-located puffs share the available background concentrations of oxidants and ammonia, which avoids overestimating chemical transformation rates due to “double counting” the influence of the background when puffs overlap.

Baseline concentration fields are important inputs to SCICHEM because the amount of ozone and secondary $PM_{2.5}$ formed from emissions from a single source depends on the reactivity of the Baseline air. A chemically evolved Baseline input field (i.e., without the new or modified Project sources) should include the following compounds consistent with the photochemical mechanism employed in SCICHEM: speciated NO_X and volatile organic compounds (VOC), sulphur dioxide (SO_2), carbon monoxide (CO), ammonia (NH_3), all needed intermediate photochemical product species (such as nitric acid and other oxidized nitrogen species), ozone, and primary and secondary $PM_{2.5}$ components (dust, sulphate, nitrate, ammonium, elemental and organic carbon, etc.). Since many of these compounds are not measured, and those that are measured are not adequately characterized in time and space for use in SCICHEM, the use of a PGM is the best approach to develop these background fields.

Advantages of SCICHEM include:

- Provides more flexible and often simpler modelling platform for assessing single source impacts;
- Requires fewer and simpler inputs than for PGMs; and
- Can be run in different modes of complexity depending on the single source application. For ozone and secondary $PM_{2.5}$, it is appropriate to use 3-D NWP model data and complete photochemistry.

Disadvantages of SCICHEM include:

- Requires information about the background chemical environment to perform nonlinear chemical calculations within puffs. This factor is easily addressed if existing PGM output fields are available covering the domain and period of concern. However, if no such datasets are available, either a set of default background values can be used or a PGM simulation would be necessary. Thus, the effort could effectively revert to running and evaluating a PGM for the domain and period(s) of interest, thereby leading to a larger effort than applying the PGM alone.

2.4 ALTERNATE MODELS

Although the models recommended here should be applicable for most LFV applications, there may be circumstances where an alternate model would be better suited. The conditions under which an alternate model could be considered include:

- The recommended models are not appropriate due to technical limitations for the application;
- The alternate model performs better than the Guideline model based on peer reviewed evidence where the proposed alternate model has been applied in a similar situation using performance indicators relevant for this application (maximum hourly concentration comparisons, exceedance threshold comparisons, spatial pattern comparisons, etc.);
- The alternate model is publicly available; and

- The use of the alternate model has been agreed upon by all interested parties.

The selection and rationale for an alternate model must be included in the Photochemical Modelling Plan.

2.5 MODIFICATIONS TO MODELS

Modifications to the model program can result in unexpected results due to the complexity of the interrelated model components. If a model is to be modified, the source code must be provided, and the following information must be included in the Photochemical Modelling Plan:

- The scientific and technical justification for such a modification;
- Documentation of the modification; and
- Thorough documentation of the evaluation of impacts on model performance.

2.6 DOMAIN SIZE AND RESOLUTION

In order to achieve a realistic characterization of ozone and secondary $PM_{2.5}$, PGMs must include chemical influences from all emission sources in the region and concentrations entering from well outside the region. Furthermore, photochemistry introduces a time “lag” in the generation of ozone and $PM_{2.5}$, which depends on the mix of precursors and environmental conditions. This lag moves peak secondary concentration impacts away from the source and extends the area over which those peaks may occur. According to the US EPA (2019), peak ozone and secondary $PM_{2.5}$ impacts most often occur within 100 km of source. All of these issues require a photochemical modelling domain that is more expansive than typically employed in simpler dispersion modelling applications. Particularly relevant to the LFV, the domain size and resolution must adequately account for the influences of Project-specific emissions, complex topography, land-water heterogeneity, related recirculation patterns, and influences from regional sources that influence secondary air pollutants in the LFV.

Selecting the appropriate 3-D grid resolution for the selected domain must provide a balance between the need to resolve important flow features and the computer resources required to run the NWP and photochemical models. It must be stressed that higher resolution is not a guarantee for improved model fidelity or performance against observed conditions. For example, very high resolution often exposes and increases uncertainty in the spatial characterization of emissions, meteorology, and other influencing factors, while dynamical treatments in PGMs are not designed to properly characterize nonhydrostatic motions at resolutions below about 1 km. Given the professional judgement involved, it is critical that the grid resolution and domain size are identified in the Photochemical Modelling Plan and discussed with the agencies involved.

2.6.1 HORIZONTAL DOMAINS

Below are recommendations for establishing the horizontal extent of the modelling domain:

- **Recommendation**: Specify the domain to cover the immediate area of the LFV, the surrounding topography and water bodies, and other large regional sources such as Seattle-Tacoma and maritime emissions (Figure 2-1 shows an example of a single modelling domain); and
- **Recommendation**: Specify the meteorological modelling domain to align with, and extend a bit beyond, the corresponding photochemical modelling domain grid(s).

The practice of defining a slightly larger NWP modelling grid alleviates numerical noise that can be introduced at the meteorological model domain boundaries. US EPA (2018) suggests at least 5 additional grid rows and columns outside each photochemical modelling grid.

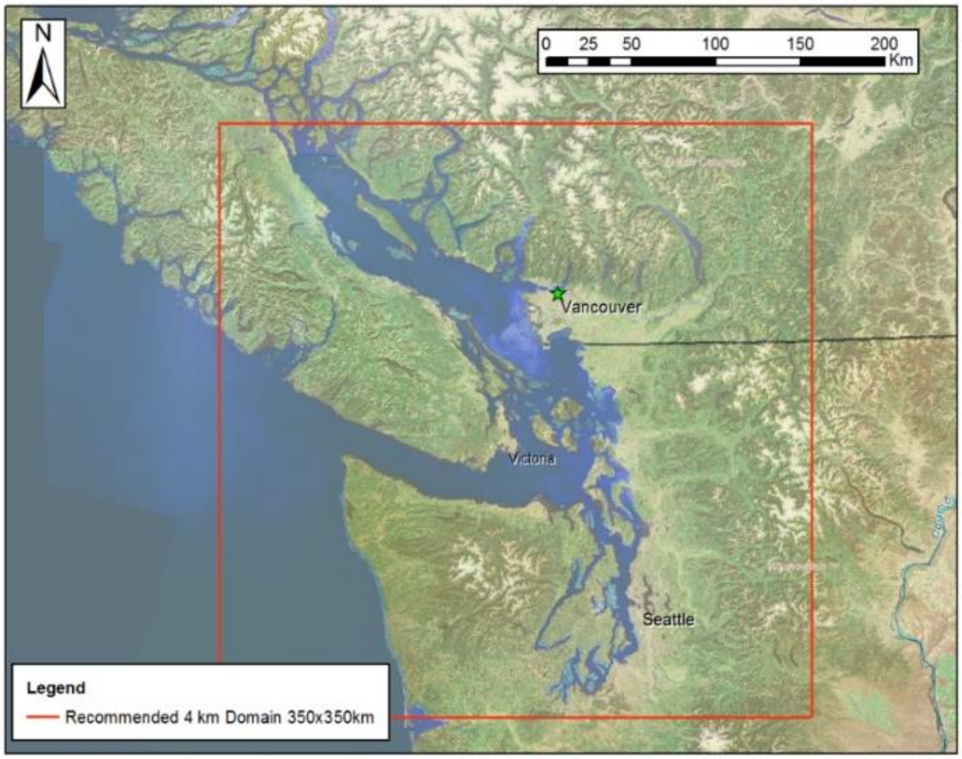

Figure 2-1. Example photochemical modelling domain (red box) centered over the LFV covering a 350 km square area with 88x88 grid cells at 4 km grid resolution.

2.6.2 SPATIAL RESOLUTION AND NESTING STRATEGIES

Below are recommendations for establishing the spatial resolution of both the meteorological and photochemical modelling grid(s):

- **Recommendation**: Establish the domain grid resolution to be no coarser than 3 to 5 km (US EPA, 2018);
- **Recommendation**: Consider a very high resolution inner nested grid (~1 km) that covers an area overlapping the MVRD emission inventory (Figure 2-2) in order to resolve source impacts near or within complex/narrow basins and valleys, or along waterways and shorelines; and/or
- **Recommendation**: Consider a coarser resolution outer grid (~9 to 15 km) to capture super-regional emission influences and to provide a more appropriate buffer zone from the imposed boundary conditions (Figure 2-3).

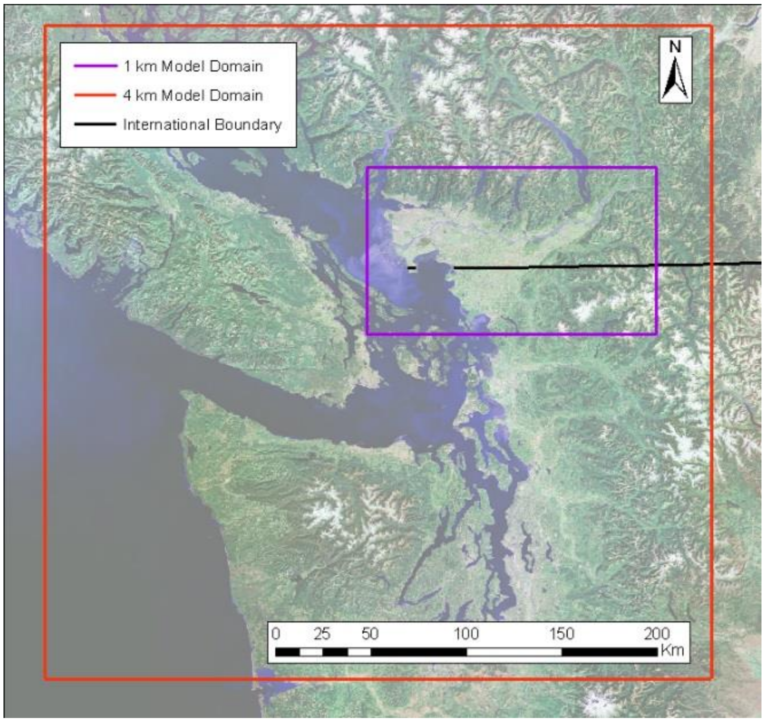

Figure 2-2. **Example photochemical modelling domain for the LFV as shown in Figure 2-1 (red box) that includes a higher resolution nested grid with 1 km grid cell size (purple box) over the MVRD emission inventory area described in Section 3.1.1.**

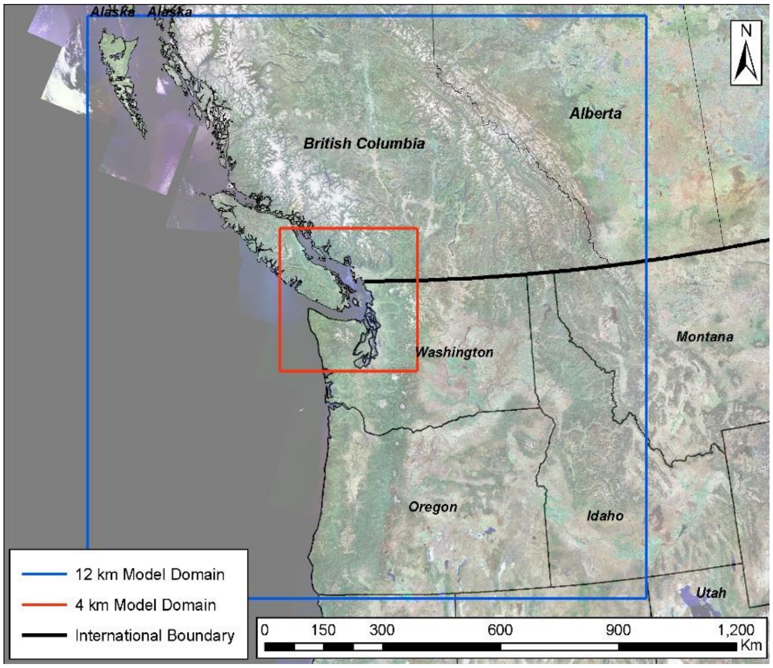

Figure 2-3. **Example photochemical modelling domain for the LFV as shown in Figure 2-1 (red box) that Is nested within a lower resolution outer grid with 12 km grid cell size (blue box).**

2.6.3 VERTICAL DOMAIN

Below are recommendations for establishing the vertical extent and resolution of the modelling domain, which are consistent with current US EPA photochemical modelling guidance (US EPA, 2018) and has been shown to be adequate for regional modelling applications:

- **Recommendation**: Define the NWP modelling grid to comprise a minimum of 30 to 50 vertical layers from the surface through the troposphere (16 to 20 km above sea level) to ensure adequate resolution of mixing depths, temperature gradients and vertical shears (Table 2-1);
- **Recommendation**: Define the photochemical grid that ideally matches the NWP model grid, but otherwise consider a minimum subset of 20 to 30 layers from the surface through the troposphere (note that CMAQ does not allow sub-setting of NWP model layers); and
- **Recommendation**: Use at least 10 layers to properly resolve the lowest 1 km in order to capture recirculation processes, boundary layer processes, thermal internal boundary layers, etc., given the region's complex coastline and topography and the prevalent stratification with the shallow marine boundary layer.

Table 2-1. Example NWP model and PGM vertical grid structures developed by the US EPA (2015) for regional modelling.

PGM Layers	NWP Layers	Sigma Levels*	Pressure (mb)	Altitude (m AGL)
25	35	0.000	50.00	17,556
	34	0.050	97.50	14,780
24	33	0.100	145.00	12,822
	32	0.150	192.50	11,282
23	31	0.200	240.00	10,002
	30	0.250	287.50	8,901
22	29	0.300	335.00	7,932
	28	0.350	382.50	7,064
21	27	0.400	430.00	6,275
	26	0.450	477.50	5,553
20	25	0.500	525.00	4,885
	24	0.550	572.50	4,264
19	23	0.600	620.00	3,683
18	22	0.650	667.50	3,136
17	21	0.700	715.00	2,619
16	20	0.740	753.00	2,226
15	19	0.770	781.50	1,941
14	18	0.800	810.00	1,665
13	17	0.820	829.00	1,485
12	16	0.840	848.00	1,308
11	15	0.860	867.00	1,134
10	14	0.880	886.00	964
9	13	0.900	905.00	797
	12	0.910	914.50	714
8	11	0.920	924.00	632
	10	0.930	933.50	551
7	9	0.940	943.00	470
	8	0.950	952.50	390
6	7	0.960	962.00	311
5	6	0.970	971.50	232
4	5	0.980	981.00	154
	4	0.985	985.75	115
3	3	0.990	990.50	77
2	2	0.995	995.25	38
1	1	0.998	997.63	19

*Sigma refers to a normalized terrain following pressure coordinate, where a value of 1 is at the surface and a value of 0 is at the top pressure surface of the model (50 mb in this case). The calculated altitude above ground level (AGL) in the rightmost column assumes a surface pressure of 1000 mb.

2.7 PERIOD TO MODEL

Elevated ground level ozone can occur during warm, stagnant, inversion conditions when precursor emissions accumulate, and ample sunlight together with higher temperatures drive photochemical reactions. Typically, elevated ozone in the LFV can occur from late spring through summer. Ozone concentrations may be elevated by factors outside the LFV, including regional sources beyond the LFV, wildfires or global influences (stratospheric intrusions, transboundary transport). Elevated $PM_{2.5}$ can also occur at the same time as elevated ozone because primary $PM_{2.5}$ emissions similarly accumulate during those conditions and many of the products of ozone chemistry form secondary $PM_{2.5}$. However, other factors can result in high $PM_{2.5}$ concentrations, including cool stagnant periods during autumn and winter when rates of residential wood combustion are at their highest and certain chemically derived compounds, such as nitrate, more readily condense and remain in particulate form, especially with high humidity. $PM_{2.5}$ events may also result from regional transport of both natural (e.g., fires, dust, and biogenic organics) and anthropogenic sources in any season. As a result, $PM_{2.5}$ episodes occur throughout the year.

2.7.1 MODELLING PERIOD

Below are recommendations for selecting the modelling period:

- **<u>Recommendation</u>**: Consider a minimum modelling period of one 3-month summer period (strictly for ozone assessments), but an entire year is recommended as this would address both ozone and $PM_{2.5}$ formation, and would also allow more direct comparisons with air quality objectives which include both a threshold and a statistical component (e.g., 4th highest 1-hour average);
- **<u>Recommendation</u>**: Consider a recent period with available emissions, monitoring and meteorological datasets that can support a robust photochemical modelling assessment. See Table 2-2 for specific information on available emission inventories in the region; details on available emission inventories are presented in Section 3; and
- **<u>Recommendation</u>**: Consider a recent year that represents typical climatological, meteorological and air quality conditions for each season – for example a summer that is not particularly cool, rainy and clean; nor hot, stagnant and polluted. Try to avoid periods with extensive contributions from atypical event-oriented sources such as wildfires. See Table 2-2 for specific considerations.
- **<u>Recommendation</u>**: Consult with reviewing agencies when selecting a year for modelling.

Table 2-2. Possible years to model over 2015-2020, considerations for whether the year is atypical, and suggested emission inventories to pair for each year. The MVRD inventory, Canadian Air Pollutant Emission Inventory (APEI), and US National Emission Inventory (NEI) are described in Section 3.1.1.

Year	Considerations	Paired Emission Inventory Years
2015	Very hot summer, wildfires	2015 MVRD 2015 Canadian APEI 2014 US NEI
2016	Cool summer	2015 MVRD 2015 Canadian APEI 2016 US NEI*
2017	Hot summer, wildfires	2015 MVRD 2015 Canadian APEI 2017 US NEI
2018	Wildfires	2020 projected or actual MVRD (as available) 2015 Canadian APEI** 2017 US NEI
2019	None	2020 projected or actual MVRD (as available) 2015 Canadian APEI** 2017 or 2020 US NEI (as available)
2020	Wildfires, COVID-19	2020 projected or actual MVRD (as available) 2015 Canadian APEI** 2017 or 2020 US NEI (as available)

*The US EPA developed a 2016 national inventory outside their standard 3-year update cycle.

** Use a more recent Canadian APEI inventory when available.

3. PHOTOCHEMICAL MODEL INPUT – EMISSIONS

This section provides guidance on selecting regional emission inventories and developing emission rate inputs for the recommended models. Any uncertainties and errors in these inputs will be reflected in the model results, so this step is critical to the quality of the photochemical modelling effort.

3.1 REGIONAL EMISSIONS

The following subsections recommend and describe existing anthropogenic and natural emission inventories, software tools and methods needed to support photochemical modelling for the LFV domain and selected modelling period.

Emission inventories covering different portions of the modelling domain should be processed and combined to represent actual conditions during the chosen recent historical modelling period. This requires careful harmonization of multiple data sources to prevent double counting sources, reporting in consistent units, reporting consistent chemical compounds, etc. The resulting set of historical emissions is often referred to as the "Baseline" scenario and should not include the specific new or modified source emissions for the proposed Project.

3.1.1 ANTHROPOGENIC INVENTORIES

Modelling should make use of the most recently available MVRD, Canadian and US emission inventories, as listed in Table 3-1, keeping in mind that it is likely that the various inventories will be valid for different years, and some sort of alignment/adjustment may be necessary in order to use them for the chosen simulation period.

- **Recommendation**: Include the MVRD (2018a) local emission inventory for the municipalities within the jurisdiction of MVRD and FVRD (Figure 3-1);
- **Recommendation**: Include the Environment and Climate Change Canada (ECCC, 2022a) National Pollutant Release Inventory (NPRI) for provincial and territorial areas levels, or the 2015 SMOKE-ready Air Pollutant Emission Inventory (APEI; ECCC, 2022b); and
- **Recommendation**: Include the US National Emission Inventory (NEI; US EPA, 2022c).

Table 3-1. Local, regional and national emission inventories available to support photochemical modelling.

Inventory	Geographic scope	Latest Year & Update Frequency	Anthropogenic Sources Included
Lower Fraser Valley Air Emissions Inventory (MVRD, 2018a)	LFV disaggregated to municipalities, plus Whatcom County, WA	2015, 5 years	All (industry, area, mobile)
Canada Air Pollutant Emissions Inventory (ECCC, 2022a,b)	Canadian national, provincial, territorial; Some estimates are available at finer geographic scale	2018, yearly 2015, as needed	All (industry, area, mobile)
US National Emission Inventory (US EPA, 2022c)	US national, state, county	2017, 3 years	All (industry, area, mobile)

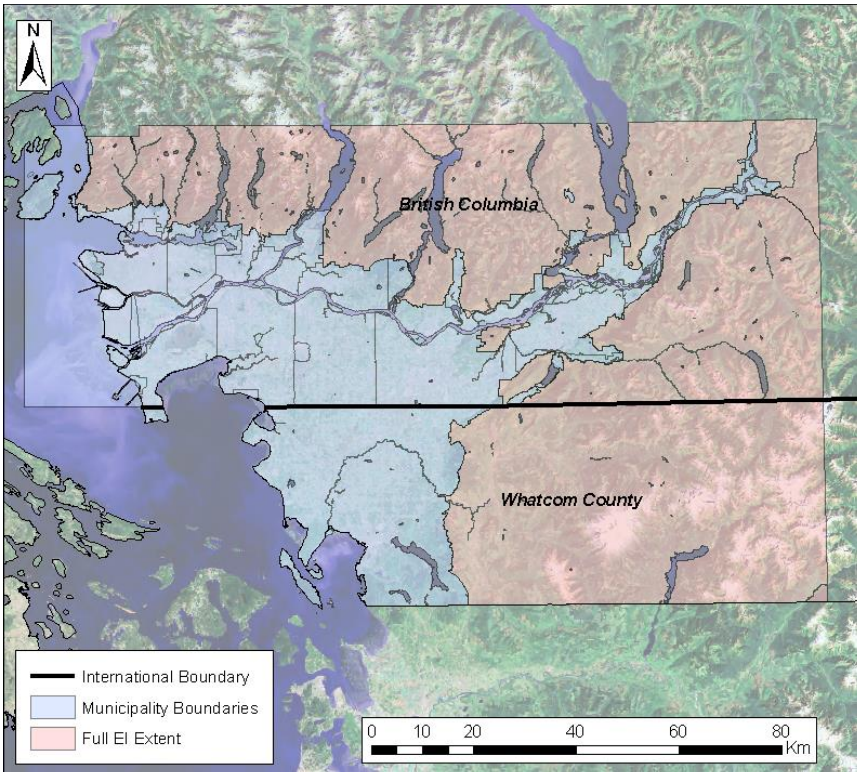

Figure 3-1. Colour shading represents the entire spatial extent of the periodic MVRD emission inventories. Blue shade indicates municipalities within the LFV and includes areas within the jurisdiction of MVRD and FVRD, and westernmost portion of Whatcom County, Washington.

The MVRD inventory includes a portion of Whatcom County, Washington, which is derived from US national inventories. Each inventory includes emission projections for the same area at 5-year increments out to 20 years (e.g., out to the year 2035 for the 2015 emissions inventory). The NPRI is developed every year and the latest is available for 2018. However, there is no set schedule for developing national inventory data in formats that can be readily used by emission processing systems such as SMOKE. The 2015 APEI is latest inventory that can be readily used by the SMOKE emission processing system. The US NEI is provided at state and county levels every 3 years.

3.1.2 CHEMICAL COMPOUNDS TO MODEL

Given the large set of chemical compounds necessary to simulate photochemistry for ozone and $PM_{2.5}$ assessments, a large set of criteria air contaminant (CAC) emission estimates must be available in the raw inventories. Using an emission processing system (Section 3.1.3 below), these CACs must be further split into the individual chemical species required by specific photochemical mechanisms employed in the models.

- **Recommendation**: Include the CACs shown in Table 3-2.

Table 3-2. Criteria air contaminants (CAC) to be included in photochemical modelling assessments.

CAC	Notes
Carbon Monoxide (CO)	
Nitrogen oxides (NO_X)	Split for modelling into nitric oxide (NO), nitrogen dioxide (NO_2) and nitrous acid (HONO);
Sulphur oxides (SO_X)	Split for modelling into sulphur dioxide (SO_2), sulphur trioxide (SO_3 or "SULF"), and sulphate (SO_4).
Volatile organic compounds (VOC)	Split for modelling into numerous classes of explicit and lumped organic gasses, depending on the model's chemistry mechanism
Ammonia (NH_3)	
PM < 10 microns (PM_{10})	Inhalable particulate matter with aerodynamic diameter less than 10 microns, may be further split for modelling by source type (e.g., natural vs. anthropogenic) for source attribution
PM < 2.5 microns ($PM_{2.5}$)	Fine particulate matter with aerodynamic diameter less than 2.5 microns ($PM_{2.5}$), which must be split for modelling into primary elemental and organic carbon components and some specific individual mineral elements to support chemical calculations; the remaining inorganic components may be further split by source type similarly to PM_{10}.

3.1.3 INVENTORY PROCESSING SYSTEM

The anthropogenic emissions inventories discussed in the previous section must be processed to convert annual emission estimates reported for large geographic areas (provincial, state, district, municipality, county, etc.) to photochemical model ready hourly emission rates of specific chemical species in each model grid cell. Model ready emissions reflect source sector-specific activity for the specific season, month, and day-of-week, which can differ significantly among individual sources within broader industrial, commercial, mobile, area and agricultural sectors. Additionally, emissions must match the chemical speciation of CACs required by the photochemical mechanism.

SMOKE is the most widely used and maintained emissions processing system in North America. The flexibility of SMOKE provides a large set of capabilities to address a wide range of source sectors including area, point, mobile (both on-road and non-road), and biogenic.

- **Recommendation**: Use the SMOKE system (CMAS, 2022b) as the primary emissions modelling tool to generate model ready emissions; and
- **Recommendation**: Process emissions separately for each major source category (e.g., vehicles, area, industrial, and marine sources) to facilitate quality assurance review. Carefully review the SMOKE log files for significant error messages and to ensure that appropriate source profiles are being used.

3.1.4 BIOGENIC EMISSION MODELS

Biogenic VOCs (most notably isoprene, sesquiterpene and other terpenes) are involved in photochemical oxidant chemistry, impacting both ozone and secondary organic aerosol components of $PM_{2.5}$. Two widely used biogenic emission systems are recommended:

- **Recommendation**: Use the Biogenic Emission Inventory System (BEIS), which is included within the SMOKE system (CMAS, 2022b); or
- **Recommendation**: Use the Model of Emissions of Gases and Aerosols from Nature (MEGAN), which is a stand-alone system developed at the National Center for Atmospheric Research (NCAR, 2022b).

BEIS generates gridded, hourly emissions of specific VOC compounds, CO and NO emissions from vegetation and soils. Given that it is part of SMOKE, the use of BEIS may be a more practical option to generate biogenic emissions. The Biogenic Emission Landuse Database (BELD) that supports BEIS extends up to northern British Columbia so be sure to check that BEIS is applicable for your modelling domain. Also, BELD often exhibits large discontinuities in land use across the Canada-US border.

MEGAN ingests data fields defining land cover/vegetation type and meteorological parameters supplied via CMAQ input files, and estimates hourly gridded biogenic emissions of specific VOC compounds and soil NO. The MEGAN land use database has global coverage at 30 seconds (approximately 1 km) spatial resolution.

3.1.5 FIRE EMISSION DATA

Large wildland fires have episodically large impacts on local ozone and $PM_{2.5}$ air quality in the LFV (MVRD, 2018b). It may not be prudent to consider modelling days when fires are active in the region and have an obvious and large contribution to monitored exceedances of air quality objectives or standards. However, given the seasonally high frequency of fires throughout western North America together with contributions from long range transport, the impacts of regional fires are inevitable and thus it is necessary to include their influences regardless of the chosen simulation period. Forest fire emissions are highly episodic and location specific. Consider including day-specific wild and prescribed fire (together called wildland fires) emission estimates when influential fires occur within the modelling domain. Use of fire emissions should be documented in the Photochemical Modelling Plan, and may consist of one or a combination of the following:

- **Recommendation**: Use the US EPA BlueSky (US EPA, 2022d) reporting and modelling framework, which provides wildland fire emissions in SMOKE format for historical years through the current US National Emission Inventory year of 2017;
- **Recommendation**: Use the Canadian SMARTFIRE2 Wildfire Smoke Forecasting System, which operationally run at the University of British Columbia (UBC, 2022) and can be used directly by the SMOKE model; and/or
- **Recommendation**: Use the Fire INventory from NCAR (FINN; NCAR, 2022c), which provides daily, 1 km resolution, global estimates of trace gas and particle emissions from open burning of biomass, which includes wildfire, agricultural fires, and prescribed burning (FINN data need to be translated into data files consistent with Bluesky/SMOKE).

3.1.6 RECOMMENDATIONS FOR OTHER NATURAL EMISSIONS

Many natural emission sources are highly dependent on space and time varying meteorological and surface conditions. It is therefore important to estimate their fluctuating emission rates based on the conditions present within the modelling domain and during the modelling period, even if certain sources are reported in emission inventories (which are usually much coarser in time and space). CMAQ includes inline calculations for oceanic, windblown dust, and lightning NO_X emissions as the model runs (US EPA, 2022b). For CAMx, stand-alone emission models are available that are developed and distributed by Ramboll (2022a). Specific recommendations include:

- **Recommendation**: Include oceanic emissions such as sea salt and certain halogens because sea salt contributes sizeable fractions to PM mass budgets in the LFV throughout the year, particularly at coastal monitoring sites, and oceanic halogens affect ozone chemistry; but
- **Recommendation**: Disregard windblown dust and lightning NO_X as they are likely to be minor to negligible contributors to ozone and $PM_{2.5}$ in the LFV.

3.2 MODELLING SCENARIOS

3.2.1 BASELINE

Baseline emissions represent the release of all CACs and other photochemically relevant emissions (NO_X, VOC, SO_X, CO) from all existing sources within the modelling domain as a function of time and space, and Baseline emissions should adequately reflect activities and rates consistent with the chosen historical simulation period. The Baseline scenario is used to:

- Assess the ability of the model to replicate the historical conditions of the period being modelled; and
- Provide a reference air quality level in the absence of the Project's new or modified sources under assessment.
- **Recommendation**: Develop inputs, model and evaluate a Baseline scenario.

3.2.2 FUTURE BASELINE

There may be situations where historical Baseline emissions for the chosen period are expected to change dramatically by the time a new or modified source is scheduled to come on line (e.g., influences of new control regulations, vehicle fleet turnover toward new technologies, new sources or decommissioning of existing sources). In such cases, the Baseline scenario may not be an appropriate characterization of the ambient environment without the Project, and a future projected Baseline should be considered. SMOKE provides the ability to project Baseline emissions to a future year based on sector and process specific factors.

- **Recommendation**: Identify the need for modelling of a future Baseline year in the Photochemical Modelling Plan and describe the approach to project Baseline emissions to the selected year.

3.2.3 NEW OR MODIFIED PROJECT SOURCES

Whether modelling a historical or future Baseline scenario, a separate set of emission inputs need to be developed that include the new or modified Project emissions to be analyzed. These emission sources can be added to existing emission inventory files, or developed as separate inventory files, for ingestion and processing by SMOKE. Guidance on determining Project source types and emission parameters, as well as source specific issues, is available in the British Columbia Air Quality Dispersion Modelling Guideline (ENV, 2022).

- **Recommendation**: Separately develop new or modified Project emissions so that they may be added or otherwise tracked during the PGM application; or

- **Recommendation**: If SCICHEM is to be used, develop background concentration fields to represent the Baseline or future Baseline emissions only (all Project new or modified emissions are to be simulated explicitly by SCICHEM).

4. PHOTOCHEMICAL MODEL INPUT - METEOROLOGICAL DATA

Photochemical models require 3-D gridded fields of wind, temperature, humidity, precipitation, turbulence (mixing) parameters, and other miscellaneous variables. These should be derived using the recommended NWP model described in this section. In order to reduce uncertainty in the model predictions, the meteorological data must be shown to accurately represent actual historical conditions over the selected domain and period.

This section recommends a particular NWP model and its preferred physics configurations, as well as available input datasets for topography and land cover. It also recommends the most appropriate large-scale meteorological analyses that can support the generation of initial/boundary conditions and the model's data assimilation or "nudging" scheme.

4.1 GENERAL RECOMMENDATIONS FOR NWP MODELLING

Below are recommendations for applying an NWP model:

- **Recommendation**: Generate meteorological fields at hourly intervals over the chosen photochemical modelling period, domain, grid resolution and mapping projection (see Section 2.5); this is done to maximize consistency between the NWP and photochemical modelling platforms and to minimize the introduction of errors resulting from translation/interpolation to different grid systems;
- **Recommendation**: Since coupled NWP/photochemical modelling applications are run for historical periods (hindcast), use weather observation data to "nudge" the model toward actual conditions thereby improving the resulting meteorological predictions; and
- **Recommendation**: Conduct QA/QC checks and analyses (see Section 7) to determine whether the NWP model output data is sufficiently accurate for use in photochemical modelling.

NWP models offer an alternative to meteorological measurements as input to SCICHEM. This approach offers many advantages:

- Provides data for any location, which is important in regions where there are few surface and/or upper air data.
- Takes less time to generate a dataset than a monitoring program.
- Avoids subjective decisions regarding the applicability of meteorological data collected in a different location (for example, adjusting/rotating winds to account for different terrain orientations).
- Provides details of the space and time variability of the meteorology in three dimensions within a modelling domain, of critical importance for LFV given the complex geophysical setting.

4.2 MODELLING SYSTEM

The Weather Research and Forecasting (WRF) model, Advanced Research WRF (ARW) core (NCAR, 2022a) is a state-of-the-science "next generation", publicly available/open source NWP system supported by global collaborative contributions to its development and testing. WRF maintenance and distribution is managed by NCAR. WRF is directly compatible with the recommended photochemical models and has a long and well vetted history in supporting photochemical modelling exercises around the world.

- **Recommendation**: use the WRF/ARW model to support photochemical modelling assessments.

Note that other NWP models (e.g., RAMS, GEM) cannot be used with the three recommended photochemical models as there are no existing interface programs to support the coupling of these models.

4.2.1 GUIDANCE ON WRF MODEL CONFIGURATION AND OPTIONS

Recommendations for setting WRF physics and nudging options are based on collective experience in applying WRF for photochemical modelling exercises in support of regulatory-oriented modelling projects conducted throughout North America over the last decade. The selections for each should be established and justified in the Photochemical Modelling Plan.

- **Recommendation**: Employ the WRF physics options and setting in Table 4-1.

Table 4-1. Recommended WRF physics options and settings.

Physics Option	Setting
Vertical coordinate system	hybrid sigma-pressure
Cloud microphysics	WRF Single-Moment 6-Class Scheme (WSM6)
Longwave radiation	Rapid Radiative Transfer Model (RRTMG)
Shortwave radiation	RRTMG
Surface layer physics	Pleim-Xiu or Revised Mesoscale Model version 5 (MM5)
Land Surface Model (LSM)	Pleim-Xiu or Noah
Planetary Boundary Layer (PBL)	Asymmetric Convective Model (ACM2) or Yonsei University (YSU)
Sub-grid Cumulus Parameterization/Shallow Convection	Multi-scale Kain-Fritsch (MSKF) or Grell-Freitas (GF) Ensemble with "scale aware" physics, no shallow convection
Urban Canopy	None
Ocean Model	Simple Mixed Layer Ocean Model

Four-dimensional data assimilation (FDDA) is a process by which third-party meteorological analyses (i.e., the same used to develop WRF's initial/boundary conditions) or individual observational data at monitoring points are ingested into the model simulation. These external datasets are used to periodically "nudge" the model predictions toward the data values, thereby controlling model drift from conditions that actually occurred. This approach has been shown to be very effective in controlling model error growth, allowing the user to have confidence that the resulting variable fields remain constrained toward observed conditions over extended simulation periods.

It is recommended that nudging toward meteorological analyses be employed with some caveats:

- **Recommendation**: Apply analysis nudging on any regional grids with 10 km resolution or larger, while on finer resolution grids, analysis nudging should be applied only above the boundary layer;
- **Recommendation**: To the extent that sufficient local observational data are available, consider point nudging to observed winds at specific monitoring locations, both at the surface and above the boundary layer (if available), but do not perform point nudging to thermodynamic variables (temperature and humidity);

- **Recommendation**: Apply the nudging strengths (coefficients) for each key variable as presented in Table 4-2; and
- **Recommendation**: Consider other point nudging parameters such as radius of influence, vertical influence, and temporal ramp-up/down periods, which depend heavily on grid resolution and the specific topography and environment in each application (document settings in the Photochemical Modelling Plan).

Table 4-2. Recommended analysis and point nudging coefficients typically used for WRF applications.

Variable	Analysis Nudging Coefficients (s-1)	Point Nudging Coefficients (s-1)
Winds	3×10^{-4}	1×10^{-4}
Temperature	3×10^{-4} (above PBL only)	Not Applied
Water Mixing Ratio	1×10^{-5} (above PBL only)	Not Applied

4.3 DATA SOURCES: REGIONAL AND GLOBAL ANALYSES

4.3.1 TOPOGRAPHY AND LAND COVER DATASETS

Below are recommendations for the use of standard terrestrial datasets:

- **Recommendation**: Use standard topography datasets available from the WRF distribution web site (NCAR, 2022a) which provides several global and North American datasets at various spatial resolutions; and
- **Recommendation**: Use high resolution satellite-based (MODIS) land cover datasets which are available from the WRF distribution web site (NCAR, 2022a) and specifically compatible with the Pleim-Xiu land surface treatment in WRF.

Note that these datasets are distributed by NCAR specifically for use in WRF and will therefore also support the photochemical models. However, they may differ from those used in the biogenic emission models or from land cover datasets used to define spatial surrogates for emissions processing in SMOKE.

4.3.2 METEOROLOGICAL ANALYSES

There are several choices available from NCAR (2022a) to develop initial conditions (used to start the model), boundary conditions (used to defined conditions on the boundaries of the outermost WRF grid), and analysis nudging inputs (FDDA to control model drift from observed conditions). Each data source offers its own mix of benefits and drawbacks, depending on spatial coverage, resolution relative to the WRF grid(s), and available variable fields. WRF results depend on the choice of large-scale analysis for initial/boundary conditions and data nudging. Many WRF applications in western North America have achieved good results with the 12 km North American Mesoscale (NAM) dataset for initial/boundary conditions and FDDA.

The following analysis datasets are recommended, depending on grid resolution and spatial extent:

- **Recommendation**: Use the National Center for Environmental Prediction (NCEP) NAM analyses (6-hourly, 12 km resolution over the US and parts of Canada);

- **<u>Recommendation</u>**: Use the NCEP North American Regional Reanalysis (NARR) dataset (3-hourly, 32 km resolution over North America); or
- **<u>Recommendation</u>**: Use the European Centre for Medium-Range Weather Forecasts (ECMWF) Reanalysis (ERA5) dataset (1 and 3-hourly, 31 and 62 km resolution globally).

The specific meteorological analysis product to be used for WRF modelling should be stated and justified in the Photochemical Modelling Plan.

4.3.3 OTHER SURFACE ANALYSES

Sea surface temperature data are available from several different sources at varying spatial and temporal scales.

- **<u>Recommendation</u>**: Use the Fleet Numerical Meteorology and Oceanography Center (FNMOC, 2022) sea surface temperature product.

The FNMOC product has horizontal resolution of about 9 km in the midlatitudes and is produced four times per day using Advanced Very High-Resolution Radiometer (AVHRR) sensors aboard Polar Orbiting Environmental Satellites, as well as in situ buoy observations.

As with the other regional and global analyses, snow cover is available from several sources:

- **<u>Recommendation</u>**: Use the Snow Data Assimilation System (SNODAS) product from the US National Snow and Ice Data Center (NSIDC, 2022), which is at 1 km resolution;
- **<u>Recommendation</u>**: Use the Canadian Meteorological Centre (CMC, 2022) northern hemispheric snow depth data consisting of daily files with a spatial resolution of 24 km; or
- **<u>Recommendation</u>**: If the WRF application uses ERA5 analysis fields, use snow depth from ERA5, which is at a slightly lower resolution (31 km) than the CMC product.

While SNODAS is recommended for high resolution modelling domains, the product extends to about 54 degrees north latitude, which may exclude parts of the outermost WRF domain. The specific sea surface temperature and snow cover dataset to be used for WRF modelling should be stated and justified in the Photochemical Modelling Plan.

4.4 DATA SOURCES: SURFACE DATA

Individual station weather data from common sources such as airports are available through NCAR. Several data formats are available, and each includes standard reporting metrics from active airports throughout North America and across the globe. Station data may be ingested into the analysis fields used to develop initial/boundary conditions and FDDA inputs to WRF, which inserts local scale influences in the larger-scale analyses. Much of the same airport surface station data available from NCAR are also provided by Canadian agencies described below. Data from non-traditional or special study networks require formatting into common data structures that the WRF system can recognize and process.

4.4.1 METEOROLOGICAL SERVICE OF CANADA (MSC)

MSC (2022) archives meteorological data collected at airports, climate stations, buoys, lighthouses, and special studies. Airport, climate, and buoy data provide most if not all of the required surface meteorological parameters for WRF and are likely already included in standard North American weather data distributed by NCAR. MSC hourly airport observation data are primarily designed to generate long term climate statistics and to satisfy aviation weather requirements. It is important to note the following issues (also applicable to data provided by NCAR):

- Wind speed is usually measured at 10 m above the ground.
- The wind measurement may not be a true hourly average but can be an observer-estimated or automated average over the last two to ten minutes of every hour.
- Wind directions are reported to the nearest 10 degrees.
- The wind direction and speed are assigned a zero when the wind speed is zero or below the anemometer starting threshold (AST).
- There can be differences in wind instrumentation from these stations – for example, some stations use sonic anemometers (with an AST of 0) and others use older instruments with an AST of 1 or 2 knots (approximately 1 m/s). If there are frequent periods when the wind speeds are less than the AST (which commonly occurs in valleys/basins), there will be an unrealistically high frequency of calms (zero wind speed). Check to confirm the lowest non-zero wind speed in the data record as this will define the AST.

4.4.2 BC AND MVRD METEOROLOGICAL DATA

ENV downloads and archives hourly meteorological data at various stations across BC outside the LFV. MVRD operates and maintain meteorological instrumentation throughout the LFV at air quality monitoring network stations in both MVRD and FVRD. The rest of the sites are operated by various industries. Wind and temperature are measured along with variables more suited for air quality analysis and modelling including relative humidity, barometric pressure, precipitation, and incoming solar radiation.

Although the data quality is maintained through a maintenance program and data quality checks, it is recommended that information on the siting, instrumentation, and data treatment are reviewed for appropriateness before using the data. Data are available online for current and historical sites in BC from the Air Data Archive website (ENV, 2022). To obtain validated data from LFV meteorological stations, an email request should be sent to: AQinfo@metrovancouver.org. While LFV data may also be available on the ENV website, it should be emphasized that such station data may not be validated and/or up to date.

Note that anemometers at most ENV and LFV sites have a starting threshold of 1 km/h (approximately 0.5 m/s). However, due to changes in the database structure along with hardware changes, there have been some historical changes to the way winds less than the AST have been reported. The following is recommended for light wind/calm treatment of the data:

- **Recommendation**: For LFV data, consult directly with Metro Vancouver; and
- **Recommendation**: For ENV data, wind speeds less than the AST should be set to zero, and wind directions should also be assigned as zero.

For BC wind data consider the following:

- Winds are typically measured at 10 m except for a few sites where measurements are made on top of a building.

For LFV wind data consider the following:

- Wind speed and direction measurements are made at various heights throughout the network. Anemometer heights range from 10 to 30 m above the ground. Also consider that some LFV stations are located on top of buildings and on top of bridges, which may not be representative or applicable. Anemometer heights can be obtained for MVRD stations in a report titled: “Station Information: Lower Fraser Valley Air Quality Monitoring Network” (Metro Vancouver, 2012).

4.4.3 OTHER SOURCES OF SURFACE (LAND AND MARINE) METEOROLOGICAL DATA

Other sources of data include the fire weather network program (Ministry of Forests), the road maintenance and avalanche forecast program (Ministry of Transportation and Infrastructure), university research programs, programs operated within national parks, marine observations (ships and buoy data) and industry operated stations. In data sparse areas, or areas where a network of meteorological data is needed to characterize complex meteorological fields, these other sources of data can be useful.

Instrument siting, type, maintenance and data formats (meta data) are very important given that these stations are set up for purposes other than air quality analysis. Such information may be lacking, so care is required before using the data from these sources.

Meteorological data collected by several agencies (along with meta data information) can be obtained from the Pacific Climate Impact Consortium data portal (PCIC, 2022). If more recent data are not available from PCIC, contact the listed agencies directly. Marine (ocean) observation data are available online from US National Data Buoy Center (NDBC, 2022).

- **Recommendation**: If data from these other sources are considered for modelling purposes:
    - Review siting to determine whether the data are influenced by obstacles or terrain features;
    - Review instrument types for thresholds;
    - Review maintenance and data quality assurance protocols;
    - Review sampling frequencies;
    - Consider if data are recorded at the top of the hour and whether wind direction is rounded to the nearest 10 degrees, similar to airport data;
    - Determine the measurement units (e.g., m/s or km/h) and whether they need to be converted for use in the WRF system;
    - Assess the validity of the data for the purposes of modelling through the generation of wind roses and frequency of calms; and
    - If documentation on the data is not available, apply tests to confirm quality and representativeness such as wind roses, time series plots and percentiles.

4.5 DATA SOURCES: UPPER AIR

The density of upper air stations in western Canada and US is sparse and use of upper air data well away from these sites, especially at lower levels (i.e., within a mountain valley) may not be applicable. However, for regional meteorological/photochemical modelling applications, upper air soundings may be needed depending on the professional judgment of a meteorologist, the specific needs for WRF, and for QA/QC evaluation of WRF results.

- **Recommendation**: Consider using the upper air stations listed in Table 4-3 and document selection and use in the Photochemical Modelling Plan.

The upper air data are available online from the National Oceanic and Atmospheric Administration (NOAA) Radiosonde Database (NOAA, 2022). Upper air data are also readily available from: http://weather.uwyo.edu/upperair/sounding.html. Data from the Aircraft Communications Addressing and Reporting System (ACARS) at Vancouver International Airport (KYVR) and Seattle-Tacoma International Airport (SeaTac or KSEA) provide hourly estimates of vertical temperature profiles (e.g., https://a.atmos.washington.edu/marka/tha.cgi?sea).

Table 4-3. Upper Air (Radiosonde) Stations in the Western/Pacific Region.

Station, Location	Latitude, Longitude (°)
Yakukat, Alaska	59.51, -139.66
Whitehorse, Yukon	60.70, -135.06
Fort Nelson, British Columbia	58.83, -122.60
Edmonton-Stony Plain, Alberta	53.53, -114.10
Prince George, British Columbia	53.90, -122.80
Kelowna, British Columbia	49.97, -119.38
Spokane, Washington	47.68, -117.63
Quillayute, Washington	47.95, -127.36
Port Hardy, British Columbia	50.68, -127.36
Annette Island, Alaska	55.03, - 131.56

4.6 PROCESSING WRF DATA TO PHOTOCHEMICAL INPUTS

This section describes the tools to process WRF output data into the input formats needed for the recommended photochemical models.

4.6.1 PROCESSING FOR CMAQ

WRF 3-D gridded output fields, land cover categories, and topography are processed into formats required by CMAQ using the Meteorology-Chemistry Interface Processor (MCIP). MCIP also diagnoses several additional meteorological fields from WRF data that are needed by CMAQ. These are mainly related to characterizing sub-grid clouds from aqueous chemistry, convective mixing, and wet scavenging.

4.6.2 PROCESSING FOR CAMX

The CAMx preprocessor called WRFCAMx translates WRF 3-D gridded output fields and 2-D topography into formats required by CAMx. It also translates WRF's land cover categories into the specific land cover types used by CAMx. WRFCAMx also diagnoses several additional fields from WRF data that are needed by CAMx, including vertical turbulent exchange coefficients (or diffusivities) and sub-grid cloud information. Several options are available to calculate diffusivities, and the user should select the approach that matches the boundary layer scheme employed in WRF and document that selection in the Photochemical Modelling Plan. WRFCAMx allows for subsets of the WRF layer structure.

4.6.3 PROCESSING FOR SCICHEM

SCICHEM meteorological requirements are flexible, and SCICHEM can handle a variety of inputs from standard surface and upper air observations to gridded meteorological fields. As recommended above, SCICHEM should be run with 3-D meteorological fields derived using WRF. WRF output files can be used directly to drive SCICHEM.

The US EPA has developed the Mesoscale Model Interface Program (MMIF; US EPA 2022e). MMIF processes WRF output to develop 3-D hourly-varying meteorological files for direct input to SCICHEM. MMIF does not perform any coordinate transformation. Therefore, SCICHEM must be run in the same coordinate system and map projection as WRF. In addition, MMIF does not provide output with a grid resolution finer than the WRF grid, and MMIF cannot process additional observation data as well. The use of MMIF should be identified in the Photochemical Modelling Plan.

5. PHOTOCHEMICAL MODEL SET UP AND APPLICATION

This section recommends available sources of data and methods to develop initial/boundary conditions and lists optimal model configurations.

5.1 INITIAL AND BOUNDARY CONDITIONS

5.1.1 PHOTOCHEMICAL GRID MODELS

Initial conditions specify the 3-D distribution of all pollutants throughout all modelling grids at the start of a simulation. Boundary conditions specify the time-varying 2-dimensional (2-D) distribution of all pollutants along the lateral boundary “walls” of the outermost modelling grid. PGM simulated results in the outermost grid are then used to define boundary conditions for any nested grids. External sources of data are needed to specify initial conditions for each grid, and boundary conditions for the outermost grid.

In the past, PGM initial/boundary conditions were grossly estimated from sparse observational data or set to typical concentration profiles, which led to large simulation errors attributed to these inputs. For more than a decade, initial/boundary conditions have been developed from the output of global chemical transport models, much like how large-scale or global meteorological analyses are used to define initial/boundary conditions for NWP models like WRF. CMAQ and CAMx preprocessors are available to process global model output to initial/boundary conditions for regional PGM applications anywhere in the world (e.g., Ramboll 2022a).

- **Recommendation**: Use output from the Community Atmosphere Model with Chemistry (CAM-Chem, NCAR, 2022d) global model to develop initial/boundary conditions for PGMs. NCAR runs CAM-Chem routinely and provides an on-line library of 6-hourly CAM-Chem output datasets going back to 2001; or
- **Recommendation**: Use output from the GEOS-Chem global model (Harvard, 2022) to develop initial/boundary conditions, if such datasets are readily available for the Baseline year, or if you are capable of running GEOS-Chem yourself. Harvard does not run GEOS-Chem operationally and does not post output files.

CAM-Chem data are available since 2001 every 6 hours on a global grid with 0.9x1.24 degree (~100 km) horizontal resolution and 56 vertical levels. Posted data are current up to about 2 years prior to the current year.

GEOS-Chem output data are usually produced every 3 hours on a global grid with 2x2.5 degree (~250 km) horizontal resolution and 72 vertical levels.

5.1.2 SCICHEM

As a single source Lagrangian puff model, SCICHEM does not require initial and boundary conditions. As discussed above, however, SCICHEM does require time-varying gridded fields of background pollutant concentrations in order to appropriately perform photochemistry. SCICHEM is flexible in how background concentrations can be specified for a single source application. It can use a single set of representative background concentrations (i.e., constant over space and time) or hourly varying 3-D background concentrations from a PGM, such as CMAQ or CAMx. Either of two approaches are recommended, and the choice of which to use should be documented in the Photochemical Modelling Plan:

- **Recommendation**: Consider using SCICHEM datasets containing horizontally uniform, vertically varying (18 layers up to 3.5 km), monthly averaged, diurnally varying (hourly) background concentrations, which have been developed for several state-level regions of the US (i.e., Washington State could be used for the LFV), processed from a 2011 simulation using CAMx (EPRI, 2021); or
- **Recommendation**: Use hourly, 3-D PGM output specific to the LFV, which provides realistic, spatial and temporally varying chemically balanced background concentration values that will result in the most credible single source ozone and $PM_{2.5}$ impacts.

The background chemistry processor distributed with SCICHEM allows users to create background concentration fields for any region of interest from available CAMx or CMAQ outputs.

5.2 RADIATION AND PHOTOLYSIS PARAMETERS

5.2.1 CMAQ

CMAQ calculates photolysis rates inline as the model runs, using an algorithm called FASTJ. The routine considers several environmental parameters including adjustments for the presence of clouds and aerosol loadings and profiles. An older CMAQ option remains to calculate photolysis rates externally using the JPROC preprocessor and to pass those calculations to CMAQ as an input file. FASTJ is the simpler option and has been shown to result in similar performance as JPROC.

- **Recommendation**: Use the FASTJ inline photolysis rate calculation method.

5.2.2 CAMX

CAMx requires an external calculation of photolysis rates for key photolytic reactions. The Tropospheric Ultraviolet and Visible (TUV) radiation model developed by NCAR has been adapted to generate a multi-dimensional look-up table of clear sky photolysis reaction rates specific to the photochemical mechanisms available in CAMx. A CAMx preprocessor called O3MAP is used to prepare daily total atmospheric ozone column data from publicly available, satellite-derived datasets for TUV and CAMx. As CAMx runs, an inline adjustment is applied to clear sky photolysis rates to account for clouds and aerosols.

- **Recommendation**: Use TUV and O3MAP to calculate clear sky photolysis inputs for CAMx.

5.2.3 SCICHEM

SCICHEM provides an input photolysis rate look-up table that consists of clear sky rates for each photolytic reaction. SCICHEM also adjusts rates for the presence of clouds.

- **Recommendation**: Use the clear sky photolysis rate table provided with SCICHEM.

5.3 MODEL OPTIONS AND SETTINGS

Key configuration options and settings for each model are listed and described below, along with recommended settings. Note that only the key chemical and physical options are listed here; numerous other options and settings related to I/O are left to the user to determine using expert judgement. Carefully consult the respective user's guides for each model and document any deviation from the recommended options and settings along with the rationale in the Photochemical Modelling Plan.

5.3.1 RECOMMENDATIONS FOR CMAQ

CMAQ requires two approaches to select major chemical and physical options: (1) as compile-time settings that fix the model configuration to the user's particular specifications, and (2) as run-time settings that are controlled in the run script that executes the model.

5.3.1.1 CMAQ COMPILE-TIME SETTINGS

To select the options listed in Table 5-1 the user must configure the "makefile" build script and recompile CMAQ to create a new executable. Several CMAQ science modules have more than one option (select only one in the makefile), while others only have a single setting that cannot be changed (not included in the Table 5-1). See the CMAQ User Manual for complete information.

Table 5-1. Recommended CMAQ compile-time settings.

Variable	Description	Recommendation
set potvortO3	A shell variable. Uncomment this line to build CMAQ with potential vorticity free troposphere ozone scaling (for hemispheric model applications).	Leave commented out with the "#" character
ModDriver	The generalized coordinate driver module. driver/wrf (default): use WRF-based scheme for mass conserving advection; select this option when using WRF meteorology. driver/yamo: use Yamartino scheme for mass conserving advection. driver: For CMAQ v5.3 and higher.	driver/wrf (CMAQ v5.2.1 and lower) driver (CMAQ v5.3 and higher)
ModCpl	Mass coupling concentration conversion module. couple/gencoor_wrf (default): Coupling scheme compatible with the WRF-based advection scheme; select this option when ModDriver is set to driver/wrf or driver. couple/gencoor: Coupling scheme compatible with the Yamartino advection scheme; select this option when ModDriver is set to driver/yamo. couple/gencoor_local_cons: Available in CMAQ v5.3 and higher, advects air density and re-diagnoses the vertical velocity field according to the layer-by-layer mass continuity equation which guarantees that the CCTM advected density matches that derived from the driving meteorological inputs (not recommended).	couple/gencoor_wrf (all CMAQ versions)
ModVadv	Vertical advection module. vadv/wrf (default): use the WRF omega calculation with the Piecewise Parabolic Method (PPM) to calculate vertical advection; this module should be used only with WRF meteorology. vadv/yamo: use the global mass conserving scheme to calculate vertical advection. vadv/wrf_cons: For CMAQ v5.3 and higher vadv/local_cons: Available in CMAQ v5.3 and higher (not recommended).	vadv/wrf (CMAQ v5.2.1 and lower) vadv/wrf_cons (CMAQ v5.3 and higher)
ModCgrds	CMAQ model species configuration module. spcs/cgrid_spcs_nml (default): namelist files used to configure model species. spcs/cgrid_specs_icl: use Fortran INCLUDE files to configure model species.	spcs/cgrid_spcs_nml
ModPhot	Photolysis calculation module. phot/inline (default): calculate photolysis rates inline using simulated aerosols and ozone concentrations. phot/table: calculate clear sky photolysis rates offline using the program JPROC.	phot/inline
Mechanism	Chemistry mechanism for gas, aerosol, and aqueous chemistry. See the CMAQ Mechanism Definitions Table in the User Manual.	cb6r3_ae6nvPOA_aq (CMAQ v5.2.1 and lower) cb6r3_ae7_aq (CMAQ v5.3 and higher)
Tracer	Specifies tracer species. Invoking inert tracer species requires defining the tracers in namelist files and compiling the CMAQ	trac0 (default)

Variable	Description	Recommendation
	programs with these files. The setting corresponds to the directory name in the $CMAQ_HOME/CCTM/src/MECHS directory. trac0 (default): do not use any tracers.	
ModGas	Gas-phase chemistry solver module. gas/smvgear: SMVGEAR chemistry solver. gas/ros3: Rosenbrock chemistry solver. gas/ebi_mechanism (default): Euler Backward Iterative solver.	gas/ebi_mechanism
ModCloud	CMAQ cloud module for modelling the impacts of clouds on deposition, mixing, photolysis, and aqueous chemistry. cloud/acm_ae6: ACM cloud processor that uses the ACM methodology to compute convective mixing with heterogeneous chemistry for AERO6 (Default in CMAQ v5.2.1 and lower). cloud/acm_ae7: ACM cloud processor that uses the ACM methodology to compute convective mixing with heterogeneous chemistry for AERO7 (CMAQ v5.3 and later). cloud/acm_ae6_mp: ACM cloud processor that uses the ACM methodology to compute convective mixing with heterogeneous chemistry for AERO6 and air toxics; this is the multipollutant mechanism in CMAQv5. cloud/acm_ae6_kmt: ACM cloud processor that uses the ACM methodology to compute convective mixing with heterogeneous chemistry for AERO6 and aqueous chemistry with kinetic mass transfer (KMT) and Rosenbrock solver. cloud/acm_ae6i_kmti: ACM cloud processor that uses the ACM methodology to compute convective mixing with heterogeneous chemistry for AERO6 and aqueous chemistry with kinetic mass transfer (KMT) and Rosenbrock solver with an extension to simulate the aqueous phase formation of SOA in cloud droplets. cloud/acm_ae7_kmt2: ACM cloud processor that uses the ACM methodology to compute convective mixing with heterogeneous chemistry for AERO7 and aqueous chemistry with the revised extended kinetic mass transfer (KMT2) and Rosenbrock solver. Available in CMAQ v5.3 and later. Recommended only for research applications because of run time penalties. cloud/acm_ae7_kmtbr: ACM cloud processor that uses the ACM methodology to compute convective mixing with heterogeneous chemistry for AERO7 and aqueous chemistry with kinetic mass transfer (KMT) and Rosenbrock solver. Available in CMAQ v5.3 and later. Suitable for simulations over marine environments; requires the selection of the “cb6r3m_ae7_kmtbr” option for the gas-phase chemistry mechanism. Recommended only for research applications because of run time penalties.	cloud/acm_ae6 (CMAQ v5.2.1 and lower) cloud/acm_ae7 (CMAQ v5.3 and higher)
DepMod	Selects module for inline dry deposition velocity calculations (CMAQ v5.3 and later).	DepMod

5.3.1.2 CMAQ RUN-TIME SETTINGS

The Linux environment variables listed in Table 5-2 are invoked during execution of CMAQ and are set in the run script by using the syntax:

```
setenv variable value
```

where each variable name is listed below with the recommended value. See the CMAQ User Manual for complete information.

Table 5-2. Recommended CMAQ run-time settings.

Variable	Description	Recommendation
MECH	Chemical mechanism; must match the Mechanism variable setting in the CMAQ build script (No default).	cb6r3_ae6nvPOA_aq (CMAQ v5.2.1 and lower) cb6r3_ae7_aq (CMAQ v5.3 and higher)
CONC_SPCS	Model species to be written to the CONC output file (all species if commented out).	Output all species
CONC_BLEV_ELEV	Vertical model layer range for output concentrations (all layers if commented out).	1 1 (only surface layer)
AVG_CONC_SPCS	Model species to be time-averaged to the ACONC file for each output time step, for any of the species output to the CONC file (all species if commented out).	Output all species
ACONC_BLEV_ELEV	Vertical model layer range for averaged output concentrations (all layers if commented out).	1 1 (only surface layer)
CTM_WB_DUST	Calculate inline windblown dust emissions (Y or N); requires certain land use input files.	N
CTM_ERODE_AGLAND	Use optional erodible agricultural land classifications for windblown dust emissions (Y or N); requires certain crop data.	N (CMAQ v5.2.1 and lower) N/A for CMAQ v5.3 and higher
CTM_LTNG_NO	Activate lightning NO emissions (Y or N); requires setting additional variables.	Y
KZMIN	Determine minimum eddy diffusivity based on urban land use fraction (Y or N).	Y
CTM_ILDEPV	Calculate inline deposition velocities (Y or N) using the M3DRY module (only in CMAQ v5.2.1 and lower). CMAQ v5.3 and higher always calculates inline deposition velocities using either the M3DRY or STAGE modules (see Table 5-1).	Y (CMAQ v5.2.1 and lower) N/A for CMAQ v5.3 and higher
CTM_MOSAIC	Calculate land use specific deposition velocities and fluxes (Y or N). In CMAQ v5.3 and higher, this option is only available when using the STAGE deposition module.	N
CTM_FST	Use MOSAIC method to get land use specific stomatal flux (Y or N).	N
CTM_ABFLUX	Activate fertilizer ammonia bidirectional flux for inline emissions and deposition velocities (Y or N); requires four additional input files that include gridded fractional crop	N

Variable	Description	Recommendation
	distributions, soil properties, fertilizer conditions, and an agricultural soil initial conditions file.	
CTM_HGBIDI	Activate mercury bidirectional flux for inline emissions and deposition velocities (Y or N).	N
CTM_SFC_HONO	Calculate surface HONO interactions (Y or N).	N
CTM_GRAV_SETL	Activate gravitational sedimentation for aerosols (Y or N).	Y
CTM_BIOGEMIS	Calculate biogenic emissions (Y or N); requires setting several other variables.	N (calculate externally)
CTM_PT3DEMIS	Calculate plume rise for elevated point sources (Y or N); requires setting several other variables (only in CMAQ v5.2.1 and lower). CMAQ v5.3 and higher always calculates inline plume rise.	Y (CMAQ v5.2.1 and lower) N/A for CMAQ v5.3 and higher
CTM_PROCAN	Activate process analysis tool (Y or N); requires configuration input files.	N
NPTGRPS/N_EMIS_PT	Number of input point source elevated emission sector file groups (NPTGRPS for CMAQ v5.2.1 and lower, N_EMIS_PT for CMAQ v5.3 and higher).	As needed
CTM_EMLAYS	Number of emissions layers for calculating elevated point source emissions (default = all, only in CMAQ v5.2.1 and lower). In CMAQ v5.3 and higher, all layers are used.	All (CMAQ v5.2.1 and lower) N/A for CMAQ v5.3 and higher
LTNGNO	Define inline or offline lightning emissions calculation: set to path for gridded lightning NO emissions file or set to “inline” which requires the LTNGPARAMS variable.	Inline
USE_NLDN	Use hourly NLDN strikes file to compute inline lightning NO emissions (Y or N).	N
LTNGPARAMS	Use lightning parameters configuration file to compute inline lightning NO emissions (Y or N); requires input hourly flash count observations and other parameters.	N
LOG_START	Convective precipitation (RC) value to transition the lightning NO emissions calculation from linear to log linear (default = 0.9, only in CMAQ v5.2.1 and lower).	0.9 (CMAQ v5.2.1 and lower) N/A for CMAQ v5.3 and higher
PX_VERSION	Indicate whether the Pleim-Xiu land-surface model was used for the input meteorology (Y or N); requires soil moisture, soil temperature, and soil type variables for use in the calculation of soil NO emissions.	Y

5.3.2 RECOMMENDATIONS FOR CAMX

All of the chemical and physical settings available in CAMx, including all Probing Tools, are chosen at run time. This simplifies the CAMx build process. The variables below are set using the Fortran “namelist” convention. The namelist syntax is:

```
variable = value,
```

where each variable name is listed in Table 5-3 with the recommended value. See the CAMx User Manual for complete information.

Table 5-3. Recommended CAMx run-time settings.

Variable	Description	Recommendation
Flexi_Nest	Allow only certain inputs for nested grid (missing input fields will be interpolated or assigned) (True or False).	False
Advection_Solver	Solver to calculate horizontal advection (PPM or Bott).	PPM
Chemistry_Parameters	Set path to the chemistry mechanism definition file.	CAMx7.0.chemparam.CB6r4_CF2
Chemistry_Solver	Numerical solver approach to calculate gas-phase chemistry (EBI or LSODE).	EBI
PiG_Submodel	Invoke Plume-in-Grid for user-selected set of point sources (None, GREASD, IRON); requires special post-SMOKE file manipulations to select point sources for the treatment. Note your choice to use PiG and rationale in the Photochemical Modelling Plan.	None
Probing_Tool	Invoke a Probing Tool (None, SA, DDM, PA, RTRAC); requires additional input files, carefully consider their use relative to "brute force" runs that may be easier to set up and evaluate for single source applications. Note your choice to use Probing Tools and rational in the Photochemical Modelling Plan.	None
Drydep_Model	Activate dry deposition calculations (None, Wesely89, Zhang03).	Zhang03
Wet_Deposition	Activate wet deposition calculations (True or False)	True
ACM2_Diffusion	Activate ACM2 vertical diffusion (True or False)	True
Surface_Model	Activate the surface chemistry model (True or False); requires addition inputs of surface reactions and rates	False
Inline_Ix_Emissions	Activate inline marine halogen emissions for ozone chemistry (True or False)	True
Super_Stepping	Activate super stepping time step calculation, which allows CAMx to run faster with negligible to minor loss of accuracy in transport calculations aloft (True or False).	True
Bidi_NH3_Drydep	Activate bidirectional ammonia flux treatment (True or False)	False
Gridded_Emissions	Use gridded 2-D and 3-D emission inputs (True or False)	True
Point_Emissions	Use elevated point source emission inputs (True or False)	True
Ignore_Emission_Dates	Ignore synchronizing emission file dates to simulation date (True or False); use for single representative day of emission inputs to represent a multiple day simulation.	False (depends on how emission inputs were developed)
Output_Species_Names	List of species to output (ALL or list each)	ALL
Average_Output_3D	Output 3-D grid of concentrations (True or False)	False
NetCDF_Format_Output	Write output to netCDF files (True or False)	True

5.3.3 RECOMMENDATIONS FOR SCICHEM

SCICHEM has relatively few user-selectable settings as compared to the PGMs, and there are no compile-time options. The SCICHEM User Manual (EPRI, 2021) provides default or recommended run-time options for most SCICHEM applications.

5.3.3.1 SCICHEM CHEMISTRY

The SCICHEM "multicomponent" file specifies the photochemical mechanism, model species, their physical and chemical properties, chemical reactions, and associated reaction rate constants, etc. The multicomponent file is specified in the SCICHEM control file (Section 5.3.3.2). There are three multicomponent files provided with SCICHEM, ranging in complexity from full photochemical modelling applications to a null-reaction mechanism for inert (tracer) modelling.

- **Recommendation**: Use the full photochemical mechanism multicomponent file.

The SCICHEM multicomponent file also provides default background concentrations for each chemical species which are used only if the user does not provide a background chemistry file name. Use of default background values from the multicomponent chemistry files is not recommended.

- **Recommendation:** Specify a background chemistry file obtained from a PGM simulation, if such information is available, or from Washington State background concentrations distributed with SCICHEM as described in Section 5.1.2.

5.3.3.2 SCICHEM CONTROL FILE

Key options in the SCICHEM control file and recommended or default values are provided in Table 5-4. For most of these options, default values are used if the parameters are not included in the control file.

5.3.3.3 SCICHEM METEOROLOGY SCENARIO FILE

A meteorology scenario file is needed that specifies the meteorological inputs (i.e., if the data are observational or gridded data from a prognostic model) and several other project dependent variables. More information is provided in the SCICHEM User Manual. Most of these variables are required and have no recommended or default values. Other variables that can be specified are recommended in Table 5-5. Note that most of these variables are related to the use of observational meteorological data in the SCICHEM simulation and are not relevant for gridded files based on NWP model (e.g., WRF) outputs.

- **Recommendation**: Do not use observational meteorological data to drive SCICHEM simulations, use NWP model output instead.

Table 5-4. Recommended SCICHEM Control File settings.

Variable	Description	Recommendation
dynamic	Flag to include momentum and buoyancy dynamics (T or F); if set to “F” then puffs are treated as passive (default = F).	T
dense_gas	Flag to include dense gas effects (T or F) (default = F).	F
static	Flag to perform quasi-steady calculation of continuous sources (T or F) (default = T)	T
run_mode	Use standard run mode (0) or fast mode (1); if set to “1” vertical and horizontal resolutions are coarsened and the merge criteria for puffs are relaxed (default = 0).	0
t_avg	Conditional averaging time (seconds) for defining diffusive component of turbulence (no default).	0
wwtrop	Minimum tropospheric vertical turbulence fluctuation (m^2/s^2) (default = 0.01).	0.01
sltrop	Tropospheric vertical length scale (m) used as the minimum value (default = 10).	10
epstrop	Tropospheric energy dissipation rate (m^2/s^3) (default = 0.0004).	0.0004
uu_calm	Minimum horizontal velocity fluctuation variance (m^2/s^2) (default = 0.25).	0.25
sl_calm	Horizontal length scale (m) associated with uu_calm (default = 1000).	1000
nzbl	Number of boundary layer vertical grid levels (default = 11).	Depends on input data
vres	Spacing parameter (m) that limits the vertical growth of a puff (default = 250).	250
hres	Spacing parameter (in horizontal domain units, e.g., km or degrees) that limits the horizontal growth of a puff. For observation-based meteorology, the default is one-tenth of the domain; for gridded meteorology the resolution is always the same as that of the meteorological fields.	Use default
mgrd	Grid resolution parameter that limits the horizontal growth of a puff. The horizontal size of the puffs will be limited to 2^{mgrd} x hres (default = 2).	1
smpfile	Path of file with sampler (receptor) locations for sampler output. Consider this setting and document in the Photochemical Modelling Plan (no default).	None

Table 5-5. Recommended SCICHEM Meteorology Scenario File settings.

Variable	Description	Recommendation
nearest_sfc	Number of nearest surface observation stations used for meteorology interpolation (if the data are observational).	Default
nearest_prf	Number of nearest upper air profile observation stations used for meteorology interpolation (if the data are observational).	Default
lmc_ua	Flag to calculate mass consistent adjustment to observational wind fields (MCWIF; T or F)	T
alpha_max	Maximum value of vertical adjustment parameter for MCWIF (if lmc_ua is “T” and a terrain file is specified).	1
alpha_min	Minimum value of vertical adjustment parameter for MCWIF (if lmc_ua is “T” and a terrain file is specified).	0
max_iter_ac	Maximum iterations allowed for MCWIF calculation using the point relaxation method.	10000
ac_eps_ac	Convergence criterion for MCWIF calculation using the point relaxation method.	0.01
max_iter	Maximum iterations allowed for MCWIF calculation using the FFT method.	30
ac_eps	Convergence criterion for MCWIF calculation using the FFT method.	0.00001
lout_met	Flat to output observed meteorological fields	F
lout_2D	Flag to output 2-D gridded meteorological fields	F
lout_3D	Flag to output 3-D gridded meteorological fields	F

5.3.3.4 SCICHEM RECEPTORS

Receptors are the locations within the model domain where the concentration/deposition predictions are output. SCICHEM saves ground-level concentrations in a spatially and temporally varying adaptive grid that is determined internally as the model runs, avoiding the need for the user to specify receptor grid information and providing a complete description of the concentration field. The information required to process gridded data for a given hour is embedded in the output file. The SCICHEM postprocessor is used to extract ground-level concentrations at any number of arbitrary receptors. The user specifies a list of receptor coordinates and the postprocessor extracts the values for user-specified averaging times (e.g., 8-hour rolling averages) and rankings (e.g., 4th highest).

The SCICHEM option to specify elevated receptors (i.e., “flagpoles”) creates a text file with values at user-specified output intervals that can be read by spreadsheet and other data processing tools.

- **Recommendation**: If elevated “flagpole” receptors are necessary to assess Project impacts, provide a list of such receptors at SCICHEM runtime. The use of elevated receptors will not be necessary in most cases.

The location and number of receptors must be judiciously selected in order to achieve a balance between enough receptors to resolve maximum concentrations and too many receptors where computer processing times and output files become unreasonable. Refer to the British Columbia Air Quality Dispersion Modelling Guideline (ENV, 2022) for additional recommendations on receptor locations. The SCICHEM receptor configuration should be defined in the Photochemical Modelling Plan.

5.4 MODEL OUTPUT AND FREQUENCIES

General recommendations for modelled output include:

- **<u>Recommendation</u>**: Configure the models to output surface concentrations hourly. This serves two purposes:
  - It allows for direct comparison to measurement data (hourly is the minimum measurement averaging period) to support the model performance evaluation.
  - It allows maximum flexibility to calculate longer term metrics ranging from daily averages (8-hour maximum, daytime average, 24-hour average) to monthly, seasonal and annual averages and frequency distributions consistent with air quality objectives and standards.
- **<u>Recommendation</u>**: Configure the models to output ozone and all aerosol chemical components that comprise $PM_{2.5}$ mass.

The minimum list of specific chemical species that should be output from each model and the methods to derive total $PM_{2.5}$ mass from each are described in sections 5.4.1, 5.4.2 and 5.4.3.

5.4.1 CMAQ

Table 5-6 lists CMAQ gas-phase model precursor and ozone species that should be output for any chosen gas-phase chemistry mechanism, while Tables 5-7a and 5-7b list minimum model species for two possible aerosol schemes.

Table 5-6. The minimum CMAQ gas-phase (ppm) model species recommended for output.

Label	Description
O3	Ozone, ppm
NO	Nitric oxide, ppm
NO2	Nitrogen dioxide, ppm
HNO3	Nitric acid, ppm
SO2	Sulphur dioxide, ppm
NH3	Ammonia, ppm

Additional recommendations include:

- **<u>Recommendation</u>**: Do not use the semi-volatile primary organic aerosol (POA) scheme – its novelty and additional complexity may not necessarily translate to dramatic improvements in the representation of organic aerosols, particularly for cool environments like the LFV where most semi-volatile POA emissions likely remain in the aerosol form;
- **<u>Recommendation</u>**: Use Table 5-7 for the list of CMAQ particulate model species that should be output when using the "AE6NVPOA" aerosol scheme; or
- **<u>Recommendation</u>**: Use Table 5-8 for the list of CMAQ particulate model species that should be output when using the "AERO7" aerosol scheme.

The aerosol size distribution in CMAQ is modelled as the superposition of three log-normal distributions or modes. These modes include the Aitken mode (I-mode) representing homogeneous gas-to-particle conversion, the accumulation mode (J-mode) representing most of the fine particle mass, and coarse mode (K-mode) representing sizes beyond $PM_{2.5}$.

- **Recommendation**: Calculate total $PM_{2.5}$ mass by summing the I- and J-mode masses for each species, which is the recommended approach by the US EPA (2018).

Table 5-7. The minimum CMAQ particle-phase (µg/m^3) model species recommended for output with the AE6NVPOA aerosol scheme.

Size Mode		Description
I-mode	**J-mode**	
ASO4I	ASO4J	Fine mode sulphate, µg/m^3
ANO3I	ANO3J	Fine mode nitrate, µg/m^3
ANH4I	ANH4J	Fine mode ammonium, µg/m^3
AECI	AECJ	Fine mode elemental carbon, µg/m^3
APOCI	APOCJ	Fine mode primary organic carbon, µg/m^3
APNCOMI	APNCOMJ	Fine mode primary non-carbon mass associated with organic carbon, µg/m^3
	AALK1J	Secondary organic mass from lower volatility products of alkanes, µg/m^3
	AALK2J	Secondary organic mass from higher volatility products of alkanes, µg/m^3
	AXYL1J	Secondary organic mass from lower volatility products of xylenes, µg/m^3
	AXYL2J	Secondary organic mass from higher volatility products of xylenes, µg/m^3
	AXYL3J	Secondary organic mass from non-volatile products of xylenes, µg/m^3
	ATOL1J	Secondary organic mass from lower volatility products of toluene, µg/m^3
	ATOL2J	Secondary organic mass from higher volatility products of toluene, µg/m^3
	ATOL3J	Secondary organic mass from non-volatile products of toluene, µg/m^3
	ABNZ1J	Secondary organic mass from lower volatility products of benzene, µg/m^3
	ABNZ2J	Secondary organic mass from higher volatility products of benzene, µg/m^3
	ABNZ3J	Secondary organic mass from non-volatile products of benzene, µg/m^3
	ATRP1J	Secondary organic mass from lower volatility products of monoterpenes, µg/m^3
	ATRP2J	Secondary organic mass from higher volatility products of monoterpenes, µg/m^3
	AISO1J	Secondary organic mass from higher volatility products of isoprene, µg/m^3
	AISO2J	Secondary organic mass from lower volatility products of isoprene, µg/m^3
	AISO3J	Secondary organic mass from non-volatile products of isoprene, µg/m^3
	ASQTJ	Secondary organic mass from semi-volatile products of sesquiterpenes, µg/m^3
	APAH1J	Secondary organic mass from lower volatility products of PAH, µg/m^3
	APAH2J	Secondary organic mass from higher volatility products of PAH, µg/m^3
	APAH3J	Secondary organic mass from non-volatile products of PAH, µg/m^3
	AOLGAJ	Non-volatile organic mass from oligomerization of anthropogenic SOA, µg/m^3
	AOLGBJ	Non-volatile organic mass from oligomerization of biogenic SOA, µg/m^3
	AORGCJ	Non-volatile organic mass from in-cloud SOA formation, µg/m^3
	AGLYJ	Non-volatile organic mass from heterogeneous uptake of glyoxal and methylglyoxal onto particles (for CB6r3 or AE6I only), µg/m^3
ACLI	ACLJ	Fine mode particulate chloride, µg/m^3

Size Mode		Description
I-mode	**J-mode**	
ANAI	ANAJ	Fine mode sodium, µg/m^3
	AMGJ	Fine mode magnesium, µg/m^3
	AKJ	Fine mode potassium, µg/m^3
	ACAJ	Fine mode calcium, µg/m^3
	AFEJ	Fine mode iron, µg/m^3
	AALJ	Fine mode aluminum, µg/m^3
	ASIJ	Fine mode silicon, µg/m^3
	ATIJ	Fine mode titanium, µg/m^3
	AMNJ	Fine mode manganese, µg/m^3
AOTHRI	AOTHRJ	Remaining un-speciated fine mode primary PM, µg/m^3

Table 5-8. The minimum CMAQ particle-phase (µg/m^3) model species recommended for output with the AERO7 aerosol scheme.

Size Mode		Description
I-mode	**J-mode**	
ASO4I	ASO4J	Fine mode sulphate, µg/m^3
ANO3I	ANO3J	Fine mode nitrate, µg/m^3
ANH4I	ANH4J	Fine mode ammonium, µg/m^3
AECI	AECJ	Fine mode elemental carbon, µg/m^3
APOCI	APOCJ	Fine mode primary organic carbon, µg/m^3
APNCOMI	APNCOMJ	Fine mode primary non-carbon mass associated with organic carbon, µg/m^3
	AAVB1J	Secondary organic mass from lower volatility products of anthropogenic VOCs (benzene, toluene, xylene, PAHs, alkanes), µg/m^3
	AAVB2J	Secondary organic mass from higher volatility products of anthropogenic VOCs (benzene, toluene, xylene, PAHs, alkanes), µg/m^3
	AAVB3J	Secondary organic mass from higher volatility products of anthropogenic VOCs (benzene, toluene, xylene, PAHs, alkanes), µg/m^3
	AAVB3J	Secondary organic mass from higher volatility products of anthropogenic VOCs (benzene, toluene, xylene, PAHs, alkanes), µg/m^3
	AMT1J	Secondary organic mass from low volatility products of monoterpene photooxidation, µg/m^3
	AMT2J	Secondary organic mass from low volatility products of monoterpene photooxidation, µg/m^3
	AMT3J	Secondary organic mass from high volatility products of monoterpene photooxidation, µg/m^3
	AMT4J	Secondary organic mass from high volatility products of monoterpene photooxidation, µg/m^3
	AMT5J	Secondary organic mass from high volatility products of monoterpene photooxidation, µg/m^3
	AMT6J	Secondary organic mass from high volatility products of monoterpene photooxidation, µg/m^3
	AMTNO3J	Semi volatile organic nitrates from monoterpene oxidation, µg/m^3
	AMTHYDJ	Organic pseudo-hydrolysis accretion product from monoterpene organic nitrates, µg/m^3

Size Mode		Description
I-mode	J-mode	
	AISO1J	Secondary organic mass from higher volatility products of isoprene, μg/m^3
	AISO2J	Secondary organic mass from lower volatility products of isoprene, μg/m^3
	AISO3J	Secondary organic mass from non-volatile products of isoprene, μg/m^3
	ASQTJ	Secondary organic mass from semi-volatile products of sesquiterpenes, μg/m^3
	AOLGAJ	Non-volatile organic mass from oligomerization of anthropogenic SOA, μg/m^3
	AOLGBJ	Non-volatile organic mass from oligomerization of biogenic SOA, μg/m^3
	AORGCJ	Non-volatile organic mass from in-cloud SOA formation, μg/m^3
	AORGH2OJ	Water associated with organic species of particulate matter, μg/m^3
	AGLYJ	Non-volatile organic mass from heterogeneous uptake of glyoxal and methylglyoxal onto particles (for CB6r3 or AE6I only), μg/m^3
ACLI	ACLJ	Fine mode particulate chloride, μg/m^3
ANAI	ANAJ	Fine mode sodium, μg/m^3
	AMGJ	Fine mode magnesium, μg/m^3
	AKJ	Fine mode potassium, μg/m^3
	ACAJ	Fine mode calcium, μg/m^3
	AFEJ	Fine mode iron, μg/m^3
	AALJ	Fine mode aluminum, μg/m^3
	ASIJ	Fine mode silicon, μg/m^3
	ATIJ	Fine mode titanium, μg/m^3
	AMNJ	Fine mode manganese, μg/m^3
AOTHRI	AOTHRJ	Remaining un-speciated fine mode primary PM, μg/m^3

5.4.2 CAMX

Table 5-9 lists the ozone, gas precursor, and $PM_{2.5}$ species that should be output by CAMx using any chosen gas-phase mechanism and using the standard “CF” aerosol scheme.

- **Recommendation**: Do not use the CAMx Volatility Basis Set (VBS) organic aerosol options for many of the same arguments discussed above for the CMAQ semi-volatile POA option; and
- **Recommendation**: Calculate total $PM_{2.5}$ mass by summing all PM components listed in the Table 5-9.

Table 5-9. The minimum CAMx gas (ppm) and particle phase (µg/m^3) model species recommended for output.

Label	Description
O3	Ozone, ppm
NO	Nitric oxide, ppm
NO2	Nitrogen dioxide, ppm
HNO3	Nitric acid, ppm
SO2	Sulphur dioxide, ppm
NH3	Ammonia, ppm
PSO4	Particulate sulphate, µg/m^3
PNO3	Particulate nitrate, µg/m^3
PNH4	Particulate ammonium, µg/m^3
NA	Particulate fine sodium, µg/m^3
PCL	Particulate fine chloride, µg/m^3
FPRM	Primary remaining un-speciated $PM_{2.5}$, µg/m^3
FCRS	Primary un-speciated crustal $PM_{2.5}$, µg/m^3
PEC	Primary fine elemental carbon, µg/m^3
POA	Primary fine non-volatile organic aerosol mass, µg/m^3
SOA1	Anthropogenic secondary organic mass from higher volatility products, µg/m^3
SOA2	Anthropogenic secondary organic mass from lower volatility products, µg/m^3
SOPA	Anthropogenic secondary organic mass from non-volatile products and polymerized semi-volatile SOA, µg/m^3
SOA3	Biogenic secondary organic mass from higher volatility products, µg/m^3
SOA4	Biogenic secondary organic mass from lower volatility products, µg/m^3
SOPB	Biogenic secondary organic mass from non-volatile products and SOA formed from aqueous reactions, µg/m^3

5.4.3 SCICHEM

Table 5-10 lists the SCICHEM gas-phase and aerosol-phase model species recommended for output. SCICHEM outputs plume increments and ambient background surface concentrations. Note that any species that are not emitted directly by the source of interest are considered in the background and omitted from the list of plume incremental concentrations. The SCICHEM postprocessor can use these outputs to report either source impacts (i.e., increments) or total (increment + background) concentrations based on a user-specified flag. Note that SCICHEM uses the same modal particle size representation as CMAQ.

SCICHEM allows the user to predefine output species groups, such as $PM_{2.5}$ and PM_{10}, in the multicomponent file. Examples of these predefined groups for $PM_{2.5}$ species are provided in Table 5-11. Note that new groups can also be defined by using previously defined groups as shown in the example for total $PM_{2.5}$ in the last entry of Table 5-11.

- **Recommendation**: Calculate total $PM_{2.5}$ concentrations by summing of all the Aitken (I) mode and accumulation (J) mode concentrations.

Table 5-10. The minimum SCICHEM gas (ppm) and particle-phase (µg/m^3) model species recommended for output.

Label	Description
O3	Ozone, ppm
NO	Nitric oxide, ppm
NO2	Nitrogen dioxide, ppm
HNO3	Nitric acid, ppm
SO2	Sulphur dioxide, ppm
NH3	Ammonia, ppm (if emitted from the modelled source, otherwise omitted)
ASO4J, ASO4I	Fine mode sulphate, µg/m^3
ANO3J, ANO3I	Fine mode nitrate, µg/m^3
ANH4J, ANH4I	Fine mode ammonium, µg/m^3
AECJ, AECI	Fine mode elemental carbon, µg/m^3
AORGPAJ, AORGPAI	Fine mode primary organic carbon, µg/m^3
AALKJ	Secondary organic mass from products of long-chain alkanes, µg/m^3
AXYL1J	Secondary organic mass from lower volatility products of xylenes, µg/m^3
AXYL2J	Secondary organic mass from higher volatility products of xylenes, µg/m^3
AXYL3J	Secondary organic mass from non-volatile products of xylenes, µg/m^3
ATOL1J	Secondary organic mass from lower volatility products of toluene, µg/m^3
ATOL2J	Secondary organic mass from higher volatility products of toluene, µg/m^3
ATOL3J	Secondary organic mass from non-volatile products of toluene, µg/m^3
ABNZ1J	Secondary organic mass from lower volatility products of benzene, µg/m^3
ABNZ2J	Secondary organic mass from higher volatility products of benzene, µg/m^3
ABNZ3J	Secondary organic mass from non-volatile products of benzene, µg/m^3
ATRP1J	Secondary organic mass from lower volatility products of monoterpenes, µg/m^3
ATRP2J	Secondary organic mass from higher volatility products of monoterpenes, µg/m^3
AISO1J	Secondary organic mass from higher volatility products of isoprene, µg/m^3
AISO2J	Secondary organic mass from lower volatility products of isoprene, µg/m^3
AISO3J	Secondary organic mass from non-volatile products of isoprene, µg/m^3
ASQTJ	Secondary organic mass from semi-volatile products of sesquiterpenes, µg/m^3
AOLGAJ	Non-volatile organic mass from oligomerization of anthropogenic SOA, µg/m^3
AOLGBJ	Non-volatile organic mass from oligomerization of biogenic SOA, µg/m^3
AORGCJ	Non-volatile organic mass from in-cloud SOA formation, µg/m^3
ACLJ, ACLI	Fine mode particulate chloride, µg/m^3
ANAJ, ANAI	Fine mode particulate sodium, µg/m^3
A25J, A25I	Remaining un-speciated fine mode primary PM, µg/m^3

Table 5-11. Examples of user defined SCICHEM PM species groups (for output only).

Group Name	Group Constituents	Description
PSO4	ASO4J, ASO4I	Total $PM_{2.5}$ sulphate, µg/m^3
PNO3	ANO3J, ANO3I	Total $PM_{2.5}$ nitrate, µg/m^3
PNH4	ANH4J, ANH4I	Total $PM_{2.5}$ ammonium, µg/m^3
PSOA	AALKJ, AXYL1J, AXYL2J, AXYL3J, ATOL1J, ATOL2J, ATOL3J, ABNZ1J, ABNZ2J, ABNZ3J, ATRP1J, ATRP2J, AISO1J, AISO2J, AISO3J, ASQTJ, AOLGAJ, AOLGBJ, AORGCJ	Total $PM_{2.5}$ secondary organic aerosol (SOA) , µg/m^3
POC	AORGPAJ, AORGPAI	Total $PM_{2.5}$ primary organic carbon, µg/m^3
PEC	AECJ, AECI	Total $PM_{2.5}$ elemental carbon, µg/m^3
P25	A25J, A25I	Total other un-speciated primary $PM_{2.5}$, µg/m^3
PM25	PSO4, PNO3, PNH4, PSOA, POC, PEC, P25, ANAJ, ANAI, ACLJ, ACLI	Total $PM_{2.5}$, µg/m^3

6. POST PROCESSING

6.1 ASSESSING INCREMENTAL PROJECT IMPACTS

This section recommends approaches to assess Project impacts from the output of photochemical models. The postprocessing methods, calculated metrics, and evaluation techniques are developed to be consistent with the forms and averaging periods specific to the local air quality objectives for 1- and 8-hour ozone concentration, and for 24-hour and annual $PM_{2.5}$ mass concentration.

Project-specific modelling involves adding a source or set of sources associated with the new Project to a “Baseline” emission inventory and assessing impacts to ozone and $PM_{2.5}$ over the requisite spatial and time scales.

6.1.1 RECOMMENDATIONS FOR SCICHEM

SCICHEM should be run for the set of new or modified source(s) and impacts should be analyzed directly from the SCICHEM output. This is possible because SCICHEM differentiates individual plume increments from specific sources and so directly provides the spatial and temporal concentration impacts. The SCICHEM postprocessor is used to report either source impacts (i.e., increments) or total (increment + background) concentrations.

6.1.2 RECOMMENDATIONS FOR PGMS

Several methods may be considered to determine Project impacts from PGM output. Either of these approaches may be acceptable provided a rationale is included in the Photochemical Modelling Plan.

The most straightforward approach (“brute force”) involves running the model twice: (1) for the “Baseline” scenario without the new or modified source(s), and (2) for the “Project scenario” that combines Baseline emissions and the Project source(s). Results from the Baseline and Project scenarios are differenced in a manner that pairs them spatially and temporally. The brute force approach is an appropriate representation of a Project’s impact and sensitivity (to the extent that it is adequately represented by the model) because it explicitly considers air quality effects from adding or changing source emissions. When considering collective impacts from a small set of sources, brute force is the easiest way to apply PGMs and the easiest to understand.

If the brute force method becomes too time or computationally consuming, then “instrumented” methods or “Probing Tools” available in both CMAQ and CAMx should be used to estimate contributions and sensitivity for multiple sources in a single model run. However, output from these tools can be voluminous in cases where many sources are tracked simultaneously. Proper interpretation of results from this tool requires some familiarization and experience.

- **Recommendation**: Use the brute force method for assessing simple Project impacts or the collective impacts from a small set of sources; or
- **Recommendation**: Use instrumented methods to estimate contributions or sensitivity for multiple or complex sources combinations.

6.1.3 STEPS FOR ASSESSING OZONE IMPACTS

Recommendations: Follow the methods below for assessing ozone impacts:

- Modelled hourly ozone concentrations should be used to compare to the 1-hour objective as well as to calculate rolling 8-hour averages (e.g., hours 0-7, 1-8, etc.) to compare to the 8-hour objectives. Project ozone increments (impacts) and total ozone concentrations (all sources) should be time-averaged in this manner. These calculations should be performed for all grid cells covering the area of interest. To limit the quantity of data, this averaging can be limited to the months of May to September (i.e., warm season months when elevated ozone concentrations may occur).
- Cumulative frequency distributions of observed and predicted 8-hour average ozone from the "Baseline" scenario should be developed at key monitoring sites and presented. Cumulative frequency distributions of predicted 8-hour ozone that include the Project scenario should also be presented to illustrate source impacts over the range of the frequency distribution and allow an immediate assessment of if and when source impacts cause exceedances of the ozone objectives.
- The spatial distribution of peak 8-hour ozone concentrations should also be analyzed to indicate if the new source(s) result in exceedances of the ozone objectives away from monitoring sites. This can be done several ways, and the list below presents approaches in general order of descending conservativism. Justification for the method chosen should be given in the Photochemical Modelling Plan:

    1) Determine the maximum 8-hour ozone impact anywhere in the innermost domain of interest (i.e., focused on the LFV), add it to the observed maximum 8-hour ozone among all sites reported for the modelling period, and determine if the objective is exceeded (a space- and time-unpaired assessment).

    2) Determine the maximum 8-hour ozone impacts in each grid cell containing a monitoring site, add them to the respective observed maximum 8-hour ozone at each site for the modelling period, and determine if the objective is exceeded at any site (a space-paired, time-unpaired assessment).

    3) Determine the 8-hour ozone impacts in each grid cell containing a monitoring site for the day of observed maximum 8-hour ozone at the respective sites, add them to the observed maximum 8-hour ozone at each site for the modelling period, and determine if the objective is exceeded at any site (a space- and time-paired assessment).

    4) (a) Determine the maximum simulated 8-hour ozone in the Baseline scenario among all grid cells within the area of interest and determine if and where the objective is exceeded (a purely simulated Baseline exceedance assessment that is subject to model bias). Compare results at specific grid cells containing monitoring sites to the respective observed maximum 8-hour ozone to assess the level of bias in peak simulated values.

        (b) Determine the maximum simulated 8-hour ozone in the Project scenario among all grid cells within the area of interest, determine if and where the objective is exceeded, and identify any new exceedances and the extent to which existing exceedances in (a) are exacerbated.

        (c) Consider adjusting maximum simulated values in (b) by the bias determined in step (a) above and repeat the analysis in (b). A single area-wide average bias might be applied, or monitor-specific biases could be applied over their respective "areas of influence".

    5) Determine the maximum simulated 8-hour ozone impacts among all grid cells within the region of interest and compare to "significance" thresholds, if the agencies choose to develop and adopt such thresholds to define significant impacts for Project assessments.

6.1.4 STEPS FOR ASSESSING $PM_{2.5}$ IMPACTS

Recommendations: Follow the methods below for assessing $PM_{2.5}$ impacts:

- For 24-hour $PM_{2.5}$ objectives, modelled hourly total $PM_{2.5}$ concentrations should be averaged to rolling 24-hour values (e.g., hours 0-23, 1-24 (0 next day), 2-25 (1 next day),…, 23-46 (22 next day)). Project $PM_{2.5}$ increments (impacts) and total $PM_{2.5}$ concentrations (all sources) should be time-averaged in this manner. These calculations should be performed for all grid cells covering the area of interest. Given the form of the $PM_{2.5}$ objectives, this averaging should be performed for the entire modelling period.
- Cumulative frequency distributions of observed and simulated 24-hour $PM_{2.5}$ from the Baseline scenario should be developed at key monitoring sites. Cumulative frequency distributions of predicted 24-hour $PM_{2.5}$ that include the Project scenario should also be presented to illustrate source impacts over the range of the frequency distribution and allow an immediate assessment of if and when source impacts cause exceedances of the $PM_{2.5}$ objectives.
- The spatial distribution of peak 24-hour $PM_{2.5}$ concentrations should also be analyzed to indicate if the new source(s) result in exceedances of the $PM_{2.5}$ objective away from monitoring sites, or if their peak impacts exceed a significance level if adopted by the agencies. This could be done using the same approaches listed for ozone above. Justification for the method chosen should be given in the Photochemical Modelling Plan:

    1) Determine the maximum 24-hour $PM_{2.5}$ impact anywhere in the innermost domain of interest (i.e., focused on the LFV), add it to the observed maximum 24-hour $PM_{2.5}$ among all sites reported for the modelling period, and determine if the objective is exceeded (a space- and time-unpaired assessment).

    2) Determine the maximum 24-hour $PM_{2.5}$ impacts in each grid cell containing a monitoring site, add them to the respective observed maximum 24-hour $PM_{2.5}$ at each site for the modelling period, and determine if the objective is exceeded at any site (a space-paired, time-unpaired assessment).

    3) Determine the 24-hour $PM_{2.5}$ impacts in each grid cell containing a monitoring site for the day of observed maximum 24-hour $PM_{2.5}$ at the respective sites, add them to the observed maximum 24-hour $PM_{2.5}$ at each site for the modelling period, and determine if the objective is exceeded at any site (a space- and time-paired assessment).

    4) (a) Determine the maximum simulated 24-hour $PM_{2.5}$ in the Baseline scenario among all grid cells within the area of interest and determine if and where the objective is exceeded (a purely simulated Baseline exceedance assessment that is subject to model bias). Compare results at specific grid cells containing monitoring sites to the respective observed maximum 24-hour $PM_{2.5}$ to assess the level of bias in peak simulated values.

       (b) Determine the maximum simulated 24-hour $PM_{2.5}$ in the Project scenario among all grid cells within the area of interest, determine if and where the objective is exceeded, and identify any new exceedances and the extent to which existing exceedances in (a) are exacerbated.

       (c) Consider adjusting maximum simulated values in (b) by the bias determined in step (a) above and repeat the analysis in (b). A single area-wide average bias might be applied, or monitor-specific biases could be applied over their respective "areas of influence".

5) Determine the maximum simulated 24-hour $PM_{2.5}$ impacts among all grid cells within the area of interest and compare to "significance" thresholds, if the agencies choose to develop and adopt such thresholds to define significant impacts for Project assessments.

- For annual $PM_{2.5}$ objectives, modelled hourly total $PM_{2.5}$ concentrations should be averaged over the entire 365-day year that was simulated. Project $PM_{2.5}$ increments (impacts) and total $PM_{2.5}$ concentrations (all sources) should be time-averaged in this manner. These calculations should be performed for all grid cells covering the area of interest.
- The spatial distribution of annual $PM_{2.5}$ concentrations should be analyzed to indicate if the new source(s) result in exceedances of the annual objective, or if their peak impacts exceed a significance level if such is adopted by the agencies. This could be done using the same approaches listed above for 24-hour $PM_{2.5}$.

6.2 WET AND DRY SULPHUR AND NITROGEN DEPOSITION

All three photochemical models recommended in this guideline can provide spatial and temporal rates of sulphur (S) and nitrogen (N) deposition. Individual deposition accumulations, from both dry and wet processes, are provided for each S and N-containing compound.

- **Recommendation**: Determine rates of total accumulated S and N deposition by summing rates for S- and N-containing chemical species with appropriate factors that account for the relative S and N fractions of their mass. For example, S deposited mass should include the sum of SO_2, SO_3 (if explicitly modeled), and SO_4. N deposited mass should include the sum of NO, NO_2, HNO_3, NH_3, NH_4, and several NO_Z compounds (intermediate oxidized NO_X products such as N_2O_5).

6.3 PHOTOCHEMICAL MODEL REPORTING

The recommended information to be submitted to the agencies for review and acceptance includes sufficient information, tables and figures that address the objectives of the study, the modelling methodology, QA/QC steps, and other supporting information to demonstrate that the model has been applied properly and the model output can be used to inform decision makers. This is crucial so that reviewers can understand the assumptions and steps involved in the work.

Recommendation: Consider the following documentation for Photochemical Modelling Assessments, which should also be specified in the Photochemical Modelling Plan:

- Site Description
  - A site plan showing location and elevation of emission sources and buildings.
  - Description of topography and land use in model domain and geophysical data used in assessment (map showing contours, residential areas, roads, prominent geographic features).
- Modelled Emissions
  - Physical attributes and dimensions of Project stacks, vents and other sources.
  - Project emission rates used in assessment, including documentation on their development or derivation.

  - Regional anthropogenic and natural emission inventory processing steps and results (tables, QA/QC steps) for the domain and period selected for modelling.
- Meteorological Data Description
  - Description of meteorological conditions leading to air quality episodes.
  - Description of observed meteorological data used in assessment, reasons for their use, and presentation of wind roses (seasonal and annual).
  - Preprocessing utilities and assumptions applied to prepare the data sets.
  - Modelling domain extent and grid resolution.
  - Configuration of WRF.
  - Examples of simulated meteorological data from WRF (winds, temperature, stability) in space and time.
  - Description of QA/QC tests undertaken and clear documentation of results to assure the quality of the WRF output and that model behaviour is reasonable.
- Photochemical Model Related Information
  - Modelling domain extent and grid resolution.
  - Receptor grid resolution and size.
  - Identification of model used for assessment, stating any assumptions and modifications and identifying settings used in the model.
  - Source of data and method to develop chemical initial/boundary conditions.
  - Description of QA/QC tests undertaken and clear documentation of results to assure the quality of the photochemical model output and that model behaviour is reasonable.
- Specific Output for All Pollutants Modelled (not all required, but depends on objectives of modelling study)
  - Baseline, Future Baseline (if applicable) and all Project scenario (permitted, normal operation and other operating conditions, as specified) concentration patterns and metrics.
  - Figures showing isopleths of maximum (for all averaging times of concern) predicted concentrations overlaid on a map of the model domain and zoomed-in maps for localized impacts.
  - Exceedance frequencies above a specified threshold concentration (if agencies develop and adopt such thresholds).
  - Model output may include scenarios of existing sources, individual new sources, and all Project sources.
  - Time series and tables of model output (Baseline and total Baseline + Project) at existing monitoring sites (including monitored concentrations for comparison) and other receptors of interest.
  - Special output required for vegetation or health risk assessments.

- Electronic copies of input and critical output files must be compiled and available upon request by the agencies.

7. QUALITY ASSURANCE AND QUALITY CONTROL

Good modelling practice involves examination of input files to ensure that specific data treatments have been applied properly. However, even with error-free input files, there is no assurance that the model output will be appropriate. A review of the output is essential as it can indicate whether the model is behaving as expected under various circumstances. Spotting odd model behaviour and errors through this type of analysis comes from experience as well as expert training.

The central goal of the evaluation process is to show that the models are "fit for purpose". Thus, the purpose of the modelling needs to be clearly agreed upon and the notion of what constitutes fitness needs to be an open discussion and part of the Photochemical Modelling Plan.

This section presents recommendations on assessing both NWP and photochemical model performance in replicating historical conditions based on comparisons to measurements. Recommendations include options to assess photochemical model sensitivity to inputs from which to understand model responses. Since every situation and model application is different, this section provides guidance in more general terms, and thus recommendations below are not as specific as in previous sections.

7.1 RECOMMENDED NWP MODEL QA/QC PROCESS

NWP model results should be evaluated with respect to operational and phenomenological considerations important to air quality applications. Generally, the model performance evaluation involves careful analysis of an initial set of model results, identification of major performance issues that could be detrimental to the photochemical model simulation, adjustments to the meteorological model configuration or its inputs, and perhaps several additional runs to alleviate or improve upon those performance issues.

A variety of qualitative and quantitative methods should be applied to evaluate model results against observed data. The observational dataset should consist of as much routine and special study (if available) measurement networks as possible that operate within the regional modelling domain. If observation nudging is employed in the meteorological model, then consider whether including those data in the performance evaluation would bias the model-observation comparison. Optionally, observations from a certain subset of the networks could be sequestered and reserved specifically for the model performance evaluation step.

7.1.1 QUALITATIVE EVALUATION

Graphical comparisons allow for a qualitative assessment of model performance by comparing results to commonly available analysis maps or imagery of key weather patterns and features. The purpose of these evaluations is to establish a first-order acceptance/rejection of the simulation in adequately replicating the gross weather phenomena in the region of interest. Thus, this approach screens for obvious model flaws and errors. Subjective model evaluations should be based on expert meteorological judgment regarding whether the model replicates the local- and small-scale features adequately, as well as the driving synoptic-scale patterns. A variety of graphical analyses should be developed to visually review the spatial/temporal evolution of wind, temperature, precipitation and boundary layer features and patterns.

Recommendation: Examples of qualitative analyses include an assessment of:

- Wind roses (seasonal and annual) produced at key locations

    - Do they make qualitative sense?
    - How well do they compare to wind roses based on actual data?
- Thermally generated flows and diurnal variations
    - Do the meteorological fields under clear sky conditions reflect the expected day and night flow fields induced by the terrain?
    - Is there any evidence of unrealistic flow given the local topography?
    - Do the meteorological fields during the spring and summer months reflect sea breeze circulation patterns on days with conducive conditions?
- Hourly time series of wind speed, direction, temperature and humidity at individual sites and for averages over multiple sites in a region.
    - Do the variables indicate systematic biases overall, or during periods of the day or night, or over specific episodes?
    - Are there unexplainable features in the model results that lead to particularly poor or questionable results?
- Vertical profiles of wind and temperature (and diurnal variations)
    - Do these vertical profiles make qualitative sense, especially as the temperature profile varies diurnally?
    - How well do they compare to nearby upper air soundings?
- The different levels of wind fields over the domain (and diurnal variations)
    - Is there evidence of unrealistic wind jets at low elevations (this has occurred in some NWP model output)?

7.1.2 QUANTITATIVE EVALUATION

A detailed model evaluation is difficult to summarize from a purely objective point of view; therefore, statistics on hourly and daily time frames must be relied upon to quantitatively characterize how well a model replicated conditions over the period and modelling domain.

The remainder of this section describes the various statistical measures that should be considered in the Photochemical Modelling Plan. The model evaluation approach should be based, at a minimum, on a quantitative analysis of bias and error statistics for wind speed, direction, temperature, and humidity at the surface.

Bias (B): the mean signed difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly or daily):

$$\frac{1}{N}\sum\left(P_j - O_j\right)$$

Subscript j represents the pairing of N observations O and predictions P by site and time.

Gross Error (E): the mean absolute difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly or daily):

$$\frac{1}{N}\sum\left|P_j - O_j\right|$$

Note that the bias and gross error for winds are calculated from the predicted-observed residuals in speed and direction (not from vector components u and v). The direction error for a given prediction-observation pairing is limited to range from 0 to ±180°.

<u>Root Mean Square Error</u> (RMSE): the square root of the mean squared difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly or daily):

$$\sqrt{\frac{1}{N}\sum\left(P_j - O_j\right)^2}$$

<u>Least Square Regression</u>: fits the observation set to a linear model that describes the prediction set for all sites with valid data within a given analysis region and for a given time period (daily or longer). The y-intercept a and slope b of the resulting straight-line fit are calculated to describe the regressed prediction $\hat{P}$ for each observation:

$$\hat{P}_j = a + bO_j$$

The goal is for a slope of 1, a y-intercept of 0, and a correlation coefficient R of 1 (a perfect regression). Correlation coefficient is calculated from:

$$\frac{\Sigma\left[\left(P_j - \bar{P}\right) \times \left(O_j - \bar{O}\right)\right]}{\sqrt{\Sigma\left(P_j - \bar{P}\right)^2 \times \Sigma\left(O_j - \bar{O}\right)^2}}$$

Where overbars represent mean predictions and observations. Note that mean observed and predicted winds are vector-averaged (for east-west component u and north-south component v), from which the mean wind speed and mean resultant direction are derived.

- **<u>Recommendation</u>**: Include a description of QA/QC tests undertaken and clear documentation of results in the Project report to demonstrate the quality of the WRF output and that model behaviour is reasonable.

7.1.3 STATISTICAL BENCHMARKS

A logical question is: “what represents acceptable vs. unacceptable statistical performance for this period and location?” To help answer this question, each statistical metric is compared to performance benchmarks established from a review of previous NWP modelling results (Emery et al., 2001). As part of a large modelling project in 2005 for the US Western Regional Air Partnership, Kemball-Cook et al. (2005) proposed updates to a few performance benchmarks for applications in complex terrain characteristic of the Rocky Mountain region and Alaska. These should be also applicable to the LFV. Both sets of benchmarks are shown in Table 7-1.

7.2 RECOMMENDED PHOTOCHEMICAL GRID MODEL QA/QC PROCESS

This section recommends a general methodology to evaluate photochemical model results for ozone and $PM_{2.5}$ with respect to operational and phenomenological considerations. Guidance developed by the US EPA (2018) is currently the most well considered and modern advice for regulatory-oriented photochemical modelling applications. Therefore, the approach described therein is briefly summarized here. Local observational datasets should be identified that can support graphical and statistical evaluation techniques. Note that many of the same concepts and considerations are consistent with those presented in Section 7.1 regarding the NWP model performance evaluation.

Table 7-1. Meteorological performance benchmarks widely used for photochemical modelling exercises throughout North America over the past 20 years (Emery et al., 2001; Kemball-Cook et al., 2005).

Parameter	Original/Simple Terrain	Complex Terrain
Temperature Bias	≤ ±0.5 K	≤ ±2.0 K
Temperature Error	≤ 2.0 K	≤ 3.5 K
Humidity Bias	≤ ±1.0 g/kg	≤ ±0.8 g/kg
Humidity Error	≤ 2.0 g/kg	≤ 2.0 g/kg
Wind Speed Bias	≤ ±0.5 m/s	≤ ±1.5 m/s
Wind Speed RMSE	≤ 2.0 m/s	≤ 2.5 m/s
Wind Direction Bias*	≤ ±10 degrees	≤ ±10 degrees
Wind Direction Error	≤ 30 degrees	≤ 55 degrees

*Value for complex terrain was not specified and the simple terrain value is duplicated here for consistency. Therefore, some flexibility in this value should be allowed.

7.2.1 OVERVIEW

Many sources of uncertainty in model predictions are considered “reducible”. That is, they can be controlled or minimized by developing input data properly, checking and rechecking for errors, correcting for odd model behaviour, and ensuring that the errors in the measured data are minimized. However, even if the reducible uncertainty could be minimized, there is always a level of inherent model uncertainty that cannot be eliminated (i.e., from discretization, parameterizations, etc.). The goal of these recommendations is to minimize the reducible error by providing direction on input data, the appropriate application of models, directions on preparing model input files and settings, and providing guidance on proper model evaluation.

Model evaluation requires considerable expertise in order to interpret model performance and likely causes for systematic biases and errors. Measurements and model predictions can be compared in a variety of ways, each providing a different perspective on model performance. A model may show competency in certain predictions (e.g., average concentrations) but inadequacy in others (e.g., the frequency of concentrations above a certain threshold).

Generally, the model performance evaluation involves careful analysis of an initial set of model results, identification of major performance issues, adjustments to the model configuration or its inputs, and perhaps several additional runs to alleviate or improve upon those performance issues. However, caution should be used in modifying inputs to achieve good model performance because arbitrarily “tuning” the model to fit the observations can introduce compensating errors, which would lead to an incorrect response to emission perturbations. A variety of objective methods should be applied to evaluate model results against observed data.

7.2.2 THE OPERATIONAL EVALUATION

The operational model performance evaluation should be conducted using available software tools that can generate statistics and graphical model-observation comparisons. One of the most comprehensive, well vetted, and publicly available tools developed specifically for the photochemical modelling community is the US EPA's Atmospheric Model Evaluation Tool (AMET; US EPA, 2022f).

The observational dataset should consist of as much routine and special study (if available) measurement networks as possible that operate within the regional modelling domain. Ambient data should include, at a minimum, the LFV surface air quality monitoring network (MVRD, 2012). The network includes widely monitored pollutants including ozone, carbon monoxide (CO), sulphur dioxide (SO_2), nitrogen dioxide (NO_2), and particulate matter. PM measurements include both particles smaller than 10 microns (PM_{10}), and particles smaller than 2.5 microns ($PM_{2.5}$). Other pollutants important for photochemical modelling are monitored at a few sites in the Canada National Air Pollution Surveillance (NAPS; ECCC, 2022c) network, including ammonia (NH_3), elemental or black carbon, and volatile organic compounds (VOC), which are measured on an every 6th or 12th day national schedule.

Calculating a single set of statistics for a very large area or time period would not yield significant insight into performance. Therefore, the statistical analyses should be refined to subregions within large modelling domains to capture their local climatic differences; plots and graphs are used to visually present these statistics on both hourly and daily time frames. The minimum set of recommended statistics are listed below. The statistical metrics to be analyzed should be identified in the Photochemical Modelling Plan.

Bias: the mean signed difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly or daily); see Section 7.1.2 for the mathematical definition.

Gross Error: the mean absolute difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly or daily); see Section 7.1.2 for the mathematical definition.

Root Mean Square Error (RMSE): the square root of the mean squared difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly or daily); see Section 7.1.2 for the mathematical definition.

Least Square Regression: fits the observation set to a linear model that describes the prediction set for all sites with valid data within a given analysis region and for a given time period (daily or longer); see Section 7.1.2 for mathematical definitions.

Normalized Mean Bias (NMB): the bias statistic is normalized by the mean observation and expressed in percent:

$$\frac{\sum\left(P_j - O_j\right)}{\sum O_j} \times 100$$

Values range from -100% to +∞, so under and over predictions are not symmetrical around 0.

Normalized Mean Error (NME): the gross error statistic is normalized by the mean observation and expressed in percent:

$$\frac{\sum\left|P_j - O_j\right|}{\sum O_j} \times 100$$

Values range from 0% to +∞.

- **Recommendation**: Include a description of QA/QC tests undertaken and clear documentation of results in the Project report to demonstrate the quality of the photochemical model output and that model behaviour is reasonable.

7.2.3 STATISTICAL BENCHMARKS

As discussed in Section 7.1 for NWP model evaluation, statistical "benchmarks" can provide important contextual linkages between statistical results of a particular application and those of past studies. Benchmarks for ozone and $PM_{2.5}$ have been established and widely used over the past three decades (US EPA, 1991; Boylan and Russell, 2006). Recently, Emery et al. (2016) updated ozone and $PM_{2.5}$ performance benchmarks for a set of the three most widely reported statistics. However, benchmarks should not be relied upon to define an acceptable model, and this Guideline reaffirms the importance of also evaluating the model via diagnostic methods.

Table 7-2 presents the recommended goals and criteria of Emery et al. (2016) for NMB, NME, and the correlation coefficient (R) for 1-hour and maximum daily 8-hour (MDA8) ozone and 24-hour total $PM_{2.5}$ and component species. The "goals" should be considered the best a model can be expected to achieve. The "criteria" indicate values achieved by a majority of past applications. Values that exceed the criteria should be considered poor performers for the particular metric and chemical species.

Table 7-2. Recommended benchmarks for photochemical model performance statistics. See the text for additional information on the metrics and benchmarks.

	NMB		NME		R	
Species	**Goal**	**Criteria**	**Goal**	**Criteria**	**Goal**	**Criteria**
1-h or MDA8 Ozone	< ±5%	< ±15%	< 15%	< 25%	> 0.75	> 0.50
24-h $PM_{2.5}$, SO_4, NH_4	< ±10%	< ±30%	< 35%	< 50%	> 0.70	> 0.40
24-h NO_3	< ±15%	< ±65%	< 65%	< 115%	None	None
24-h POC	< ±15%	< ±50%	< 45%	< 65%	None	None
24-h PEC	< ±20%	< ±40%	< 50%	< 75%	None	None

No recommendations are provided for correlation benchmarks for NO_3, elemental carbon (PEC), and organic carbon (POC) because of few published data available and large statistical uncertainty. The list below includes additional recommendations from that study and are reemphasized in this guidance:

- **Recommendation**: For 1-hour ozone NMB and NME, include only prediction-observation pairings when the observations are above 40 ppb (commonly referred to as a "cut-off") as a general demarcation between nocturnal ozone destruction and daytime ozone production regimes. (the choice of 40 ppb is not absolute and should consider the chemical climatology of the region being modelled);
- **Recommendation**: Do not apply a cut-off for statistics generated for MDA8 ozone;
- **Recommendation**: Do not exceed temporal scales for ozone statistics beyond 1 month; spatial scales should range from urban to ≤1000 km;
- **Recommendation**: Do not apply cut-offs for any statistics reported for 24-hour total and speciated PM; and
- **Recommendation**: Do not exceed temporal scales for 24-hour total and speciated PM should beyond 3 months (or 1 season); spatial scales should range from urban to ≤1000 km.

7.2.4 DIAGNOSTIC EVALUATION

Diagnostic evaluations typically involve sensitivity tests, source apportionment, and process analysis. These types of analyses should be conducted where practical. The diagnostic evaluation assesses the model's ability to properly simulate physical and chemical processes and, to the extent possible, the sensitivity to input changes. This Guideline summarizes a few tools and methods that should be considered for PGM applications (specific issues related to SCICHEM are discussed in Section 7.3).

- **Recommendation**: Carefully consider diagnostic analyses and describe methods in the Photochemical Modelling Plan.

7.2.4.1 PROCESS ANALYSIS

Both CMAQ and CAMx include process analysis tools that generate diagnostic information on individual chemical reactions and physical processes that spatially and temporally evolve all chemical concentrations addressed in the model. Computational cost to produce these additional outputs are minimal but they can be voluminous. Accessible sets of process analysis outputs are available from these models in the same format as the concentration output files, and so they can be visualized using the same graphics tools.

7.2.4.2 SOURCE APPORTIONMENT

Source apportionment methods are available in CAMx and CMAQ to identify emission sources that contribute to secondary pollutant concentrations (ozone and $PM_{2.5}$) in specific areas and times. These tools use chemical "tracers" that undergo the same chemistry, transport and removal processes as the standard chemical species. Emission tracers are set according to emissions from specific source categories and specific source regions. Secondary tracers are chemically produced from the emission tracers (accounting for nonlinear interactions), as well as from intermediate product tracers such as organic nitrates. The resulting tracer "concentrations" indicate the attribution of a particular pollutant to the selected source sectors and regions. Results are easily reviewed and are straightforward to interpret.

7.2.4.3 SENSITIVITY ANALYSIS

These are useful to identify model sensitivity to various inputs (e.g., to assess the role of potential error in each type of input), and to identify sensitivity to "what if" scenarios, which usually involve emission perturbations. Sensitivity analyses can also be useful to identify causes for poor model performance beyond what Process Analysis can provide. There are two widely used sensitivity approaches. So-called "brute-force" simulations involve modifying a model input, rerunning the model, and comparing to a "Baseline" simulation. Such tests are straightforward to implement and analyze, but they can be resource intensive if many tests are to be conducted. The Direct Decoupled Method (DDM), implemented in both CAMx and CMAQ, allows for sensitivity to emission changes to be calculated inline as the models run, reducing or alleviating the need for multiple explicit brute-force runs.

- **Recommendation**: Include a description of any sensitivity tests undertaken and clear documentation of results in the Project report to demonstrate the quality of the photochemical model output and that model behaviour is reasonable.

7.3 CONSIDERATIONS FOR SCICHEM

The model evaluation steps outlined above for PGMs are not entirely applicable to plume/puff models like SCICHEM. While those steps are useful to evaluate the background concentration fields provided to SCICHEM (assuming they were derived from PGMs such as CAMx and CMAQ), SCICHEM simulates only the plume concentrations from specific sources, which are often hypothetical or projected and thus not yet realized. Therefore, evaluation of SCICHEM simplifies to assessing the veracity of the resulting prospective secondary pollutant concentration fields when the sources in question are simulated.

Karamchandani et al. (2020) describe a model inter-comparison study (SCICHEM, CMAQ and CAMx) of secondary pollutants from emissions from a hypothetical coal-fired power plant. The hypothetical stacks were located in 4 separate regions of the US, including the Seattle area. Annual simulations were conducted to determine the frequency distribution of source impacts over each of the 4 regions. Information from the Seattle case could be used to assess, in a relative way, the results from Project-specific SCICHEM applications.

- **Recommendation**: Include a description of QA/QC tests undertaken and clear documentation of results in the Project report to demonstrate the quality of the photochemical model output and that model behaviour is reasonable.

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APPENDIX A: PHOTOCHEMICAL MODELLING PLAN

A.1 GENERAL INFORMATION

Date:

Facility Name, Company, Location/Area (Address, Latitude, Longitude):

Air Quality Consultant and Contact Information:

Agency Contact:

Rationale for Level 3 Assessment using advanced photochemical modelling:

Does this plan follow a modelling approach similar to that taken in a previously reviewed and accepted air quality assessment? If so, provide the Project name and agency contact:

A.2 PROJECT DESCRIPTION

Provide an overview of the Project, including purpose and steps involved in the photochemical modelling study:

State which secondary contaminants will be modelled (e.g., ozone and/or secondary $PM_{2.5}$), which ambient air quality standards and objectives will be addressed, and which directly-emitted pollutants are involved (e.g., SO_X, NO_X, VOC, and/or $PM_{2.5}$):

List the specific model output parameters to be generated for reporting to decision makers and stakeholders (e.g., impacts to air concentration standards and objectives, deposition to sensitive ecosystems, other):

A.3 PHOTOCHEMICAL MODEL/VERSION AND CONFIGURATION

<u>Selected Photochemical Model</u>

- Specify model and version (Section 2):
- Specify any non-guideline models or versions (i.e., beta test versions) planned for use (Section 2.4.1), and provide rationale:
- Specify any modifications to the selected model (Section 2.4.2), and provide rationale:

<u>Model Configuration Settings</u>

- Specify configuration settings (Section 5.3), note those that differ from the Guideline recommendations and provide rationale:
- Specify source of data for initial/boundary conditions and describe processing methodology (Section 5.1):
- Specify approach to derive photolysis rates (Section 5.2):

A.4 DOMAIN AND RECEPTOR DEFINITION

Domain Configuration

- Describe the extent of the NWP and photochemical modelling domains (Section 2.5), including the use of any nested grids, and provide rationale:
- Specify map projection to be used by NWP/photochemical models (name, projection parameters, domain-specific parameters):
- List resolution (km) for each grid by NWP/photochemical model:
- List size (number of grid cells in X and Y directions) for each grid by NWP/photochemical model:
- List number of vertical levels and their altitudes (m AGL) by NWP/photochemical model:
- Provide domain maps that characterize the topography, land use distribution and key site locations (facility, air quality and meteorological monitoring sites, receptors):

SCICHEM Receptors (if applicable, Section 5.3.3.4)

- Proposed receptor grid spacing:
- Anticipated sensitive receptor locations:
- Anticipated flagpole receptor locations and heights (m AGL):

A.5 PERIOD TO BE MODELLED AND BASELINE AIR QUALITY LEVELS

Consult with reviewing agencies when selecting a year for modelling. State which calendar year is selected for photochemical modelling and rationale, and list specific months to be modeled if the analysis is performed only for ozone (Section 2.6):

Describe the general air quality conditions that occurred during the selected period (is an MVRD air quality summary report available for the chosen year?):

A.6 SOURCE OF REGIONAL EMISSION INPUTS

State whether new emission processing will be conducted for this Project, or existing model-ready emission dataset will be used (specify original data source, model and version, and any notable considerations):

Emission Sectors

- Specify source and year of anthropogenic emission inventories for LFV, BC, and US (Section 3.1.1, Table 2-2):
- Specify model and version to generate biogenic emissions:
- Specify source of wildland fire emission dataset:
- Specify oceanic emission model (if not estimated by the photochemical model):

Emission Scenarios

Describe the anticipated regional modelled emission scenarios (Baseline and/or future Baseline) and rationale (Section 3.2):

If modelling a future Baseline scenario, list any other projects that are expected to be operational and included in the emission inventory (name, location, industry sector):

A.7 PROJECT EMISSION SOURCES AND CHARACTERISTICS

Provide a map showing the source locations, buildings, and facility fence line:

Model Emission Scenarios

- Describe the different model emission scenarios required for the assessment, if multiple options are under consideration:
- Describe anticipated abnormal emission scenarios (start-up, shut-down, upsets), their anticipated frequency of occurrence, and how they will be modelled:
- Describe approach to assess air quality implications under the 25, 50, 75% emission scenarios:

Source Characterization

Provide the following details of the sources to be modelled in a table:

- Source ID
- Type (point, area)
- Process source category code(s) (for use in speciating VOC and PM)
- List specific emitted pollutants (e.g., SO_X, NO_X, VOC, CO, NH_3, $PM_{2.5}$, PM_{10})
- Basis for emission rate (proposed/approved emission limit, manufacturer specification, emission factor, CEM, modelled emission rate, stack sampling, other)
- Expected frequency of operation, temporal profile/variability (hourly, day-of-week, seasonal)
- Expected variability in emission parameters (flow rate, temperature, etc.)
- If modelling a future Baseline scenario, provide similar information on any other projects that are expected to be operational and will be included in the modelling (as listed above):

A.8 METEOROLOGICAL MODEL CONFIGURATION

State whether new WRF modelling will be conducted for this Project, or existing NWP model output will be used (specify original data source, model and version, and any notable considerations):

Model Configuration Settings

- Specify WRF version (Section 4.2):
- Specify configuration settings (Section 4.2.1), note those that differ from the Guideline recommendations and provide rationale:

Topography and Land Use Data

- Specify source of topographic data:
- Specify source of land cover/use data:

Large Scale Meteorological Analyses:

- Specify source of meteorological analyses used for initial/boundary conditions and/or FDDA:
- Specify source of sea surface temperature analyses:
- Specify source of snow cover analyses:

Meteorological Monitoring Data

Specify surface weather monitoring networks to be used in a table:

- Network name/source
- Number of sites
- Use of data (enhance large scale analyses, FDDA, model performance evaluation)
- Period of record (note any major data outages during the modelling period)

Specify upper air radiosonde networks or profiler sites to be used in a table:

- Network name/source or profiler location/operator
- Location
- Use of data (enhance large scale analyses, FDDA, model performance evaluation)
- Period of record (note any major data outages during the modelling period)

Processing NWP Data for Photochemical Modelling

- Specify the NWP-photochemical interface tool to be applied:
- Specify selection of processing options/parameters for the selected interface tool:

A.9 MODEL OUTPUT AND POSTPROCESSING

List the individual species that will be output by the selected photochemical model and how PM components will be combined to total PM mass (Section 5.4):

Describe how Project-level emission impacts are to be determined (e.g., brute force differences from multiple runs, source apportionment, sensitivity analysis), and rationale (Section 6.1):

Describe approach to assess ozone impacts relative to local objectives and standards (Section 6.1.3):

Describe approach to assess PM impacts relative to local objectives and standards (Section 6.1.4):

Describe approach to assess S and/or N deposition loads (if applicable) to various areas of the domain and by critical land use types:

Data Reporting (Section 6.3)

- Baseline, Future Baseline (if applicable) and all Project scenarios (permitted, normal operation and other operating conditions, as specified) concentration patterns and metrics:
- Figures showing isopleths of maximum (for all averaging times of concern) predicted concentrations overlaid on a map of the model domain:
- Exceedance frequencies above a specified threshold concentration:
- Model output may include scenarios of existing sources, individual new sources, and all Project sources:
- Time series and tables of model output for Project sources at existing monitoring sites (including monitored concentrations) and other receptors of interest:
- Special output required for vegetation, health risk or visibility assessments:
- Other (specify):

A.10 QUALITY ASSURANCE/QUALITY CONTROL

Model Input Data

Indicate which checks below will be conducted to assure the quality of the photochemical model inputs:

- Review SMOKE emission processing scripts, cross-reference and profile/surrogate input files, and output logs to ensure proper execution and processing of raw inventory data to model-ready inputs.
- Review other emission model and program scripts, inputs and output logs to ensure proper execution and processing of model-ready emission inputs (biogenic, oceanic, etc., as applicable).
- Review WRF preprocessing and runtime scripts, input files, and output logs to ensure proper execution of the entire NWP system.
- Review all photochemical model preprocessor scripts, input files and output logs to ensure proper execution and processing of model-ready inputs (initial/boundary conditions, photolysis rates, etc., as applicable).

NWP Model Performance Evaluation

Indicate the checks that assure the quality of the NWP model results:

- Wind roses (seasonal and annual) produced at meteorological monitoring sites.
- Thermally generated flows and diurnal variations

- Hourly time series of predicted and observed wind speed, direction, temperature and humidity at individual sites and for averages over multiple sites in the domain.
- Vertical profiles of wind and temperature (and diurnal variations).
- Spatial plots of wind and temperature fields over the domain at several vertical levels.

Indicate the checks that quantitatively measure NWP model performance in replicating actual historical conditions:

- Calculate statistical agreement with observed wind, temperature and humidity at specified weather stations throughout the domain.
- Compare and report statistical results against historical benchmarks (Section 7.1.3).

Photochemical Model Results

Indicate the checks that assure the quality of the photochemical model results:

- Review photochemical model scripts and output logs to ensure proper execution and generation of output.
- Hourly time series of predicted and observed ozone, $PM_{2.5}$ and applicable precursor concentrations (e.g., NO_X, VOC, CO as available) at individual monitoring sites and for averages over multiple sites in the domain.
- Spatial plots of concentration fields over the domain.
- Regression plots of simulated vs. observed ozone and $PM_{2.5}$ for all sites over the domain.

Indicate the checks that quantitatively measure photochemical performance in replicating actual historical conditions:

- Calculate statistical agreement with observed ozone and $PM_{2.5}$ concentrations at specified monitoring sites throughout the domain.
- Compare and report statistical results against historical benchmarks (Section 7.2.3).

Indicate any diagnostic tests planned to assess robustness and sensitivity of photochemical results:

- Process Analysis, physical and/or chemical processes.
- Source Apportionment, and apportionment of which emission sectors/regions.
- Brute force or DDM Sensitivity, and sensitivity to which inputs or emission sectors/regions.

Submission of all computer files associated with the modelling may be required upon request.

A.11 REVIEW OF PLAN AND REVISIONS

A Photochemical Modelling Plan can change over the course of developing the air quality assessment so acceptance of the initial submission of the plan is on the basis of the best information provided to date. Changes to the plan (additions, modifications) should be noted and agreed to with the authorizing agency, as necessary. An updated Photochemical Modelling Plan may be necessary.

Agency Acceptance of Original Plan (Name): __________________________

Date: ____________________