A COMPARISON OF THE PERFORMANCE OF GRAL AND CALPUFF IN THE MODELLING OF FUMIGANT EMISSIONS FROM SHIPPING CONTAINERS

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Abstract

GRAL has a number of advantages over many traditional models (e.g. CALPUFF, AERMOD) in the assessment of air quality impacts. In particular, its integrated micro-scale flow-field model allows it to simulate the effect of structures and buildings on pollutant dispersion. This feature has led to it becoming a popular air dispersion model for the assessment of a range of air emission source types in a complex environment.

One scenario where GRAL has specific use and advantage over a traditional model is in the modelling of fumigant venting from shipping containers. The dispersion of pollutants is effected by a combination of factors, including the direction and size of the container opening, and wind flow around the containers and other local structures.

Trinity Consultants Australia previously prepared a vent management plan for shipping container fumigation operations based on CALPUFF modelling. This study examines the performance of GRAL compared to CALPUFF for the same project. The results are also compared to monitoring data and the differences in vent management plan outcomes are reviewed.

Keywords: GRAL, CALPUFF, wind flow field, fumigation, shipping containers.

1. Introduction

GRAL presents several advantages over traditional models such as AERMOD and CALPUFF in assessing air quality impacts. Its integrated micro-scale flow-field model allows it to effectively simulate how structures and buildings influence pollutant dispersion, making it a popular choice for assessing diverse emission sources in complex environments.

While GRAL was initially developed to address the unique challenges of low wind speed conditions in Austria's inner-Alpine basins and the need to assess impacts from tunnel portal sources, its applications extend beyond this context. Numerous studies have compared GRAL with traditional models, often focusing on point source scenarios such as generators in built-up areas. For instance, a study by Ward and Rollings (2021) compared GRAL and CALPUFF odour concentration predictions for a sewer vent stack in an inner-city suburban location, finding similar performance but noting GRAL's results were likely more realistic due to its consideration of wind flow around buildings (Ward & Rollings 2021).

Extensive work has been undertaken for road emissions in New South Wales, such as a comparative study conducted by Boulter et al., where road traffic emissions for a study area in Western Sydney were modelled using GRAL and CAL3QHCR (Boulter et al. 2017). Overall, GRAL performed better spatially and provided preferable results from an air quality point of view with slight overestimations of concentrations, whilst CAL3QHCR presented slight underestimations.

Ward, Clarke, and Rollings conducted a performance study between GRAL and AERMOD, the recommended regulatory air dispersion model for assessing freeway traffic emissions in Victoria. They concluded that GRAL appears to provide the most realistic results for road projects, especially where noise barriers are present (Ward, Clarke & Rollings 2020). On the other hand, AERMOD over-predicted short and long-term concentrations, with slightly improved results when using the adjusted U*-star method.

There is limited information regarding GRAL's performance and applications specifically for industrial settings in Australia. However, a review of existing literature suggests that GRAL tends to provide more realistic predictions in complex built environments compared to traditional models. Given this, it would be valuable to assess whether similar outcomes apply to industrial settings where complex structures and varied emission sources often present unique challenges for air quality modeling. Therefore, this study aims to address this gap by focusing on a unique industrial scenario, characterised by distinct dispersion patterns and physical configurations, further highlighting GRAL's versatility and applicability in diverse contexts.

2. Project Example

The GRAL and CALPUFF comparison was undertaken for a fumigation operation at a grain production facility in NSW.

CALPUFF was previously adopted for the assessment to derive a vent management procedure, which controlled methyl bromide emissions by managing the number of containers opened and vented based on prevailing wind conditions. Full details of this assessment and the CALPUFF modelling are presented in the study by Wong (2018).

The on-site fumigation area that was considered comprises of four bays, which are situated between 30 metres to 130 metres from the northern boundary. Fumigation and venting only occurs in a single bay at any time, with one bay holding up to 54 shipping containers (18 containers x 3 high).

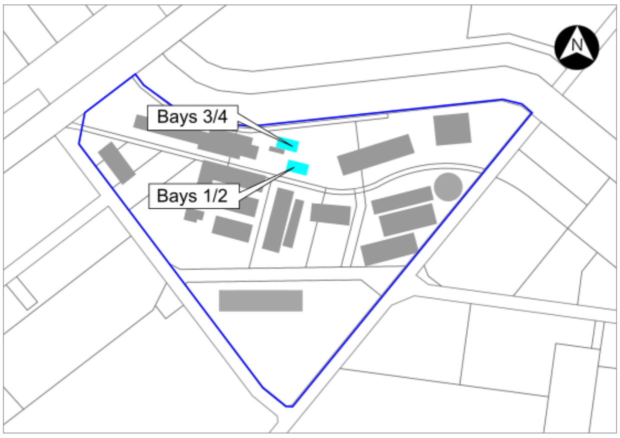

Figure 1. Site Layout

The vent management plan was developed based air dispersion modelling for two scenarios:

1. Calibration modelling - comparison of predicted results with the continuous boundary monitoring results, which provided a basis for establishing the accuracy of CALPUFF and for making adjustments to results, if considered necessary.
2. Compliance modelling - modelling of emissions to determine the maximum allowable containers vented for a given wind condition.

Based on the results of the CALPUFF modelling, two vent management plans were prepared – one for Bays 1 and 2 (furthest from the site boundary) and a second for Bays 3 and 4 (nearest to the site boundary).

3. Modelling Scenarios for Comparison

The calibration and compliance modelling scenarios were run in both CALPUFF and GRAL, and the results were compared to determine the differences in the vent management plan. For the purpose of this comparative study, a vent management plan was developed using GRAL for Bay 4 only.

3.1. Calibration Model

Key inputs and features of the calibration model are summarised as follows:

- Six venting events were modelled. The six venting scenarios considered occurred between December 2016 to February 2017. These scenarios were selected as they corresponded to wind conditions resulting in the highest boundary concentrations. Wind conditions were determined from the nearest Bureau of Meteorology station, as shown in Figure 2.

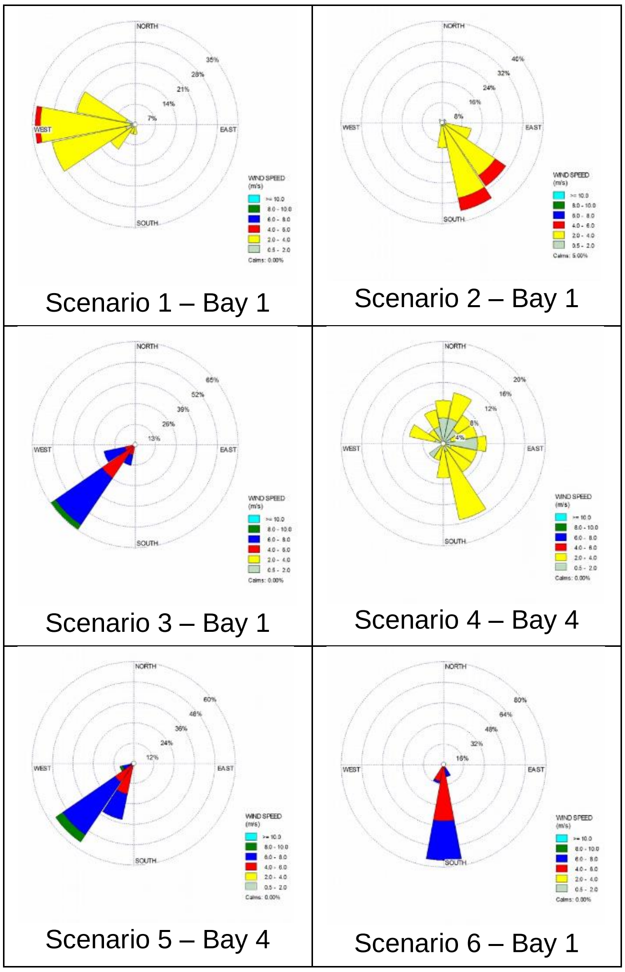

Figure 2. Wind Rose for Calibration Scenarios

- The emission rates were derived using the field sheet data provided by the site, which identified the amount of methyl bromide used in each container.
- The total number of containers being vented and their specific location within the fumigation bay were provided in operator field sheets.
- Predictions were assessed and compared to measured results. From this information, it was

determined whether the model was over- or under-predicting methyl bromide concentrations at the site boundary.

3.2. Compliance Modelling

A synthetic single-point meteorological file was developed for the purpose of predicting pollutant dispersion under a range of conditions, consistent with the Level 1 screening meteorological dataset defined in the NSW Methods for Modelling and Assessment of Air Pollutants in NSW (NSW EPA 2016). The Level 1 data set covers a range of wind speeds, wind direction and mixing heights. With regards to wind direction, a full range of directions were considered at 10 degree increments.

Predictions were made at various discrete receptors along the whole site boundary (north, east, south and west). The results of the modelling were then analysed to identify the maximum number of containers that could be vented under different wind conditions before the methyl bromide air quality goal was exceeded.

3.3. GRAL vs CALPUFF Model Configuration

The main purpose of this study was to investigate how GRAL would perform compared to CALPUFF, while utilising it's unique modelling features directly applicable to the project example. These features include the micro-scale flow-field model for simulating building structures and the vertical area source option ('tunnel portal'), which can be used to represent emissions from the vertical/opened shipping container doors. Besides this, GRAL was set up so as to replicate the CALPUFF model as much as possible for other inputs, such as meteorology and topography, for both the calibration and compliance modelling scenarios.

3.3.1. Meteorology

Single point meteorological files were developed for each modelling scenario. As discussed previously, the calibration modelling utilised data from the nearest Bureau of Meteorology station, while the compliance modelling utilised a synthetic data set considering a range of wind speeds over a full range of wind directions.

The majority of parameters required in the CALPUFF meteorological file were also required in GRAL. These parameters include wind speed, wind direction and stability class. It is noted that, when using a single point meteorological file, GRAL does not require mixing height or temperature.

3.3.2. Source characteristics

In CALPUFF, each container was modelled as an individual volume source with an initial sigma Y and Z of 1.0 m. A height of either 1.3 m, 3.9 m or 6.5 m was adopted depending on the level of the container above ground.

In GRAL, container openings were modelled using the "tunnel portal" option, with the following inputs:

- 7.8 m high source, representing the height of 3 containers
- 1.3 m wide source, representing one door typically being opened during venting
- Minimal exit velocity of 0.1 m/s
- Temperature difference compared to ambient of 0^{o}C

As noted above, three containers stacked on top of each other were modelled as a single source. This approach was taken to reduce the number of model runs to cover 54 containers for Bay 4 (resulting in 18 runs instead of 54). For the facility being considered, it is noted that the operator first fills a bay vertically (up to 3 high) at the starting end, before moving horizontally across the bay to the other end. Therefore, the modelling scenarios adopted in GRAL are consistent with on-site practices.

3.3.3. Building topography

CALPUFF can include the influence of turbulence associated with building wake on dispersion from point sources, but does not model the changes in wind direction due to buildings or their effect on dispersion from volume sources, which was identified as one of the limitations of using the model in the original air quality assessment.

In GRAL, all building structures on the subject site were included. In addition to this, the containers being vented were included, as the presence of these containers is expected to affect air dispersion directly around the source of emissions.

Flow fields were modelled for a total of 24 building scenarios to represent each modelled scenario (6 calibration scenarios and 18 venting scenarios). Each building/flow field scenario differed in terms of the number and location of the shipping containers. For the calibration scenarios, the shipping containers were modelled as per information provided in photos. For the compliance modelling of Bay 4, shipping containers were increased from 3 containers at the western end up to 54 containers at the eastern end.

4. Results

4.1. Calibration Modelling

Error! Reference source not found. presents the calibration modelling results for CALUFF and GRAL.

Table 1. Predicted vs Measured Results – 1-hr AVG

Vent Scenario	Bay	Predicted:Measured Ratio	
		CALPUFF	GRAL
1	1	2.7	< 0.1
2	1	14.6	3.3
3	1	67.6	3.4
4	4	33.9	8.6
5	4	78.0	47.8
6	1	108.0	113.8

A comparison of the results in Table 1 shows that both models over-predict compared to the measured boundary concentrations. The extent of over-prediction is less for GRAL, with predicted to measured ratios being lower compared to CALPUFF for 4 of the 6 vent scenarios. The ratio for Vent Scenario 6 was slightly higher for GRAL, but only by a small margin (5% higher). For Vent Scenario 1, a very low concentration was predicted at the boundary (<1 μg/m^3), resulting in a predicted to measured ratio of less than 0.1.

Figure A1 in Appendix A presents concentration plots as heat maps for each calibration scenario. The plots for Calibration Scenarios 3 and 5 do show a modelling artefact being an unusual narrow, high concentration area, extending immediately east from the shipping containers. Otherwise, the plots show dispersion patterns as expected for the associated wind conditions (as per Figure 2).

4.2. Compliance Model

The outcomes of GRAL and CALPUFF were compared by analysing the frequency of venting restrictions occurring throughout the year. A venting restriction refers to the maximum number of containers that can be vented before exceedance of the air quality goal at the site boundary occurs.

The number of containers that can be vented for a given hour is determined based on the observed wind speed and wind direction (obtained from the local BoM station) and the results of the GRAL/CALPUFF compliance modelling (which provide predicted concentrations/max containers for a wide range of wind speed/direction conditions).

Ultimately, it is this practical outcome relating to container restrictions that has the most relevance to the operator. The annual wind rose used to calculated the frequency of venting restrictions is presented in Figure 3. Table 2 presents a comparison of the venting restrictions using GRAL and CALPUFF.

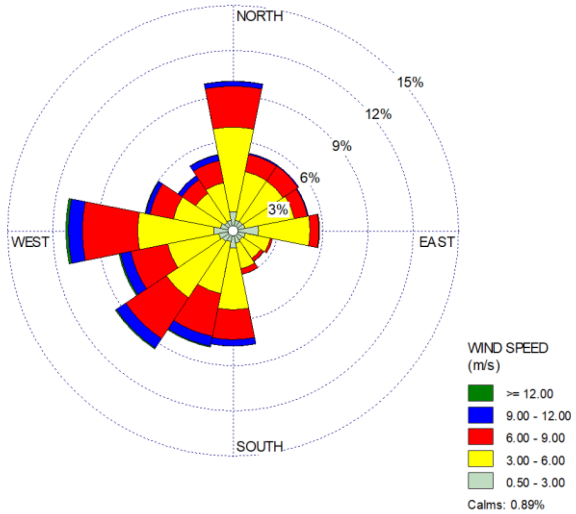

Figure 3. Annual Wind Rose (7 am to 5 pm)

Table 2. Frequency of Venting Restrictions for Bay 4 – CALPUFF vs GRAL

No. of Containers Allowed to Vent	% of Time	
	GRAL	CALPUFF
<10	29%	39%
11-20	6%	4%
21-30	4%	4%
31-40	1%	2%
41-50	2%	2%
51-54	58%	48%

Table 2 shows that GRAL provides a lower frequency of more restrictive conditions (i.e. < 10 containers) and higher frequency of less restrictive conditions (i.e. 51-54 containers). These outcomes are consistent with the results of the calibration modelling, which showed that GRAL was predicting lower results than CALPUFF. The frequency of venting restrictions for container categories between 11 and 50 are similar between the two models. In practice, the main implication of Table 2 is that improved operational efficiencies can be achieved by the fumigation operator, since the maximum number of containers (54) can be vented for the majority of the year (58% of the time).

Concentration plots for 6 different meteorological conditions with 18 containers venting are presented in Appendix A (wind speeds of 0.5 m/s and 3 m/s combined with wind directions of 80º, 180º and 270ºC). The concentration plots show a shielding effect provided by the containers being vented and surrounding buildings.

Further analysis has been undertaken to compare predicted concentrations under different wind speeds and directions. Table 3 and Table 4 present the proportion (%) of meteorological conditions for which GRAL is predicting higher than CALPUFF (for the 18 container scenario).

Table 3. Proportion (%) of GRAL Predictions Higher than CALPUFF Predictions (Categorised by Wind Speed)

WS (m/s)	Freq %	WS (m/s)	Freq %
0.5	31%	6	10%
1	8%	7	14%
1.5	6%	8	11%
2	6%	10	17%
2.5	5%	12	25%
3	6%	14	19%
3.5	8%	16	14%
4	6%	18	19%
4.5	8%	20	14%
5	6%		

Note: Each wind speed category includes a range of wind directions and stability classes

Table 4. Proportion (%) of GRAL Predictions Higher than CALPUFF Predictions (Categorised by Wind Direction)

WD (º)	Freq %	WD (º)	Freq %	WD (º)	Freq %
10	8%	130	0%	250	0%
20	12%	140	0%	260	0%
30	14%	150	0%	270	0%
40	18%	160	0%	280	0%
50	29%	170	0%	290	0%
60	45%	180	47%	300	8%
70	37%	190	10%	310	8%
80	47%	200	0%	320	18%
90	35%	210	0%	330	14%
100	2%	220	0%	340	10%
110	0%	230	0%	350	12%
120	0%	240	0%	360	10%

Note: Each wind direction category includes a range of wind speeds and stability classes

From Table 3 and Table 4, it can be seen that GRAL is predicting higher than CALPUFF for only a small proportion of modelled meteorological conditions, for the majority of wind speeds and wind direction categories. For many of the wind directions, GRAL is always predicting lower than CALPUFF (i.e. frequency 0%). However, there are certain conditions when GRAL is predicting higher concentrations more frequently. For example, GRAL results in more frequent higher predictions (29% to 47% of the time) for wind directions 50º to 90º. This is likely due to the presence of an elongated building immediately west of Bay 4 and very close to the northern boundary of the site. Winds blowing from these directions disperse pollutants towards this building and pollutants are subsequently concentrated on the northern facade along the northern side boundary. At a wind direction of 180⁰, GRAL is predicting higher than CALPUFF for 47% of the modelled meteorological conditions. In both instances, the higher predictions generally occur under higher wind speeds and more stable conditions. The results demonstrate that the presence of structures can have a positive and negative effect on concentrations depending on the specific meteorological conditions being considered.

5. Conclusion

This study has analysed the performance of GRAL compared to CALPUFF in an industrial setting, specifically relating to the venting of methyl bromide from shipping containers. This scenario provided a useful context for applying GRAL's micro-scale flow-field model in a built-up industrial environment. Overall, GRAL predicted lower than CALPUFF for the range of wind conditions and stability classes adopted in the modelling. GRAL was also the more accurate of the two models when comparing predictions with measured data collected at the boundary of the container fumigation site.

These outcomes highlight the importance of model selection in air quality assessments. While regulatory guidelines may formally approve the use of traditional models, the model selection process should not be limited to these models alone. For industrial assessments, in which complex building structures are often relevant, GRAL may be the preferred choice over traditional air dispersion models. For the project example used in this study, the use of GRAL would have also resulted in improved operational efficiencies for the site operator.

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Appendix

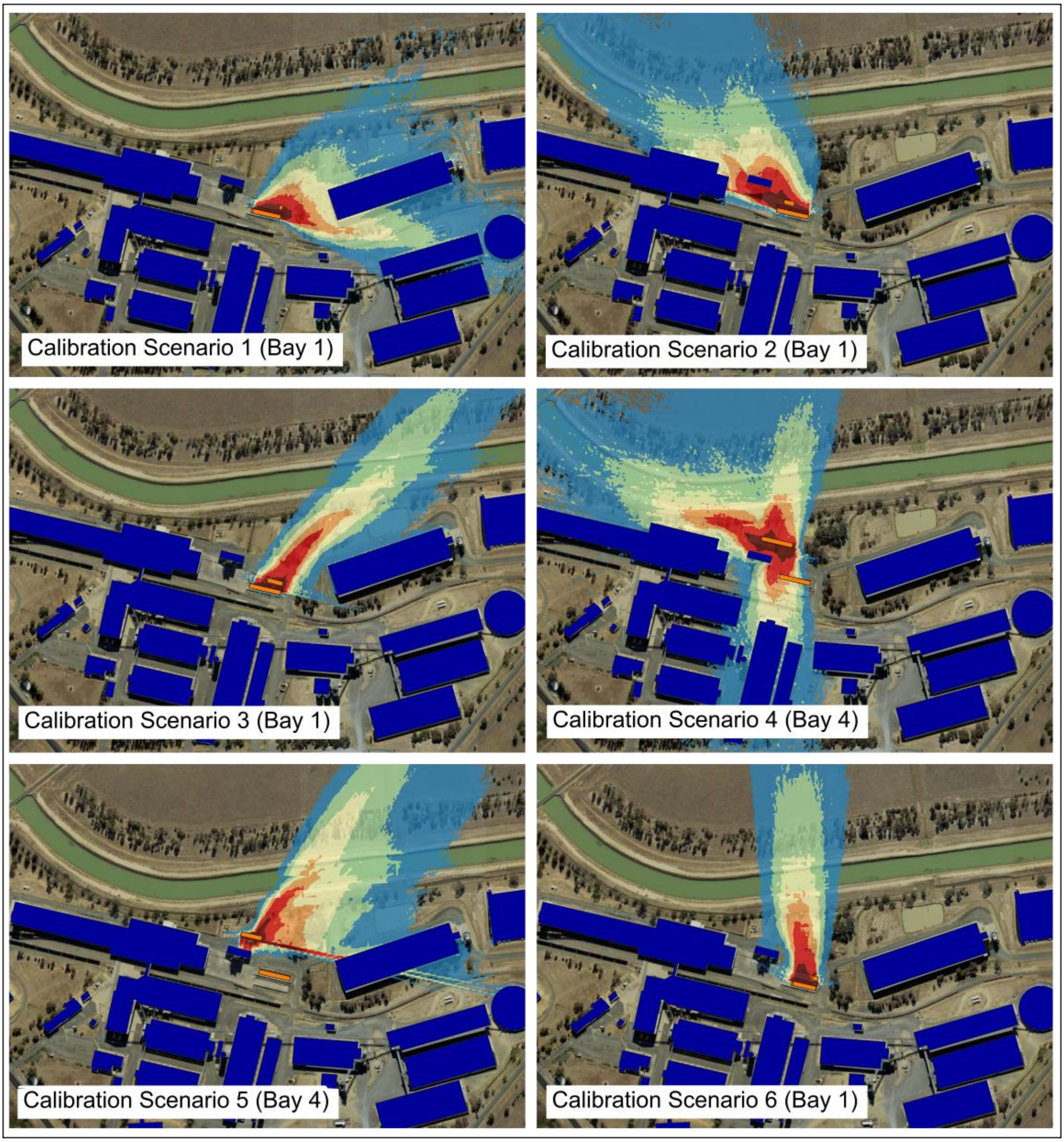

Figure A1. Concentration Plots (Heat Map) for Calibration Scenarios

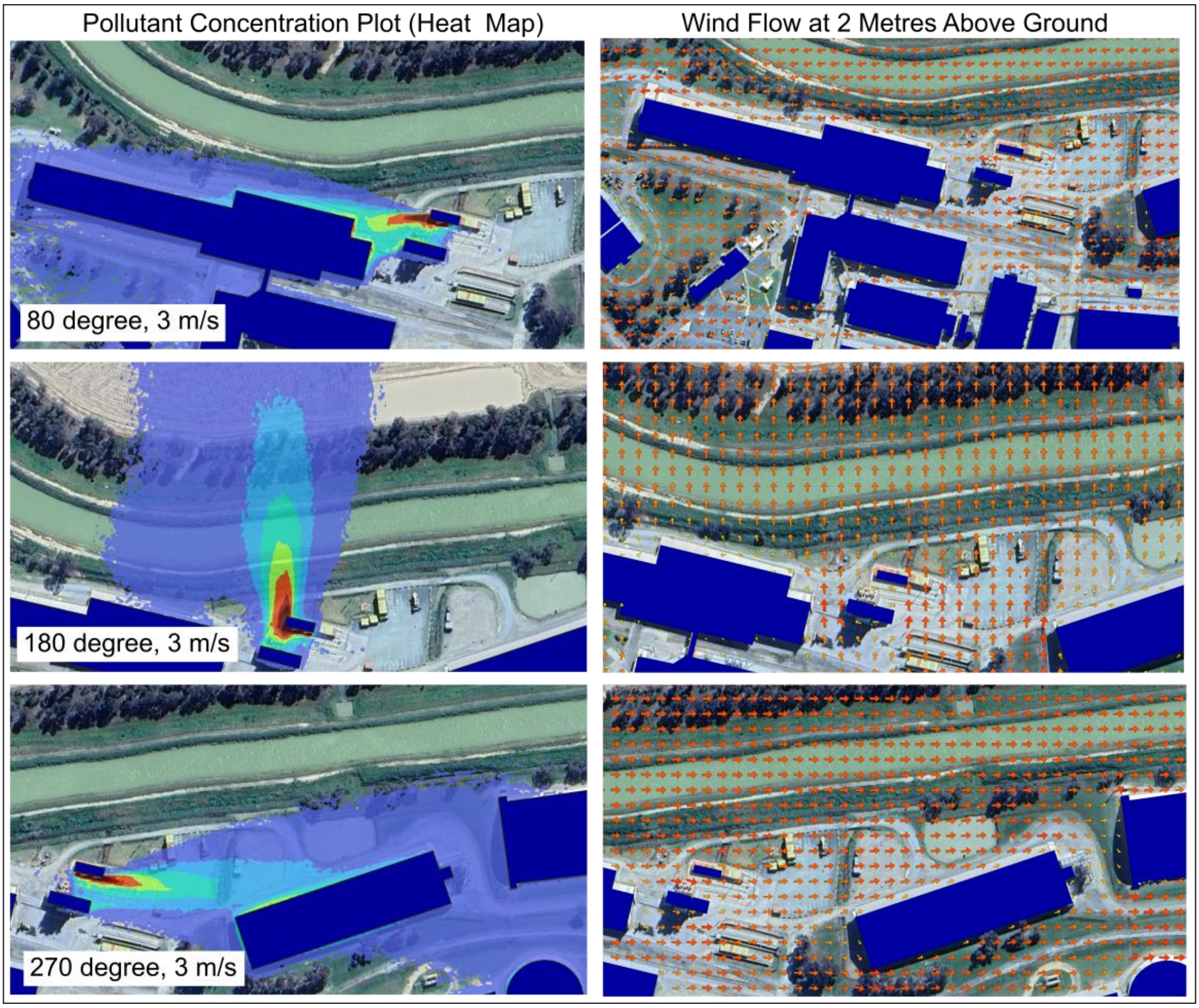

Figure A2. Concentration Plots (Heat Map) and Wind Flows for Select Wind Conditions