Atmospheric Chemistry in Existing Air Atmospheric Dispersion Models and Their Applications: Trends, Advances and Future in Urban Areas in Ontario, Canada and in Other Areas of the World

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ABSTRACT

Air quality is a major concern for the public. Therefore, the reliability in modeling and predicting the air quality accurately is of a major interest. This study reviews existing atmospheric dispersion models, specifically, the Gaussian Plume models and their capabilities to handle the atmospheric chemistry of nitrogen oxides (NO_x) and sulfur dioxides (SO_2). It also includes a review of wet deposition in the form of in-cloud, below cloud, and snow scavenging. Existing dispersion models are investigated to assess their capability of handling atmospheric chemistry, specifically in the context of NO_x and SO_2 substances and their applications to urban areas. A number of previous studies have been conducted where Gaussian dispersion model was applied to major cities around the world such as London, Helsinki, Kanto, and Prague, to predict ground level concentrations of NO_x and SO_2. These studies demonstrated a good agreement between the modeled and observed ground level concentrations of NO_x and SO_2. Toronto, Ontario, Canada is also a heavily populated urban area where a dispersion model could be applied to evaluate ground level concentrations of various contaminants to better understand the air quality. This paper also includes a preliminary study of road emissions for a segment of the city of Toronto and its busy streets during morning and afternoon rush hours. The results of the modeling are compared to the observed data. The small scale test of dispersion of NO_2 in the city of Toronto was utilized for the local hourly

meteorological data and traffic emissions. The predicted ground level concentrations were compared to Air Quality Index (AQI) data and showed a good agreement. Another improvement addressed here is a discussion on various wet deposition such as in cloud, below cloud, and snow.

Keywords: Air quality data, Air dispersion modeling, Gaussian dispersion model, Dry deposition, Wet deposition (in-cloud, below cloud, snow), Urban emissions

1. INTRODUCTION

Over the past few years, the smog days in Ontario, Canada have been steadily increasing. Overall, longer smog episodes are observed with occurrences outside of the regular smog season. Air pollution limits the enjoyment of the outdoors and increases the cost of the health care [1] and [2]. To combat this problem, the Ontario Ministry of Environment (MOE) introduced new tools to reduce emissions as well as improved communication with the public on the state of the air quality. The communication policy has been implemented by the introduction of an Air Quality Index (AQI) based on actual pollutant concentrations reported by various monitoring stations across Ontario. One major concern is the spatial distribution of pollutants not captured by monitoring stations.

To further enhance the understanding of pollution in an urban area, studies involving computational fluid dynamics (CFD) for street canyons, the land use regression (LUR), and the use of dispersion models have been conducted [3]. For a number of cities across the world dispersion models were applied to urban areas to understand pollution in a given city [4], [5], [6], [7] and [8]. The objective of these studies was to develop new air quality standards. These studies compared modeled ground level concentrations of NO_x, SO_2, and CO to the monitored data and showed a good agreement between observed and predicted data.

Therefore, the main objectives of this study are to review the developments of Gaussian dispersion model, to review the dispersion modeling applied to urban areas, and to conduct a small scale test for the city of Toronto, Ontario, Canada.

Over the years, the dispersion models have been used by the policy makers to develop air quality standards, an approach applicable to the city of Toronto, Ontario, Canada [10] and [11]. In 2005, fifteen smog advisories, a record number covering 53 days, were issued during smog season [12] in Toronto, Ontario, Canada. This is also a record number of days covering smog since the start of the Smog Alert Program in Ontario in 2002. Even more prominent was an episode that lasted 5 days in February 2005 and occurred outside smog season due to elevated levels of particulate matter with diameter less than 2.5 micrometers ($PM_{2.5}$) followed by the earliest smog advisory ever issued during the normal smog season in April, 2005. As shown in Table 1, there has been an increase in smog advisories since 2002 [12], [13], [14] and [15].

TABLE 1: Summary of smog advisories issued from 2002 to 2005 in Ontario, Canada [12-15]

Year	Number of Advisories	Number of Days
2002	10	27
2003	7	19
2004	8	20
2005	15	53

Since 1999, each air quality study completed states that the air quality in Ontario is improving [12-18]. In 2005, the Ontario Medical Association (OMA) announced air pollution costs were estimated to be $507,000,000 in direct health care costs [1]. The OMA deems the cost to be an underestimate and a better understanding of air pollution and its effect on human health is required. In the past few years, a number of air initiatives have been established by the Ontario Ministry of the Environment (MOE). The initiatives include recently improved means of how the state of air quality is reported to the general public, the implementation of new regulations and mandates to reduce industrial emissions, and the review of the air quality standards for the province. For many that live in and around the Great Toronto Area (GTA), checking the AQI became a daily routine [19]. In recent years, AQI was reported to public using a new scale with a range of 1 to 100, good to very poor, respectively. Along with the quantitative scale, AQI lists the primary contaminant of greatest impact on human health which results in a poor air quality. Furthermore, the public is provided with a brief summary warning of how the pollutants affect vulnerable population so that necessary precautions may be undertaken. At the present time, the Ministry of the Environment utilizes data from Environment Canada's Canadian Regional and Hemispheric Ozone and NO_x System (CHRONOS), NOAA's WRF/CHEM and NOAA-EPA NCEP/AQFS models to forecast air quality for the City of Toronto [20]. The primary objective is to forecast smog episodes.

The AQI information is obtained via a network of 44 ambient air monitoring stations and 444 municipalities across Ontario [12] and [21]. In addition to improving public communication on the status of the air quality, the MOE established a set of new regulations targeting industries with the direct objectives to reduce emissions. Since the early 70's, the MOE established a permitting system that set ground level limits. All industrial emitters were required by law, Section 9 of Canadian Environmental Protection Act (CEPA), to utilize an air dispersion model (Appendix A: Ontario Regulation 346 (O.Reg. 346)) and site specific emissions to demonstrate compliance against set ground level concentrations for the contaminants of interest. With time, the tools used to demonstrate compliance were clearly becoming out of date [22]. As the regulation aged, limitations began to slow the approval process and prevent certain applicants from obtaining permission to conduct work. It became apparent that in order to address the public concern, i.e., poor air quality, and pressure from industry, the MOE began to look into alternative solutions. In the 90's, the MOE introduced a number of alternative permits and an Environmental Leaders program. The new permits (i.e. streamline review, the use of conditions in permits, and the comprehensive permits) were becoming ineffective as shown by the internal review of MOE's work. Specifically, work was conducted by Standards Compliance Branch (SCB), former Environmental SWAT Team, and Selected Targets Air Compliance (STAC) department. The SCB's work on regular basis demonstrated that approximately 60% of an industrial sector was found to be in non-compliance with provincial regulations [23]. The Environmental Leaders program is a program where companies are invited to sign up and are included under following conditions [24]:

a) commitment to voluntary reduction of emissions; and
b) making production and emission data available to the public.

In exchange, Environmental Leaders program members are promised:

a) the public acknowledgement in MOE's publications; and
b) the recognition on the Ministry's web site.

Currently, there are nine members listed on the MOE's website [24]. As stated by the Industrial Pollution Team, the program was not effective in Ontario [24]. The report prepared by the Industrial Pollution Team specifically addresses the need to update tools (i.e. air dispersion models) utilized in the permitting process. Poor air quality, aging permitting system, and industries not committing to reduce emissions resulted in an overhaul of the system by implementation of the following new regulations:

1. Ontario Regulation 419/05, entitled "Air Pollution – Local Air Quality", (O.Reg. 419/05) replaced O.Reg. 346 allowing companies to utilize new dispersion models: Industrial Source Complex – Short Term Model [Version 3]-Plume Rise Model Enhancements (ISC-PRIME), the American Meteorological Society/Environmental Protection Agency Regulatory Model Improvement Committee's Dispersion Model (AERMOD) along with the establishment of new air standards [25];
2. Ontario Regulation 127/01, entitled "Airborne Contaminant Discharge Monitoring and Reporting", (O.Reg. 127/01) which is an annual emissions reporting program due by June 1st each year [26];
3. Data from annual reporting programs was utilized to implement Ontario Regulation 194/05, entitled "Industrial Emissions – Nitrogen Oxides and Sulphur Dioxide", (O.Reg. 194) which caps NO_x and SO_x emissions of very specific industries with set reduction targets [27]. The targets are intensity based. For industries that do not meet their targets, options of trading or paying for the emissions exist;
4. On the federal level, a National Pollutant Release Inventory (NPRI), a program similar to O.Reg. 127/01 which requires industries to submit an annual emissions report by June 1st each year [28];
5. On the federal level, Canadian Environmental Protection Act Section 71 (CEPA S. 71) requires for specific industries, as identified within the reporting requirement, to submit annual emissions by May 31 due [29] with the objective to set future targets that will lower annual emissions. Due May 31st 2008 are the annual 2006 values; and
6. On the federal level, a Greenhouse Gases Release (GHG) inventory was introduced for larger emitters (> 100 ktonnes/year) of CO_2 which requires annual reporting. [30]

With the rise of the poor air quality in Ontario that causes high health cots, the MOE began to update its 30 year old system. This improvement is coming about in forms of various new regulations with objectives to reduce overall emissions. The current reforms and expansion of regulations within the province of Ontario have a goal in common to reduce emissions that have a health impact. Other Canadian provinces such as British Columbia [31] and Alberta [32] are also undergoing reforms to improve their air quality. These provinces are moving to implement advanced air dispersion models to study the air quality.

The annual air quality studies, new regulations, and air standards all published by the MOE do not link together at the present time. The AQI warnings issued to the public in most cases are based on readings from one monitoring station within a region [33]. Uniform air quality across the municipality of interest is the main assumption undertaken with the AQI warnings. Data used to establish the AQI is not processed or reviewed for quality control [33]. Historical data, statistical analysis, decay rate, or predicted future quality of air is not provided. Data used to establish the AQI undergoes minimal review for quality control [33]. Both assumptions of uniformity and minimal quality check have been recognized in the most recent Environmental Commissioner of Ontario report [34] as providing a "false sense of security".

The AQI notification program can be refined by completing air dispersion modeling for a city. This approach incorporates a reduced gird size, utilization of local meteorological conditions, input of actual emissions from surround sources, and predicted concentration contours at various time frames, i.e., sub hourly and hourly, to better represent the state of air quality within the area of interest. There are a number of similar approaches currently conducted in other countries [4], [5], [6], [7], [8] and [9], of which all share the same objective to utilize air dispersion models for a city and use the information to understand air quality and provide information to develop air quality standards for that city.

In order to understand the limitations of the air dispersion models, next section provides an overview of the Gaussian Plume model. Subsequently, a discussion follows with a review of standard methods applied to handle dry and wet deposition specifically in box models. This is followed by a review of other wet deposition (i.e. in-cloud, below cloud, and snow scavenging) not necessarily already implemented in box models. Section 4 takes the knowledge from previous discussion and concentrates on how the dispersion models have been applied up to date to urban areas with a review of five studies. The studies show that Gaussian dispersion model should be used to urban areas and yields good results. Finally, in our own study, a small scale study was conducted for the city of Toronto, Ontario, Canada, utilizing local meteorological and traffic data. This is a preliminary study which confirms Gaussian dispersion could be applied to the city of Toronto and it can be expanded to include other factors, such as wet deposition, scavenging, and reactions, in the model.

2. CURRENT AIR DISPERSION MODELS

The atmospheric dispersion modeling has been an area of interest for a long time. In the past, the limitation of studying atmospheric dispersion was limited to the data processing. The original dispersion models addressed very specific situations such as a set of screen models (SCREEN3, TSCREEN, VISCREEN etc.) containing generated meteorological conditions which were not based on measured data. There are also models which apply to specific solution, a single scenario such as point source (ADAM), spill (AFTOX), and road (CALINE3). With the advancement of computing power, the box type of air dispersion models became widely available (ISC-PRIME, AEMOD, CALPUFF). The advantage of the box type models is not only being readily available in most cases but also is capable of handling multiple emission sources. At the present time, the most of the box dispersion models are under the management of the US Environmental Protection Agency (US EPA) [35]. Many of these box models are widely used in other countries and recently a number of environmental governing bodies set these air dispersion models on the preferred list [25], [31], [32] and [36] The box models allow the user to enter information about meteorology, emission sources, and in some instances topography. The information is processed by the box models to provide concentrations of the pollutant of interest. With the recent expansion of computing speeds and the ability to handle large data, dispersion modeling has been expanded. In many cases, the models are used to simulate urban areas or emergency situations. The new tools allow for the evaluation of past events and the prediction of future events such as poor air quality days (i.e. smog) in the cities. This study concentrates on the revaluation of such dispersion model, Plume model and its capability to handle atmospheric chemistry, specifically how the chemistry of NO_x and SO_2 contaminants have been treated in a Gaussian Plume model for an urban area.

2.1. Gaussian Dispersion Model

The concepts of the Gaussian Plume model, dispersion coefficients, characterization of sources (i.e. volume, line, and area sources), limitations of the model, and the capabilities to handle atmospheric chemistry are discussed in this section. The discussion revolves around concepts that apply to urban type of sources.

2.1.1. Basic Gaussian Plume Model

Between the seventeenth and eighteenth centuries, a bell-shaped distribution called “Gaussian-distribution” was derived by De Moivre, Gauss, and Laplace [37]. Experiments conducted by Shlien and Corrsin [38] related to dispersion of a plume related Gaussian behaviour. This discovery has since been used to provide a method of predicting the turbulent dispersion of air pollutants in the atmosphere. The basic Gaussian Plume is as follows [37]:

$$C(x,y,z) = \frac{Q_p}{2\pi U \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{z^2}{2\sigma_z^2} \right) \quad (1)$$

where C, Q_p, σ_y, σ_z, and U are average mass concentration [g/m^3], strength of the point source [g/s], dispersion coefficient in y-direction [m], dispersion coefficient in z-direction [m], and wind velocity [m/s], respectively. This equation applies to an elevated point source located at the origin (0,0) and the height of H, in a wind-oriented coordinate system where the x-axis is the direction of the wind, as shown in Figure 1.

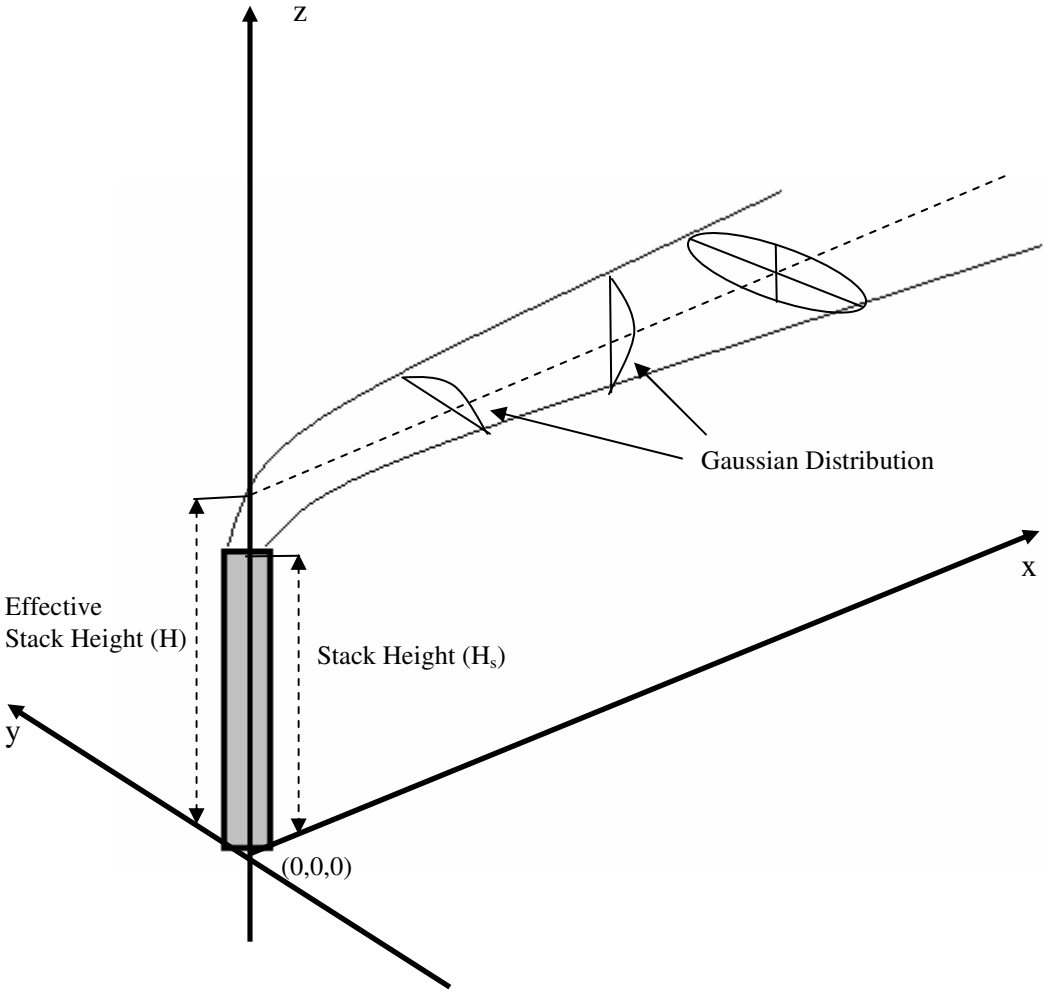

FIGURE 1: Elevated point source described by Gaussian Plume model

is the effective height of the stack, which is equal to the stack's height plus the plume rise (Figures 1 and 2). As dictated by the Gaussian Plume equation, the maximum concentration lies in the centre of the plume.

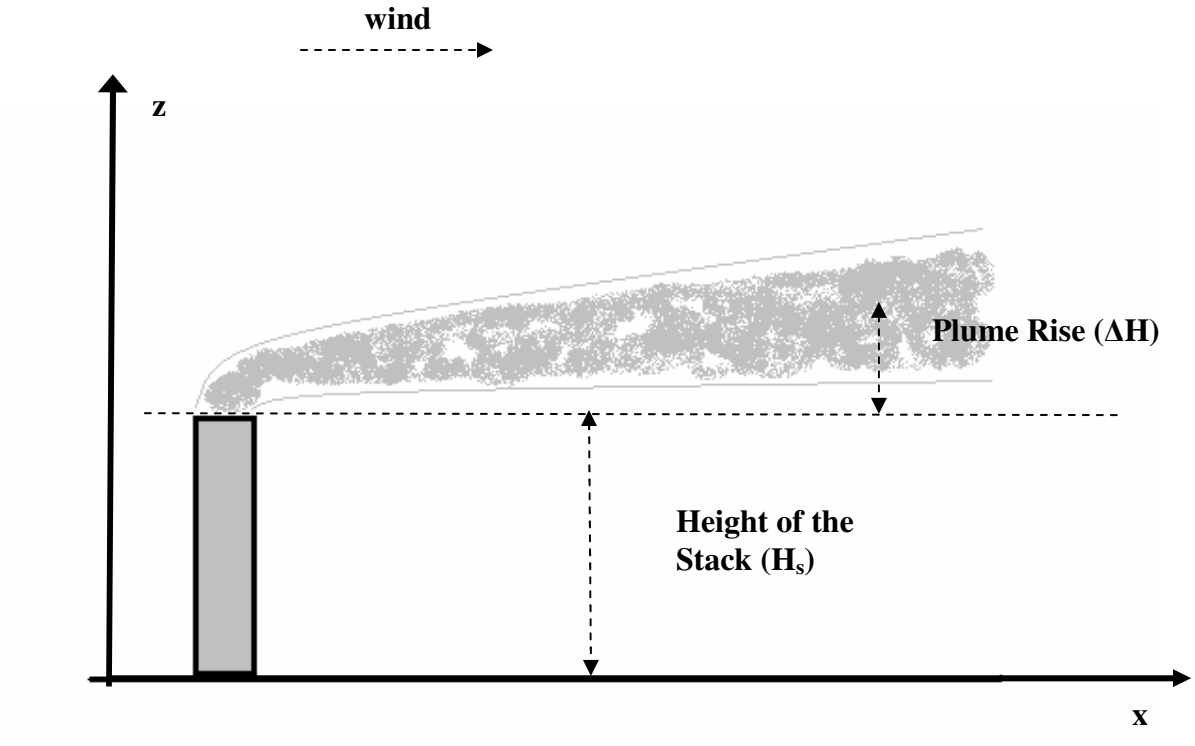

FIGURE 2: Effective stack height of a point source is a sum of the stack height and plume rise. The momentum and thermal rise add up to the physical height of the stack creating an effective stack height

The plume disperses in the horizontal direction following the Gaussian distribution. The distributions are described by the values of σ_y and σ_z. Average wind speed, U, is a function of the height, z. If this value is not known, the first estimate could be made utilizing the following power law velocity profile at elevation z_1 [39]:

$$U = U_1\left(\frac{H}{z_1}\right)^n \tag{2}$$

where n, U_1, z_1, and H are a dimensionless parameter, wind velocity at reference elevation of z_1 [m/s], elevation [m], and stack height [m], respectively.

The basic Gaussian Plume model is for a point source, i.e., the tall stack in space that emits without set barrier. The ground level concentrations can be evaluated to infinity. At some point in time, the plume disperses in the vertical direction and touches the ground. The basic formula can be further modified to account for the plume reflection from the ground, considered a zero flux or impenetrable surface. This was accomplished by creating an image source component in basic Gaussian Plume formula, as shown in Equation (3).

$$C(x,y,z) = \frac{Q_p}{2\pi U\sigma_y\sigma_z}\exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left\{\exp\left[-\frac{(z-H)^2}{2\sigma_z^2}\right]+\exp\left[-\frac{(z+H)^2}{2\sigma_z^2}\right]\right\} \tag{3}$$

The reflection source is shown in Figure 3.

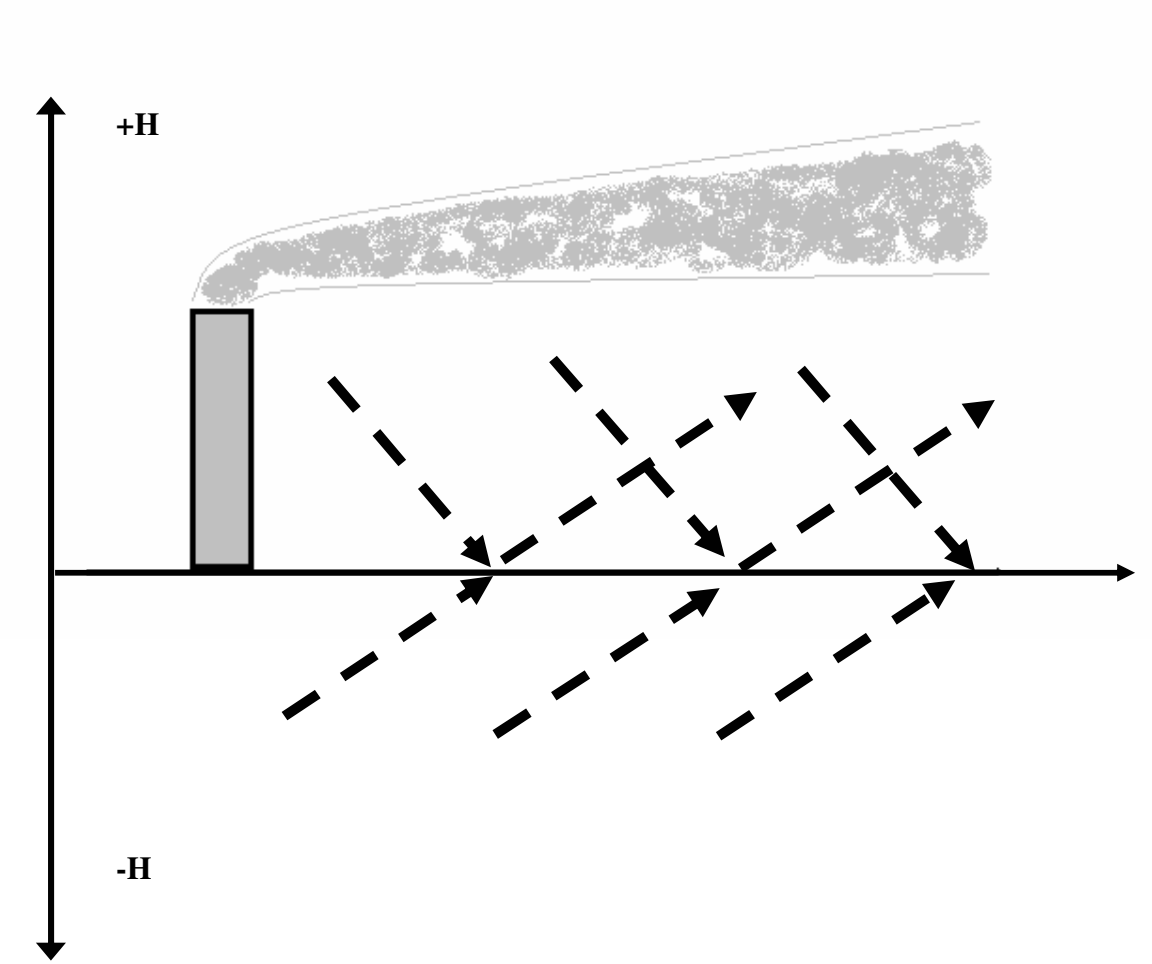

FIGURE 3: Side of image source which allows for the reflection of plume off ground

The result is the Gaussian dispersion equation for a continuous point-source. This equation provides the downwind concentration from an isolated point source located at (0,0,z) to infinity. There are a number of simplified forms of the Gaussian Plume formula for situations such as maximum concentration/first touchdown of the plume and ground level sources [37].

2.1.2. Dispersion Coefficients

The dispersion coefficients, σ_y and σ_z in Equation (1), are used in the dispersion model to provide the dispersion effect of the plume. These coefficients describe how well the atmosphere is mixed. Ideally, high mixing of air in the atmosphere which surrounds a source is sought. High mixing results in good dispersion of the pollutants and thus, lower ground level concentrations. The state of the atmosphere depends on few variables such as mechanical mixing induced by winds and thermal mixing induced by solar insulation. The most commonly used descriptive of the atmosphere's state is provided by Pasquill Stability classes. There are six classes labeled A to F, ranging from unstable or most turbulent to most stable or least turbulent conditions,

respectively [37]. Table 2 provides the Pasquill Stability classes which describe the state of the atmosphere.

TABLE 2: Pasquill dispersion classes related to wind speed and insulation [37] (Adopted from Turner 1970)

Surface Wind Speed[d]	Day Incoming Solar Radiation[a,c]			Night Cloudiness[b,c]	
(m/s)	Strong[e]	Moderate[f]	Slight[g]	Cloudy	Clear
<2	A	A-B	B	-	-
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
>6	C	D	D	D	D

A. Insulation, incoming solar radiation: Strong > 143 cal/m2/sec, Moderate = 72-143 cal/m2/sec, Slight < 72 cal/m2/sec.
b. Cloudiness is defined as the fraction of sky covered by clouds.
c. A – very unstable, B – moderately unstable, C – slightly unstable, D – neutral, E – slightly stable, F – stable. Regardless of wind speed, Class D should be assumed for overcast conditions, day or night.
d. Surface wind speed is measured at 10 m above the ground.
e. Corresponds to clear summer day with sun higher than 600 above the horizon.
f. Corresponds to a summer day with a few broken clouds, or a clear day with sun 35 – 600 above the horizon.
g. Corresponds to a fall afternoon, or a cloudy summer day, or clear summer day with the sun 15 – 350.

The Pasquill dispersion coefficients are based on the field experimental data, flat terrain, and rural areas. The plots allow for the user to read off dispersion coefficient at specific distance for selected stability class extracted from Table 2. The graphical plots of the dispersion coefficients become useless when solving Gaussian dispersion using a box model on a computer platform.

A number of analytical equations have been developed that express dispersion coefficients for rural and urban areas. These algebraic solutions are fitted against the dispersion coefficient plots and provide a few methods to calculate each dispersion factor. One of the methods is the use of power law to describe dispersion coefficients [37] and [40]:

$$\sigma_y = ax^b \qquad (4)$$
$$\sigma_z = cx^d + e$$

where x and variables a through e are distance [m] and dimensionless parameters, respectively. Parameters a through e are functions of the atmospheric stability class and the downwind is a function to obtain dispersion coefficients or a combination of power law and another approach. Another approach, most commonly used in dispersion models is shown as follows [40]:

$$\sigma_y = \left(\frac{x}{2.15}\right)\tan\theta \qquad (5)$$

where $\theta = f - g(\ln x)$ and θ , f and g are angle [0] and two dimensionless parameters, respectively. McMullen [41] developed the following dispersion coefficients as the most representative of Turner's version of the rural Pasquill dispersion coefficients for rural areas. The advantage of the McMullen's equation is its application to both vertical and horizontal dispersion coefficients.

$$\sigma = \exp\left(g + h\ln x + i(\ln x)^2\right) \qquad (6)$$

Constants g through i are dimensionless parameters as provided in Table 3. There also exist dispersion coefficients suitable for urban areas. Experimental data obtained from urban areas result in higher dispersion coefficients [42] and [43]. The plume encounters turbulence due to buildings and relatively warmer temperatures associated with urban areas. These can alter the atmospheric conditions for a small localized area when compared to the prevailing meteorological conditions. A higher dispersion coefficient results in a closer maximum ground-level concentrations as demonstrated in Figure 4.

TABLE 3: Constants g, h, and i in McMullen's Equation (6) for rural dispersion coefficients [37]

Pasquill Stability Class	To obtain σ_z			To obtain σ_y		
	g	h	i	g	h	i
A	6.035	2.1097	0.2770	5.357	0.8828	-0.0076
B	4.694	1.0629	0.0136	5.058	0.9024	-0.0096
C	4.110	0.9201	-0.0020	4.651	0.9181	-0.0076
D	3.414	0.7371	-0.0316	4.230	0.9222	-0.0087
E	3.057	0.6794	-0.0450	3.922	0.9222	-0.0064
F	2.621	0.6564	-0.0540	3.533	0.9191	-0.0070

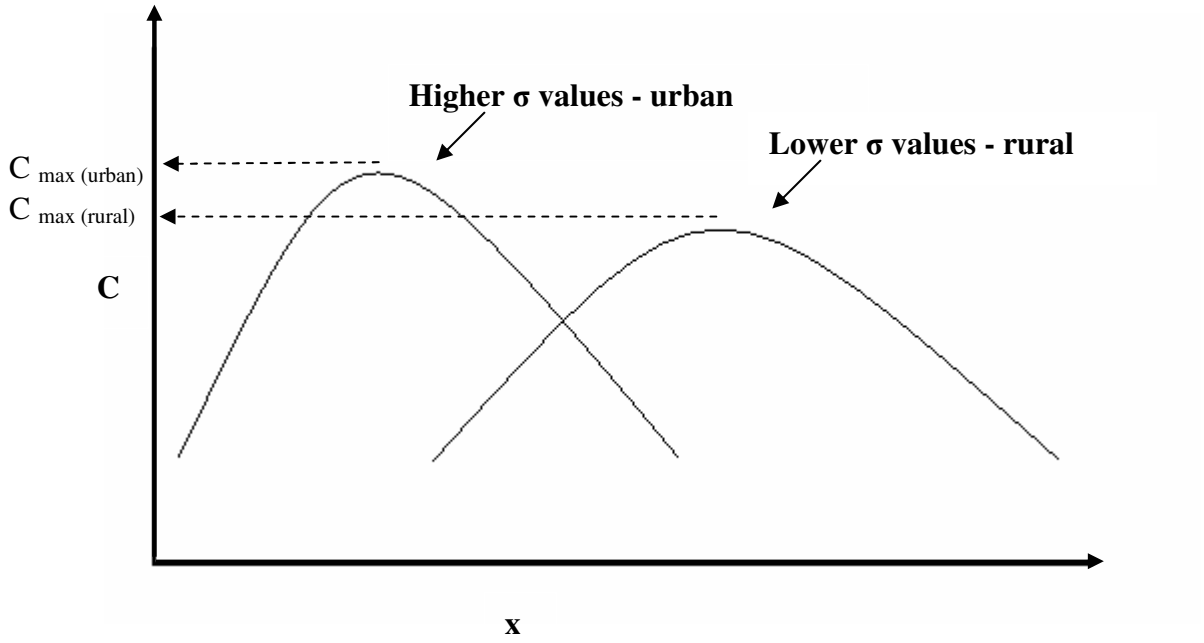

FIGURE 4: Effect of urban and rural dispersion coefficients. For urban areas a higher maximum ground level concentration, i.e. $C_{max(urban)}$, is observed and closer to the source. For rural areas a lower maximum ground level concentration, i.e. $C_{max(rural)}$, is observed and it occurs further from the source

For a plume passing through an urban area, the maximum ground-level concentration not only occurs closer to the source but also appears at a higher concentration than if modeled in rural area. In addition, further away from the urban area, a plume results in a lower ground level concentration than that if modeled in rural area. Initial mixing induced by the turbulence in a city

results in a better dispersion. For urban areas, the dispersion coefficients can be expressed by previously mentioned power law, with corrected constants, as shown in the following equation:

$$\sigma = jx(1+kx)^{l} \quad (7)$$

Constants j through l are dimensionless parameters are provided in Table 4. There seems to not be a single better solution, therefore, when selecting a method, one should evaluate the various approaches [44].

TABLE 4: Constants j, k, and l for estimation of Briggs urban dispersion coefficients in Equation (7) [37]

Pasquill Stability Class	To Obtain σ_z			To Obtain σ_y		
	j	k	l	j	k	l
A-B	240	1.00	0.50	320	0.40	-0.50
C	200	0.00	0.00	220	0.40	-0.50
D	140	0.30	-0.50	160	0.40	-0.50
E-F	80	1.50	-0.50	110	0.40	-0.50

2.1.3. Characterization of Various Emission Sources in Gaussian Dispersion Model

The Gaussian Plume model originally developed for point sources (i.e. tall stacks) can be also applied to other types of emission sources. These emission sources are most commonly described as volume, line, and area sources. The box dispersion models are also capable of handling sources below grade and flares. These sources (e.g. quarries or flares) are not typical of Toronto city and therefore, will not be discussed. Toronto is mainly characterized by sky scrapers and highways, which can translate to volume sources and line (or area) sources.

Volume Source

A building structure is characterized in an air dispersion model as a volume source. The solution proposed under the Gaussian Plume model is to model the volume source as a point source at a distance with matching dispersion coefficients to the dimensions of the virtual source [40], as shown in Figure 5. The initial lateral and vertical dimensions are modified dimensions of source width and height, as shown in Table 5.

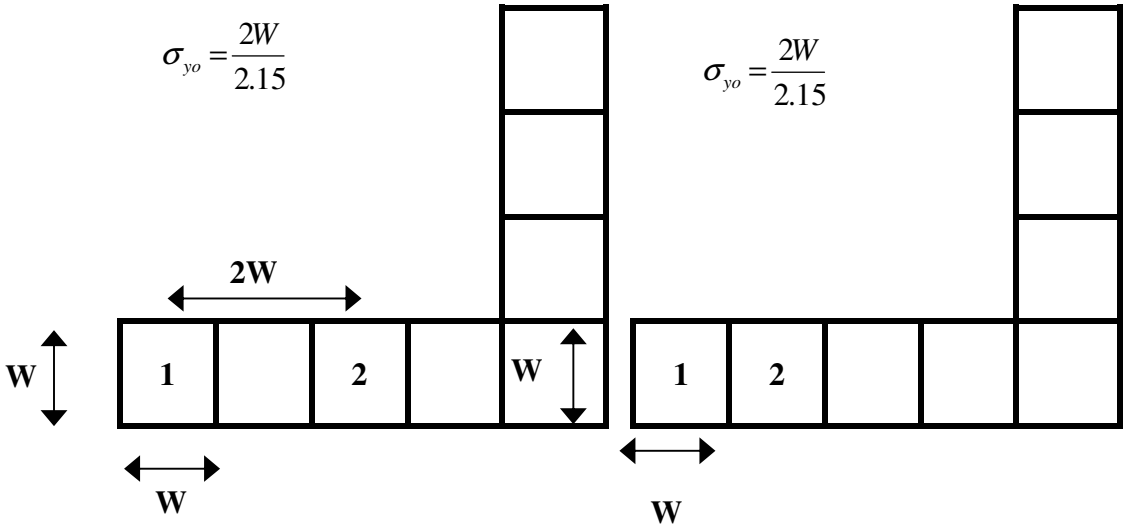

FIGURE 5: (Upper) Line source represented by adjacent volume source. (Lower) Line source represented by separated volume source

TABLE 5: Initial dimensions for a virtual source [40]

Type of Source	Procedure for Obtaining Initial Dimension
Initial Lateral Dimension (σ_{yo})	
Single Volume Source	$\sigma_{yo} = \frac{L}{4.3}$
Line Source Represented by Adjacent Volume Source (Figure 5)	$\sigma_{yo} = \frac{L}{2.15}$
Line Source Represented by Separate Volume Source (Figure 5)	$\sigma_{yo} = \frac{A}{2.15}$ [A – centre to centre distance]
Initial Vertical Dimension (σ_{zo})	
Surface-Based Source (H=0)	$\sigma_{zo} = \frac{B}{2.15}$ [B – vertical dimension]
Elevated Source (H >0) on or Adjacent to Building	$\sigma_{zo} = \frac{C}{2.15}$ [C – building height]
Elevated Source (H>0) not on or Adjacent to a Building	$\sigma_{zo} = \frac{A}{4.3}$

Line Source

Line source is characterized by being a surface based source at grade-level. Road emissions can be modeled as line sources. Figure 6 shows a line source of length L and strength Q_l normal to the wind vector. The emissions, Q_l, arise from a small segment of a line, dy', and are expressed as $Q_l dy'$. The receptor is located at point (x, y) downwind of the line source. One of the solutions to represent line sources by Gaussian Plume formula is given by [45].

$$C = \frac{Q_l}{\sqrt{2\pi} U \sigma_z} \left[erf\left(\frac{\frac{L}{2} - y}{\sqrt{2\sigma_y}} \right) + erf\left(\frac{\frac{L}{2} + y}{\sqrt{2\sigma_y}} \right) \right] \quad (8)$$

and are source strength [g/s] and length [m], respectively. This equation is used to estimate the concentration downwind of an infinite line source normal to the mean wind vector.

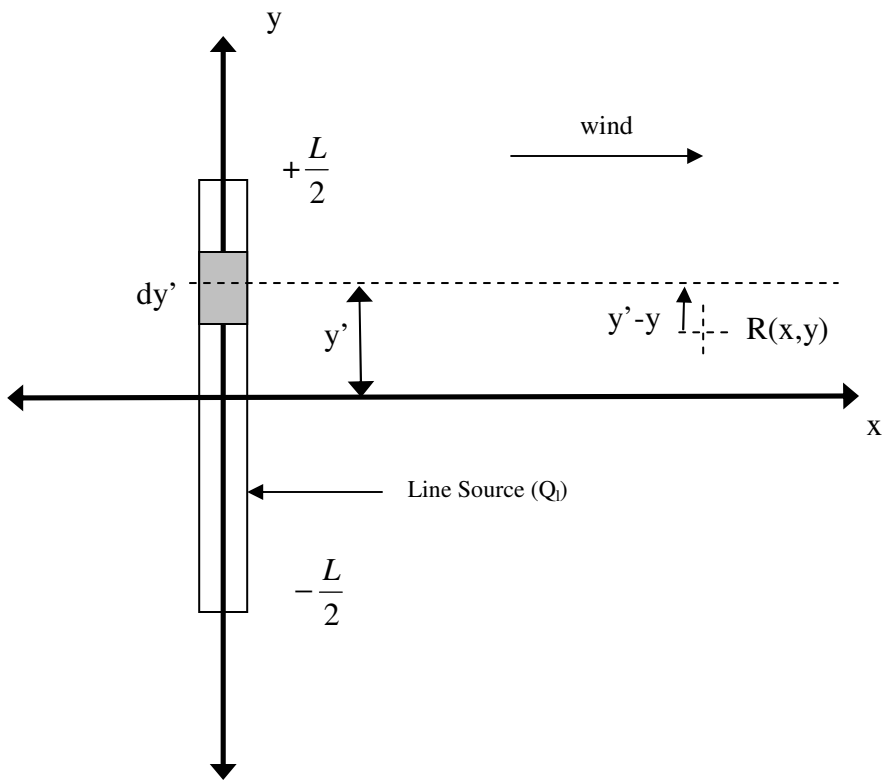

FIGURE 6: A line source of length L and strength Q_l

The governing equation of a line source oriented at an oblique angle, as shown in Figure 7, to the mean wind vector was developed by Calder [43]. The perpendicular distance, d_p, is the distance between the receptor and the line source. Angle θ is the angle between its normal and the wind vector and applies to angles as large as 75° [46].

This solution is shown in Equation (9) [45]:

$$C = \sqrt{\frac{2}{\pi}} \frac{Q_l}{U \cos\theta \sigma_z \left(\frac{d_p}{\cos\theta} \right)} \tag{9}$$

where d_p is perpendicular distance [m]. A limitation of this approach includes its inability to account for mixing due to heated exhaust [47].

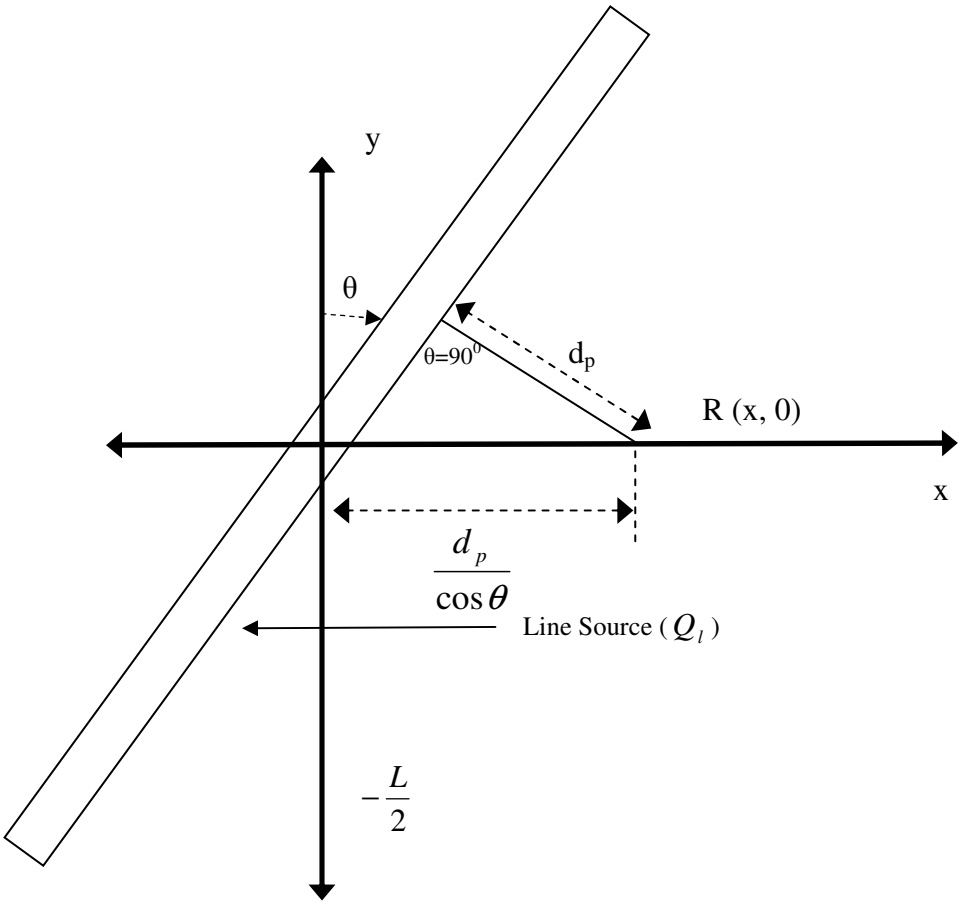

FIGURE 7: Infinite line source with strength Q_l at an oblique angle (θ) to the wind

Area Source

An alternative method that can be used to model emissions from a road is by describing the road as area source. Open fields from which wind erosion occurs is another example of an area source. In essence, a line source with width x_1 normal to the wind direction can be used to represent an area source as shown in Figure 8. The area source (considered to be long enough to be infinite) is a sum of smaller line sources, each of strength $Q_a dx'$ per unit length, where emission rate is Q_a. There are two descriptions of area sources that follow the Gaussian Plume model.

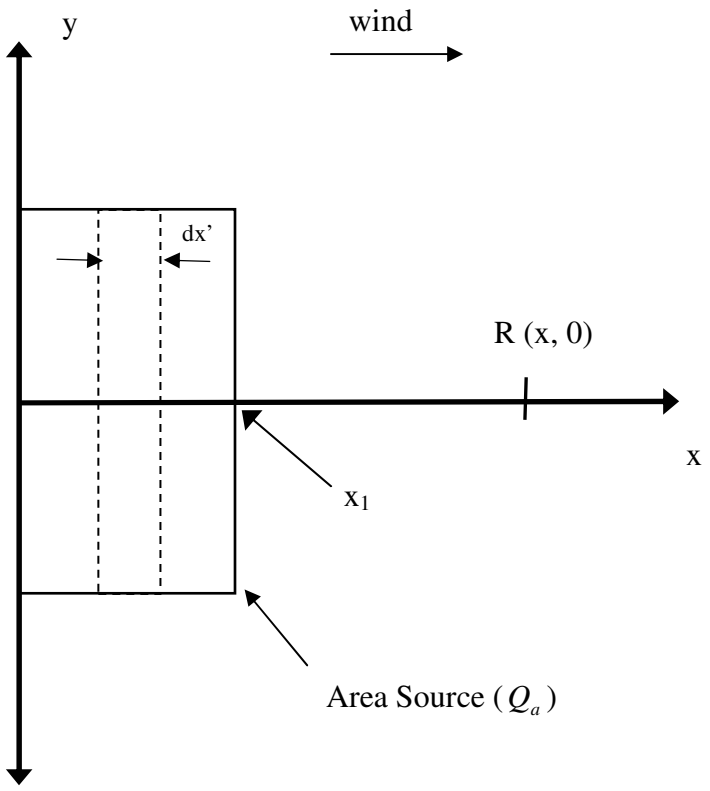

FIGURE 8: An area source with strength Q_a and width x_1

In the case of area sources, dispersion coefficients are evaluated using power law as shown in Equation (10). The dispersion coefficient in the z-direction is to be evaluated for a distance of $x - x'$ (concentration at a receptor) and thus, it is expressed in a power law form [45]:

$$\sigma_z = m(x - x')^n \tag{10}$$

where $(x - x')$, m, and n are distance [m] and two dimensionless parameters, respectively. Dimensionless parameters are a function of atmospheric stability and selected from Table 6.

TABLE 6: Power law constants used to calculate the dispersion coefficients in Equation (10) [45]

Dispersion Class	σ_{ya}		σ_z (0.5 – 5 km)		σ_z (5 – 50 km)	
	a	b	m	n	m	n
A	0.3658	0.9031	2.5×10^{-4}	2.1250	-	-
B	0.2751	0.9031	1.9×10^{-3}	1.6021	-	-
C	0.2089	0.9031	0.20	0.8543	0.5742	0.7160
D	0.1474	0.9031	0.30	0.6532	0.9605	0.5409
E	0.1046	0.9031	0.40	0.6021	2.1250	0.3979
F	0.0722	0.9031	0.20	0.6020	2.1820	0.3310

[a] *Use power law mentioned previously to evaluate horizontal dispersion.*

The following equation [45] is used to determine concentrations at receptor from a downwind edge. The source height, H, allows one to utilize this approach to road sources where emissions are released at the above ground at the height of the truck.

$$C = \frac{Q_a}{\pi U} \int_{y'=-\frac{L}{2}}^{+\frac{L}{2}} \int_{x'=0}^{x_1} \frac{\exp\left[-\frac{(y-y')^2}{2\sigma_y^2} - \frac{H^2}{2\sigma_z^2} \right]}{\sigma_Y \sigma_Z} dx'\, dy' \tag{11}$$

where Q_a and $(y - y')$ are strength of area source [g/m^2/s] and distance [m], respectively, $\sigma_Y = \sigma_y(x - x')$ and $\sigma_Z = \sigma_z(x - x')$. This solution is time consuming when evaluated numerically, therefore, often an approximation developed by Calder [48] is used. This solution is called the narrow plume approximation as shown in Equation (12):

$$C = \sqrt{\frac{2}{\pi}} \frac{Q_a}{U} \int_0^{x_1} \sigma_z^{-1} \exp\left(-\frac{H^2}{2\sigma_z^2} \right) dx' \tag{12}$$

where parameters are defined as before.

2.1.4. Limitations of Gaussian Plume Dispersion

There are a number of limitations that must be observed before applying the basic Gaussian Plume model to air dispersion problems. Following is a description of each limitation [37]:

a) vertical and crosswind diffusion occur according to Gaussian distribution;
b) downwind diffusion is negligible compared to downwind transport;
c) the emissions rate, Q, is continuous and constant;
d) the horizontal wind velocity and the mean wind direction are constant;
e) there is no deposition, washout, chemical conversion or absorption of emissions, and any emissions diffusing to the ground are reflected back into the plume (i.e. all emissions are totally conserved within the plume);
f) there is no upper barrier to vertical diffusion and there is no crosswind diffusion barrier;
g) emissions reflected upward from the ground are distributed vertically as if released from an imaginary plume beneath the ground and are additive to the actual plume distribution; and
h) the use of σ_y and σ_z as constants at a given downwind distance and the assumption of an expanding conical plume require homogeneous turbulence throughout the x, y and z-directions of the plume.

It is important to note that many of these limitations have been resolved by studies conducted in the application of Gaussian Plume dispersion model to urban areas. Additional limitations can arise in following situations, identified by this study, such as decision over election of source type (i.e. line, area or volume) adequate to be assigned to an emission source e.g. road sources. Another limitation of the model is its under performance during cooler months of the year. This can be potentially resolved through the modification of dispersion coefficients.

2.1.5. Chemistry in Gaussian Plume Dispersion

One of the most commonly used Gaussian Plume model is ISC-PRIME. [49][31][32][36] This box model handles NO_x and SO_x in following ways:

a) decay term;
b) dry deposition; and
c) wet deposition.

The use of decay term D [s^{-1}] is one way of including the removal of a pollutant in the Gaussian Plume model as follows [40]:

$$C(x,y,z) = \frac{Q_p D}{2\pi U \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2} \right) \left\{ \exp\left[-\frac{(z-H)^2}{2\sigma_z^2} \right] + \exp\left[-\frac{(z+H)^2}{2\sigma_z^2} \right] \right\} \tag{13}$$

where D is decay term [s^{-1}]. The decay term in the ISC-PRIME model is defined as follow:

$$D = \exp\left(-\psi \frac{x}{U}\right) \tag{14}$$

where $\psi = \frac{0.693}{T_{1/2}}$ and $T_{1/2}$ is the pollutant half life (s^{-1}) [50].

Furthermore, the box model utilizes a decay term of 4.81×10^{-5} s^{-1} for SO_2 concentrations when modeled in urban area. There is no similar decay term assigned to NO_x pollutant in this box model [40].

There also exists a dry deposition option available in the box model ISC-PRIME. It is applied to particulate formed by gaseous pollutants. These emissions are characterized by a high fraction of particulate $\text{over } 2\ \mu\text{m in}$ diameter. The following approach estimates deposition velocity and must be evaluated for each mass fraction and each particle category [51].

$$v_d = \left(r_a + r_d + r_a r_d v_g\right)^{-1} + v_g \tag{15}$$

where v_d, r_a, r_d, and v_g are deposition velocity [cm/s], aerodynamic resistance [s/cm], deposition layer resistance [s/cm], and gravitational settling velocity [cm/s], respectively. The distance closer to the ground can be divided into two phases:

a) fully turbulent region with vertical fluxes constant;
b) a thick quasi-laminar sub-layer.

Both regions can be identified using Monin-Obukhov length, L, an implicit function of friction velocity. Iteration is used to evaluate L until the solution converges [51]. The iteration is completed using Equation (16):

$$u_* = \frac{k u_{ref}}{\ln\left(\frac{z_{ref}}{z_0}\right) - \Psi_m\left(\frac{z_{ref}}{L}\right) + \Psi_m\left(\frac{z_0}{L}\right)} \tag{16}$$

where:

$$\Psi_m\left(\frac{z_{ref}}{L}\right) = 2\ln\left(\frac{1+\mu}{2}\right) + \ln\left(\frac{1+\mu^2}{2}\right) - 2\tan^{-1}\mu + \frac{\pi}{2}$$

$$\mu = \left(1 - 16\frac{z_{ref}}{L}\right)^{\frac{1}{4}}$$

$$\Psi_m\left(\frac{z_0}{L}\right) = 2\ln\left(\frac{1+\mu_0}{2}\right) + \ln\left(\frac{1+\mu_0^2}{2}\right) - 2\tan^{-1}\mu_0 + \frac{\pi}{2}$$

$$\mu = \left(1 - 16\frac{z_0}{L}\right)^{\frac{1}{4}}$$

$$L = -\frac{\rho c_p T_{ref} u_*^3}{kgH}$$

In the above equations, $u_*, z_{ref}, z_0, k, u_{ref}, L$, and Ψ_m are surface friction velocity [cm/s], reference elevation [m], elevation [m], surface roughness length [m], unit-less von Karman constant [0.40], wind speed at reference elevation [m/s], Monin-Obukhov length [m], and decay coefficient [s^{-1}], respectively. Also, μ, ρ, c_p, T_{ref}, and g are absolute viscosity of air

[1.81×10^{-4} g/cm/s], particle density [g/cm^3], specific heat of air at a constant pressure, reference temperature [K], and acceleration due to gravity [cm/s^2], respectively.

For the turbulent region, the dominant is the aerodynamic resistance. For the turbulent region following equation applies, where L is > 0:

$$r_a = \frac{1}{ku_*}\left[\ln\left(\frac{z_d}{z_o}\right) + 4.7\frac{z}{L}\right] \tag{17}$$

For L <0, the following equation applies:

$$r_a = \frac{1}{ku_*}\left[\ln\frac{\left(\sqrt{1+16\left(\frac{z}{|L|}\right)}-1\right)\left(\sqrt{1+16\left(\frac{z_0}{|L_0|}\right)}+1\right)}{\left(\sqrt{1+16\left(\frac{z}{|L|}\right)}+1\right)\left(\sqrt{1+16\left(\frac{z_0}{|L|}\right)}-1\right)}\right] \tag{18}$$

where u_*, z_d, and L_0 are surface friction velocity [cm/s], surface roughness [m] and initial length [m], respectively.

A minimum value of 1 m for Monin-Obukhov lengths is assumed for rural locations. The deposition layer resistance is expressed as:

$$r_d = \frac{1}{\left(Sc^{-\frac{2}{3}} + 10^{-\frac{3}{St}}\right)u_*} \tag{19}$$

where S_c and S_t are Schmidt and Stokes numbers, respectively.

The Schmidt number has an impact on the deposition rate of small particles, particles that follow Brownian motion. The parameter with the Stokes number is a measure of inertial impact, dominated by intermediate sized particles (2-20 μm). [51] The gravitational settling velocity is expressed as:

$$v_g = \frac{(\rho - \rho_{air})gd_p^2 c_2}{18\mu} S_{CF} \tag{20}$$

where $v_g, \rho, \rho_{air}, d_p, c_2$, and S_{CF} are gravitational settling velocity [cm/s], particle density [g/cm^3], air density [1.2×10^{-3} g/cm^3], particle diameter [µm], air units conversion constant [1×10^{-8} cm^2/µm^2], and dimensionless slip correction factor, respectively. Finally the slip factor can be estimated as follow:

$$S_{CF} = 1 + \frac{2x_2\left(a_1 + a_2\exp\left(-a_3\frac{d_p}{x_2}\right)\right)}{10^{-4}d_p} \tag{21}$$

where x_2, a_1, a_2, and a_3 are all dimensionless constants [6.5×10^{-6}, 1.257, 0.4, and 0.55×10^{-4}, respectively]. A user of a box model who wishes to utilize acid rain can accomplish it by use of wet deposition syntax. The settling velocity and a product of the concentration as expressed in Equation (3) give dry deposition [40]:

$$C = v_d \frac{Q_p}{2\pi U \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left\{\exp\left[-\frac{(z-H)^2}{2\sigma_z^2}\right] + \exp\left[-\frac{(z+H)^2}{2\sigma_z^2}\right]\right\} \quad (22)$$

where v_d is deposition velocity [cm/s]. The wet deposition is estimated using scavenging ratio approach [52]. The ratio shown in Equation (23) is a function of scavenging coefficients and precipitation rate (cloud water droplets):

$$\Lambda = \lambda R \quad (23)$$

where Λ, λ, and R are scavenging ratio [s^{-1}], scavenging coefficient [h/mm/s], and precipitation rate [mm/h], respectively. The scavenging coefficients are influenced by pollutant characteristics such as solubility and reactivity for gases, size distribution for particles, and the nature of precipitation: liquid or frozen. Meteorological processors such as PCRAMMET use precipitation rate and precipitation type data to estimate scavenging ratio. Finally, this ratio is used in Equation (24), where t is the plume time traveled [s], to estimate wet deposition:

$$C = C_0 \exp(-\Lambda t) \quad (24)$$

where C_0 is initial average mass concentration [µg/m^3].

2.1.6. Treatment of Inversion Layers

Winter months not only give poor dispersion conditions but inversion layers can also trap pollutants. The Gaussian Plume model can be modified to include inversion layers. The approach is similar to that used in augmenting basic Gaussian Plume to include ground reflection.

A more rigorous approach in modeling inversion layers is shown in Equation (25) [53].

$$C = \frac{Q_p}{2\pi U \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left\{\exp\left[-\frac{(z-H)^2}{2\sigma_z^2}\right] + \exp\left[-\frac{(z+H)^2}{2\sigma_z^2}\right] + A\right\} \quad (25)$$

where:

$$A = \exp\left(\frac{-(z+2H_{bl}-H)^2}{2\sigma_z^2}\right) + \exp\left(\frac{-(z-2H_{bl}+H)^2}{2\sigma_z^2}\right) + \exp\left(\frac{-(z-2H_{bl}-H)^2}{2\sigma_z^2}\right)$$

is the height of the boundary layer [m]. A separate type of inversion layer fumigation is when the inversion layer is located above the effective stack height and acts as a barrier. This barrier prevents the plume from dispersing in the vertical direction and forces the emissions to the ground as shown in Figure 9. This is an extreme case of poor dispersion and often is a result of off-shore sea breeze. A ground based inversion, fumigation could also be expressed by modifying Gaussian Plume model. Fumigation as it can be handled by Gaussian Plume is shown in Equation (26) [40].

$$C(x,y,z) = \frac{Q_p}{(2\pi)^{\frac{1}{2}} U \sigma_y H} \exp\left(-\frac{1}{2}\frac{y^2}{\sigma_y^2}\right) \quad (26)$$

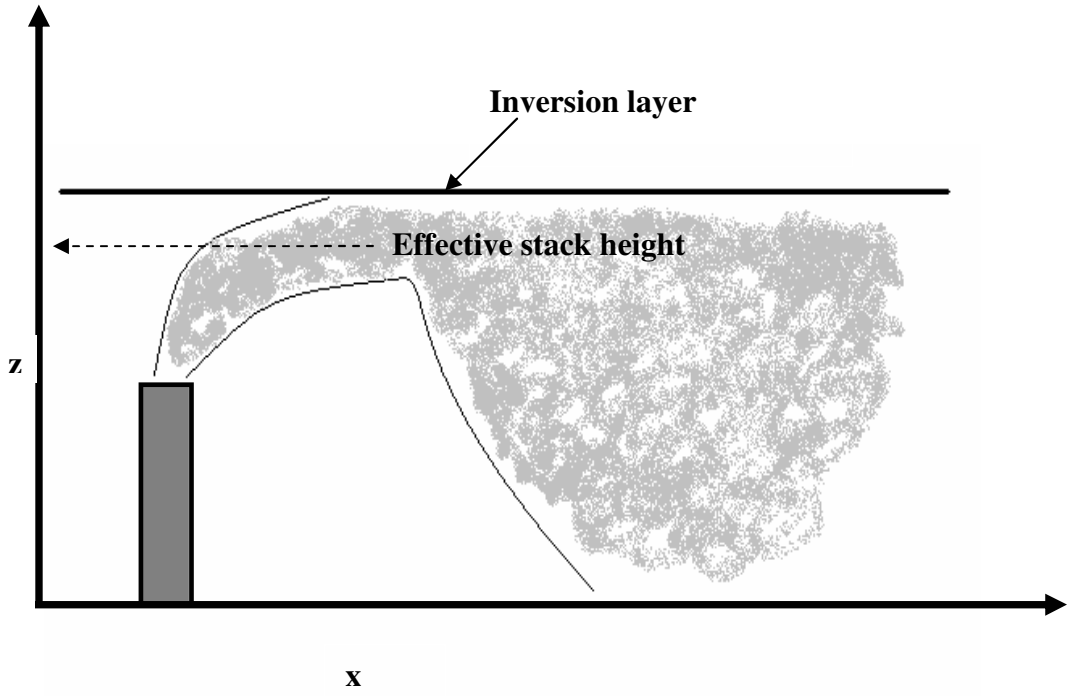

FIGURE 9: Fumigation induced by an inversion layer located above the effective stack height. The inversion layer acts similar to a mirror sealing and forces the plume to the group which result in poor dispersion and higher maximum ground level concentrations at the ground level

There are a number of other inversion layers and some assist the dispersion. Lofting is a reverse of fumigation as shown in Figure 9 [54]. The inversion layer is located below the top of the stack and therefore, forces the plume to disperse in the upward direction [50].

3. ATMOSPERHIC CHEMISTRY OF NO_x AND SO_x

In an urban area, the main sources of NO_x and SO_x emissions arise from the road traffic, emissions from fuel fired equipment which provides power/electricity, and fuel fired equipment which provides power/electricity, and industries. At the present time, the most complete databases (i.e. National Pollutant Release Inventory (NPRI)) available in Canada contain the emissions of NO_x and SO_x from industrial sources only. Most recent publication shows that transportation contributes to 40% of NO_x (transportation) and 28% NO_x (road vehicles) and 4% SO_x (transportation) annually [55]. Emissions of NO_x into the atmosphere due to combustion of fuel are driven by the nitrogen in the atmosphere. Approximately 90% of emissions due to combustion of fuel result in NO [53]. NO can potentially convert to NO_2, therefore, it is often referred to as NO_x and NO_2 when estimating emissions. In addition, for urban areas, diurnal variations in NO_x are observed due to morning and afternoon traffics. Emissions of SO_x into the

atmosphere due to combustion of fuel are strictly related to sulphur content in the fuel. Regulations are put in place to control the content of sulphur in fuel, result for the annual and diurnal cycles to be significantly reduced in comparison to that of NO_x [56].

There are a number of deposition mechanisms that can be identified with NO_x and SO_2 such as dry deposition, wet deposition, and cloud water deposition. These mechanisms are discussed in the following with means to further augment existing Gaussian Plume model.

3.1. Dry Deposition

The surface concentration always tends towards the atmospheric concentration. This tendency can be disrupted by three processes which move the gasses down the gradient between the atmosphere and the surface. Turbulent diffusion moves the gas to the surface. Molecular diffusion transfers the gas across the laminar boundary layer next to the surface. Gas molecules dissolve or react with the surface itself. All three must be present for dry deposition to occur. Dry deposition is a function of deposition velocity and the transfer resistance. Formation of sulphuric acid and nitric acid are two dry reactions of importance to emissions from urban areas. Some measurements of dispersing plumes show a 4% per hour, on a sunny day for the conversion of SO_2 to H_2SO_4 [53]. Production of nitric acid occurs at night as the radical is photolytically unstable.

Deposition Velocity

Given there is a flux due to a gradient between the atmospheric concentration at 1-2 m above the ground and zero concentration at the surface, the deposition velocity is given as [57]:

$$v_g = \frac{F_g}{C_z} \tag{27}$$

Where v_g, F_g, and C_z are deposition velocity [m/s], flux to surface [kg/m^2/s] and atmospheric concentration [kg/m3], respectively [53]. The concentration in Equation (27) is evaluated at known height, z.

Transfer Resistance

Transfer resistance is considered as a part of the concept of conductance to describe particulate deposition from atmosphere to surface. Deposition velocity is defined as conductance.

$$r_t = \frac{1}{v_g} \tag{28}$$

Where r_t is the total transfer resistance [s/m]. Total resistance is calculated using Equations (28) and (29), and incorporating ground level concentration:

$$r = \frac{C_z - C_S}{F_g} + \frac{C_S}{F_g} = r_{rain} + r_{surface} = r_a + r_s \tag{29}$$

Where r, C_z, C_s, F_g, r_a, and r_s are resistance [s/m], atmospheric concentration [kg/m^3] at reference height, surface concentration [kg/m^3], flux to surface [kg/m^2/s], aerodynamic resistance [s/m], and surface resistance [m/s], respectively. The aerodynamic resistance, r_a, can be added as two resistors in series: turbulent resistance transfer and by eddies and molecular diffusion of the gas through the laminar boundary layer to the surface itself. For urban area, an area with high surface roughness and strong winds, the aerodynamic resistance becomes low. Table 7 summarizes typical aerodynamic values used for r_a. The surface resistance values have been widely studied and are readily available [57].

TABLE 7: Typical aerodynamic resistance values (r_a) for various wind speeds and vegetation [53]

Aerodynamic Resistance (r_a) [s/m]	Condition
200	Wind speed < 1 m/s, vegetation 10 cm tall
20	Wind speeds > 4 m/s, over 1 m vegetation
20	Wind speeds of < 10 m/s, forest canopy

The resistances that related to stomata: deposition to dry leaf surface, deposition to liquid water on leaf surface and deposition to the soil, are additional paths that might be considered. Each path having its own resistance component adds to the equation. Suggested values of v_g are 10 mm/s during the day time and 5 mm/s at night for NO_2 and SO_2 [57].

Dry deposition, Equation (29), was expanded by Wesely [58] for SO_2. This equation is augmented to include a term which represents bulk surface resistance, r_c. The r_c includes not only vegetated surfaces but the range of surface conditions. Bulk surface resistance for seasonal categories and land use may be estimated using equation augmented in Equation 29. As the temperature drops (< -2 °C), the surface resistance increases. Therefore, Wesely [58] briefly discussed surface uptake of HNO_3, SO_2, and NO_2 by the following term for each substance.

$$\text{Surface Uptake} = 1000e^{-(T_S+4)} \tag{30}$$

where T_S is the surface temperature [K].

3.2. Wet Deposition

Sulphur and nitrogen are incorporated into cloud droplets, raindrops and snow flakes, which are deposited on ground. The reactions of sulphur and nitrogen in water form a complex set based on presence of gaseous O_3 and H_2O_2, and catalysts Mn and Fe at surface of aerosol particles. These reactions last for days, thus deposition may occur thousand kilometers from the source [53].

3.3. Cloud Water Deposition

Scavenging below and in-cloud of gases is yet another transport phenomenon which should be accounted for in air dispersion models. The SO_2 gas can dissolve in clouds as it is considered a moderately soluble gas [59].

One approach to estimate below-cloud scavenging is proposed by Asman [59]. The equations are limited to rain and do not include "snow" type of precipitation. Below cloud scavenging coefficient, Λ_b, is a function of rain fall, I, as described in Equation (31). Temperature, $T_a(0)$, and relative humidity, rh (0), are measured at ground level.

$$\Lambda_b = aI_{mm}^{b_{av}} \tag{31}$$

where:

$$a = aa + bbD_g(1298.15)$$

$$aa = a_0 + a_1 rh(0)$$

$$bb = b_0 + b_1 rh(0)$$

$$b_{av} = b_{av0} + b_{av1} rh(0)$$

In these equations, Λ_b, I_{mm}, D_g, $rh(0)$, $T_a(0)$, a, b, aa, bb, a_0, b_0, b_1, b_{av0} and b_{av1} are cloud scavenging coefficient [s^{-1}], rain fall [mm/h], relative humidity at ground level [%], temperature at ground level [K], and remaining are parameters with individual functions shown in Tables 8 and 9.

TABLE 8: Below-cloud scavenging constants [59]

Constant	Formula
a_0	$4.476\times10^{-5} - 1.347\times10^{-7} T_a(0)$
a_1	$-3.004\times10^{-7} + 1.498\times10^{-9} T_a(0)$
b_0	$8.717 - 2.787\times10^{-2} T_a(0)$
b_1	$-5.074\times10^{-2} + 2.894\times10^{-4} T_a(0)$
b_{av0}	$9.016\times10^{-2} + 2.315\times10^{-3} T_a(0)$
b_{av1}	$4.458\times10^{-3} - 2.115\times10^{-5} T_a(0)$

TABLE 9: Scavenging coefficients for temperature of 10 °C [59]

Gas	a	b_{av}
NH_3	9.85×10^{-5}	0.616
HNO_3	7.70×10^{-5}	0.616
N_2O_5	5.23×10^{-5}	0.616

A second approach to calculate below-cloud scavenging was developed by Chang [60]. A simpler approach which utilizes one equation and applies to rain and snow fall is as follows:

$$\Lambda_b = 0.33\times10^{-4} I_{mm}^{0.42} + 1.0\times10^{-4} I_{mm}^{0.58} \quad (32)$$

Furthermore, the following equation was also proposed to be used for in-cloud removal of HNO_3:

$$\Lambda_c = 4.6\times10^{-4} I^{0.86} \quad (33)$$

where Λ_c is in-cloud removal [s^{-1}]. Snow scavenging can be expressed in a similar manner as shown in Equation (34):

$$\Lambda_S = 0.88\times10^{-4} I_{mm}^{0.33} + 0.6\times10^{-4} I_{mm}^{0.76} \quad (34)$$

where Λ_S is snow scavenging [s^{-1}]. Chang [60] poses a question for NO_2 scavenging by liquid cloud. NO_2 is considered to be slow due to low NO_2 solubility in water. The study points out that in snow NO_2 dissolves well.

4. APPLICATIONS OF GAUSSIAN PLUME MODEL TO URBAN AREAS

The evaluation of emissions for an urban area depends on emission summary, meteorological data, and surroundings. This information can be embedded into a dispersion model to estimate concentrations of various chemicals across the area of interest. The predicted concentrations can further be compared to the monitored data of the area. There are a number of approaches applied to dispersion of pollutants around a city which include the study of street canyons, forecasting type of modeling, and applications of statistical distribution to describe behaviour of a plume. This section evaluates the applications of Gaussian dispersion to five cities around the world and provides a critique of different applications of Gaussian dispersion for urban areas. Two studies have been completed on predicting ground level concentrations of various pollutants for the City of Toronto, one using land use regression and second a Gaussian dispersion model. The final subsection contains a description of a small scale study conducted for the city of Toronto, Ontario, Canada, and emissions due to traffic specifically emissions of NO_2. The ground level concentrations were predicted using ISC-PRIME model and compared to the monitored data. The dispersion modeling was conducted for the first few days of February 2005, days leading to the earliest smog season recorded in Toronto [12].

4.1. Dispersion Modeling of the City of Kanto, Japan

Kitabayashi et al. [4] studied NO_x emissions for a mega city, Kanto, Japan. The main sources included mobile sources (trucks), an electric power plant, and ventilation towers that service automotive tunnels. In that study, the Gaussian plume model was augmented with a chemical reaction module and incorporated concentrations for background gases. The integrated model was tested against a typical stack gas (point source). Results were stated as reliable with no analysis provided. This would quantify the relationship of data that led to a conclusion of the model's reliability. Proposed investigations for the future include inclusion of more data (i.e. monitoring stations) for the area of interest and comparison of observed concentrations to the predicted by the integrated Gaussian plume model.

The above model lacks statistical analysis in the form of comparing percentiles of modeled concentrations to monitored data for different time frames. The study overcomes one of the Gaussian dispersion limitations: the equation of continuity assumes dispersion of a chemically stable material that did not deposit to the ground [53]. The model could be augmented by the addition of dry and wet deposition for the NO_x and SO_x species using methods described in the open literature [61], [62], [63] and [64]; thus, improving the overall mass balance.

4.2. Dispersion Modeling of the City of London, UK

Two dispersion models were studied for the city of London, UK.

First Model

Owen et al. [5] utilized an existing air dispersion model which incorporated skewed – Gaussian distribution, ADMS-URBAN, along with meteorological data from one meteorological station, background concentrations of pollutants of interest for the 1995, year and emissions inventory from 1997 for the city of London. The model covered a domain of approximately 40 km by 40 km in the city of London and estimated ground level concentrations of NO_x and NO_2. The main sources of emissions (75 wt%) were roads characterized as line sources and industrial sources characterized as point sources.

The modeled concentrations were compared to the monitored data for the summer and winter of 1995. Concentrations of NO_x and NO_2 were predicted utilizing the empirical function derived by Derwent and Middleton [65]. The modeled concentrations showed an under-prediction for winter months with a conclusion that the overall model's performance was reasonable when compared to the monitored data.

For the predicted occurrences of the highest concentrations, the meteorological data during the winter season was reviewed and reasons for possible under predictions were provided. The under prediction in the cooler season was due to (cold stable conditions) the poor dispersion. In addition, the average daily traffic flow was used while the remaining information was set in the model on an hourly basis. The cold stable conditions may be described by using the approach of Milliez and Carissimo [66] and Owen et al. [5] commented on missed smaller sources (i.e. winter emissions due to combustion related to heating of homes). Perhaps if hourly data of traffic were available, the correlation would have been improved.

The study did include review of modeled concentrations for the top percentiles against the observed data. The statistical analysis included the calculation of mean, standard deviation, correlation, and fraction of data within a factor of two.

A description of the model setup and grid density, chemistry, building effect and dry and wet deposition was not discussed in the above model. The chemistry may be approached using methods of Asman, Chang, Wesely and Cana-Cascallar [59], [60], [58] and [67]. The building effect on the dispersion and modification to the dispersion code can be set as per any of the proposed solutions by Milliez and Carissimo, Xie et al., Baker et al., Baik et al. [66], [68], [69] and [70]. Treatment of slow winds may be approached by the method used by Goyal et al. [71]. All these approaches would have been refined the algorithm and possibly lead to a better correlation. The study did not also comment on the use of various years for input into the model. Obtaining input data and meteorological information for the same year as the observed ambient concentrations would yield refined correlations.

Second Model

Seika et al. [6] transformed the German dispersion model IMMAUS designed for the former city of west-Berlin into a computer platform formulated for the city of London, UK. The emission inventory included traffic, non traffic point, and area sources. Concentrations were evaluated on a gird of various densities from 1 to 10 km spatial separation. The model included hourly meteorological data and background concentrations. The Gaussian plume included total reflection. The dispersion model handled dry and wet deposition for area sources only. The modeled concentrations showed a good agreement to the monitored data observed for the year 1993.

The study also provided an in depth review of the physics behind the assumed dispersion, meteorology, and emissions inventory. An observed limitation was the need to improve how the Gaussian plume diffusion applied to wind speeds below 1 m/s, varying wind speeds and need a module which calculated mid-day boundary layer depths. The dry deposition for area sources was simulated using Chamberlain's source depletion formulation. The study did not provide statistical analysis of the comparison for the modeled concentrations and observed values.

4.3. Dispersion Modeling of the City of Helsinki, Finland

The NO_x emissions, dispersion, and chemical transformation for Helsinki metropolitan area was also modeled by Karppinen et al. [7] and [8]. Its objective was to study traffic-originated NO_x and to compare the results to four local monitoring stations for the year 1993. The domain of the city of Helsinki is approximately 30 by 30 km. Concentrations were modeled on a receptor grid with a network having dense grid (50 by 50 m) in the vicinity of the major roads and largest grid interval of 500 by 500 m around the perimeter of the city. Results were plotted as iso-concentration curves.

The hourly traffic emissions were based on EEME/2 transportation planning system (INRO 1994) and new emission factors that related to Helsinki city traffic. Pollutant concentrations were computed using the road network dispersion model CAR-FMI and urban dispersion modeling system UDM-FMI. Road sources were modeled as line source and remaining sources were

assigned characteristics of point sources. The meteorological data was obtained from two YTV meteorological stations and the mixing height of the atmospheric boundary layer was evaluated from a sounding station 90 km North-West of the city.

The 1998 study compared predicted annual average concentration to the observed data, showing a good agreement. There was a good agreement between the modeled data and three of the 4 YTV stations, however, there was a poor agreement with the 4th station. Road emissions contributed less than 50% of total emissions. Their analysis showed traffic sources have greater effect than industrial sources on the ground-level concentrations. In another study [8], the evaluation of seasonal and monthly concentrations was included. The results still contain severe under prediction of the modeled NO_x for the same 4th monitoring station as identified in the 1998 study. Furthermore, within the later study, the under prediction has been recognized for the winter months [8].

That study, comments on the variation between the modeled and observed concentrations. The statistical analysis included root mean squared error, index of agreement, correlation coefficient, normalized mean square error, and fractional bias. These parameters were applied to predicted and observed data sets as suggested by Willmott [38].

Both studies did not provide a review of all data provided by external bodies (meteorology, traffic, and ambient concentrations) utilized. The review of meteorology (i.e. wind roses, wind speeds, and stability classes) could provide an insight into variables that drive dispersion. Review of the calms and the treatment of calm conditions were not addressed. The study did not discuss traffic data to asses its limitations in the analysis. The review of ambient concentrations can give an insight of sampling methods and their limitations. Finally, the study did not address review data that did not pass quality control and thus, was not included in the modeling.

Furthermore, Karppinen et al. [8] proceeded to compare modeled hourly average concentrations to the observed data. A discussion was not given on the shortcomings of the data. The hourly average concentrations did not have a good agreement with the monitored data. A preferred approach can include a review of more than 1 year of modeled, selecting a year that best represents the meteorological conditions. A further look at the hourly averages on a daily basis along with the review of the meteorological conditions for these hours and traffic data may have provided an insight into why certain hourly averages did not match the modeled values (e.g. reduced traffic due to shutdown of a street would have resulted in lower observed concentrations but was not seen by the model). The monitored data was obtained at 4 m for two stations and 6 m for the fourth station. The study did not specify at what heights the concentrations were predicted and if those heights relate to the monitored data.

The study commented on road emissions being below 50% of the total emission and having a great impact on the final concentrations. It did not provide an explanation for this observation and it can be explained by source characteristics. Roads modeled as area sources are ground based and therefore, do not disperse as well as tall sources which have thermal and momentum rise (i.e. industrial sources). Tall sources, even though made more than 50% of the total emissions, disperse better than sources which behave as ground based sources. [40], [53], [37] and [45] In addition, road sources could have also been modeled as smaller virtual sources (i.e. width/length) as proposed in US EPA [51]. This approach is time consuming but addresses the dispersion associated with the traffic.

The lack of agreement between the modeled concentrations and the observed data at the 4th monitoring station may be explained by building downwash effect. The severe under prediction could be explained by a possible plume trap (i.e. busy intersection with tall buildings) around the area thus, resulting in higher observed concentrations. By reviewing the traffic data and locations of the monitoring stations, adjustments could have been made to correct the study to account for a better representation of the dispersion around the 4th monitoring station.

4.4. Dispersion Modeling of the City of Prague, Czech Republic

Brechler [9] developed a Gaussian dispersion model for the city of Prague. Sources were characterized as point (stacks of thermal power plants), line (traffic sources), and area sources (cross roads, petrol stations, parking sites, railway, and bust stations). Emissions due to furnaces which heat homes were included. Brigg's formula was used to define plume rise [72]. A complex network of monitors maintained by Czech Hydrometeorological Institute and hygienic service of the Prague city includes 27 monitors. The model was used to estimate concentrations of various pollutants for years 1994, 1996, and 1998.

The study did not explain the selection of non-consecutive years for which concentrations were evaluated. The model did resolve a limitation of a Gaussian dispersion model, inability to resolve flow field due to complex terrain. This was resolved by dividing the domain into smaller segments with individual meteorological conditions computed by a mesoscale model. Gaussian dispersion was selected primarily due to time limitations and simplicity of the model. An alternative approach to describing stability of the atmosphere was done by utilizing Bubnik – Koldovsky classification and not Pasquill [73]. This approach uses a classification based on the value of vertical gradient of temperature and splits all possible conditions of vertical temperature stability into 5 categories for each vertical segment. Pasquill-Gifford approach utilized solar insulation and wind speed [37]. The study did not discuss statistical analysis of the predicted values and monitored data.

4.5. Historical Work Completed on the Simulation of Pollution Type of Studies Completed for the City of Toronto, Canada

Remarkably, little work has been published on simulating ground level concentrations of various pollutants for the City of Toronto [74], [75] and [76] All three studies look at the emissions from the city using various tools and on various domain sizes.

First Study

The 1996 publication by Lin et al. was a study of a single poor air quality episode observed on April 6, 1992, at some distance away from the City of Toronto. This publication was a result of a program entitled Southern Ontario Oxidants Study (SONTOS 92). The objective of the SONTOS 92 program was to study the impact of emissions from the City of Toronto on the ozone levels in two areas: the first one located 140 km North-East of the City of Toronto in the city of Hastings and the second one 80 km South-West of Toronto in the city of Binbrook. Lin et al. [74] applied a one dimensional photochemical transport model along with Lagrangian calculations to model the emission of pollutants from the city. The City of Toronto was assumed to be a box of 20 by 30 km. The model predicted concentrations of various contaminants in Hastings and compared them to the observed data on April 6, 1992. The study concludes that the City of Toronto has an impact on the ozone levels downwind and further studies on regional scale were to be completed. No results were published for the city of Binbrook. It is important to note that no other results or analysis of data collected under SONTOS 92 have been published.

Second Study

Yang et al. [75] conducted a smaller in domain exercise by looking at pollution around a specific intersection located in the core of the City of Toronto at Bay Street and King Street. The study concentrated on the street canyon effect, similar to CFD type of exercises. This study was designed with a dense grid and included an area with very tall buildings (i.e. 330 m above grade). A non-steady state dispersion model (CALPUFF) was used to predict concentrations at the ground level and at various heights above grade. The meteorological data was predicted using MM5-a prognostic model. This publication did not study any particular air quality event that occurred in the city and did not compare results to measured data. The study concluded that CALPUFF is a potentially adequate tool which can simulate flow fields.

Third Study

Unlike the two previous mentioned studies by which dispersion models were utilized, the study conducted by Jerrett et al. considered traffic pollution in the City of Toronto and utilized a land use regression (LUR) approach to predict ground level concentrations of NO_2. The study was conducted in 2002 for a period of 2 weeks with numerous air samplers deployed across the City of Toronto. A regression of 0.69 was determined with the intention to include other sources and meteorological data to improve the results. In addition, the authors propose to generate more data to encompass a full year.

4.6. Preliminary Dispersion Modeling of the City of Toronto, Canada

In our own study, the Gaussian dispersion model along with local meteorological data was applied to road network with the objective to predict 1-h ground level concentrations of NO2. Furthermore, the objective of this study was to compare the predicted concentrations to those recorded by a local monitoring station.

Description of the Event and Modeling Domain

The timing of study was selected to be the first few days of February 2005, coinciding with the beginning of the earliest episode of smog recorded in Toronto. The area of study was selected to be two blocks of major streets surrounding a monitoring station located at Finch Avenue and Yonge Street, station I.D. 34020 [77], an approximate area of 36 km^2. The monitoring station did not capture full data for the entire smog episode. The 1-h concentrations of SO_2, NO_2, NO_x, $PM_{2.5}$ and O_3 observed at the monitoring station could be obtained from the historical depository [77]. The hourly meteorological data were obtained from a meteorological station at Toronto's Lester B. Pearson International Airport [78], approximately 30 km away from the selected area of study shown in Figure 10. The meteorological data was collected 10 m above the ground. For the time under consideration, there were two predominant wind directions, with the winds occurring at 2 m/s from south-south-east and at 5.7 m/s from north-north-west, shown in Figure 11. Morning and afternoon peak-traffic times were modeled to occur from 7 am to 9 am and from 4 pm to 6 pm, respectively. Traffic data from 2001 [79] and the Environment Canada's emission factors [80] for various vehicles were used to estimate emission rates of NO_2.

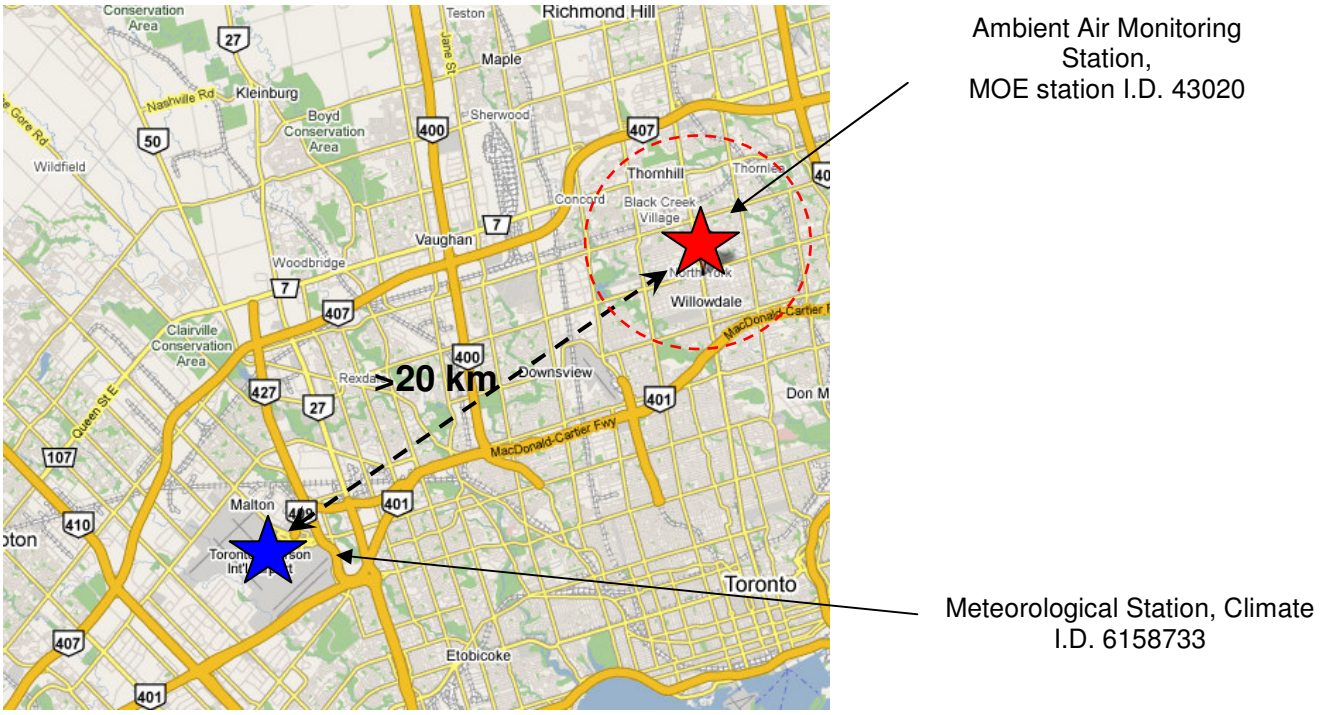

FIGURE 10: The preliminary study was conducted by simulating emissions from a 3 block sector around Yonge Street and Finch Avenue intersection located more than 20 km from the nearest source of meteorological data (Toronto Pearson International Airport)

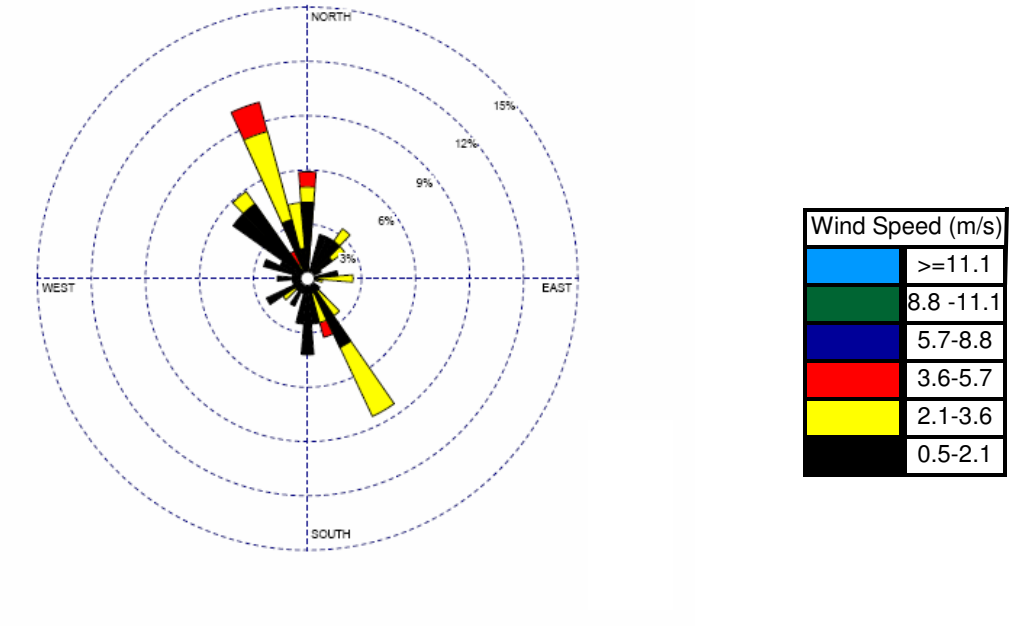

FIGURE 11: February 1 to 5, 2005 - wind rose from Toronto Lester B. Pearson International Airport (WMO Identifier 6158733) for the period associated with the study of emissions from a road network located in the city of Toronto, Ontario, Canada. Wind direction is to be read FROM

Dispersion Model Setup

The study area, shown in Figure 12, was set in ISC-PRIME dispersion model (version 04269) to evaluate 1-h ground level concentrations of NO_x in urban area. Selection of urban option allowed for the model to utilize urban dispersion factors.

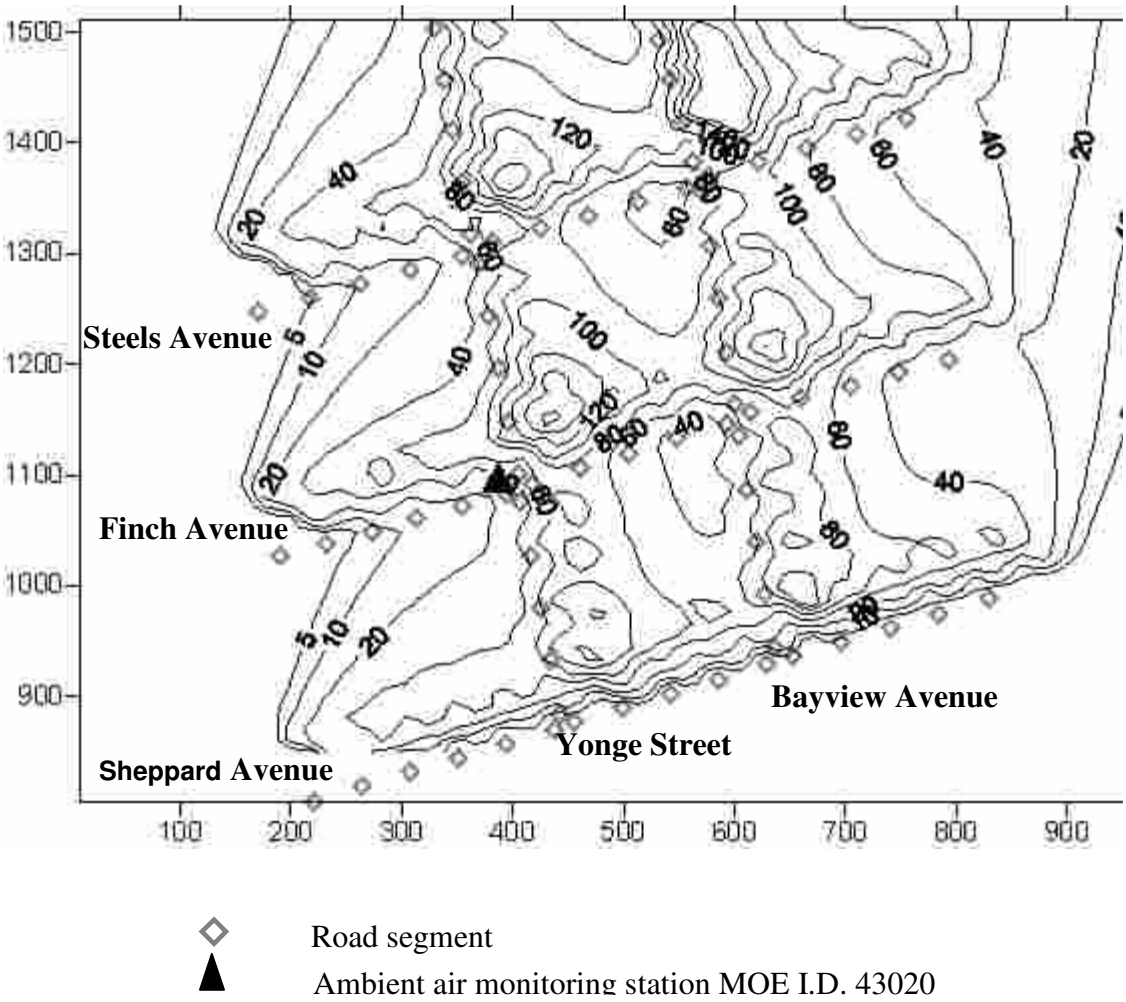

FIGURE 12: Area of study located in the city of Toronto, Canada, and modeled contour plots of ground level concentrations, NO_x µg/m^3 (4 pm, February 4, 2005)

The characterization of road within the dispersion model was based on three options: as line been studied as potential methods to characterize road emissions within the Gaussian dispersion model. The limitation of a line source as mentioned earlier arises when winds approach at angles greater then 75^o. The area source has a limit on the length to width ratio 10:1. Furthermore, the use of line or area sources yields an over prediction of the ground level concentrations [81] therefore, it was not evaluated in this study. A third option of setting up a road in a Gaussian dispersion model is to use numerous volume sources along the stretch of the path that follows road [51]. Sometimes this method is referred to as “equivalent line” source where the width of the

road becomes the basis for the initial lateral dimension. Inclusion of the plume spread factors allows to account for the mixing due to the elevated temperature of the exhaust gas [82]. In addition, each virtual source is separated by the width of the road (25 m) resulting in a series of volume sources. The height of the mobile equipment present on the road (3 m) was used to define the initial vertical dimension. The use of a volume source with embedded dispersion factors (σ_y, σ_z) allows the code to account for vehicle induced turbulence.

Results and Discussion

The modeled and monitored concentrations for the peak traffic times between 7 am and 9 am are provided in Table 10. Preliminary statistical analysis summarized in Table 11 shows a good agreement between predicted and measured data. Plot of monitored data versus observed data yields a regression of 0.5. It was observed that both the morning and afternoon of day 1 had the least correlation. Note, the sample size is relatively small and further work is required to increase it.

TABLE 10: Summary of morning and afternoon peak time average concentrations of NO_2 for the City of Toronto obtained in this study

Concentration (µg/m^3)	Day 1	Day 2	Day 3	Day 4	Remarks
			Morning		
Monitoring Station I.D. 43020	79	**88**	**81**	**120**	Good agreement for days 2, 3 and 4
Results from the Simulation in ISC-PRIME	55	**87**	**56**	**88**	
			Afternoon		
Monitoring Station I.D. 43020	41	**90**	**111**	**100**	Good agreement for days 2,3 and 4
Results from the Simulation in ISC-PRIME	106	**105**	**173**	**114**	

TABLE 11: The statistical analysis of the predicted and measured hourly time series of NO_2 concentrations for the City of Toronto modeled by this study. Morning and afternoon Traffic Peak Hours for February 1-4, 2005

Statistic	Predicted	Measured
Mean	55	84
Maximum	88	120
Standard Deviation	22	15

Two additional observations with regards to the relationships between the modeled concentrations and road traffic emissions could be made from the results. For the morning traffic, the model under-predicted the ground level concentrations. This can be explained by the presence of calm meteorological conditions that have limited mixing [5]. The afternoon traffic model over-predicted the ground level concentrations. This over-prediction could be a result of the presence of fog/clouds in the afternoon hours however, further study is necessary.

To further refine calculations, one can add emissions from local industrial sources as well as the nearby 400 series highways in addition to updating the traffic information with a 2005 traffic count. The meteorological conditions, specifically the presence of fog and clouds, could be accounted via the inclusion of the wet deposition. The analysis of hourly and 24 hour averages would be of interest and allow one to further refine the results. As indicated in the previous sections, the Gaussian dispersion model did not perform accurately when simulating during the winter period.

5. CONCLUSIONS

The air quality in Ontario is on a decline and causes the province additional cost in health care as well as limits enjoyment of the outdoors. The provincial governing bodies introduced regulations to reduce air emissions; and communication tools in the form of AQI however, this communication tool has its own limitations. One major limitation of the AQI is that for many cities, the local air quality, often over 50 km in radius, is evaluated by a single monitoring station. This lack of resolution results in large areas being declared with “poor” air quality when in fact the situation may be highly localized. Another limitation is that the air quality is based on unprocessed data from the monitoring stations. Without some appreciation of the quality of the data, and an understanding of the data in context with the region, it is difficult to fully trust that predictions of air quality are accurate. Finally, the program is costly in maintenance. With governments at all levels experiencing budgetary limits, a costly environmental system is much more difficult to run and manage when the return is rarely visible.

An improved set of methods to determine the AQI should include canyon effects, land regression modeling, and dispersion modeling. Canyon effects and land regression modeling have their own limitations since they only cover a small geographical area of study and require extensive pre-processing and manipulation of large data sets. Dispersion modeling is not a new approach and has been carried out in major cities across the world and showed a good agreement with monitored data for the area of interest.

In the preliminary study shown in this paper, a small scale dispersion model for the city of Toronto, Ontario, Canada, was carried out. The results showed a reasonable agreement with the monitoring data with respect to predicting localized contaminant concentrations. Furthermore, by super-imposing the hourly concentrations over the modeled area, the results showed locations of localized hot spots (i.e. poor air quality).

The readily available tools and data combined with a dispersion model provide a more accurate representation of the air quality at a lower cost than the existing systems in place. A dispersion model applied to the city of Toronto removes the assumption of uniform air quality within the vicinity of a monitoring station. This clearly addresses one of the key limitations of the AQI. The preliminary results are encouraging to apply existing air dispersion model, available emissions data for assessing air quality in the city of Toronto.

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