


Project Acronym	Web-SCADIM
Project Title	WEB-BASED SCREENING AIR QUALITY DISPERSION MODEL FOR INDUSTRIAL SITES
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1. Executive Summary

The scope of this project is to develop a screening model for evaluating the impact of emissions released by industries on air quality. This model should be user-friendly and easily accessible online. Since the users may not be experts in the concerned field, the model contains instructions and detailed information for data interpretation. The model also guides the user to achieve valid results by providing information on its limitations. The results so obtained helps to decide whether or not further evaluation and action is required.

For this purpose, Gaussian plume model was chosen as an underlying model. This model provides a simple approach to achieve results in a short span of time, which makes it the most commonly used model for air dispersion modelling. It was modified in order to integrate meteorological data which gives additional information on the wind pattern. Wind Rose diagram is used to understand the wind behavior and its subsequent impact on emissions. The model was tested and verified with other models to ascertain the accuracy of the results. Finally, the model was transformed into a web-based model with the help of excel online and embedded onto the concerned website.

The web-based model provides instruction for use. Accordingly, the user can insert all the inputs and run the model for result. In case of invalid input, user will be notified so that error in the result is not mistaken as accurate. Along with the result, the user also gets recommendation on the further course of action. This is a very practical resource for industries as a screening tool to assess the impact of their emissions on the quality of air. The use of this model will greatly benefit the industries and indirectly contain the effects of air pollution due to unchecked emissions.

2. Context, Position and Objectives of the Project

2.1. Context, Scientific, Social and Economic Issues

Air pollution, being both an environmental and a social problem, leads to a multitude of adverse effects on the ecosystem, the climate and human health. The industrial revolution had and still has a positive impact on the standard of living of human beings but the environment pays a costly price for this advancement. One of the foremost aspects of our environment to suffer this industrialization was air quality. Due to the lack of foresight and proper planning, pollutant dispersion from various industrial activities have led to numerous deaths and illnesses over the years. Pollutant dispersion models are now important to governments, organizations and individuals alike in order to prepare and guard against future disasters (*BC air quality, 2013*).

Dispersion models are increasingly being used to answer pertinent questions like ‘if a factory should be built’ or ‘how far it should be from the receptors (populated areas)’ but it is not an exact science. Simple and complex equations are generally used to predict these dispersion scenarios but the results are never perfect and always evolving (*Capelli et al, 2013*). The proper interpretation of these results depend on experience and expertise. Scientific knowledge of how the pollutants disperse through the atmosphere,

farthest impact distance from site and the quantity/concentration is critical for air pollution dispersion modelling.

Detailed screening information with positive and reliable results should ideally be carried out under strict conditions without the effect of external factors, the use of reliable software, large amounts of data and analyst participation charges. Factors like these could include vehicular emissions and industrial emissions (*BC ministry, 2015*).

In many cases, especially with the small and medium scale enterprises (SME), screening models are not used because they are not affordable due to the need of skilled technicians for data interpretation. Regulations concerning flue gas emissions from the stacks of industrial sites are continuously updated due to technological development such as gas monitors and analyzers which constitute a cost and nuisance for already established industries which are taxed to ensure that pollution caused by them is well under applicable regulations and environmental controls.

2.2. Position of the Project

The aim of this project is to bridge the gap between complexity, accuracy and reliability. The Gaussian plume model is one of the well-known air dispersion screening models with a lot of limitations and is the basis for this project. Another goal of this project is to eliminate one of the limitations with a proposed improvement by the integration of meteorological data (wind rose) to get more accurate results which will be carried out using Microsoft Excel for all necessary programming. The meteorological data will help us to see the impact in terms of wind direction that changes continuously. The wind rose diagram can represent yearly wind activity, condition and direction in a specific area. To be able to integrate this with the new parameter, the existing model should be modified and subsequently tested. The University of Manchester has a working Gaussian plume model in MATLAB which takes into account various wind variables for scenarios with multiple stack emissions occurring simultaneously with effects of humidity over an annual cycle. (*U of M, 2016*). Other open source web models by individuals and educational institutions exist with attempts at integrating wind speed and direction like the California State University's model which focuses on concentration values at the center of the plume and average wind speed which could result in false values with large deviations. (*CSUN 2016*)

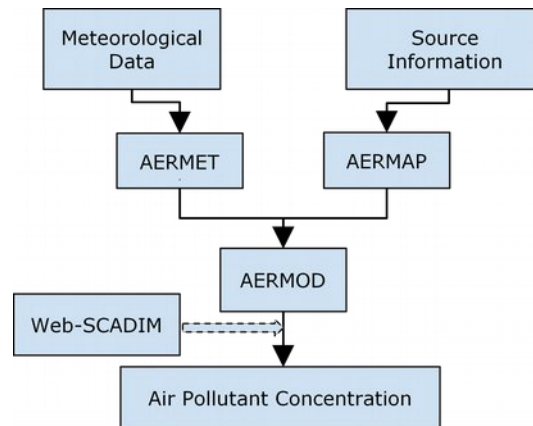


Figure 2. 1 Web-SCADIM position in the value chain

The plume model is used to calculate the concentration of a pollutant at a certain point and assumes dispersion in the horizontal and vertical direction. The Pasquill-Gifford model is a classic equation used for determining the concentration of pollutant in the air using predefined parameters like effective stack height, wind speed, distance and emission rates. The need for improvement comes from the assumptions set for the use of the plume model. For example, emissions are assumed to be constant and continuous for steady state analysis over a relatively flat terrain and pollutant degradation does not occur (chemically inert pollutants) and are not absorbed by any surfaces but reflected. Wind speed is assumed to be constant in time and elevation with pollutant concentrations having a normal distribution and a fixed concentration of one-tenth at the edge of the plume (MFE, 2004) (RPI, 2016)

2.3. State of the art

1.1.1. Air Dispersion Model

An air dispersion modelling problem can be solved with various numerical methods. Assuming a homogenous, steady-state flow and point source, the well-known Gaussian plume distribution can be used. The greatest advantage of Gaussian models is that they have an extremely fast, almost immediate response time, because their calculation is based only on solving a single formula. The Gaussian plume dispersion model used to calculate plume contaminant concentration at a point in space.

$$C(x, y, z) = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \left[\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right) \right] \dots (1)$$

Where,

- c = concentration at a given position [grams/m³]
- x = downwind [m]

y	= crosswind [m]
z	= vertical direction [m]
u	= wind speed [m/s]
H	= effective stack height [m]
σ_y, σ_z	= standard deviation of the concentration [m]

Equation 1 shows the formula for calculating the concentration of pollutants, in the downwind, crosswind and vertical directions, released based on the wind speed, effective height and the mass flowrate of the gas released. Atmospheric stability class will affect σ_y and σ_z of the main equation. In a stable atmosphere, when an air parcel sinks, pressure and temperature changes, and the temperature inside the air parcel will be greater compared to the surrounding and it will move upward since it is less dense than the surrounding. In a simple way, a stable atmosphere suppresses a vertical motions of air parcels and an unstable atmosphere will favor vertical motion of air parcels. There are six different stability classes that represent the atmosphere condition. The most popular stability classification is Pasquill method that defines from the very unstable F to the very stable A class. Pasquill took into account wind speed, sun elevation and cloud cover data to determine the stability class that provided pre-defined mixing efficiency values (*Turner, 1997, Sriram et al., 2006*).

The schematic below shows a Gaussian probability of encountering a puff of pollutant using the Pasquill method:

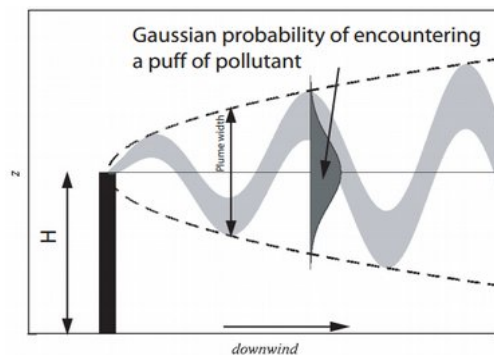


Figure 2. 2 Pasquill method modelled schematic

An advanced Gaussian model that was developed by US EPA (Environmental Protection Agency) is called AERMOD. It has a high-end turbulence parameterization based on the Monin–Obukhov-theory, and can handle complex terrain (*Cimorelli et al., 2005*).

1.1.2. Meteorological Data: Wind Rose

Wind Rose is a speed distribution diagram that summarizes the frequency and speed of wind blowing from each direction in radial scale and is the most common way of displaying wind data. As it grows

outward on the radial scale, the frequency associated with wind coming from that direction increases. The radial length around the circle is the percentage of time that the wind blows from that direction.

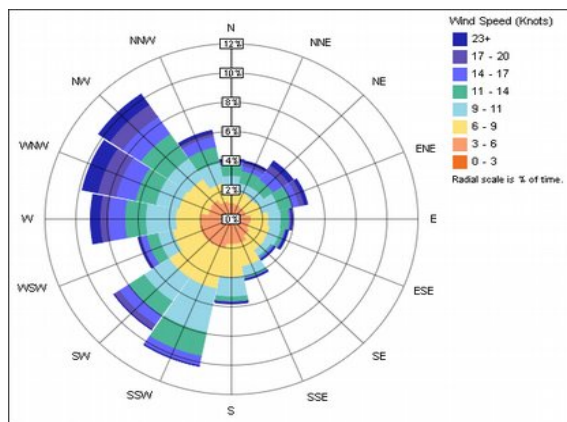


Figure 2. 3 Wind rose meteorological data example

The contribution of the project on the state of the art are to integrate the widely known wind rose data to improve the screening air quality dispersion tool based on Gaussian plume model, to make the tools available to be used online by any user.

1.1.3. Dispersion Measurements and Analysis

1. Pollutants Measured (Gas and Particulates):

Air pollutants may be categorized as either primary air pollutants (i.e. pollutants directly emitted to the atmosphere) or secondary air pollutants (pollutants formed in the atmosphere from 'precursor gases' such as secondary PM, O₃ and secondary NO₂) (Gemmer and Xiao, 2013). The pollutants which may be present in an industrial site vary from dust or particulate matter (PM₁₀, PM_{2.5}), acid gases and other gases including NO_x and SO_x, heavy metals and carbon compounds. European standard for industrial site have a regulation to ensure each site has a proper monitoring of its stack emission and to treat its emission before discharging it into the atmosphere. An advanced model can use this parameter as an optional input but it will not make any difference while using gaussian plume model.

2. Emission Factors

An emission factor is a representative value that attempts to relate the quantity of a pollutant released to the atmosphere with an activity associated with the release of that pollutant. Some important parameters to be noted are emission velocity, emission rate, source type, stack diameter and stack height plus plume rise that will be known as effective stack height.

3. Emission Zones and Standards

Table 2.1 below shows the European Union and World Health Organization's corresponding air quality target and limit values for major air pollutants such as particulate matter, NO_x, SO_x, CO, Ozone and PAHs.

Table 2. 1 Air quality target and limit values for air pollutants under EU legislation (EEA, 2015)

S/ N	Pollutant	Averaging Period	EU Air Quality Guideline	Permitted Concentration Each Year	WHO Air Quality Guidelines
1	PM _{2.5}	1 year	25µg/m ³	Not applicable	
2	PM ₁₀	24 hours	50µg/m ³	50µg/m ³ not to be exceeded 35 days per year	
		1 year	40µg/m ³	Annual average ≤ 40µg/m ³	
3	SO ₂	1 hour	350µg/m ³	≤ 350µg/m ³ in 24 hours per day (Alert threshold is at 500µg/m ³)	500µg/m ³ in 10 minutes
		24 hours	125µg/m ³	≤ 125µg/m ³ in 3 days per year	20µg/m ³
4	NO ₂ and NO _x	1 hour	200µg/m ³	≤ 200µg/m ³ in 18 hours per year (Alert threshold is at 400µg/m ³)	200µg/m ³
		1 year	40µg/m ³	Annual average ≤ 40µg/m ³	40µg/m ³
5	Lead	1 year	0.5µg/m ³	Annual average ≤ 0.5µg/m ³	0.5µg/m ³
6	CO	Maximum daily-8 hours (mean)	10µg/m ³	Maximum daily 8-hour mean ≤ 10µg/m ³	10µg/m ³ ; 30µg/m ³ per hour
7	Benzene	1 year	5µg/m ³	Annual average ≤ 5mg/m ³	
8	O ₃	Maximum daily 8 hours (mean)	120µg/m ³	120µg/m ³ not to be exceeded on more than 25 days per year averaged over 3 years	100µg/m ³
9	Arsenic	1 year	6ng/m ³	Annual average ≤ 6ng/m ³	
10	Cadmium	1 year	5ng/m ³	Annual average ≤ 5ng/m ³	
11	Nickel	1 year	20ng/m ³	Annual average ≤ 20ng/m ³	
12	PAHs	1 year	1ng/m ³	Annual average ≤ 1ng/m ³	

2.4. Objectives, originality and innovative nature of the project

The main objectives of this project were to:

- Transform an existing Gaussian plume-based air dispersion model available in XLS format into a user-friendly web-based one which is also the end product.
- Integrate meteorological data with the aid of a wind rose to create a more dynamic air screening model

The other objectives included:

- Identifying the key meteorological parameters and data required for the screening assessment.
- Attempt to reduce or lift the technical barriers by proposing a simplified approach to fill in the new meteorological data
- Providing data interpretation, validity, limitations and necessary documentation as a complement to the model results.

1.1.4. Innovation

The innovation of the project is the integration of meteorological data into the screening model. Such data include wind, temperature and air density but our focus is on wind speed which is more likely to affect pollution dispersion than the others. There are several available user models with wind speed integration online but our approach is more detailed and user oriented. Our aim is to improve on such models by also incorporating different aspects of data interpretation into one single model.

Our ingenuity lies in highlighting the accumulation concentration of pollutant in specific area for a whole year, sensitivity analysis for all our recorded data to make room for errors and the addition of user documentation in the form of comments, standards and data interpretation to reduce reliance on outside sources and the web to interpret the results obtained from the model.

1.1.5. Limitations

Web-SCADIM answers basic air pollutant modelling questions such as the annual exposure concentration and annual decayed (accumulated) concentration based on the hours of exposure and wind speed prevalent in the direction of interest but is limited to:

- Determining only the effects of pollutant from a single source point.
- Considering emissions only from stacks in industries without considering flare sources or the geometry of the stack.
- Not accounting for the possibility of the occurrence of downwash of the release gas.
- Not integrating a mapping database, as of yet.
- Not accounting for the possibility of a more complex terrain as it is only applicable for a flat terrain.

3. Methodology

3.1. Scientific methodology

The methodology to achieve the project's objectives is as follows:

- Task 1: Selection of key parameters
- Task 2: Integration of the parameter into the XLS model
- Task 3: Testing the new model with basic cases
- Task 4: Transformation of XLS spreadsheet into dynamic web page
- Task 5: Testing and restructuring of web-based model
- Task 6: Addition of comments and data interpretation

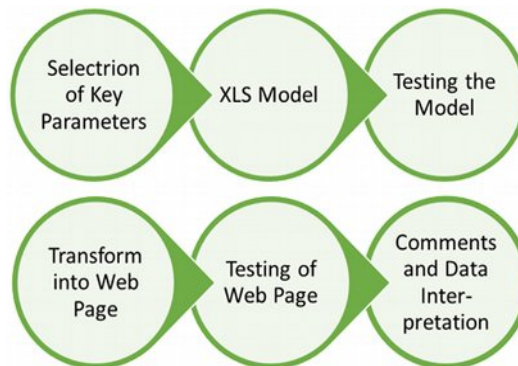


Figure 3. 1 Scientific Methodology

Task 1 Selection of key parameters

The basic parameters necessary for the implementation of the model include:

- **Effective stack height** (stack height + plume rise) - The plume rise from a stack is vertical before it disperses therefore the height needs to be considered in order to obtain reliable results of pollutant concentration. In other words, the centreline of the gaussian plume is higher than the stack height. The lowest acceptable stack height for industries is at 30m and the plume rise is dependent on the gas exit temperature, gas exit velocity and the atmospheric stability. The formulas used to calculate plume rise include Davidson-Bryant formula, Briggs equation, Holland equation, Carson and Moses equation and Concawe among others.

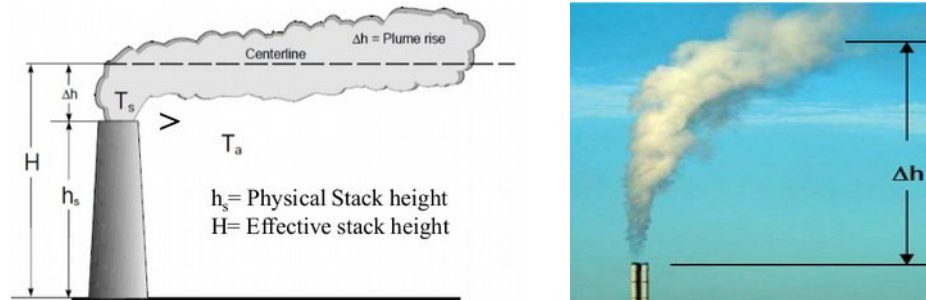


Figure 3. 2 Pictorial description of the difference between stack height and effective stack height due to plume rise

Every industry is in charge of determining its effective stack height as long as it meets requirements.

- **Gas mass flux** - This is the mass flowrate of the gas as it exits the stack. This value is measured, provided and determined by each industry in the aim of remaining within standard air quality conditions. The unit is in g/s.
- **Receptor height** - This is the height of residential zones and also the breathing zone located near the ground level. This parameter is very important in order to quantify the pollutant concentration that might affect the populace. A value of 1 m was chosen for this model including a receptor distance of 1km.
- **Meteorological data** - This includes the wind speed ranges and wind direction. Three variable ranges were provided (2-4 m/s, 4-8 m/s, >8m/s) with similar wind characteristics for each range. The wind rose data contained the matrix of percentage of each wind speed category in each direction and the receiver direction in degrees was varied to obtain various linear solutions.

Dir.	2 - 4 m/s	4 - 8 m/s	> 8 m/s	Total
020	3.0%	0.7%	0.0%	3.7%
040	2.9%	1.5%	0.1%	4.5%
060	2.6%	2.2%	0.2%	5.0%
080	2.6%	2.1%	0.3%	5.0%

Figure 3. 3 Excerpt from the wind rose data in matrix percentage.

In order for it to be user-friendly, the meteorological data to be used as the input parameter should be common and well-known which means it should be available for the SMEs to access. The data used for our simulation was already provided but another reliable source is the meteorological station of the respective industrial areas.

Task 2 Integration of the parameter into the XLS model

The wind rose data could not be used as represented therefore an accumulated wind rose graph was developed before being converted from percentage to duration. The accumulation was determined by subtracting the recorded value from each speed range from the total value for one direction.

Direction - 360°
 $>8\text{m/s} - 2.9\% - 0.0\% = 2.9\%$
 $4-8\text{m/s} - 2.9\% - 0.0\% = 2.9\%$
 $2-4\text{m/s} - 2.9\% - 0.6\% = 2.3\%$

Direction °	> 8 m/s	4 - 8 m/s	2 - 4 m/s
360	2.9%	2.9%	2.3%
020	3.7%	3.7%	3.0%
040	4.5%	4.4%	2.9%
060	5.0%	4.8%	2.6%
080	5.0%	4.7%	2.6%

Figure 3. 4 Excerpt from the wind rose accumulated data.

The wind speed duration was a more acceptable parameter than its percentage and it was calculated for 1 year using a per hour basis. Each percentage was multiplied by the total number of hours in a year (8760 hours) to find out the number of hours each wind speed category blows.

Direction °	2 - 4 m/s	4 - 8 m/s	> 8 m/s	Total
20	251	251	199	700
40	320	320	259	899
60	389	380	251	1,020
80	432	415	225	1,071
100	432	406	225	1,063

Figure 3.4 Excerpt from wind rose in duration

The first step was single direction integration which involved focusing on results for a particular direction, justifying them and then improving it into a more complex model which is the full 360° data integration. The stability class constant was used to determine the standard deviations of y and z for the final calculation of the gas concentration. The decayed concentration was calculated using a reference of every 2 hours and the total concentration for the year was determined.

Task 3 Testing the new model with basic cases

The model was tested in order to obtain a verification of the results in comparison with all the necessary formulas. Free source models by AJ designer and Screen View were used. The sensitivity analysis was performed also in this step by testing the robustness of the results of the model which is its ability to cope with errors at the input and execution stages.

The outputs of the screening model are the maximum concentration, cumulative concentration at a specific point, decayed concentration all for a year in $\mu\text{g}/\text{m}^3$ and the interrelationship between the

emission rates and the health regulation limits for work and residential areas. These were all represented with a graph of concentration (g/m^3) against distance (m) for 2 km. The detailed table showing the calculations with the various concentrations at different wind set points and standard deviations were used to obtain the necessary graphs.

Task 4 Transformation of XLS spreadsheet into dynamic web page

In order to make the excel sheet accessible online as an interactive tool, it was uploaded on excel online as the newer versions of excel do not support interactivity. By doing so, the user can input the data directly onto the sheet and get the required results. Once the sheet was uploaded on excel online, it was edited to include features that lets users type into the available cells. Subsequently, the file was embedded onto the website, from where it is ready for use by the interested individuals/parties.

Task 5 Testing and restructuring of web-based model

The web-based model was tested and the results were favourable. There was no need for restructuring.

Task 6 Addition of comments and data interpretation

In order to make the screening model more user-friendly, comments and data interpretation were added for further explanation of the results and also recommendations. Suggestions for wind stability classes were also provided to help the user making choices. For key inputs, a guidance to put values was provided.

3.2. Project management

The project was a collaboration between a group of students from Ecole des Mines de Nantes with Atmoterra, an independent environmental consultancy. Mr Adrien Bouzonville from Atmoterra supervised the project. The interaction between both parties was achieved through face-to-face meetings, information exchange through email and through an online sharing application (Google Drive).

The project itself took place from April until the end of June 2016. Having limited time, a projected timeline shown below was designed to be a guide throughout the period. Regular meetings with the supervisor were also used as avenues to give progress report. In the first meeting, the scope and objectives of the project were clarified. After determining these, the work between the students were divided and put into the designated timeline. Minutes of meeting of each meeting will be available in the appendix of this report. In the end of the project period, a poster which contains the summary of the whole project was made.

%	ITEM	April				May				June				July	
		8	15	22	29	6	13	20	27	3	10	17	24	1	4
10%	TASK 1. Select key parameters of meteorological data (wind rose)	2.0%	2.0%	2.0%	2.0%	2.0%									
25%	TASK 2. Integration of the parameter into the XLS model			5.0%	5.0%	5.0%	5.0%	5.0%							
7%	TASK 3. Testing the new model with basic cases						3.3%	3.3%	3.3%						
23%	TASK 4. Transformation of XLS spreadsheet into dynamic web page								5.0%	5.0%	5.0%	5.0%			
10%	TASK 5. Testing and restructuring of web-based model										5.0%	5.0%			
10%	TASK 6. Addition of comments and data interpretation										5.0%	5.0%	5.0%		
15%	FINAL REPORT												3.3%	3.3%	3.3%

Figure 3. 5 Excerpt from project schedule

4. Exploitation of Results

4.1. User Input

There are 3 sections in the input phase: wind speed categories, input parameters and wind rose data. The three categories of wind speed ranges were chosen during this project: 2 - 4 m/s, 4 - 8m/s and >8m/s from the meteorological data, from which the matrix percentage of each speed category was also obtained and inputted in the software. The upper and lower limits of each wind speed range are changeable for the user. Other input parameters included the pollutant mass flux, stack height, direction and distance of the concentration to be calculated, stability classifications, receiver altitude and basic wind rose data for the particular site. Users can also choose the pollutants of interest to see its yearly average concentration limit. Figure 4.1 below shows the excel user interface for inserting the parameters.

The cells in green are highlighted to mark the input area. Wind speed categories were divided into 3 different speed ranges with each having its respective stability class varied according to prevailing conditions. A set point was used because of the wind speed ranges and this was the average of each range. Users can change the scenario for this particular set point, whether it is worst case, average or best case scenario. Worst case scenario will choose lower wind speed and put it as the set point for each category.

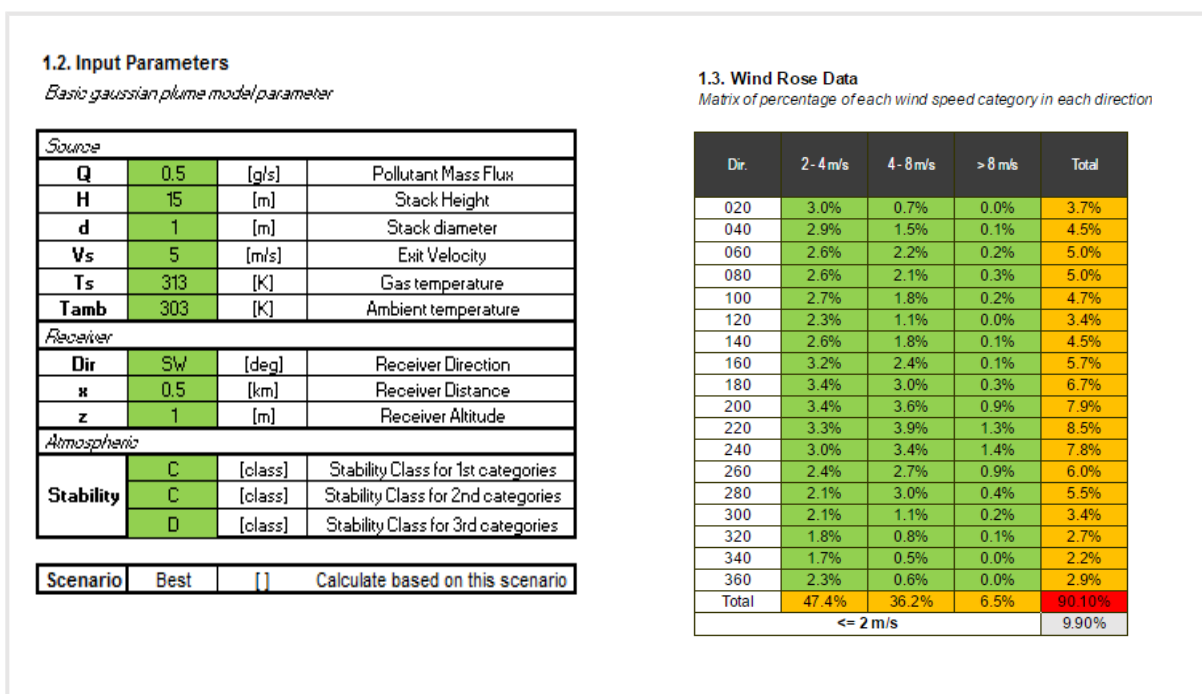


Figure 4. 1 Excel Screening Air Quality Dispersion Tools Input Parameters

SetPointA	3	ms-1	2 - 4 m/s
SetPointB	6	ms-1	4 - 8 m/s
SetPointC	8	ms-1	> 8 m/s

Figure 4. 2 Wind Speed Set Point

The wind rose data was divided into 18 classes of 20 degrees each to total 360 degrees. The Pasquill stability classes from A to F for each wind speed range were varied. There is a possible combination of wind speed and atmospheric stability as shown in table 4.1. Web-SCADIM will give users this information automatically and they can choose between the possible classes for specific wind speed that has been set.

Table 4. 1 Pasquill's Wind Speed Stability Classification

Wind Speed	A	B	C	D	E	F
1	X	X				
2	X	X	X		X	X
3	X	X	X	X	X	X
4		X	X	X	X	
5			X	X		
6			X	X		
7				X		
8				X		
9				X		
10				X		

Empirically, it can be estimated from information like cloudiness, time of day and wind speed or by using the Richardson number over a significant height difference or the vertical temperature gradient. -

$$R_i = \frac{g \left[\frac{T(z_1) - T(z_2)}{z_1 - z_2} \right]}{T(z_1) \left[\frac{u(z_1) - u(z_2)}{z_1 - z_2} \right]^2}$$

Where,

T(z) is the temperature in K at height z,

u(z) is the wind speed in m/s at height z, and

G is the gravitational constant (9.81m/s²)

The wind rose graph was generated using the accumulated wind rose data and was also converted into duration as shown in figure 4.3 below:

Accumulated Wind Rose

This table will be used to generate a wind rose graph

Dir.	> 8 m/s	4 - 8 m/s	2 - 4 m/s
360	2.9%	2.9%	2.3%
020	3.7%	3.7%	3.0%
040	4.5%	4.4%	2.9%
060	5.0%	4.8%	2.6%
080	5.0%	4.7%	2.6%
100	4.6%	4.5%	2.7%
120	3.4%	3.4%	2.3%
140	4.5%	4.4%	2.6%
160	5.7%	5.6%	3.2%
180	6.7%	6.4%	3.4%
200	7.9%	7.0%	3.4%
220	8.5%	7.2%	3.3%
240	7.8%	6.4%	3.0%
260	6.0%	5.1%	2.4%
280	4.3%	3.9%	2.1%
300	3.4%	3.2%	2.1%
320	2.7%	2.6%	1.8%
340	2.2%	2.2%	1.7%
Total	88.8%	82.4%	47.4%

2.2. Wind Rose Converted into Duration

To know how many hours each wind speed categories blows per year

Dir.	2 - 4 m/s	4 - 8 m/s	> 8 m/s	Total
20	263	61	-00	324
40	254	131	9	394
60	228	193	18	438
80	228	184	26	438
100	237	158	18	412
120	201	96	-00	298
140	228	158	9	394
160	280	210	9	499
180	298	263	26	587
200	298	315	79	692
220	289	342	114	745
240	263	298	123	683
260	210	237	79	526
280	184	263	35	482
300	184	96	18	298
320	158	70	9	237
340	149	44	-00	193
360	201	53	-00	254
Total	4,152	3,171	569	7,893
<= 2 m/s				867

Figure 4. 3 Accumulated Wind Rose and its conversion into duration per year

The stability class input is then converted into dispersion coefficients by using figure 4.4 which gives 6 different constants that are used to calculate it. The constants also depend on the distance from source. Because each wind speed category can have different stability classes, the dispersion coefficients (σ_y and σ_z) are calculated separately for each category.

Stability Class	a	x<1km			x>1km		
		c	d	f	c	d	f
A	213	440.8	1.9	9.3	459.7	2.09	-9.6
B	156	106.6	1.1	3.3	108.2	1.10	2.0
C	104	61.0	0.9	0.0	61.0	0.91	0.0
D	68	33.2	0.7	-1.7	44.5	0.52	-13.0
E	51	22.8	0.7	-1.3	55.4	0.31	-34.0
F	34	14.4	0.7	0.4	62.6	0.18	-48.6

Figure 4. 4 Stability Class Constant

> 8 m/s		4 - 8 m/s		2 - 4 m/s	
Constant	Value	Constant	Value	Constant	Value
a	68.00	a	50.50	a	104.00
c	44.50	c	55.40	c	61.00
d	0.52	d	0.31	d	0.91
f	(13.00)	f	(34.00)	f	-00
Std Deviation		Std Deviation		Std Deviation	
σ_Y	97.71	σ_Y	72.56	σ_Y	149.44
σ_Z	41.86	σ_Z	28.69	σ_Z	88.26

Figure 4. 5 Stability Class Constant for each Wind Speed Range

The effective stack height is also automatically calculated by simply inputting the stack height information. It takes into account wind speed and a higher wind velocity will change the plume direction quicker so it will give a lower plume rise. This calculation part is important to model the dispersion better. Without the plume rise, there is no correlation between plume initial speed, which is a vector and have its y-axis element, with wind direction which is assumed to be parallel to the ground. Figure 4.6 below shows the calculation result for a stack height of 15 m:

	Delta H	Stack Effective Height
1st	1.38	16.38 m
2nd	1.16	16.16 m
3rd	0.98	15.98 m

Figure 4. 6 Result of effective stack height calculation for 15m stack height

The delta H values were calculated using the formula below:

$$\Delta H = d \left(\frac{V_s}{u} \right)^{1/4} \left(1 + \frac{\Delta T}{T_s} \right) \quad \text{- Davidson-Bryant formula}$$

Where

- ΔH = plume rise above the stack in m
- D = diameter of the stack in m
- V_s = stack gas velocity in m/s
- U = wind speed in m/s
- ΔT = stack gas temperature - ambient temperature in Kelvin
- T_s = stack gas temperature in Kelvin

After calculating dispersion coefficients, effective stack height, together with the other user inputs, the pollutant concentration for each wind speed category can be calculated. The pollutant accumulation can be calculated using the averaging period provided in table 1.2 over a period of 24 hours or annually depending on requirements. Figure 4.7 gives an example of the logic used in the calculation. The parameter that needed to be calculated other than direct exposure of pollutant brought by the wind, was the decaying concentration. When wind is blowing in the desired direction, the concentration at that time can be known with gaussian plume equation (shown in orange), but when the wind is blowing to other directions, it does not mean there is no concentration in the place of interest, in fact, the previous hour's concentration will reduce by time with a decaying factor (shown in blue). A first order decay equation is chosen for this model (Thomas J). To simplify the calculation, in this screening tool, two assumptions were used. First, there is no difference between the different pollutants in this model, and second, the time where the pollutant reduced into half is assumed to be 2 hours.

$$c(t) = c_0 \exp\left(-0.693 \frac{t}{t_{1/2}}\right).$$

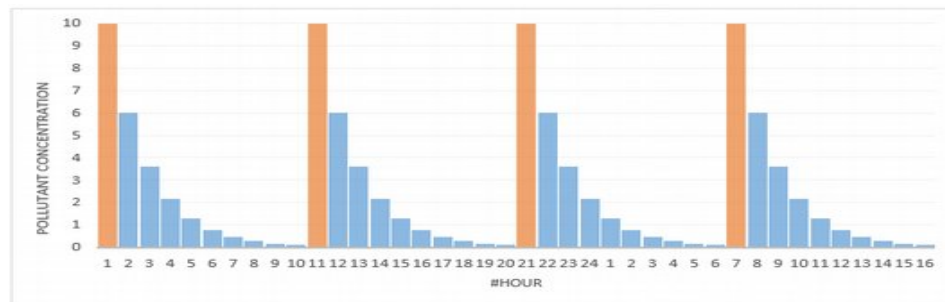


Figure 4. 7 Calculation for Pollutant Concentration

4.2. Output of the Model

The outputs of the screening model were:

- 1) short term concentration in the desired direction and coverage distance,
- 2) number of hours of exposure to the pollution concentration in a year.
- 3) accumulation of the pollutant in a year, 24 hours on yearly average.
- 4) plot of gaussian model for the 3 wind speed ranges.
- 5) plot of the influence of each wind speed category for the accumulation concentration.

For better analysis, one direction of wind speed was chosen for linear results (**50 degrees**). The analysis covers a distance of 1 km for pollutant decay and the initial concentration is in g/m³ hour.

The **hours exposed** denotes the number of hours in a year when the wind speed was in the same velocity range and direction with concentrated amounts of the decaying pollutant.

The **exposed concentration** is the total value of pollutant concentration for the year and is derived by multiplying the concentration per hour with the total number of hours it was exposed in the year. Unit in g/m³ for a year.

The **average decayed concentration** is the average decaying concentration for the pollutant. It is the average of blue bars shown in figure 4.7. Unit in g/m³ for a year.

The **total accumulation** for each range is the addition of the exposed concentration and decayed concentration. The accumulation of the pollutant is only the one caused by the source emission. It doesn't take into account the other possible sources present around the receiver. Each wind speed category has a different contribution to the total annual accumulation where the lower wind velocity gives more concentration for the same stability class.

Table 4. 2 Excel's Results Table

	Hour	Concentration	Exposed	Aver. Decayed	Decayed Exposed	Not Exposed	Total
	A	B	C	D	E	Remaining unexposed	SUM C + E
			A * B		B * D		
For 2 - 4 m/s	254.04	0.000059	0.015073	0.000014	0.035260	0	0.0503
For 4 - 8 m/s	131.4	0.000163	0.021429	0.000038	0.046002	0	0.0674
For > 8 m/s	8.76	0.000045	0.000396	0.000011	0.000927	0	0.0013

[g/m³]

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

Where,

c = concentration at a given position [grams/m³]

Q = source term [g/s]
 x = downwind [m]
 y = crosswind [m]
 z = vertical direction [m]
 u = wind speed [m/s]
 H = effective stack height [m]
 σ_y, σ_z = standard deviation of the concentration [m]

$$\sigma_y = a x^{0.894}$$

$$\sigma_z = f + c * x^d$$

The results can be compared with table 2.1 to determine if the dispersion meets with standards and regulations for the different pollutant types. The total concentration for a particular direction was calculated by adding the individual contributions from the 3 wind speed ranges and the compilation can be seen below. It helps the user to see in which distance the pollutant is concentrated and how it disperses throughout the interested direction.

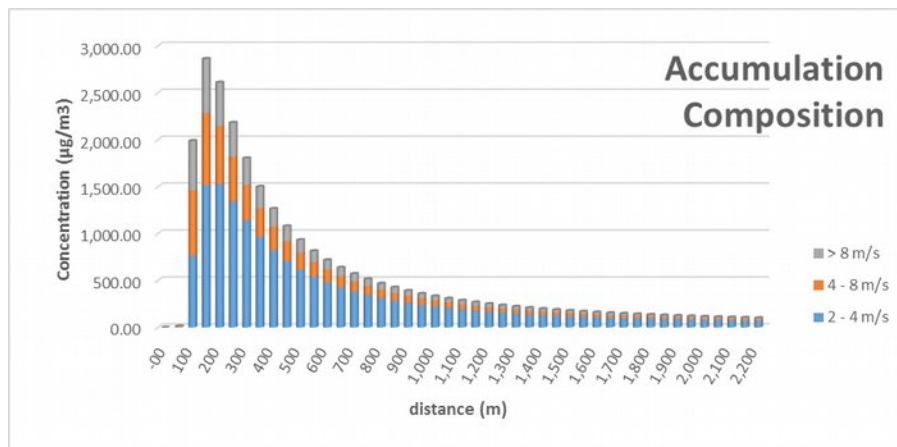


Figure 4.8 Typical graph showing the total concentration of pollutant in one direction for a year

Figure 4.9 is another graphical output that the user can get. It shows how each selected wind velocity (based on scenario) from each wind speed category disperses throughout the x-axis. Users can also view the effects of different stability classes on the dispersion profile: with stability class A giving a shorter dispersion but higher maximum settling concentration and class F giving a smoother dispersion profile in downwind direction. Users can choose to show or hide each wind speed range and analyse it separately on the graph.

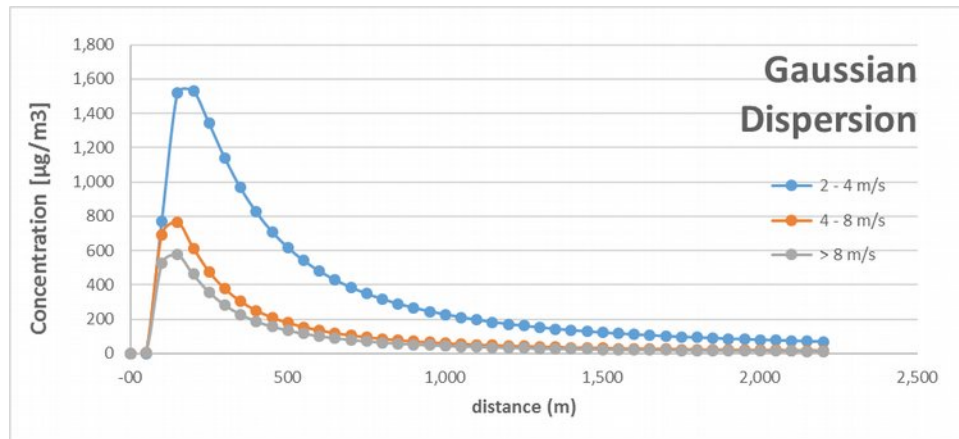


Figure 4. 9 Graph showing the three wind speed ranges

The wind rose graph below aids in visualizing the complete view of the speed ranges and the percentage of time in a year they blow in different directions. Users can see in which direction the wind blows mostly each year and make another calculation based on their interests.

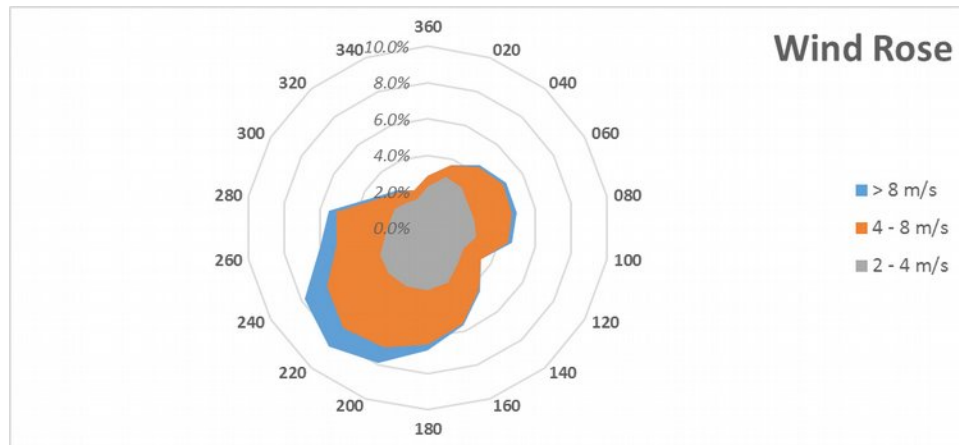


Figure 4. 10 360-degree view of the wind rose data for a year

The graphs below show the different levels of concentration in a 2 km range and the decay can clearly be seen as the plume concentration decreases with an increase in distance. They depict how the effective stack height can affect the plume shape and dispersion. A higher stack height decreases the peak concentration and also increases the distance of the plume from the source.

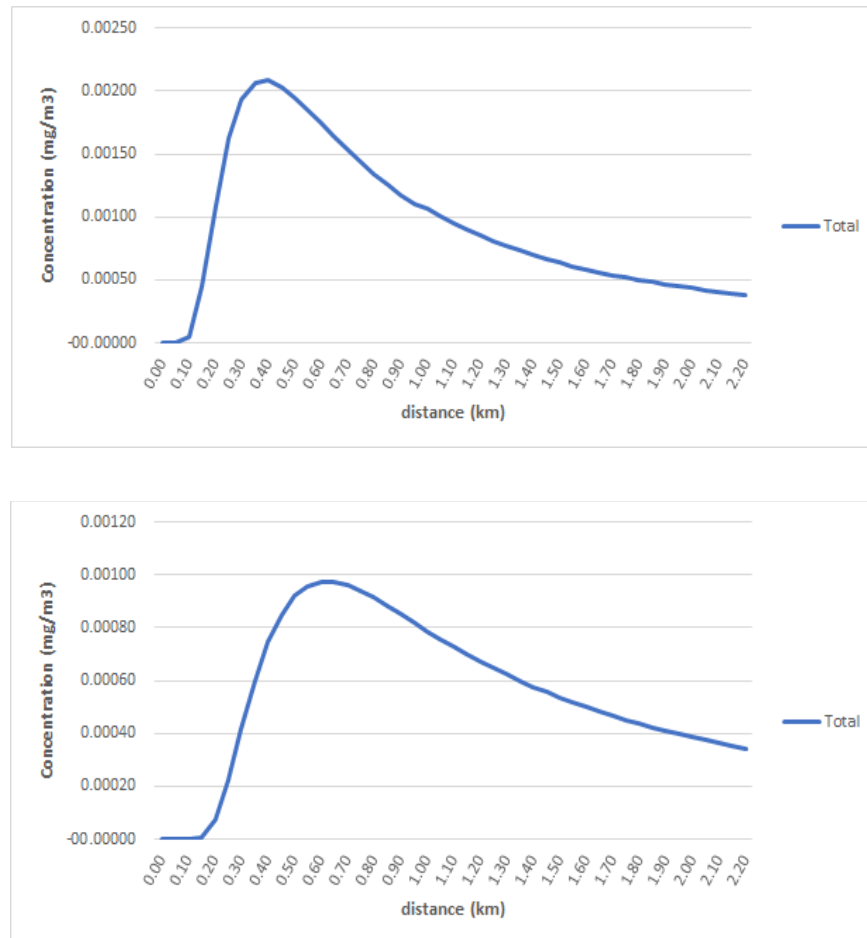


Figure 4. 11 Excel Screening Air Quality Dispersion Output Result at stack heights of 30m and 60m respectively

The calculated annual concentration is shown in figure 4.12. The tool also shows the daily (yearly average) concentration from EU and automatically compares it with the calculation and then shows a comment on whether it's over limit or acceptable.

O.3. Annual Accumulation and Average Concentration

Pollution concentration profile along the x downwind distance

Receiver Direction	SW	[direction]
Receiver Distance	0.5	[km]
Annual Concentration	22.13	[mg/(m ³ *year)]
Average Daily Concentration	60.63	[µg/(m ³ *day)]
EU Daily Limitation	40.00	OVER LIMIT
Average 8 Hours Concentration	20.21	[µg/(m ³ *8h)]

Figure 4. 12 Table of annual accumulation and average concentration

4.3. Web-based Screening Model

A simplified web-based version was developed by using excel online. An automatically generated HTML code was embedded into a web page and any user can have access to the tool. Users can only access limited spreadsheet which aims to make it more convenient for them. Web-SCADIM's description, assumptions and user guidance are available for ease of use. Further instructions for each input parameter is also available with mouse over. The section for input parameters is very similar to the excel version with the provision of brief explanations for the parameters.

I.2. Input Parameters

Basic gaussian plume model parameter

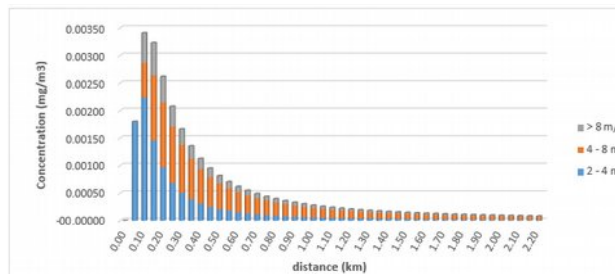
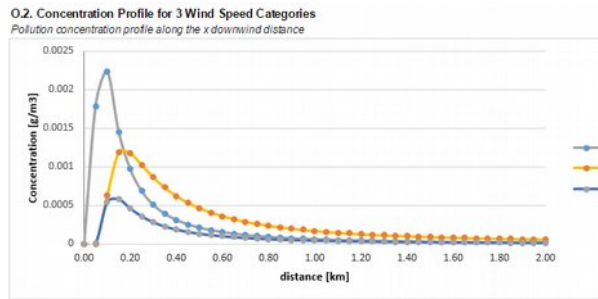
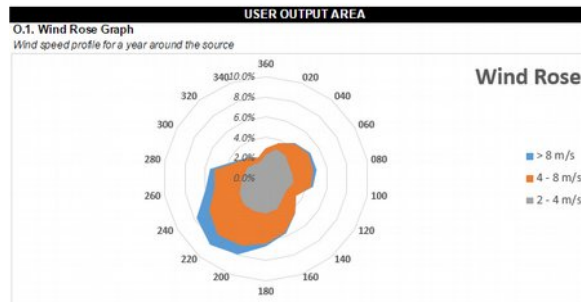
Observed Pollutant			
Type	PM2.5		Type of Pollutant
EU Yearly Limit	25	[µg/m ³]	Average Pollutant Mass Flux
Source Parameter			
Q	5	[g/s]	Pollutant Mass Flux
H	15	[m]	Stack Height
d	1	[m]	Stack diameter
Vs	15	[m/s]	Exit Velocity
Ts	40	[C]	Gas temperature
Tamb	20	[C]	Ambient temperature
Receiver Parameter			
Type	2		1: Degree (#) ; 2: Direction
Dir.	SW	[direction]	Receiver Direction
	225	[degree]	Receiver Direction
x	2	[km]	Receiver Distance
z	1	[m]	Receiver Altitude
Atmospheric Parameter			
Stability Class	E	[class]	Stability Class for 2 - 4 m/s
	D	[class]	Stability Class for 4 - 8 m/s
	D	[class]	Stability Class for > 8 m/s
Scenario	Average	[-]	Calculate based on this scenario

Figure 4. 13 Section for input parameter



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0.3. Annual Accumulation and Average Concentration

Pollution concentration profile along the x downwind distance

Receiver Direction	SW	[direction]
Receiver Distance	0.5	[km]
Annual Concentration	36.89	[mg/(m³*year)]
Average Daily Concentration	101.06	[µg/(m³*dav)]
EU Daily Limitation	40.00	OVER LIMIT
Average 8 Hours Concentration	33.69	[µg/(m³*8h)]

Figure 4. 14 The Web Result Interface

The output in this case was very compact because the major tables were filtered out to the background. The results included the wind rose graph, linear graph and numerical values which can be seen above. In addition to the output, the EU recommendations were added as a comment for faster comprehension of the results.

5. Discussion

It is generally and scientifically accepted that in most cases, the gas exiting a stack rises before it disperses. This is known as the plume rise (Theodore L & Theodore M., 2009) (Barratt R., 2001). Based on the exit temperature, wind speed of the air and exit velocity of the gas, the gas rises first and a plume shape is formed. This is taken into account by incorporating the plume rise and adding it to the physical stack height to obtain the effective stack height. The plume can be lower than the physical stack height by the effect of aerodynamic downwash, eddies caused by the flow around buildings and/or the stack and evaporative cooling of moisture droplets (USEPA, 1974).



Figure 5. 1 Downwash as a result of unstable conditions.

It is also proven that the concentration of the gas reduces as it disperses as can be seen in this picture where the colour of the plume thins out and is also a function of time, wind speed and distance. Where there is only one emission source and no other factors that interact with the plume, it is expected to follow the gaussian plume model, which is a Eulerian representation. This is proven in our results where the concentration reduces.

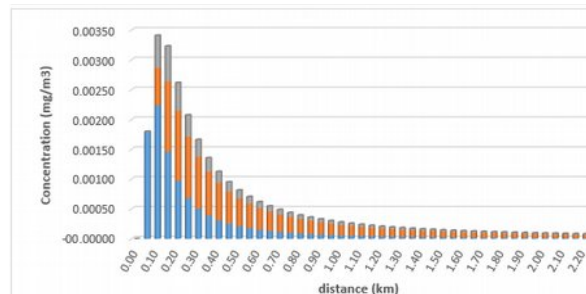


Figure 5. 2 Domtar paper mill, US. <http://goo.gl/SSGihK> & model result

From the knowledge of industries and their activities, it is known that gas exiting the stack can have pollutants which are harmful to the environment and people and this is why ideally, industries should not be located close to residential areas or ecosystems, endangered or likewise. Even though regulations about stack emissions for every pollutant exists, which each company should follow, some different values of pollutant limit for air quality exist where people's health are concerned. With the screening tool, one of the input parameters for the model include the type/mass of pollutant and the corresponding emission standards (per year, day, hour) for European countries.



Figure 5. 3 US capitol dome in the vicinity of the Capitol Power plant which has caused mercury and metal poisoning in fish and birds. <http://goo.gl/1pOISF>

In some extreme cases, the gas doesn't disperse fully and creates a pocket of high concentration close to the stack. Occurring mostly in unstable conditions our graph shows that the bulk of the gas is retained close to the stack within a distance of 300 meters.

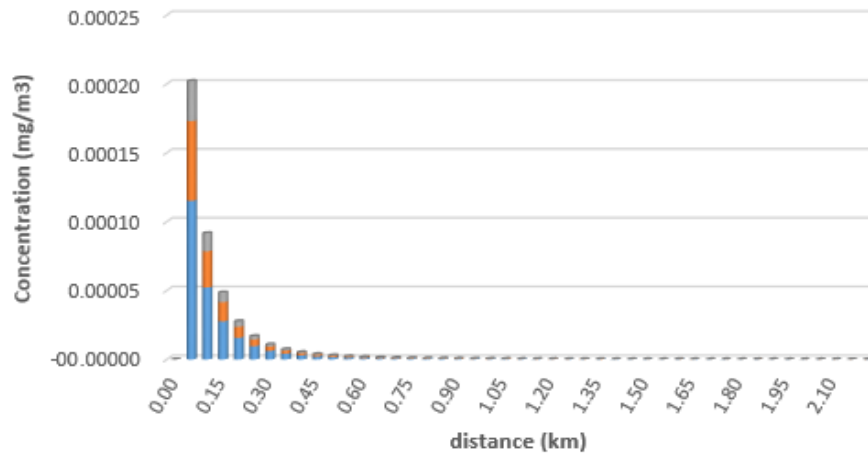


Figure 5. 4 Model result in unstable conditions

The dispersion of gas is greatly affected by some certain factors. The relationship with these factors is inversely proportional, that is, as their values increase, the concentration of the gas decreases.

The minimum acceptable stack height is 30 meters. The best way to disperse the gas to avoid trapping below the inversion layer is by dispersion during stable to neutral conditions and ensuring that the exit temperature is high enough to cause a buoyancy effect in which the gas rises vertically. The trapping occurs at the temperature inversion layer when warmer and less dense air moves over cooler and denser air. It occurs mostly during the night, early morning as the ground heats up, and in the winter months. This trapping will block the gas from moving in a vertical direction. In this case, the plume is dispersed towards the ground.



Figure 5. 5 Unstable condition resulting in tack emission trapped below the inversion layer at Lochcarron, Scotland.

<https://goo.gl/pR9t8w>

Another way to ensure a desired dispersion would be to use a sufficient exit velocity which can overcome the force of the prevailing winds or by reducing the pollutant mass flux. All these solutions can be utilized but are dependent on the budget of the industry or its location. Stable conditions which may occur in late afternoon is very effective for dispersion. It is favourable because the plume remains aloft and downwash is suppressed by the stable conditions below. A neutral atmosphere will also produce a coning shape of the plume and prevent downwash.

The results and interpretations of the model were also compared with other models for clarity. The AJ designer model had the capability of calculating only the concentration at a point and the results obtained were identical. Screen View, another free source model was used. Figure 5.6 shows the concentration profile for both models considering a point source emission in an urban area, same stack parameters, in a simple terrain, with no downwash, for C stability class and 4 m/s wind speed. There is no other available free source model that takes into account a wind rose diagram.

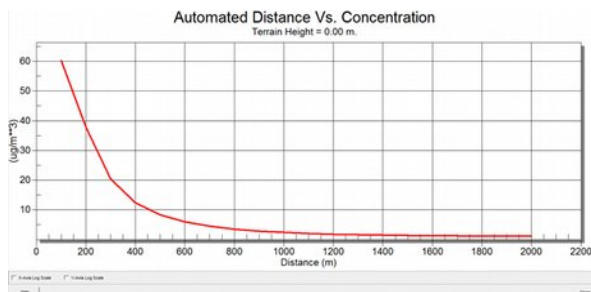
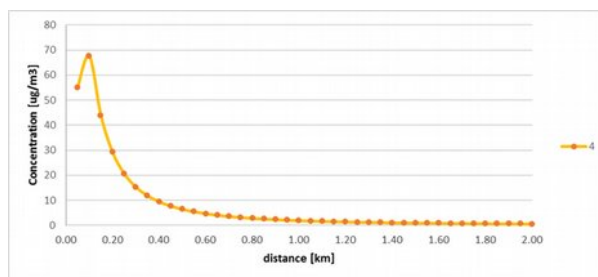


Figure 5. 6 Web-SCADIM and Screen View with similar results respectively.

A sensitivity analysis was done for different scenarios (worst, average and best) to see how each scenario affects the result of the calculation. These scenarios do not exist in the real world, where the wind velocity always changes over time. To accommodate this, the worst scenario will choose only the lower wind velocity for each wind range and give the highest concentration possible, whereas, the best scenario will choose the highest wind speed for each wind range and give the minimum concentration as the result. By observing these values, users can have a better understanding of possible situations and make the required adjustments.



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Table 5. 1 Sensitivity Study - Comparison of Results

GAS EMISSION	5 g/s of PM2.5		
STACK PARAMETER	30 m stack height, 1 m diameter, 15 m/s velocity, 40° C gas temperature		
STABILITY CLASS	Neutral for all		
	SCENARIO		
	WORST	AVERAGE	BEST
Max value at 500 m	1200 µg/m3	800 µg/m3	600 µg/m3
At 500 m	776 µg/m3/day	552 µg/m3/day	437 µg/m3/day
At 1 km	1024 µg/m3/day	710 µg/m3/day	550 µg/m3/day
At 2 km	599 µg/m3/day	410 µg/m3/day	315 µg/m3/day

The influence of each parameter change to the final concentration was also discussed. When changed, the level of impact each parameter makes on the output varies from low to high. Users can modify each parameter and find the most satisfying solution for them.

Table 5. 2 Sensitivity Study - Influence of each Parameter

Doubling the gas emission	Simply doubles the final concentration for all scenarios
Doubling the stack height	Tremendously reduces the final concentration
Doubling the stack diameter or exit velocity	Slightly reduces the final concentration
Doubling the gas temperature in °C	The effect on the final concentration can be neglected

6. Conclusion

Different air quality dispersion models with various levels of complexity were studied to select the most feasible model for the project. Based on the scope of this project, Gaussian plume model was chosen due to its simplicity, ease of computation and quick result generation. In order to create an exhaustive screening model, the model was modified to integrate more variables, such as meteorological data, to get

more accurate results which was carried out using Microsoft Excel. Wind rose diagram was used to visualize the wind patterns from the obtained meteorological data and thereby, understand the impact in terms of wind direction that changes continuously. Subsequently, Web-SCADIM was tested and compared with other similar models to verify the accuracy of the results.

The emphasis of this model was to give its users a simple, yet powerful, screening tool to assess the impact of their emissions before choosing to opt for more detailed evaluation of the impact of their emission sources. The model successfully integrates four main parameters which are effective stack height, atmospheric stability class, dispersion coefficient and several possible atmospheric scenarios. Moreover, the model had to be developed keeping in mind the requirement of its users, i.e. the industries. Accordingly, it was uploaded on excel online and was transformed into a web-based model and finally embedded onto the website allowing easy access to the industries. The online model was developed to be user-friendly for everyone and therefore, it contains comprehensive information that allows the users to interpret the data. The assumptions used in the calculation are also provided. Furthermore, it includes the validity along with the various limitations where the model may fail to deliver accurate results. Based on the inputs given by the user, the model provides the result and will recommend whether further evaluation is needed or not.

Considering the critical role of industrial emissions towards air quality, the model developed as part of this project has tried to contribute towards better understanding and control of air quality. Implementing it as a preliminary screening tool will definitely benefit the industries in the long run.

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8. Appendixes

- A. Minutes of meeting
- B. Project Timeline

MINUTES OF MEETING

PROJECT : A web based screening air quality dispersion model for industrial sites

DATE : 03/31/2016

LOCATION : B 107

AGENDA : Kick Off Meeting

LIST OF ATTENDANCE

No.	NAME	POSITION/ ORGANISATION
1	BOUZONVILLE Adrien	Project Supervisor
2	ABUDU Aderonke	Project member
3	ADEBAMBO Francis	Project member
4	BURHAN Salwa Syed	Project member
5	KEVIN Andre	Project member

POINT DISCUSSED

1. Introduction of the persons present: educational background, work experiences, knowledge base regarding air dispersion modelling, etc.
2. Discussion of aims and objectives of the project, so as to ensure proper comprehension of the questions to be answered by the project.
3. The students had the following questions:
 - a. Do we need to have a programming knowledge to carry on the project?
 - b. Is there any specific existing model that we have to work with?
 - c. Could more explanation be given on the Gaussian plume and excel modelling types?
4. Mr Bouzonville addressed each of the questions by stating that no coding knowledge was required at the initial phase and more emphasize should be on the methodology and integrating the software with meteorological data and mapping platforms such as Google Maps and OpenStreet.

He further explained that the aim of the project is to make available to the 'lay-man' a simplified web-based software which can give basic

pollutant dispersion information without a need to employ an external consultant. He gave basic knowledge with regards how the Gaussian plume modelling works.

5. The meeting was concluded with an understanding to work on methodology first, while awaiting further source documents from Mr Bouzonville.
6. Modalities for the next meetings are to be agreed upon and corresponded to the involved parties via mail.

MINUTES OF MEETING

PROJECT : A web based screening air quality dispersion model for industrial sites

DATE : 04/19/2016

LOCATION : B 108

AGENDA : Progress Meeting

LIST OF ATTENDANCE

No.	NAME	POSITION/ ORGANISATION
1	BOUZONVILLE Adrien	Project Supervisor
2	ABUDU Aderonke	Project member
3	ADEBAMBO Francis	Project member
4	BURHAN Salwa Syed	Project member
5	KEVIN Andre	Project member

POINT DISCUSSED

1. Point 2.1.1. until 2.1.3. in the presentation are more suitable for 1st section of report
2. For 2nd section of report, focus more direct on tasks
3. The modified XLS should be able to calculate total exposure for a point in specific distance from (0,0) in any direction, taking into account (1) the exposure concentration and (2) exposure duration, (3) dilution exposure and (4) non-exposed duration. In total: 8640 hours a year for residence people, and 8 hours per day for worker.
4. Sensitivity analysis should be put in main tasks.
5. Mr Adrien will provide us with english-translated XLS file soon.

PROJECT SCHEDULE

		ITEM															X			Y			Z						
%		April							May			June							July										
		8	15	22	29	6	13	20	27	3	10	17	24	31	7	14	21	28											
10%	TASK 1. Select key parameters of meteorological data (wind rose)																												
	1% Basic knowledge about Air Dispersion Models																												
	1% Key parameters of Wind Rose																												
	2% Progress Meeting																												
	1% Writing Chapter 1																												
	1% Scientific Methodology																												
	1% Project Management																												
	2% Progress Meeting																												
	1% Writing Chapter 2																												
	25%	TASK 2. Integration of the parameter into the XLS model																											
7%	6% One direction integration																												
	5% Submission of Interim Report																												
	7% 360 degree integration																												
	3% Writing Chapter 3 (1/2)																												
	4% Progress Meeting																												
	TASK 3. Testing the new model with basic cases																												
	3% Case Trial, Selectivity Analysis																												
	4% Writing Chapter 3 (2/2)																												
	23%	TASK 4. Transformation of XLS spreadsheet into dynamic web page																											
	5% Comparison of options available																												
10%	12% Implementation																												
	6% Writing Chapter 4 (1/3)																												
	TASK 5. Testing and restructuring of web-based model																												
	6% Case Trial, Selectivity Analysis																												
	4% Writing Chapter 4 (2/3)																												
	10%	TASK 6. Comments, Data Interpretation and Sensitivity Analysis																											
	4% Presentation Meeting																												
	3% Sensitivity Analysis																												
	3% Writing Chapter 4 (3/3)																												
	15%	FINAL REPORT																											
100%	7% Poster and Final Report Writing																												
	4% Final draft meeting																												
	4% Submission of Poster and Final Report																												