Generating an Hour-By-Hour Model-Ready Marine Emission Inventory

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ABSTRACT

This paper provides an overview of the tools and techniques used to develop hourly, SMOKE model-ready emission inputs for ocean-going marine vessels calling ports in British Columbia, Canada.

The authors were provided a number of unique marine emissions datasets, the most notable of which contained more than four million vessel track records from the 2005-2006 B.C. Ocean-Going Vessel Emissions Inventory prepared by the Chamber of Shipping of B.C. Detailed vessel information (vessel type, voyage ID, location, etc.) and emissions activity data (engine type, engine speed, fuel type, etc.) were provided at high spatial and temporal resolution for a full one-year period. The data were imported into a SQL Server database and then manipulated using a variety of GIS and database techniques to arrive at hourly emission files (CEM-like) for a very large 4.0 km resolution SMOKE / CMAQ model domain. Although time consuming to prepare and computationally expensive to model, preliminary results indicate that the adoption of high spatial and temporal resolution emissions inputs has an impact on the overall model performance for a number of chemical species, especially when being modelled at relatively high spatial resolutions (e.g., 4.0 km or finer).

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BACKGROUND

Over the last several years, the authors (under contract to Environment Canada) have developed a sophisticated and comprehensive air quality modelling system for use over the Pacific Northwest. The modelling system, hereafter referred to as the PNW-CMAQ system, is based on Environment Canada meteorological models, the SMOKE emissions processing system, and the CMAQ air quality model. This system has been used successfully to evaluate the impact of a number of different emission change scenarios on the ambient air quality over the Pacific Northwest for air quality management plan and policy-making purposes.

In support of a joint Canada-US Sulphur Emission Control Area (SECA) application, the authors used the PNW-CMAQ system previously to conduct numerical modelling of the impacts of sulphur (SO_x) emissions from marine vessels on air quality over the Pacific Northwest at high spatial and temporal resolutions. Sensitivity studies were completed previously for two base cases for the Georgia Basin/Puget Sound area (in August 2001 and December 2002). Emission change scenarios designed to assess air quality impact associated with both removing and doubling all marine vessel emissions were also performed. This work determined that the modelling system is suitable for evaluating marine emission impacts. However, it was also determined that greater spatial and temporal resolution in the emissions inputs, in particular for marine vessels, could assist in making better informed decisions.

Since that time, a number of more scenarios have been developed that more realistically reflect the emission changes and geographical extent that need to be analysed in support of the SECA application. A standard 2002 base case run is being performed primarily for model evaluation and comparison purposes. Detailed emission change scenarios relating to sulphur fuel content are being carried out for the year 2020. The resulting analyses will provide invaluable insight into broad decision making that is being undertaken in relation to a Canadian SECA application.

The overall purpose of the work is to evaluate potential impacts on air quality and acid deposition associated with emission changes that might arise from implementing a SECA along the coast of British Columbia, Canada.

To undertake this work, a number of enhancements and modifications have been incorporated into the PNW-CMAQ modelling system. These are mentioned briefly below to provide context to the overall project. The focus of the remainder of this paper is on the methods employed to generate an ultra-high spatial and temporal resolution marine emissions inventory for ocean-going vessels suitable for input to regional atmospheric / chemistry models.

MODEL CONFIGURATION

In addition to the marine emissions inventory pre-processing and integration into SMOKE, various other components of the base PNW-CMAQ modelling system were upgraded by the authors as described in the bulleted lists below.

Model Domain and Episodes Modelled:

- The same summer (August 09-31, 2001) and winter (December 01-13, 2002) time periods used in previous modelling exercises were adopted for comparative and model evaluation purposes.
- The model domain was expanded considerably to cover the major marine shipping routes along which goods are conveyed to and from the port of Vancouver. The expanded model domain covers an area of approximately 350,000 km^2 at a horizontal grid resolution of 4.0 km (321 columns x 271 rows = 86,991 grid cells). For comparative purposes, this domain contains approximately four times as many grid cells as the previous PNW-CMAQ 4.0 km domain and more than seven times the number of grid cells as the US EPA's 36 km national model domain.
- Figure 1 presents a graphic of the expanded 4.0 km domain.

Meteorology

- Execution of the GEM-LAM meteorological model at a horizontal resolution of 2.5 km for both summer and winter episodes as a replacement to the previously integrated MC2 meteorological model outputs generated at a 3.3 km resolution for a smaller domain.
- Modification of Environment Canada's GEM-MCIP converter to: a) make use of the latest MCIP code (version 3.3); and, b) incorporate pass-through options for a number of variables, most specifically PBL height and related parameters.

Emissions Processing

- Generation of biogenic emissions using MEGAN (ver 2.04) with updated land coverage data generated using ArcGIS.
- Migration from SMOKE version 2.1 to version 2.3.
- Use of EIGIS to generate spatial surrogates over the expanded model domain.

Chemistry Model

- Migration from CMAQ version 4.4 to version 4.6.
- Migration from the SAPRC-99_ae3_aq chemical mechanism to the SAPRC-99_ae4_aq mechanism to include the sea salt algorithms.

Base year emissions inventories for land-side activities were obtained from Environment Canada (2002 CAC EI) and the US EPA (2001 NEI). Local improvements (replacements) for several census divisions (counties) were made to these datasets using inventories generated by the Greater Vancouver Regional District (GVRD; now "Metro Vancouver") and inputs provided by individuals with local knowledge of emission sources in the region.

MARINE EMISSIONS

The marine emissions data adopted in this work were actually derived from a number of sources. Emissions associated with all inland waters and ocean-going fishing and recreational vessels, ferries, and harbour support vessels (e.g., tugs) were obtained from national inventories and allocated to the model grid using spatial surrogates developed for the region as part of previous PNW-CMAQ work.

The remainder of the ocean-going vessel emissions were compiled from three highly unique inventories. Each of the inventories was generated using different techniques and hence were provided in different formats, contained different parameters in different units, etc. In certain locations, the spatial extents of the inventories also overlapped, meaning spatial adjustments had to be made in order to prevent double counting of emissions.

The three primary marine inventories adopted include: a North American marine inventory compiled by Dr. J. Corbett at the University of Deleware (Corbett inventory); a Puget Sound (Puget) emissions inventory; and, the BC Chamber of Shipping (COS) inventory. The remainder of this paper is focused on the methods and techniques developed by the authors to integrate these disparate inventories into an ultra-high resolution marine emissions inventory for the Pacific Northwest.

Corbett Inventory

The 2005 Corbett marine emissions inventory was compiled by Dr. J. Corbett at the University of Deleware. The inventory data and accompanying reports can be downloaded from: http://coast.cms.udel.edu/NorthAmericanSTEEM/. Development on the inventory was partially funded by the California Air Resources Board (ARB), and the Commission for Environmental Cooperation of North America (CEC). The intent was to develop an inventory of commercial marine emissions for North America that would support ARB, CEC, western regional states, United States federal, and multinational efforts to quantify and evaluate potential air pollution impacts from shipping in U.S, Canadian, and Mexican coastal waters.

The Corbett inventory was compiled using the Waterway Network Ship Traffic, Energy and Environment Model (STEEM); a system designed to characterize ship traffic, estimate energy use, and assess the environmental impacts of shipping. A ship traffic module within STEEM geographically and temporally allocates ship traffic based on an empirical waterway network, historical ship movement data, and ship attributes data.

The Corbett inventory contains a set of geographically resolved annual gridded emissions for the following pollutants: Sulfur (SO_x as SO_2), Nitrogen (NO_x), Carbon dioxide (CO2), Particulate Matter (PM), Hydrocarbons (HC), and Carbon monoxide (CO). Monthly gridded inventories for each pollutant are also available.

Although the emissions are provided in GIS compatible format at a 4.0 km horizontal grid spacing, it was first necessary to remap the gridded emissions to align with the PNW-CMAQ 4.0 km grid definition. A map depicting gridded annual SO_x emissions from the Corbett inventory (once spatially trimmed to prevent overlap with the Puget and COS inventories) is shown in Figure 2.

Once the gridded emissions were remapped to the PNW-CMAQ domain, the centre of each PNW-CMAQ grid cell was calculated and used to create an inventory of distributed point sources in

SMOKE ORL format. Emissions were modelled as points so that it would be possible to take advantage of computed stack heights and plume rise within SMOKE. The following stack parameters (recommended by EPA/ARB/ EC) were assumed for all marine vessels modelled as points for all three marine inventories (i.e., Corbett, Puget, and COS inventories):

- Stack Height: 20.0 m (65.6 ft)
- Stack Diameter: 0.80 m (2.6 ft)
- Gas Exit Velocity: 25.0 m/s (82.0 fps)
- Gas Exit Temperature: 282 °C (539.6 F)

Puget Inventory

The Puget Sound emissions inventory was developed by Starcrest Consulting Group under contract to the Puget Sound Maritime Air Forum, a voluntary association of private and public maritime organizations, air agencies, and other parties with operational or regulatory responsibilities related to maritime industry air quality impacts. This 2005 base year inventory was provided in database format, with corresponding latitude / longitude coordinate pairs to allow for allocation to the model grid using a GIS. A number of modifications had to be made to the raw data tables prior to integration into a GIS (i.e., correct for missing coordinate pairs, correction of misplaced coordinates, etc.). A major limitation of this dataset is the lack of both spatial and temporal resolution.

The spatial allocation method used resulted in there being very few points along the primary shipping route from the mouth of the Puget Sound through the Strait of Juan de Fuca (i.e., at key vertices only). Further, the routes used were assumed to be identical throughout the year (i.e., the same grid cells receive emissions year-round). This results in a focusing of emissions into a few grid cells along the shipping route, causing localised hot-spots in the emissions field. Similarly, although individual vessels are identified in the database, some call to port several times per year yet there are no temporal (month, date, hour) records contained within the database. As such, emissions were compiled as annual totals and converted to hourly emissions in SMOKE using a default flat temporal profile.

As with the Corbett inventory, the resulting gridded, annual emissions were converted to SMOKE-ready point sources in ORL format using the same stack parameters presented above. A map depicting annual gridded emissions of SO_x from the Puget inventory (once trimmed to prevent overlap with the Corbett and COS inventories) is presented in Figure 3.

Chamber of Shipping (COS) Inventory

The 2005-2006 BC Ocean-going Vessel Emissions Inventory was compiled by the BC Chamber of Shipping, in collaboration with Environment Canada, the Greater Vancouver Regional District, and other key stakeholders. The spatial coverage of the COS inventory includes all ocean waters that are within the Marine Communications and Traffic Services Association (MCTSA); an area that extends from the coast to about the 50 nm limit offshore.

Extensive details on the compilation of the inventory (i.e., emission estimation methods, inputs, etc.) are not provided in this paper as they are provided elsewhere, most notably in a companion paper also presented at the 17th International Emission Inventory Conference - "Inventory Evolution - Portal to Improved Air Quality" (Portland, Oregon, June 2 - 5, 2008). Additional information can also be obtained from the BC COS website (http://www.cosbc.ca/index.php). The focus for this paper is how the raw inventory was manipulated to arrive at an ultra-high spatially and temporally resolved inventory for input to SMOKE / CMAQ. Some highlights from the 2005-2006 BC COS inventory preparation process are presented below to provide adequate context.

Highlights of the 2005-2006 BC COS Emissions Inventory

- The inventory was compiled using high-resolution Coast Guard Vessel Traffic Operation Support System (VTOSS) Track Data (vessel location and speed at 3-7 minute intervals).
- The same VTOSS data were used to determine time in mode, main engine load factors per voyage segment (using separate algorithms for cargo and cruise ships), and geographic and temporal information.
- All commercial deep-sea vessels over 20 metres in length which called at a BC port were inventoried in this manner for a period spanning from April 1, 2005 to March 31, 2006 during which time 1,428 ships made 3,565 voyages.
- The COS issued a survey and collected data on engine, boiler and fuel characteristics for each vessel making a port call in BC during the study period. These data were used to determine aux engine power, aux engine load factors, boiler fuel use, and fuel sulphur content.
- Follow-up surveys were administered to clarify auxiliary engine use at berth and to obtain unique engine power information at variable speeds for each individual cruise ship.
- Lloyd's Marine Intelligence unit data were used to compute main engine power.
- Emissions factors were derived primarily from ENTEC or IPCC for all engines and boilers in all modes of activity.
- Pollutants inventoried included: nitrogen oxides (NO_x), sulphur oxides (SO_x), volatile organic compounds (VOCs), coarse particulate matter (PM_{10}), fine particulate matter ($PM_{2.5}$), carbon monoxide (CO), ammonia (NH_3), carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O).

COS inventory Data Pre-processing

The COS inventory was provided to RWDI AIR Inc. by Environment Canada in a 4.0+ Gb ASCII flat file containing a total of more than four million data elements. These data were first imported into an enterprise level relational database (SQL Server 2003). A number of filtering routines were then developed to assist in cleaning the data of spurious and missing values.

Due to the size of the database, separate tables were developed by month of year and vessel activity (manoeuvring, underway, anchored, and berthed). These data tables were then imported into ArcGIS for spatial analysis, retaining all of the engine load information, emission estimates, voyage IDs, etc.

Once in ArcGIS, the locations of each ship for each hour were overlaid onto the expanded PNW-CMAQ model grid. A series of geoprocessing routines were then written and executed to sum all emissions by Voyage ID, per grid cell, on an hour by hour basis. In other words, if en route from Vancouver to the open sea a ship's location (and hence engine load, emissions, etc.) were recorded three times in a given 4.0 by 4.0 km grid cell over the coarse of an hour, these were summed to arrive at the total emissions from that ship on that voyage occurring in that grid cell during that hour. This same technique was used to handle occasions where a ship remained in one grid cell (sometimes at one location, sometimes at several locations within the same grid cell) for more than one hour at a time. This process was completed for each set of vessel activities, such that the product was a set of hourly, gridded, emissions tables that also contained all of the native voyage IDs and other information. A map depicting the raw tracked vertices (i.e., emission points) along the travel route for a single voyage (i.e., one vessel "underway") is shown in Figure 4 to illustrate the methodology described above.

The next step involved developing "cut-lines" between the various inventories to remove overlapping emissions where double counting was expected to occur. Spatial queries were used in combination with an inclusion / exclusion field in the database to automate the bulk of this process. Some manual review and editing was also required in a few select locations.

Having completed this process, a series of routines were developed to develop SECA-related emission change scenarios (i.e., fuel switching to 0.1% sulphur content when within 100 nm or 50 nm). Scenario changes were applied at the engine class and voyage ID level using a series of emission scenario look-up tables developed by Environment Canada.

For each scenario, emissions were adjusted and then summed across all voyages for each hour to arrive at an aggregate gridded emissions field. The centre of each grid cell was then computed and used in combination with the stack parameter assumptions detailed previously to develop an hourly varying point source emissions file. For integration into SMOKE, a custom export routine was developed to generate the output files in EMS-95 CEM format. Figure 5 is a map indicating the total number of sources and spatial extent of the COS inventory.

The SMOKE pre-processor itself also had to be modified to handle the large number of point sources: Corbett = 11,794 point sources with annual average emissions; Puget = 142 point sources with annual average emissions; and, COS = 5038 point sources with hourly varying emissions (i.e., the approximate equivalent of 5038 points x 24 hours for each day of SMOKE runs = 120,912 sources per day). During testing, SMOKE model execution times were seen as a limiting factor. A series of unique run-time scripts were developed to improve execution times and load balancing on RWDI's massively parallelized 122 CPU Linux computing cluster.

Figure 6 is a 3-D representation of SO_x emissions from the COS inventory, representing the high degree of spatial variability achieved in this highly unique emissions inventory.

RESULTS

Preliminary SMOKE and CMAQ modelling was underway at the time of writing. Initial results, however, suggest that the increased spatial and temporal resolution of the marine emissions inventory (especially the hourly COS emissions data) has a dramatic affect on the location and timing of emissions and hence location, magnitude, and timing of air pollution events (both macro- and micro-scale).

CLOSING

Highly spatially and temporally resolved activity data were used to generate emission inputs to regional atmospheric chemistry models. Although time consuming to prepare and computationally expensive to model, the adoption of high spatial and temporal resolution emissions inputs are expected to affect the overall model performance for a number of chemical species, especially when being modelled at high spatial resolutions (e.g., 4 km or finer).

This paper describes a snapshot in time of the status of an ongoing work in progress. The following items have been identified by the authors for future development:

- Completion of scheduled CMAQ modelling and model evaluation exercises.
- Integration of improved spatial and temporal emissions data for marine vessel activities in the Puget Sound (inventory under construction).
- Development of refined emission scenarios based on inputs from MARPOL.
- Integration of new emissions inventory data for other sources (e.g., migrate to an updated 2005 base year inventory for area, on-road mobile, and point sources).

KEYWORDS

Marine, Emissions, Inventories, SMOKE, CMAQ, GIS, Database, Canada

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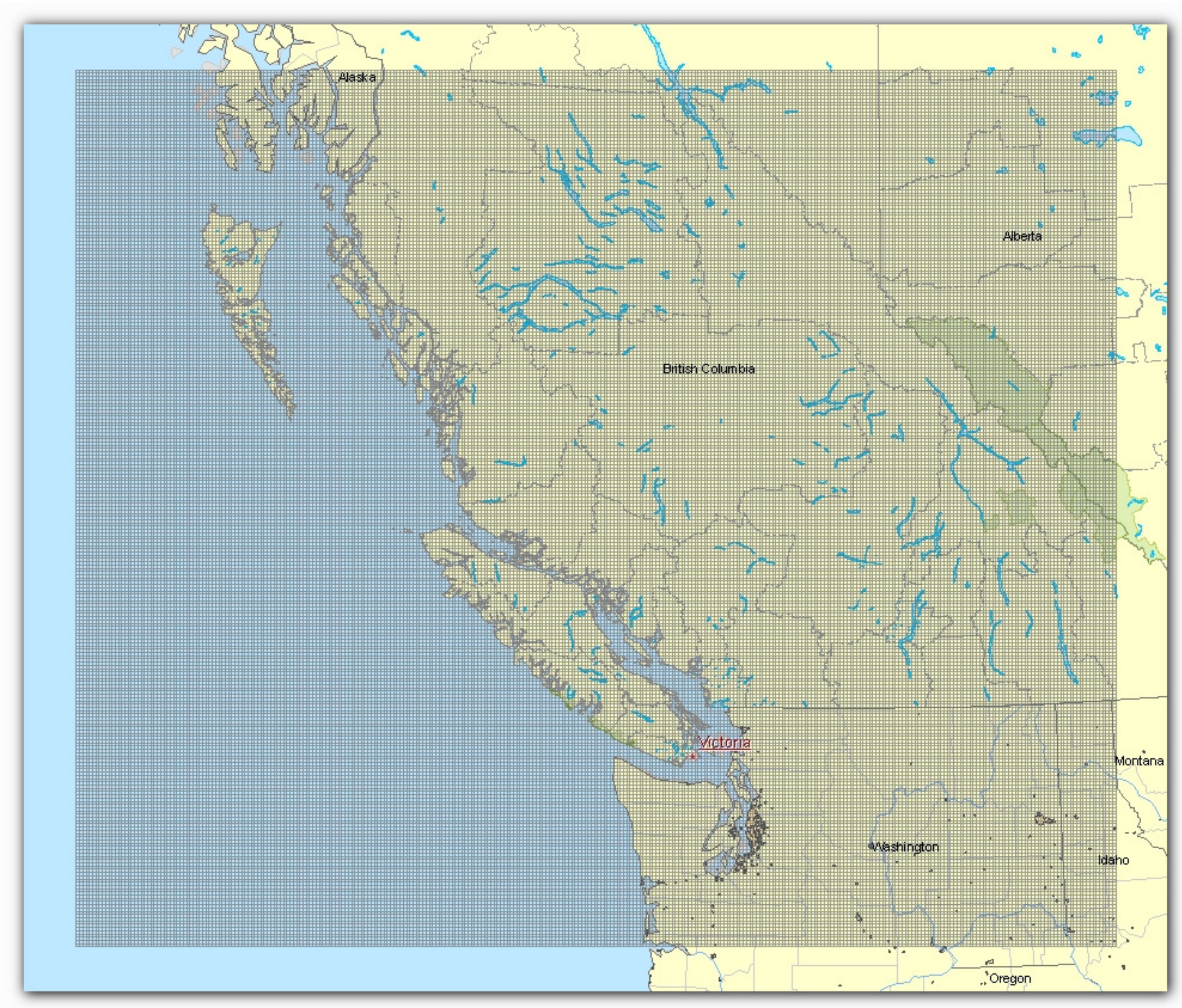

Figure 1. Expanded 4.0 km domain and revised MCTSA (50 nm limit).

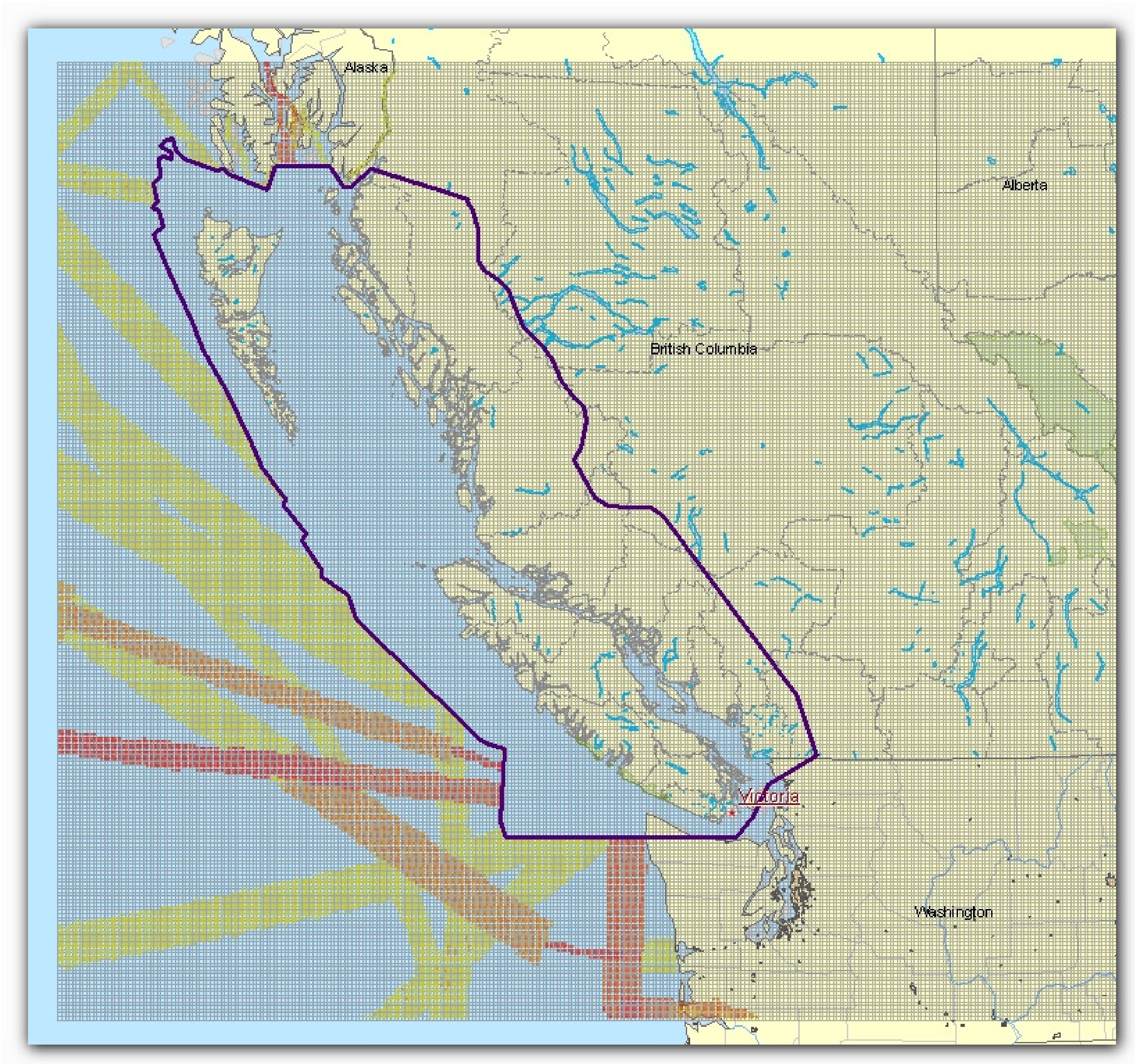

Figure 2. Gridded annual SO_x from the Corbett inventory.

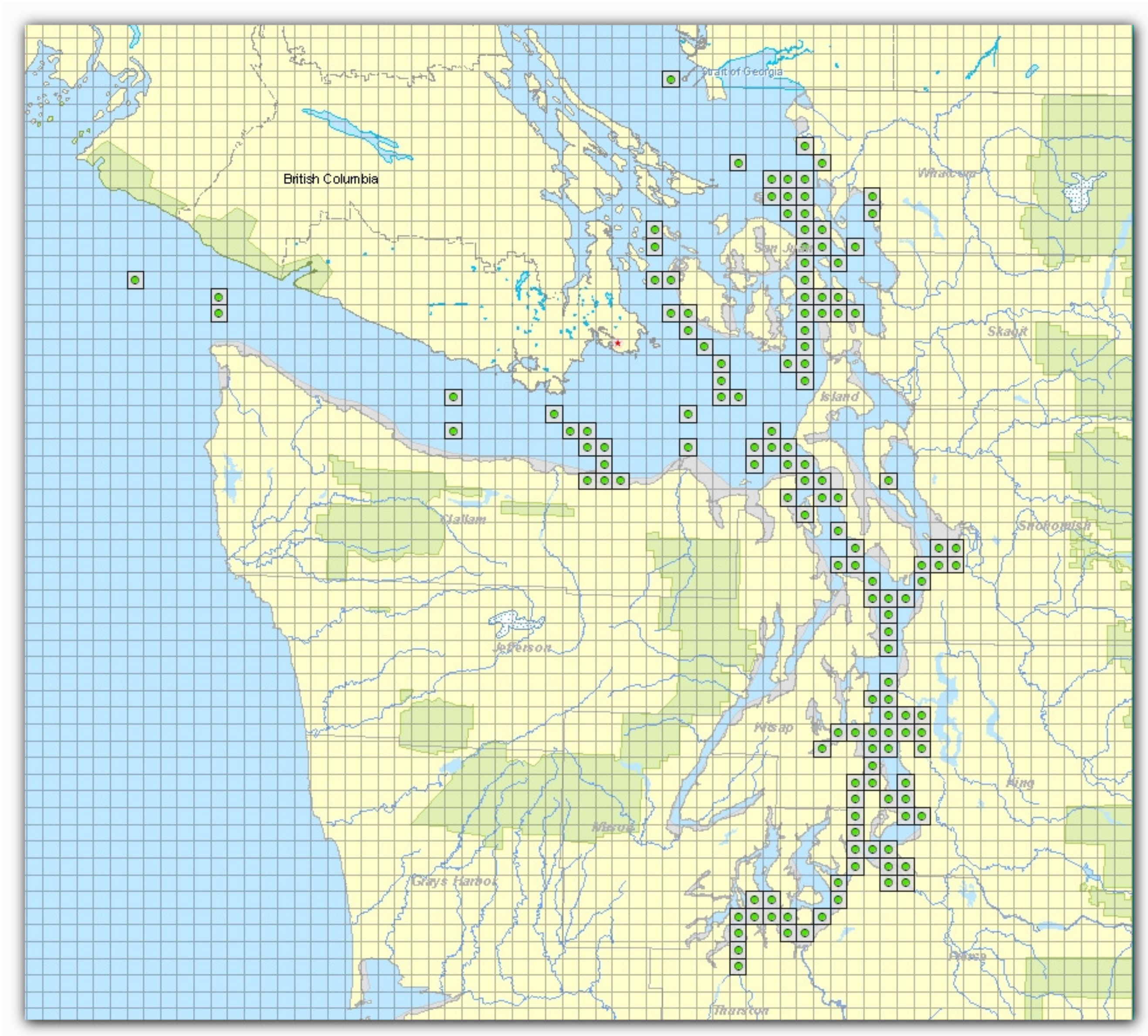

Figure 3. Gridded annual SO_x from the Puget inventory.

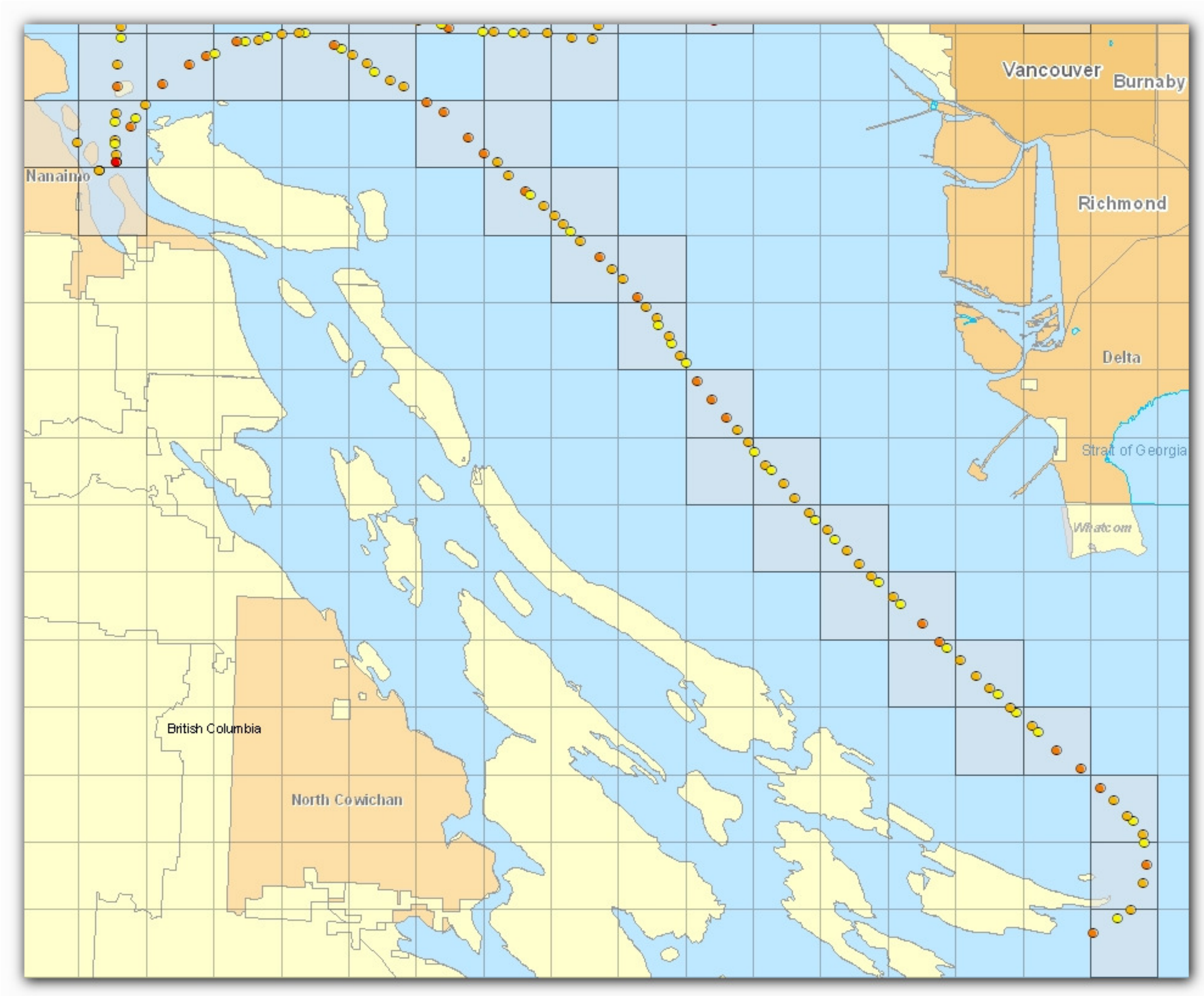

Figure 4. Example of spatial summation (geo-processing) method used to derive hourly total emissions by grid cell from the individual vessel track data in the COS emissions inventory.

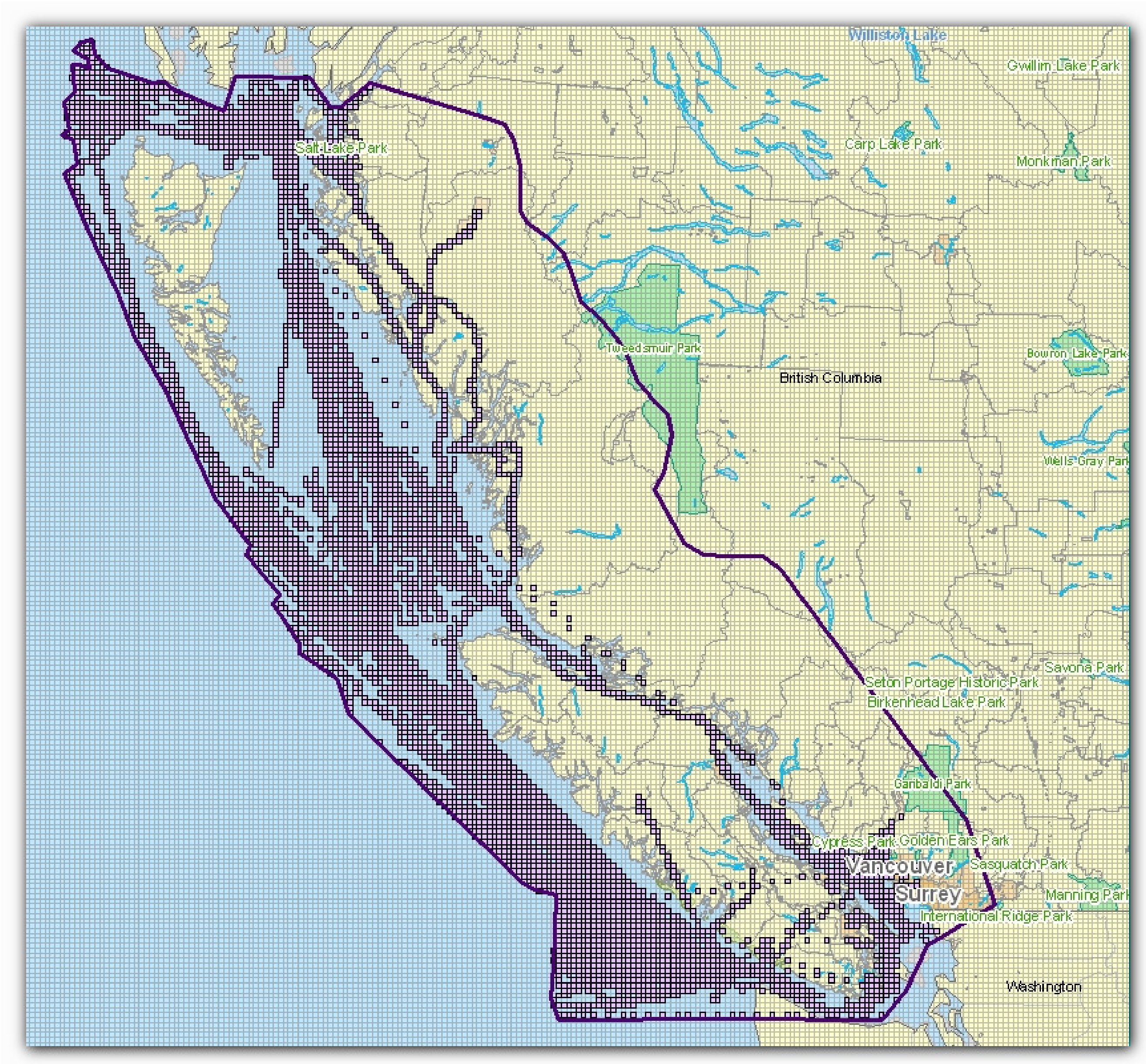

Figure 5. Map of COS point sources and spatial extent (cut-lines definition lines shown).

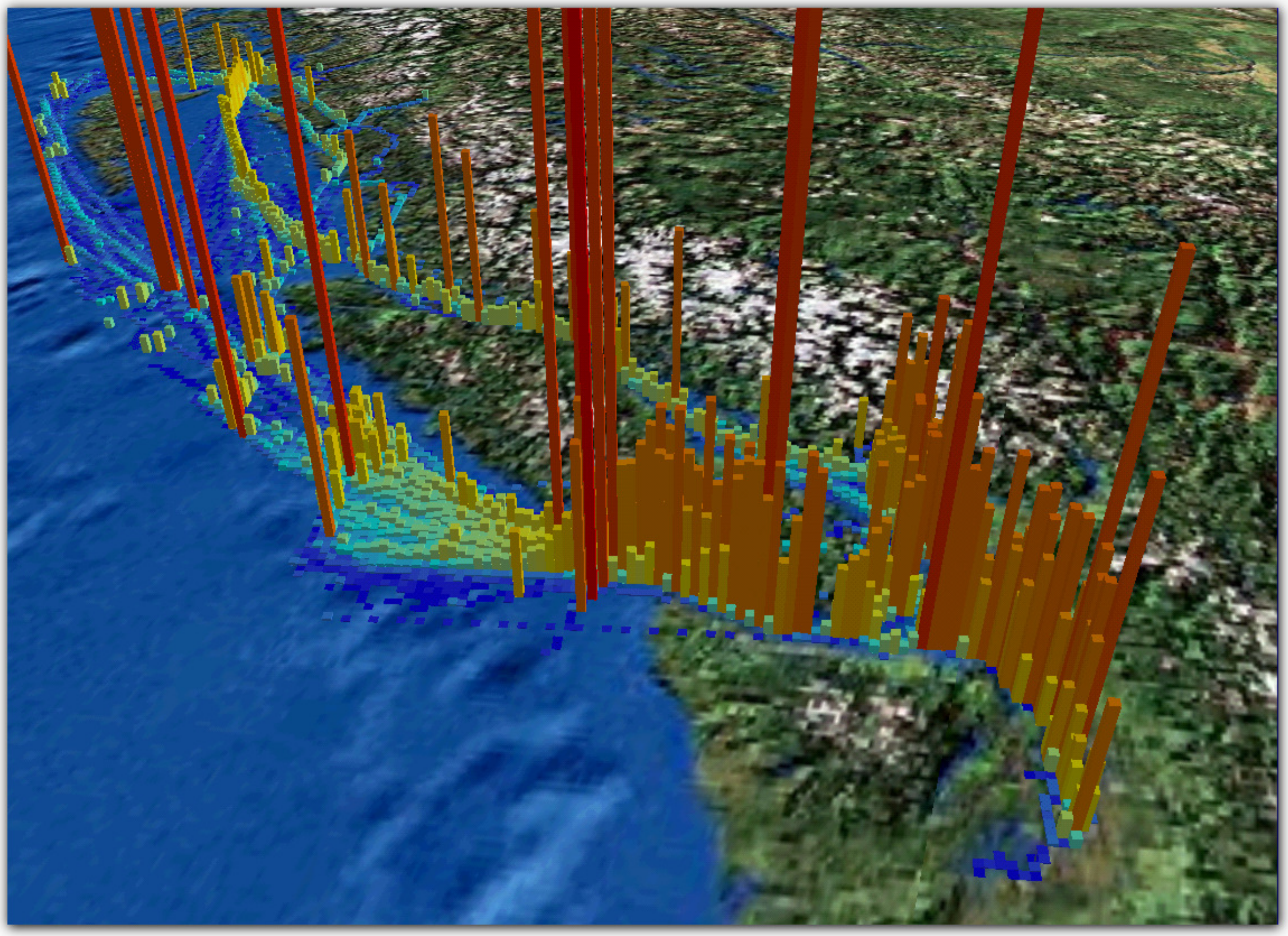

Figure 6. A 3-D representation of SO_x emissions from the COS inventory.