Modelling the Effects of E10 Fuels in Canada

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ABSTRACT

In May 2003, Health Canada held an expert panel on ethanol-blended gasoline and how its widespread use might affect human health risks from exposure to vehicle exhaust pollutants in Canada. One of the key topics of discussion was the availability of existing atmospheric photochemistry and air quality modelling results. Most of the published information was embedded in more general studies of reformulated gasoline in the U.S. and is not directly applicable to Canada because of differences in fuel formulation, vehicle fleet, and climatic conditions. Based on this information gap, the authors have undertaken a modelling exercise to quantify the effects of E10 (10% ethanol blend gasoline) splash and tailor blended fuels on the formation of smog and air toxics. Modelling is being performed over two model domains (eastern North America and the Pacific Northwest) covering two meteorological episodes for different base year emission inventories (2000 and 2010). An integral part of the emission processing has included the use of the recently 'Canadianized' version of the MOBILE emission model and a modified version of the SMOKE emission processor that is capable of handling toxic species (specifically benzene and 1,3-butadiene) explicitly using a modified version of the SAPRC99 chemical mechanism. Air quality modelling will be performed using a modified version of CMAQ capable of tracking primary and secondary toxic chemical species. This paper presents an overview of the emission inventory development and processing steps completed to date to model splash and tailor blended E10 fuel scenarios in Canada.

BACKGROUND

In May 2003, Health Canada held an expert panel on ethanol-blended gasoline and how its widespread use might affect human health risk from exposure to vehicle exhaust pollutants in Canada. The authors participated on the panel, providing input on atmospheric photochemistry and air quality modelling. This input was based on a review of published air quality modelling studies related to ethanol-blend gasoline. Most of the published information was embedded in more general studies of reformulated gasoline in the U.S. and is not directly applicable to Canada because of differences in fuel formulation and climatic conditions between the U.S. and Canada. The only air quality modelling study performed in Canada to date for ethanol-blend gasoline was simplified photochemical box modelling undertaken by the National Research Council of Canada (NRC) in the early and mid-1990's. This work focused on a historical smog event that occurred in Southern Ontario and predicted the effect that widespread use of E10 (10% ethanol-blend) would have had on pollutant levels during that event (Singleton *et al.*, 1997).

Since that time, a number of modellers have been involved in more sophisticated 3-dimensional modelling of regional smog in various parts of Canada. The Meteorological Service of Canada (MSC) has been developing a new unified model called AURAMS that treats both the gas-phase and aerosol-phase chemical transformations in the atmosphere that influence the secondary formation of pollutants during smog events. At the same time, the U.S. EPA's Models-3/CMAQ has been adopted by a number of Canadian modellers (RWDI, NRCC, Environment Canada P&NR and P&YR, Ontario MOE, etc.) and applied to various policy scenarios in eastern and western Canada. As a result of the modelling efforts that have been undertaken over the past few years, Models-3/CMAQ has been tested and evaluated for a number of representative historical smog events in various parts of Canada.

Following the Expert Panel, Health Canada initiated a detailed study of the health effects that would be associated with the use of E10 (10% ethanol blend gasoline) in Canada. As part of this work, the authors have begun an air quality modelling program that will make use of an air-toxics version of Models-3/CMAQ. This paper provides a description of the workplan for the air quality modelling and the associated emission inventory work, and presents the work that has been completed to date.

STUDY DESIGN

The following sections outline the study approach and methodology, including a description of the models used, domains and episodes, and emission scenarios.

Pollutants and Metrics of Interest

The key air pollutants potentially affected by the use of ethanol-blend gasoline are: benzene, carbon monoxide (CO), formaldehyde (HCHO), acetaldehyde (CCHO), 1,3-butadiene, peroxyacetyl nitrate (PAN), ground-level ozone (O_3), and possibly also NO_2 and fine particulate matter $PM_{2.5}$. Regional air quality modelling will be used to evaluate the relative change in air quality associated with changes in emissions resulting from the introduction of ethanol-blend fuels.

With respect to $PM_{2.5}$, the complexities of the formation of secondary aerosols are such that regional air quality models are still in need of development. This is particularly true in the case of secondary organic aerosols, such as those arising from chemical transformation of VOC emissions in vehicle exhausts. Furthermore, $PM_{2.5}$ is actually treated by two interacting sub-distributions (or modes) in CMAQ: the nuclei or Aiken (i) mode and the accumulation (j) mode. These modes include aerosol components such as sulfates, nitrates, ammonium, water, anthropogenic and biogenic organic carbon, elemental carbon and other unspecified anthropogenic origins. In this light, CMAQ does not generate actual $PM_{2.5}$ concentrations. However, the sum of these aerosol species can be used to generally represent $PM_{2.5}$ from the CMAQ modelling and, despite the high degree of uncertainty, will still be of interest to examine for "demonstration" and "guidance" purposes.

The CMAQ air quality model provides predicted hourly concentrations at each grid cell. These data will be processed to obtain spatially and temporally averaged mean and maximum concentrations for the averaging periods of interest. Model results will also be post-processed for use in subsequent human exposure and health risk analyses.

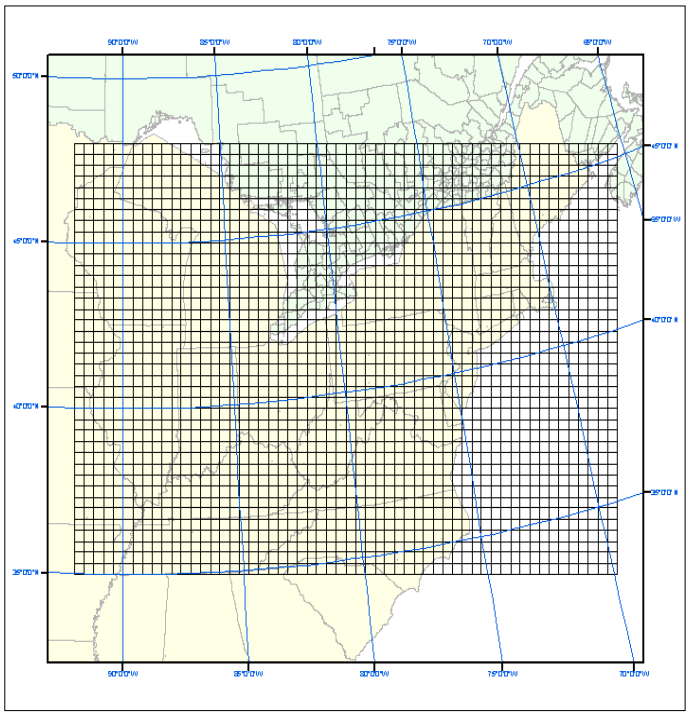
Model Domains & Episodes

Two meteorological 'Episodes' covering two geographic regions ('Domains'), and two 'Base Year' emission inventories were assessed as part of this project. Table 1 provides a summary of the meteorological Episode dates, model Domains, grid cell resolutions, and emission inventory Base Years used. Figures 1 and 2 depict graphical representations of the Eastern North America and Pacific Northwest modelling Domains, respectively.

Table 1. Model domains, grid cell resolutions, episode dates, and base year emission inventories adopted in the air quality modelling exercise.

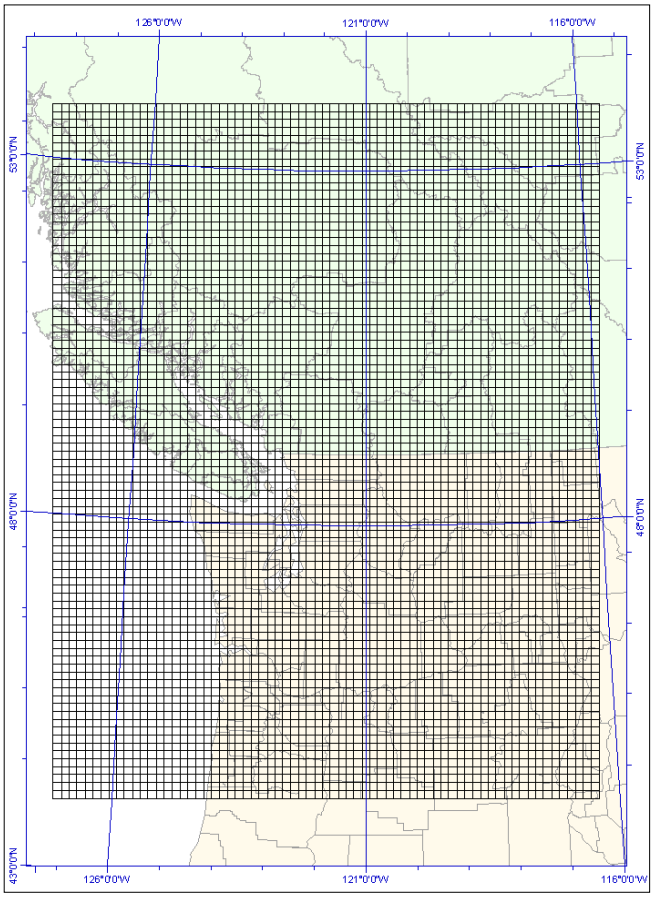
Study / Model Domain	Grid Cell Resolution	Episode Dates	Emission Inventory Base Year
Pacific Northwest	12 km	Aug. 09 to 20, 2001	Canada: 2000 US: 1999 / 2000
			Canada: 2010 (grown from 2000) US: 2010 (grown from 1999 / 2000)
Eastern North America	36 km	July 10 to 19, 1999	Canada: 1995 (grown to 2000) US: 1999

Figure 1. Eastern Canada domain.



For Eastern Canada, the model domain covers the majority of the northeastern U.S. and the most densely populated areas of southeastern Canada with a horizontal grid spacing of 36-km, which has been demonstrated to perform reasonably well at predicting ground-level ozone and fine particulate matter during the 1999 episode. The July 1999 episode extends from July 11 to 19, 1999 and coincides with a high ozone and fine particulate matter episode that occurred over southern Ontario and Quebec. Meteorological conditions during this period were dominated by a high pressure system over the southeastern U.S., resulting in southwesterly winds, predominantly clear skies, and high temperatures (daytime highs > 30ºC) over much of the northeast.

Figure 2. Pacific Northwest domain.



The Pacific Northwest model domain covers most of the northwestern region of Canada and the U.S. at a 12-km grid cell resolution. The domain extends beyond the western shore of Vancouver Island in the west to the B.C. / Alberta border in the east, and ±500 km of the Canada / U.S. border in the north-south. The domain was initially selected to allow for the assessment of regional transport between Canada and the U.S., and to study air quality impacts over the populated areas of the Lower Fraser Valley in Southern B.C. The study period (August 9 to 20, 2001) was originally selected to align with the Pacific 2001 field study. The weather affecting this period was comprised of three regimes: a dry stable blocking pattern; a wet period; and, a transient period. The dry weather (blocking pattern) lasted until August 20, during which pollutant levels became elevated, with the highest observed pollutant concentrations occurring during the August 10 to 15 stagnant phase (Snyder, 2002; Boulton *et al.*, 2004; Qiu *et al.*, 2004; di Cenzo *et al.*, 2004).

Prior to running the E10 emission scenarios, "Base Case" runs will be performed for each domain / episode combination. Results from these runs will be used as a benchmark against which to compare the scenario model results. A 2000 Base Year Emission Inventory was developed for the PNW region as part of previous work (Boulton *et al.*, 2004; Qiu *et al.*, 2004; di Cenzo *et al.*, 2004; Boulton *et al.*, 2003). However, not all sources used in that modelling have the same base year. The raw emission data used to compile the inventory ranged from 1995 to 2002 and were calculated using revised estimates, growth factors, and other techniques, depending on the data source. Nonetheless, it is considered a reasonable approximation for a year 2000 emission inventory in that region. Because the 2000 CAC EI was unavailable at the time of project initiation, growth factors provided by Environment Canada were used to develop the 2000 Base Year emission inventory for the eastern domain.

E10 Emission Calculation and Processing

Two unique emission scenarios were modelled:

1) 100% introduction of E10 fuel through Splash blend mixing, and
2) 100% introduction of E10 fuel through Tailor blend applications.

Prior to undertaking the air quality modelling portion of the work, an assessment of the relative differences between the Base Year and the two emission scenarios was performed. The purpose of this exercise was to determine which method of E10 fuel introduction (Splash or Tailor blend) would result in the greatest difference in emissions relative to the Base Case and hence is expected to have the greatest impact on air quality.

Emission estimates attributed to on-road vehicles are generated using the US EPA's MOBILE model. The latest official release of MOBILE is version 6.2 (US EPA, 2002). Through contacts with Environment Canada, the authors were able to obtain and use the recently Canadianized version of the model, MOBILE6.2C (Environment Canada, 2004). Emissions were calculated for the following pollutants of interest: NH_3, $PM_{2.5}$, CO, NO_X, SO_2, benzene, 1,3-butadiene, acetaldehyde (CCHO), formaldehyde (HCHO) and total VOCs.

The approach for this study was to perform a number of MOBILE6.2C runs to develop scaling factors based on Canadian specific data that can then be applied to the regional (census-division wide) emissions by vehicle type. These scaling factors will then be used to adjust the Base Year (i.e., gasoline fleet) emissions to a 100% E10 fleet. Table 2 presents the MOBILE6.2C model inputs adopted to produce the necessary emission estimates. Having completed the MOBILE6.2C runs, emission rates by vehicle type, speed, and ambient temperature were compared between the two E10 scenarios and the "Base Case" results on a pollutant-by-pollutant basis.

Modelling System

The model grid resolutions, meteorological inputs, and raw emission data are unique to each Episode being modelled as defined in Table 1. The following specifics of the modelling system are both domain and episode independent:

Meteorological Model and Pre-processor

- For the Pacific Northwest model Domain, MC2 model outputs (generated by the University of British Columbia (UBC) under contract to Environment Canada) were pre-processed using RWDI's MC2 → MM5 converter.
- For the Eastern Canada Domain, the MM5 model was used to generate the requisite meteorological fields.
- MCIP, version 2.2 was used in both cases to reformat and collapse the modelled meteorological fields for input to the emission processing and air quality models.

Emission Processor

- Sparse Matrix Operating Kernel Emission (SMOKE) modelling system, version 2.0
- Biogenic emissions generated using BEIS3 within SMOKE.
- Base Year emissions for mobile sources have been generated using a mix of both the MOBILE5C and MOBILE6 emission models. For the E10 emission scenarios, modified emission inventories for on-road mobile sources will be generated using as previously described. To allow for between-run intercomparisons to be made, mobile emissions for both the Base Year and E10 emission scenarios will be modelled as spatially and temporally varying area source emissions (e.g., top-down approach).

Table 2. MOBILE6.2C Workplan and model inputs.

MOBILE6.2C Parameter	Base Case		Splash Blend	Tailor Blend	
Oxygenate (Ethanol)	0% (Volume) 0% (Market Share)		10% (Volume) 100% (Market share)	10% (Volume) 100% (Market Share)	
Aromatics (%)	WEST 23.6	EAST 28.4	WEST 21.2	WEST 20.3	EAST 24.8
Olefins (%)	WEST 10.1	EAST 10.3	WEST 9.1	WEST 7.6	EAST 7.8
Benzene (%)	WEST 0.7	EAST 0.8	WEST 0.6	WEST 0.7	EAST 0.8
E300 (%)	WEST 86.6	EAST 83.3	WEST 87.9	WEST 86.6	EAST 83.3
E200 (%) W = Winter S = Summer	WEST W = 55.6 S = 48.6	EAST W = 53.7 S = 47.3	WEST W = 60.0 S = 53.7	WEST W = 55.6 S = 48.6	EAST W = 53.7 S = 47.3
Fuel RVP W = Winter S = Summer	WEST W = 13.7 S = 7.9	EAST W = 14.7 S = 8.9	WEST W = 14.7 S = 8.9	WEST W = 13.7 S = 7.9	EAST W = 14.7 S = 8.9
Gasoline Sulphur* (ppm) [1] = 2000 [2] = 2010	WEST [1] = 225 [2] = 30	EAST [1] = 456 [2] = 30	WEST [1] = 203 [2] = 30	WEST [1] = 225 [2] = 30	EAST [1] = 456 [2] = 30
Vehicle Reg. Distribution	WEST (British Columbia, 2000)		EAST (Ontario, 2000)		
Min / Max Temperature (Degrees F)	WEST (Vancouver, Normals) January: 33, 43 April: 42, 56 July: 56, 71 October: 44, 56		EAST (Toronto, Normals) January: 13, 28 April: 34, 53 July: 59, 80 October: 39, 57		
Absolute Humidity (grains/lbs)	WEST (Vancouver, Average) January: 28 April: 38 July: 61 October: 44		EAST (Toronto, Average) January: 20 April: 28 July: 69 October: 37		
Sunrise, Sunset (range: 5:00-9:00)	WEST (Vancouver, Mid Month) January: 8 AM, 5 PM April: 5 AM, 7 PM July: 5 AM, 9 PM October: 7 AM, 5 PM		EAST (Toronto, Mid Month) January: 8 AM, 5 PM April: 6 AM, 7 PM July: 6 AM, 9 PM October: 7 AM, 6 PM		
Pollutants	NH_3, $PM_{2.5}$, CO, NO_X, SO_2, Benzene, 1,3-Butadiene, Acetaldehyde (CCHO), Formaldehyde (HCHO), Total VOCs				
Average Speed	50 km/h, 80 km/h, 100 km/h				
Calendar Year	2000, 2010				
Altitude	Low				
Cloud Cover	0%				
Peak Sun	Between 10 AM - 4 PM				

Note: * Valid input range = 30 ppm to 1000 ppm

Photochemical Air Quality Model

- Modified Community Multiscale Air Quality (CMAQ) model (2003).
- Because some of the pollutants of interest to this study are unique (i.e., 1,3-butadiene and acetaldehyde (CCHO), a modified version of the Statewide Air Pollution Research Center (SAPRC-99) mechanism is being adopted. The SAPRC-99 mechanism contains more VOC species than other mechanisms and is capable of handling the pollutants of interest for this study explicitly. The disadvantages to using this mechanism are that: a) model run times for the SAPRC-99 mechanism can be more than twice as long compared to the CB-IV mechanism (due to the larger number of chemical species treated explicitly); b) additional effort is required to prepare the emission inventory-specific speciation cross-reference files and input variables; and, c) model performance evaluations have not been performed using this mechanism for the model domains or episodes being used in this study.
- A modified, 'toxic' version of SAPRC-99 for CMAQ, being developed with assistance from CE-CERT, University of California Riverside, will be used.

Modelling for this project will be performed on a PC/Linux cluster running Redhat LINUX v7.3. The cluster is configured as follows:

- One master drive node with a Pentium 4, 1.7 GHz CPU, 1.0 Tb RAID hard drive system (SAMBA enabled) and a large-capacity tape backup system.
- Five dual-processor compute nodes, four with 1.0 GHz CPUs and one with 750 MHz CPUs (10 CPUs in total) and a combined memory of 7.0 Gb RAM.
- 100Mbps Fast Ethernet connection and external UPS power supply.
- High Performance Portland Group Fortran90/C++ compiler (PGI CDK Cluster Development Kit for up to 256 CPUs).

RESULTS

At the time when this document was prepared, the MOBILE6.2C runs had been completed and the modification of the CMAQ source code to handle the air toxics explicitly was underway. The following presents an overview of the preliminary results generated and analysed to date.

Preliminary MOBILE6.2C and Emission Inventory Results

In total, 20 independent runs of the MOBILE6.2C model were performed. Model results were output using the 'Spreadsheet' option, which provides the most comprehensive list of model outputs in tab-delimited ASCII file format. From the model results, a series of tables were created that would allow for the analysis an intercomparison of model results between runs. In total, 144 individual tables were created.

Tables were organized by geographic location, vehicle type, average speed, month, and year. Both absolute emission rates, absolute change in emission rates relative to the Base Case, and percent change in emission rates relative to the Base Case were calculated and tabulated on a pollutant-by-pollutant basis.

Table 3 shows a sample set of emission tables for the Pacific Northwest Domain; light duty gasoline vehicles (LDGVs); 100, 80, and 50 km/h vehicle speeds; month of July; and the Base Case, E10 Tailor, and E10 Splash fuel scenarios.

Table 3. MOBILE6.2C results for: Pacific Northwest Domain; LDGVs; 100, 80, and 50 km/h vehicle speeds; July; and the Base Case, E10 Tailor, and E10 Splash fuel scenarios.

Pacific Northwest, LDGV, 100km/h, July, Year 2000 (g/VMT)

Pollutant	Base Case	E10 Tailor	E10 Splash	E10 Tailor		E10 Splash	
				Abs. Change	% Change	Abs. Change	% Change
CO	27.5	22.3	22.1	-5.2	-18.9%	-5.4	-19.6%
NO_X	2.0	2.0	2.0	0.0	0.0%	0.0	0.0%
VOC [1]	1.8	1.6	1.7	-0.1	-7.4%	-0.1	-5.1%
$PM_{2.5}$	0.004	0.004	0.004	0.000	0.0%	0.000	0.0%
NH_3	0.091	0.091	0.091	0.000	0.0%	0.000	0.0%
SO_2	0.052	0.052	0.047	0.000	0.0%	-0.005	-9.6%
Formaldehyde	0.0193	0.0201	0.0197	0.0008	4.1%	0.0004	2.1%
Acetaldehyde	0.0065	0.0154	0.0151	0.0089	136.9%	0.0086	132.3%
Benzene [1]	0.0563	0.0431	0.0416	-0.0132	-23.4%	-0.0147	-26.1%
1,3-Butadiene	0.0079	0.0061	0.0060	-0.0018	-22.8%	-0.0019	-24.1%

Pacific Northwest, LDGV, 80km/h, July, Year 2000 (g/VMT)

Pollutant	Base Case	E10 Tailor	E10 Splash	E10 Tailor		E10 Splash	
				Abs. Change	% Change	Abs. Change	% Change
CO	25.8	20.8	20.6	-5.0	-19.4%	-5.2	-20.2%
NO_X	1.9	1.9	1.9	0.0	0.0%	0.0	0.0%
VOC [1]	1.9	1.8	1.8	-0.1	-6.9%	-0.1	-4.8%
$PM_{2.5}$	0.004	0.004	0.004	0.000	0.0%	0.000	0.0%
NH_3	0.091	0.091	0.091	0.000	0.0%	0.000	0.0%
SO_2	0.052	0.052	0.047	0.000	0.0%	-0.005	-9.6%
Formaldehyde	0.0202	0.0211	0.0208	0.0009	4.5%	0.0006	3.0%
Acetaldehyde	0.0068	0.0161	0.0158	0.0093	136.8%	0.0090	132.4%
Benzene [1]	0.0589	0.0451	0.0436	-0.0138	-23.4%	-0.0153	-26.0%
1,3-Butadiene	0.0083	0.0064	0.0063	-0.0019	-22.9%	-0.0020	-24.1%

Pacific Northwest, LDGV, 50km/h, July, Year 2000 (g/VMT)

Pollutant	Base Case	E10 Tailor	E10 Splash	E10 Tailor		E10 Splash	
				Abs. Change	% Change	Abs. Change	% Change
CO	23.8	19.1	19.0	-4.7	-19.7%	-4.8	-20.2%
NO_X	1.9	1.9	1.9	0.0	0.0%	0.0	0.0%
VOC [1]	2.2	2.0	2.1	-0.2	-6.9%	-0.1	-4.2%
$PM_{2.5}$	0.004	0.004	0.004	0.000	0.0%	0.000	0.0%
NH_3	0.091	0.091	0.091	0.000	0.0%	0.000	0.0%
SO_2	0.052	0.052	0.047	0.000	0.0%	-0.005	-9.6%
Formaldehyde	0.0223	0.0234	0.0229	0.0011	4.9%	0.0006	2.7%
Acetaldehyde	0.0075	0.0178	0.0175	0.0103	137.3%	0.0100	133.3%
Benzene [1]	0.0649	0.0496	0.0479	-0.0153	-23.6%	-0.0170	-26.2%
1,3-Butadiene	0.0092	0.0071	0.0070	-0.0021	-22.8%	-0.0022	-23.9%

Note: [1] Includes tailpipe and evaporative emissions

A review of the MOBILE6.2C model results allowed for the following general conclusions to be drawn:

Pollutant	Conclusions
All modelled pollutants	• Change in emissions for E10 Splash and E10 Tailor relative to the Base Case are not affected significantly by average vehicle speed or season (ambient temperature);
NO_X, $PM_{2.5}$ NH_3, and SO_2	• Emission rates unchanged by the addition of E10; • SO_2 emissions slightly lower for E10 Splash due to the displacement of gasoline by ethanol;

CO	• Lower emissions for E10 Tailor and E10 Splash Scenarios relative to Base Case (Splash slightly lower than Tailor); • Change in emissions affected by calendar year (less reduction in 2010); • Change in emissions affected by vehicle type (less reduction for HDGV);
VOC	• Lower emissions for E10 Tailor and E10 Splash Scenarios relative to Base Case (Tailor slightly lower than Splash); • Changes in emissions affected by calendar year and vehicle type (highest reduction for HDGV);
Formaldehyde	• Higher emissions for E10 Tailor and E10 Splash Scenarios relative to Base Case for year 2000 (Tailor higher than Splash); • Lower emissions for E10 Tailor and E10 Splash Scenarios relative to Base Case for LDGV and LDGT for year 2010 (Splash less than Tailor);
Acetaldehyde	• Much higher emissions for E10 Tailor and E10 Splash Scenarios relative to Base Case for year 2000 (Tailor slightly higher than Splash); • Change in emissions affected by calendar year (less increase in future year for LDGV and LDGT, and more increase in future year for HDGV);
Benzene, and 1,3-Butadiene	• Lower emissions for E10 Tailor and E10 Splash Scenarios relative to Base Case (Splash slightly lower than Tailor); • Change in 1,3-Butadiene emissions for HDGV affected by calendar year (more decrease in future year);

Because the percent change in emissions for the E10 Scenarios relative to the Base Case are not affected significantly by average vehicle speed or season, the 80 km/h emission rates for the month of July will be used to develop the scaling factors required for the air quality modelling. Having said this, further review of the MOBILE6.2C results is currently ongoing.

A direct comparison of the MOBILE6.2C results from this study to those from other similar studies (e.g., ARB, 1997; and Singleton *et al*., 1997) was not feasible as each study was conducted using different inputs, emission factor models, etc. However, general comparisons can be made to help understand and explain the results.

A study conducted by the National Research Council of Canada (NRC) in 1997 estimated that emissions from LDGVs operating on ethanol blend fuels, relative to emissions from LDGVs operating on industry average gasoline, would result in an increase in total organic gases (TOG) by 9%, a decrease in carbon monoxide (CO) emissions by 15%, and no change in oxides of nitrogen (NO_X) emissions (Singleton *et al*., 1997). Although the results for CO and NO_X are similar, the results for the NRC study show an increase in TOG emissions, whereas the results for VOC emissions in the present study show a decrease with the introduction of ethanol.

The NRC results for TOG indicate that exhaust emissions decrease while evaporative emissions increase for the ethanol blend scenarios. This finding is generally consistent with the results for VOCs in the present study. However, there are differences in the combined (i.e., total) exhaust and evaporative emissions between the studies. It is expected that this is in part due to the relative magnitude and proportions of the increases/decreases in emissions from the exhaust versus evaporative components between the two studies. This assumption is supported in that

the emission factors from the NRC study are based on emissions measurements taken from vehicles representative of 1989 model year technology, in conjunction with the MOBILE5C model. Since 1989, emission control technologies, including evaporative emission controls, have improved and are accounted for in the MOBILE6.2C model.

Next Steps

Having completed the Base Case and E10 MOBILE6.2C runs, the next steps will be to complete the modification of he SMOKE and CMAQ code, update the speciation profile and cross-reference files, scale the emission inventories accordingly, and perform the corresponding SMOKE and CMAQ runs.

CONCLUSIONS

Based on the results from the MOBILE6.2C runs, it is difficult to forecast how the E10 air quality simulations will fair. One point of uncertainty lies in whether the relatively small changes to the emissions, when placed in a regional context, will be sufficient to affect change in some of the air pollutants, specifically ozone and $PM_{2.5}$.

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KEYWORDS
MOBILE6, CMAQ, SMOKE, mobile emissions, ethanol, smog, air toxics