2.0 AIRSHED MODELLING SYSTEM DESCRIPTION

The scientific community has developed advanced numerical air quality models (AQMs) to understand the interactions among meteorology, emissions (both manmade and biogenic), and pollutant chemistry and dynamics. Emissions data from emissions models and regulatory inventories are one of the most important inputs for these air quality models. Scientists use air quality modeling for a number of purposes: for provincial and federal emission reduction plans, for research on improved air characterization methods and for air quality forecasting. In all of these cases, the trend has been to model larger regions, at a finer grid resolution, with more emissions sources, and more substances (e.g., ozone, particulates, toxics). These needs require a computationally efficient, user-friendly, and flexible emissions data processing system.

There are two fundamental elements involved in the prediction of ambient air pollution concentrations. It is necessary first to determine the sources of the pollution emissions and the rates at which it is emitted, and secondly, to determine how it is transported, dispersed and transformed in the atmosphere after its release. In its simplest form, a model requires information on the emission sources, including pollution emission rates, and meteorological data. Air quality models generate air pollutant concentrations for a particular averaging time, usually at specific receptor locations. Once an air pollution model has been validated, it can be used to predict the changes in ambient air quality due to different pollution control strategies. These data provide the basis for the formulation and implementation of the most cost effective measures to improve air quality. The ultimate objective in air pollution modelling is to accurately predict the air pollution level at any point in the region of interest. That information can then be used to assess long-term or short-term exposure levels. Long-term (usually 1 year or more) exposure levels are important for chronic exposure studies while acute exposure studies use short-term changes in air pollution over time (usually 1-5 days).

In general, air quality models can be categorized by their spatial scale as macro-scale, meso-scale and micro-scale models. The macro-scale models usually refer to global scale, or regional-to-continental scale, spatial grid scales (for example: grids that are 1,000 km square). At this scale, the atmospheric flow is mainly associated with synoptic phenomena (the geographical distribution of pressure systems), attributable to large-scale inhomogeneities of the surface energy balance. The next scale is local-to-regional scale (meso-scale) modelling that includes local (community) scale studies. The flow configuration at this scale requires meteorological models capable of simulating local circulation systems, such as sea and land breezes. Atmospheric flow depends on hydrodynamic effects, such as flow and roughness as well as the inhomogeneities of the energy balance due to the spatial variation of area characteristics, such as differences of land use, vegetation types and presence of water. For a very small spatial scale (micro-scale) ranging from a few metres to 100s of metres, air flow modeling is very complex due to the more detailed surface characteristics incorporated. The atmospheric processes at this scale are typically described by using simple models for practical applications, such as street canyon models, or by using very complex computational fluid dynamic (CFD) models.

There is no single model that can address all spatial scales. Meteorological and topographical complexities at different scales are extremely difficult to address in a single mathematical representation of the transport and dispersion of pollutants.

The USEPA CALPUFF/CALMET modelling system was selected for the Toronto airshed primarily for is robust capabilities to handle a wide-range of emission source types over varying land use. It is also an officially recognized model by the Ontario Ministry of the Environment (MOE).

The CALPUFF (Scire, et al., 2000) model is a multi-layer, multi-species Lagrangian Gaussian puff dispersion model that can simulate the transport, transformation, and removal of pollutants under time- and space-varying meteorological conditions. The CALPUFF model can be used for both steady-state and non-steady-state meteorology. CALPUFF is extremely useful for situations in which straight line, steady-state assumptions inherent in plume models are invalid. Such situations arise, for example, in cases of long distance transport (>10 km) having temporally and/or spatially varying wind flow fields caused by complex terrain, non-uniform land use patterns or coastal effects, and also in conditions involving calm or very low wind speeds with variable wind directions.

The CALPUFF modelling system was used to directly predict ambient concentrations of the 29 contaminants selected for analysis However, the CALPUFF model does not include an oxidant chemistry model to estimate ozone levels. Therefore, ozone modelling was carried out with the aid of site-specific Observation Based Model (OBM) as described in Section 6.0.

The main components of the CALPUFF/CALMET Modelling System consists of

- CALMET - the meteorological model (that develops hourly wind and temperature fields on a three dimensional gridded modelling domain),
- CALPUFF - the transport and dispersion model (that transports “puffs” of material emitted from sources considered for modeling) and generates hourly concentrations, or hourly deposition fluxes, that are evaluated at receptor(s) of interest), and
- CALPOST as the post processor (that is used to process CALPUFF output files).

The complete CALPUFF modelling system is shown in Figure 2-1. A complete summary of the capabilities and features of CALMET and CALPUFF is provided in Section 2.1 and 2.2, respectively.

2.1 Major Features of CALMET

CALMET is a diagnostic meteorological model that produces three-dimensional wind fields based on parameterized treatments of terrain effects, such as slope flows, terrain blocking effects, and kinematic effects. Meteorological observations are used to determine the wind field in areas where the observations are representative. Gridded hourly meteorological data produced by MM5 can be used as the initial guess for the wind fields. The diagnostic wind module in CALMET will determine fine scale terrain effects.

The CALMET meteorological model consists of a diagnostic wind field module and micrometeorological modules for overwater and overland boundary layers. When using large domains, the user has the option to adjust input winds to a Lambert Conformal Projection coordinate system to account for Earth's curvature. The diagnostic wind field module uses a two-step approach to the computation of the wind fields. In the first step, an initial-guess wind field is adjusted for kinematic effects of terrain, slope flows, and terrain blocking effects to produce a Step 1 wind field. The prognostic grid of meteorological data can be used for the initial guess field. The second step consists of an objective analysis procedure to introduce observational data into the Step 1 wind field to produce a final wind field.

The major features and options of the meteorological model are summarized in Table 2-1. The techniques used in the CALMET model are briefly described below.

Figure 2 1: *CALPUFF Modelling System*

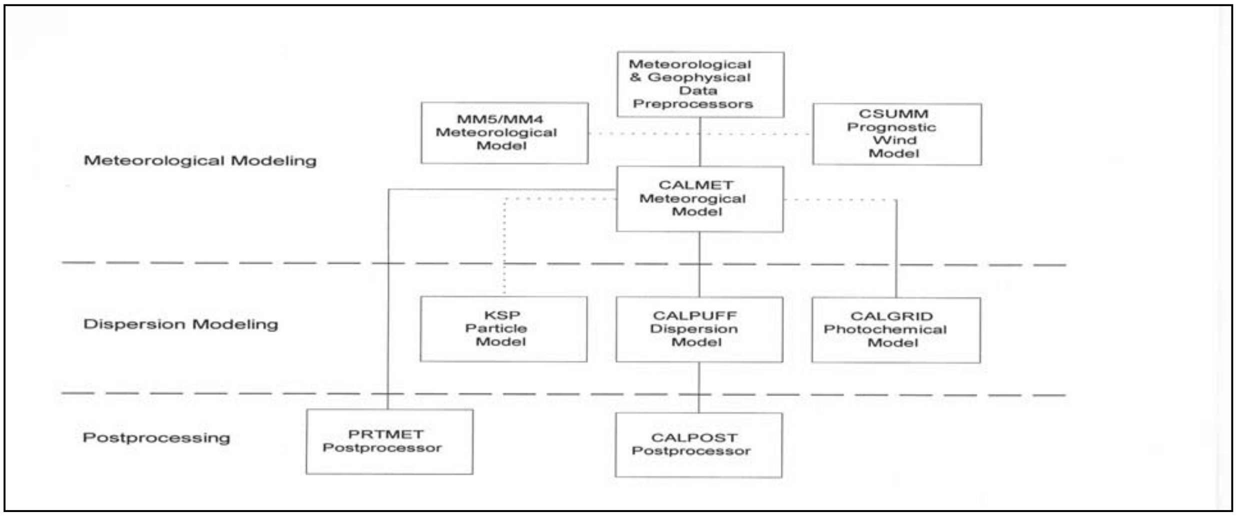

Table 2-1:Major Features of the CALMET Meteorological Model

- Boundary Layer Modules of CALMET
- Overland Boundary Layer - Energy Balance Method
- Overwater Boundary Layer - Profile Method
- Diagnostic Wind Field Module of CALMET
- Terrain Blocking Effects
- Kinematic Terrain Effects
- Divergence Minimization
- Produces Gridded Fields of U, V, W Wind Components
- Inputs Include Domain-Scale Winds, Observations, and Coarse-Grid Prognostic Model Winds (optionally)
- Lambert Conformal Projection Capability

2.1.1 Initial Wind Field

2.1.1.1 Kinematic Effects of Terrain

The approach of Liu and Yocke (1980) is used to evaluate kinematic terrain effects. The domain-scale winds are used to compute a terrain-forced vertical velocity, subject to an exponential, stability-dependent decay function. The kinematic effects of terrain on the horizontal wind components are evaluated by applying a divergence-minimization scheme to the initial guess wind field. The divergence-minimization scheme is applied iteratively until the three-dimensional divergence is less than a threshold value.

2.1.1.2 Blocking Effects

The thermodynamic blocking effects of terrain on the wind flow (i.e., wind deflecting over and around obstacles) are parameterized in terms of the local Froude number (Allwine and Whiteman, 1985). If the Froude number at a particular grid point is less than a critical value and the wind has an uphill component, the wind direction is adjusted to be tangent to the terrain.

2.1.2 CALMET Boundary Layer Models

The CALMET model contains two boundary layer models; one for application to separate overland situations and the other for application to overwater situations. As the City of Toronto is on Lake Ontario, the use of this option was selected.

2.1.2.1 Overland Boundary Layer Model

Over land surfaces, the energy balance method of Holtslag and van Ulden (1983) is used to compute hourly field grids of the sensible heat flux, surface friction velocity, Monin-Obukhov length, and convective velocity scale. Mixing heights are determined from the computed hourly surface heat fluxes and observed temperature soundings using a modified Carson (1973) method based on Maul (1980). The model also determines field grids of Pasquil-Gifford-Turner (PGT) stability class and optional hourly precipitation rates.

2.1.2.2 Overwater Boundary Layer Model

The aerodynamic and thermal properties of water surfaces suggest that a different method is best suited for calculating the boundary layer parameters in lakeshore environment. A profile technique, using air-lake temperature differences, is used in CALMET to compute the micro-meteorological parameters in the lakeshore boundary layer. An upwind-looking spatial averaging scheme is optionally applied to the mixing heights and 3-dimensional temperature fields in order to account for important advective effects.

2.2 Major Features of CALPUFF

CALPUFF adopts a non-steady-state, or dynamic, modelling approach, which evaluates the effects of spatial changes in the meteorological and surface characteristics, to properly evaluate the air quality impacts of the emissions sources (Scire et al., 2000a,b). The U.S. Environmental Protection Agency (USEPA) has formally accepted CALPUFF as an Appendix A Guideline Model (Federal Register, November 9, 2005). CALPUFF is also recommended for source-receptor distances greater than 50 km, and for use on a case-by-case basis in complex flow situations for shorter distances.

CALPUFF is a non-steady-state puff dispersion model that dynamically tracks emissions from source to receptor within areas. It accounts for spatial changes in the CALMET-produced meteorological fields, variability in surface conditions (elevation, surface roughness, vegetation type, etc.), chemical transformation, wet removal due to rain and snow, dry deposition, and terrain influences on plume interaction with the surface.

By its puff-based formulation and through the use of three-dimensional meteorological data developed by the CALMET meteorological model, CALPUFF can simulate the effects of time-varying and space-varying meteorological conditions on pollutant transport from sources in complex terrain. The major features and options of the CALPUFF model are summarized in Table 2-2.

2.2.1 Puff Sampling Functions

Included in CALPUFF is a set of accurate and computationally efficient puff sampling routines which solve many of the computational difficulties encountered when applying a puff model to near-field releases. For near-field applications during rapidly varying meteorological conditions, an elongated puff (slug) sampling function may be used. An integrated puff approach may be used during less demanding conditions. Both techniques reproduce continuous plume results under the appropriate steady state conditions.

2.2.2 Dispersion Coefficients

Several options are provided in CALPUFF for the computation of dispersion coefficients (rate of spreading of matrial), including the use of turbulence measurements (Φv and Φw), the use of similarity theory to estimate Φv and Φw from modelled surface heat and momentum fluxes, the use of Pasquill-Gifford (PG) or McElroy-Pooler (MP) dispersion coefficients. Options are available to apply an averaging time correction or surface roughness length adjustments to the PG coefficients.

2.2.3 Overwater and Coastal Interaction Effects

The CALMET meteorological model contains both overwater and overland boundary layer algorithms and the effects of water bodies on plume transport, dispersion, and deposition can be simulated with CALPUFF. The puff formulation of CALPUFF is designed to handle spatial changes in meteorological and dispersion conditions, including the abrupt changes, which occur at the coastline of a major body of water, such as Lake Ontario.

2.2.4 Dry Deposition

A full resistance model is provided in CALPUFF for the computation of dry deposition rates of gases and particulate matter as a function of geophysical parameters, meteorological conditions, and pollutant species. Options are provided to allow user-specified, diurnally variable deposition velocities to be used for one or more pollutants instead of the resistance model (e.g., for sensitivity testing) or to by-pass the dry deposition model completely.

2.2.5 Wind Shear Effects

CALPUFF contains an optional puff splitting algorithm that allows vertical wind shear effects across individual puffs to be simulated. Differential rates of dispersion and transport among the "new" puffs generated from the original well-mixed puff can substantially increase the effective rate of horizontal spread of the material.

Table 2-2:Major Features of the of the CALPUFF Model

- Emission source types
    - Point sources (constant or variable emissions)
    - Line sources (constant or variable emissions)
    - Volume sources (constant or variable emissions)
    - Area sources (constant or variable emissions)
- Non-steady-state emissions and meteorological conditions
    - Gridded 3-D fields of meteorological variables (winds, temperature)
    - Spatially-variable fields of mixing height, friction velocity, convective velocity scale
    - Monin-Obukhov length, precipitation rate
    - Vertically and horizontally-varying turbulence and dispersion rates
    - Time-dependent source and emissions data for point, area, and volume sources
    - Temporal or wind-dependent scaling factors for emission rates, for all source types
- Efficient sampling functions
    - Integrated puff formulation
    - Elongated puff (slug) formulation
- Dispersion coefficient (Φ_y, Φ_z) options
    - Estimated values of σv and σw based on similarity theory
    - Vertical wind shear
    - Puff splitting
    - Differential advection and dispersion
- Plume rise
    - Buoyant and momentum rise
    - Stack tip effects
    - Building downwash effects
    - Partial penetration
    - Vertical wind shear