Tiered Procedure for Estimating Ground-Level Ozone Impacts from Stationary Sources

ENVIRON

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Executive Summary

ENVIRON Australia Pty Ltd was commissioned to undertake a consultancy on behalf of the Office of Environment and Heritage (OEH) to evaluate ground-level ozone impacts associated with stationary sources within the NSW Greater Metropolitan Region (GMR).

The objective of the study is to develop a tiered ozone impact assessment procedure for estimating ground-level ozone impacts from stationary sources of oxides of nitrogen (NO_X) and /or volatile organic compounds (VOC).

The scope of the study includes three key components, namely:

Part 1: Develop the analysis methodology, including a detailed literature review;

Part 2: Conduct analysis and develop analysis tools; and

Part 3: Document the tiered procedure.

Overview of Ozone Precursor Licence Requirements

The literature review of licence requirements for stationary sources of ozone precursors in OECD member countries concentrates on current licensing requirements within the United States (US) and Europe Union (EU), as the regulation of ozone precursors from stationary sources has been implemented principally in these jurisdictions.

In the US, regulatory requirements differ for stationary sources that satisfy national ambient air quality standards (NAAQS) for ozone (“attainment areas”) compared with those that do not (“non-attainment areas”). Similarly, regulatory requirements differ for existing stationary sources compared with those being newly constructed or modified. The level of control technology required depends on the ambient ozone concentrations within the receiving environment relative to the NAAQS for ozone.

Given that demonstrating best practice control technologies is emphasised within the US permitting process, modelling of the photochemical transformation associated with ozone precursors is not an explicit requirement.

The EU has a similar approach for permitting major sources of ozone precursors. This approach requires that facilities adopt Best Available Techniques (BAT) as prescribed within the EU BAT Reference documents (BREFs). The recent EU Industrial Emissions Directive makes the use of BREFs effectively mandatory. The BREFs provide information on the emissions achievable with BAT, often as a range of emissions. The Industrial Emissions Directive requires these should be used to set emission limits in the facility operating permit.

The EU uses organic solvent thresholds for different industries and processes to determine whether or not the emissions from stationary sources are controlled. Each installation has to comply with industry-specific emission limit values or alternatively, industry can use a reduction scheme, that is, use substitute products with no or minimal organic solvents content.

The literature review has not identified ozone concentration increments for the evaluation of impacts associated with new or modified stationary sources.

While ozone concentration increments (i.e. Prevention of Significant Deterioration (PSD) increments) are not used in the US, the relationship between PSD increments and NAAQS for other air pollutants may be used as a guide for developing them. For short-term (i.e. 24-hour or less) averaging periods, the PSD increment for a given pollutant is generally between 1% and 6% of the NAAQS. If this relationship is applied to *National Environment Protection (Ambient Air Quality) Measure* (Air NEPM) standards for ground-level ozone, PSD increments of between 1 and 6 ppb (expressed as a 1-hour average) and between 1 and 5 ppb (expressed as a 4-hour average) would apply.

The ground-level ozone PSD increments of between 1 and 6 ppb are consistent with US modelling practice. When the USEPA evaluated ozone transport between States for the Clean Air Interstate Rule, ozone transport contributions associated with a 2 ppb increment in daily maximum 8-hour ozone were considered insignificant.

In this study, an incremental increase of greater than or equal to 1 ppb ozone (expressed as either a 1-hour or 4-hour average) has been selected as the level which represents a significant increase in ground-level ozone. This metric has been selected on the basis of the rationale detailed above, and that the 1 ppb concentration represents a measurable change using conventional ambient monitoring instrumentation.

Overview of Ozone Screening Procedures

The use of the Scheffe Tables represents the only known applicable screening procedure used for the evaluation of ozone impacts from stationary sources.

However, the Scheffe Tables have been deemed by their author as technically unsound because the plume model used to derive these tables could not adequately resolve the non-linear chemical relationships between secondary ozone and the primary ozone precursor emissions.

Notwithstanding the above, it is noted the Scheffe Tables are still referenced in the air quality impact assessment guidance of several jurisdictions in the US, including Oklahoma and City of Albuquerque.

Overview of Photochemical Mechanisms

Seven chemical mechanisms for modelling tropospheric ozone and smog have been reviewed, namely: CB4, CB05, S99, S07B, CS07A, CRI v2-R5 and MELCHIOR2. Key attributes of each mechanism have been documented. Use of any of these mechanisms for modelling tropospheric ozone in Australia are justified because all mechanisms have been peer-reviewed and/or used in peer-reviewed ozone modelling studies.

- The mechanisms reviewed may be ordered from most compact to least compact as follows: CB4, MELCHIOR2, CS07A, CB05, S99, S07B and CRI v2-R5.

- The CB4 mechanism has been superseded, and largely replaced, by CB05. CB05 should be used rather than CB4 whenever possible.

- The S07B mechanism has superseded S99 but has yet to be used in regional modelling studies. In addition, S07B is a larger mechanism than S99 and will demand more computational resources than S99. Continued use of S99 is appropriate until the impacts of changing to S07B have been tested and evaluated.

- The CS07A and CRI v2-R5 mechanisms have not yet been used in urban/regional ozone modelling studies and, if used, they should be compared to other mechanisms.

- The MELCHIOR2 mechanism is expected to be computationally efficient and it has been used extensively in one air quality model (i.e. CHIMERE). Using MELCHIOR2 is reasonable but comparison with other current mechanisms (e.g. CB05 and S99) would be useful.

- The LCC mechanism was not reviewed because documentation was not available. LCC dates from the 1980s and it is a predecessor to the SAPRC mechanisms (i.e. S99, S07B and CS07A). If the LCC mechanism is used, it should be compared to more current mechanisms (e.g. CB05 and S99) and if results are different a scientifically defensible explanation should be developed.

Overview of Photochemical Models

A summary of the key features of the following models has been documented:

- CAMx;

- CMAQ;

- CHIMERE;

- TAPM/TAPM-CTM; and

- CIT.

The CAMx and CMAQ models account for virtually all of the ozone assessment modelling currently performed in the US. The CIT and TAPM models are relevant because they are used in Australia. The CHIMERE model is probably the most widely used photochemical model that has been developed in Europe.

Although, there are some important differences among the models listed above, they also share some common features. For example, all these models are source-oriented, Eulerian models that represent the atmosphere as a three-dimensional fixed grid, and simulate the transport, transformation and removal of air pollutants by solving the conservation of mass equation for this grid.

All the models incorporate atmospheric chemistry modules to describe the conversion of emitted pollutants to secondary pollutants such as ozone. The above models are also referred to as “third-generation” chemical transport models.

The differences among the models are in the models:

- Representation of the governing processes, such as transport, chemistry and removal;
- Numerical solution of the transport and chemistry equations;
- Meteorological inputs;
- Grid configurations; and
- Ancillary capabilities such as source attribution, grid-nesting, and resolution of point source plumes.

Analysis and Development of Level 1 – Screening Procedure

The Level 1 screening procedure has been developed from CAMx simulations for the GMR. Simulations have been performed for two ozone seasons (i.e. December 2003 and January 2004; and December 2004 and January 2005) with and without new sources added to identify days on which the new sources have high ozone impacts. The days have been selected on the basis of enhanced ozone in the GMR and a demonstration of acceptable model performance. The selected high ozone impact days have then been used for CAMx simulations with the higher order Decoupled Direct Method (HDDM) used to calculate sensitivity coefficients of ozone to the additional NO_X and VOC emissions from a new source. These ozone sensitivity coefficients enable ozone impacts to be estimated for any new source of NO_X and/or VOC emissions within the GMR.

The CAMx modelling uses meteorological and emission inventory data provided by OEH, and supplemented by additional data derived by ENVIRON (e.g. date-specific biogenic emissions and model boundary conditions) as required.

The Level 1 screening procedure tool can estimate increases in 1-hour and 4-hour ozone for new sources of NO_X and/or VOC emissions within the GMR. Five source locations are included within the tool, including West Sydney, Central Sydney, East Sydney, Newcastle and Wollongong.

VOC emissions can be specified either as total VOC for screening purposes only, in which case default VOC composition is used, or as source-specific VOC, in which case source-specific VOC composition is used. Source-specific VOC emissions data is required to meet OEH requirements. If non-default VOC emissions are provided, ozone impacts are adjusted for VOC reactivity by using reactivity factors calculated specifically for each source location.

The Level 1 screening procedure tool is applicable for assessing the impact of sources with emissions of up to 5,500 tonnes/annum of NO_X and/or 7,000 tonnes/annum of VOC (using the default VOC composition). If source-specific VOC composition is used, the tool estimates the reactivity-weighted VOC emissions and compares them to the reactivity-weighted VOC emissions using the default composition. If source emissions exceed the upper bound emission rate range of the tool, a Level 2 refined procedure may be required.

Analysis and Development of Level 2 – Refined Procedure

A Level 2 refined procedure case study has been performed to demonstrate OEH expectations for this form of assessment. This case study is not intended to be prescriptive of the approach or models to be adopted. The Level 2 refined procedure uses the model inputs developed for the Level 1 screening procedure. Two CAMx runs have been performed, with and without the new source emissions, to directly assess the ozone impact of the new source.

The Level 2 refined procedure is closely related to the Level 1 screening procedure to provide consistent evaluations of new source ozone impacts. The intent of directly modelling the source using the Level 2 refined procedure is to eliminate any uncertainties attributable to the parameterisation of model results using the Level 1 screening procedure tool.

The modelling performed using the Level 2 refined procedure should not be less detailed than the modelling used to develop the Level 1 screening procedure tool. One option is the Level 2 refined procedure can use the modelling databases used to develop the Level 1 screening procedure tool.

The same criteria should be used to evaluate the significance of new source ozone impacts for the Level 1 and Level 2 procedures. The criteria are detailed below.

Framework for Ozone Impact Assessment

The ozone impact assessment is intended for those “scheduled” activities listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* which emit ozone precursors and are located or proposed to be located within the Greater Metropolitan Area (GMA) as defined within the *Protection of the Environment Operations (Clean Air) Regulation 2010*.

A stationary source refers to a premises undertaking “scheduled” activities listed in Schedule 1 of the *Protection of the Environment Operations Act 1997*, and may comprise one or more emission units. As defined within the *Protection of the Environment Operations (Clean Air) Regulation* 2010, an emission unit means an item of plant that forms part of, or is attached to, some larger plant, being an item of plant that emits, treats or processes air impurities or controls the discharge of air impurities into the atmosphere.

The ozone impact assessment procedure is illustrated by means of a flowchart in **Figure 1** and briefly described in subsequent subsections.

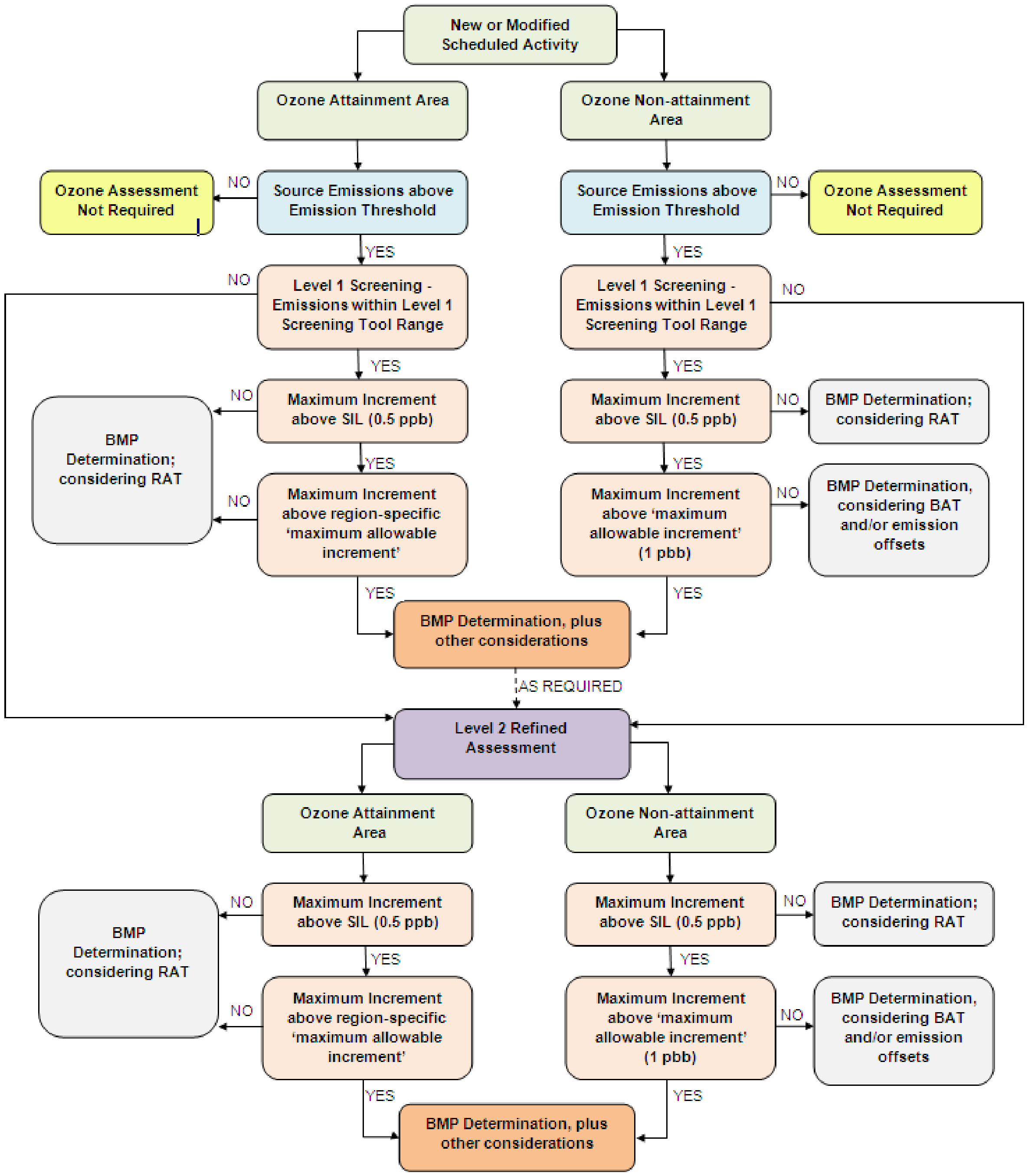

Figure 1: Ozone impact assessment procedure for new or modified scheduled activities located within the NSW GMA

Classification of Region as Ozone Attainment or Non-attainment Area

The initial step involves the classification of the region within which the source is to be located as either an ozone "attainment area" or "non-attainment area".

In determining whether an area is classifiable as an ozone attainment or non-attainment area, reference should be made to measured ambient ozone concentrations from Office of Environment and Heritage (OEH) ambient air quality monitoring stations which have been recorded over the past 5 years.

The maximum 1-hour and 4-hour average ozone concentrations recorded over the most current 5 year period should be averaged to obtain the 5-year average 1-hour and 4-hour maximum ozone concentrations for each monitoring station. Reference should then be made to the highest 5-year average maximums recorded across monitoring stations in the region within which the source is located.

The 5-year average 1-hour and 4-hour maximums for the source region should be compared to the screening procedure acceptance limits for ozone, expressed as 82% of the Air NEPM Standard(1).

Areas where the 5-year average 1-hour maximum ozone concentration is greater than 0.082 ppm, and/or where the 5-year average 4-hour maximum ozone concentration is greater than 0.0656 ppm, are classified as non-attainment areas. Similarly, areas where the 5-year average 1-hour maximum ozone concentration is less than 0.082 ppm, and/or where the 5-year average 4-hour maximum ozone concentration is less than 0.0656 ppm, are classified as attainment areas.

The Level 1 screening procedure tool contains measured ozone concentrations for the 2006-2010 period for three regions, including Sydney, Illawarra and Lower Hunter. Each region is classified as an ozone attainment or non-attainment area using the Air NEPM screening procedure acceptance limits. The results are presented in **Table 1**.

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1 *NEPC (Ambient Air Quality) Measure Technical Paper No. 4, Revision 1 – January 2007, Screening Procedures.*

Table 1: Classification of Regions based on Maximum 5-year average Ozone Concentrations recorded at OEH Stations during 2006-2010

Station	Maximum 5-year average 1-hour Ozone Concentration (ppb)	Air NEPM Ozone Standard (ppb)	Difference between Standard and Ambient (ppb)	25% of Residual	Region Classification
Sydney	116.8	100	-16.8	NA(a)	Non-attainment
Illawarra	89.0	100	11.0	NA(a)	Non-attainment
Lower Hunter	78.4	100	21.6	5.4	Attainment
Station	**Maximum 5-year average 4-hour Ozone Concentration (ppb)**	**Air NEPM Ozone Standard (ppb)**	**Difference between Standard and Ambient (ppb)**	**25% of Residual**	**Region Classification**
Sydney	98.2	80	-18.2	NA(a)	Non-attainment
Illawarra	79.4	80	0.6	NA(a)	Non-attainment
Lower Hunter	71.6	80	8.4	NA(a)	Non-attainment

(a) Maximum allowable increment specified as 1 ppb for ozone non-attainment areas.

Evaluate Source Emissions based on Emission Thresholds

The second step in the procedure involves the evaluation of the source's emissions against the new or modified source thresholds for NO_x and VOC emissions, as specified in **Table 2** for sources within ozone attainment areas and in **Table 3** for sources within ozone non-attainment areas.

Total emissions from the new or modified source, from all individual emission units, should be compared to the emission thresholds.

For a source with emissions below the relevant emission threshold, an ozone impact assessment is not required but the source should assess air quality impacts for other air pollutants as required by the *Approved Methods for the Modelling and Assessment of Air Pollutants in NSW* (DEC, 2005).

Where source emissions are above the relevant emission threshold, a Level 1 assessment should be undertaken using the Level 1 screening procedure tool. In the event the source emissions exceed the upper emission range of the tool, a Level 2 assessment may be required.

Table 2: NO_X and VOC Emission Thresholds for New or Modified Sources within Ozone Attainment Areas

Source Type	**NO_X / VOC Emission Rate tonnes/year**
New Source	
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997*	>90
Modified Source	
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997*	>35

Table 3: NO_X and VOC Emission Thresholds for New or Modified Sources within Ozone Non-attainment Areas

Source Type	**NO_X / VOC Emission Rate tonnes/year**
New Source	
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in all Other Areas	>90
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in Serious Ozone Non-attainment Area (Area has a 5-year average 1-hour maximum ozone concentration in the range of 0.13 to 0.15 ppm, and/or a 5-year average 4-hour maximum ozone concentration in the range of 0.11 to 0.12 ppm.)	>45
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in Severe Ozone Non-attainment Area (Area has a 5-year average 1-hour maximum ozone concentration in the range of 0.15 to 0.23 ppm, and/or a 5-year average 4-hour maximum ozone concentration in the range of 0.12 to 0.19 ppm.)	>25
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in Extreme Ozone Non-attainment Area (Area has a 5-year average 1-hour maximum ozone concentration in the range of 0.23 ppm and above, and/or a 5-year average 4-hour maximum ozone concentration in the range of 0.19 ppm and above.)	>10
Modified Source	
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in all Other Areas	>35
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in Serious or Severe Ozone Non-attainment Area	>25
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in Extreme Ozone Non-attainment Area	Any Increase

Evaluating the Significance of Level 1 Screening or Level 2 Refined Procedure Results

To evaluate the significance of emissions from a source and its impact on ground-level ozone in the GMR, the results of the Level 1 screening procedure should be compared to recent ambient monitoring data for ozone in the GMR. Comparisons should not be restricted to the ozone monitor nearest to the source because ozone impacts occur downwind of the source at locations that vary from day to day. Comparisons within the subregion (i.e. Sydney, Illawarra/Wollongong and Lower Hunter/Newcastle) containing the source are appropriate. Comparing the source impacts to ozone in other subregions would also be appropriate if that subregion is considered to be downwind of the source on high ozone days.

Criteria for determining the significance of predicted incremental increase in ambient ozone concentrations comprise primarily the following:

- Evaluation of sources located within ozone attainment areas against a screening impact level (SIL) of 0.5 ppb and against the maximum allowable increment for each region.
- Evaluation of sources located within ozone non-attainment areas against a SIL of 0.5 ppb and against the maximum allowable increment of 1 ppb.

In cases where the maximum ozone increment is below the SIL and/or below the relevant maximum allowable increment, further ozone impact assessment is not required but a best management practice (BMP) determination should be undertaken for the source.

In the event the impacts are greater than the maximum allowable increment, the EPA may consider the impact of the source on local and regional air quality having regard to the following matters:

i. The outcomes of the BMP determination;

ii. The frequency and duration of ground-level ozone impacts;

iii. Any pollution reduction programs established or agreed to;

iv. Any control equipment installed or agreed to;

v. Any load reduction agreement entered; and

vi. The principles of ecologically sustainable development.

The EPA may require that a Level 2 refined assessment be undertaken for the source at any time or the licensee may choose to conduct a Level 2 refined assessment rather than 1 Level 1 screening assessment. In this event, results from the Level 2 refined assessment should be compared to the relevant SIL and maximum allowable increment as required for the Level 1 screening assessment.

1. Introduction

ENVIRON Australia Pty Ltd was commissioned to undertake a consultancy on behalf of the Office of Environment and Heritage (OEH) to evaluate ground-level ozone impacts associated with stationary sources within the NSW Greater Metropolitan Region (GMR).

A stationary source refers to a premises undertaking “scheduled” activities listed in Schedule 1 of the *Protection of the Environment Operations Act 1997*, and may comprise one or more emission units. As defined within the *Protection of the Environment Operations (Clean Air) Regulation* 2010, an emission unit means an item of plant that forms part of, or is attached to, some larger plant, being an item of plant that emits, treats or processes air impurities or controls the discharge of air impurities into the atmosphere.

1.1 Study Context

The *Approved Methods for the Modelling and Assessment of Air Pollutants in NSW* (“Approved Methods for Modelling”; DEC, 2005) does not currently contain a documented procedure for predicting impacts associated with the release of precursors of ozone, primarily oxides of nitrogen (NO_X) and volatile organic compounds (VOC).

Above all, the study seeks to develop and document a tiered approach to ozone impact assessment for stationary sources of NO_X and/or VOC in NSW.

The assessment procedure which has been developed is consistent with the Level 1 and 2 philosophy contained within the Approved Methods for Modelling.

Ozone concentrations in the Sydney region have exceeded either or both of the Air NEPM ozone standards every year since 1994 (DECCW, 2010a). The number of days when the 1-hour standard was exceeded in Sydney ranged from none in 1995 to 19 in 2001. Concentrations can be as high as double the Air NEPM standards.

Ozone exceedences are less frequent in the Illawarra, occurring on up to 7 days a year. The lower Hunter region has recorded only two exceedences of the 1-hour standard since 1999.

Presently, the *Protection of Environment Operations (Clean Air) Regulation 2010* (“Clean Air Regulation”) contains minimum performance standards for both NO_X and VOC. However, these values are generic and do not relate to the sensitivity of the receiving airshed.

Additionally, the Approved Methods for Modelling does not currently contain a procedure for predicting the impacts associated with ozone precursors.

This study addresses the potential need for additional, location-specific stationary source controls, combined with scientifically defensible methods to efficiently assess which sources will have a significant impact.

Ultimately, the aim of developing a tiered ozone impact assessment procedure is to provide direction about:

- When an ozone impact assessment needs to be conducted;

- Whether an ozone impact assessment is considered to be technically robust; and/or
- The extent to which additional ozone precursor controls are required at the proposal stage.

Efficient methods for determining these outcomes are required to ensure that the development application process is conducted in a timely, transparent and scientifically rigorous manner.

1.2 Study Objective

The objective of the study is to develop a tiered ozone impact assessment procedure for estimating ground-level ozone impacts from stationary sources that emit precursor emissions of carbon monoxide (CO), methane (CH_4), NO_X and VOC.

In line with the Clean Air Regulation, VOC means any chemical that:

(a) Is based on carbon chains or rings, and

(b) Contains hydrogen, and

(c) Has a vapour pressure greater than 0.27 kPa at 25°C and 101.3 kPa, and

include any such compound containing oxygen, nitrogen or other elements, but does not include methane, carbon monoxide, carbon dioxide, carbonic acid, metallic carbides and carbonate salts.

1.3 Scope of Study

The scope of the study which reflects the Technical Brief issued by OEH, as provided in **Appendix 1**, includes three key components. These components and their respective tasks are as follows:

Part 1: Develop the analysis methodology

Task 1.1: Conduct a literature review of licence requirements for stationary sources of ozone precursors with particular emphasis on best available technology and air quality impact assessment definitions and requirements in OECD member countries, new source review (NSR) requirements implemented by USEPA and permitting guidance developed in various states in the US;

Task 1.2: Conduct a literature review of screening procedures for estimating ground-level ozone impacts from stationary sources of ozone precursors. Discuss the merits and drawbacks of each procedure, data requirements, its ease of use and any practical limitations of applying it in NSW.

Task 1.3: Conduct a literature review of photochemical mechanisms for estimating ground-level ozone impacts from stationary sources of ozone precursors. Discuss the merits and drawbacks of each mechanism, data requirements, its ease of use and any practical limitations of applying it in NSW.

Task 1.4: Conduct a literature review of photochemical models for estimating ground-level ozone impacts from stationary sources of ozone precursors. Discuss the merits and drawbacks of each model, data requirements, its ease of use and any practical limitations of applying it in NSW.

Task 1.5: Using the outcomes of the literature review, document the methodology for developing a Level 1 - screening procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors, including the photochemical mechanism and photochemical model that will be used.

Task 1.6: Using the outcomes of the literature review, document the methodology for developing a Level 2 - refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors, including the photochemical mechanism(s) and photochemical model(s) that will be used.

Part 2: Conduct analysis and develop analysis tools

Task 2.1: Conduct analysis and develop a Level 1 screening procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors; and

Task 2.2: Conduct analysis and develop a Level 2 refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors.

Part 3: Document the tiered procedure

Task 3.1: Develop detailed guidance for inclusion in the *Approved Methods for Modelling* for Level 1 – screening procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors; and

Task 3.2: Develop detailed guidance for inclusion in the *Approved Methods for Modelling* for Level 2 – refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors.

1.4 Report Outline

The findings from the literature review are documented in **Section 2**.

An overview of the analysis and development of the Level 1 screening procedure and the Level 2 refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors are documented in **Section 3** and **Section 4**, respectively.

The framework for ozone impact assessments and guidance on the Level 1 screening procedure and the Level 2 refined procedure is provided in **Section 5**.

2. Literature Review

2.1 Literature Review of Ozone Precursor Licence Requirements

This section documents licence requirements for stationary sources of ozone precursors in OECD member countries. The literature review concentrates on current licensing requirements within the United States (US) and European Union (EU), as the regulation of ozone precursors from stationary sources has been implemented principally in these jurisdictions.

2.1.1 United States

The following provides a summary of licence requirements for ozone precursors in the US as they relate to Prevention of Significant Deterioration (PSD, www.epa.gov/NSR/psd.html), New Source Review (NSR, www.epa.gov/nsr/index.html) and Minor Source Permits.

2.1.1.1 Basic Concepts

Areas in the US not meeting the National Ambient Air Quality Standards (NAAQS, www.epa.gov/air/criteria.html) are called “non-attainment areas”. NAAQS are reviewed regularly and updated periodically. Designations of “non-attainment areas” for ozone are listed at: www.epa.gov/ozonedesignations/.

Permitting and regulatory requirements differ for stationary sources in either “attainment” or “non-attainment areas”.

Permitting and regulatory requirements differ for existing stationary sources and sources being newly constructed or modified.

2.1.1.2 Existing Sources in Ozone Attainment Areas

In general, there are no Federal requirements specific to ozone that States would be obliged to impose on existing sources in ozone “attainment areas”.

However, there could be general emission standards in State rules along with Federal emissions standards that would apply to existing sources that were built or modified after specific dates (e.g. US New Source Performance Standards (NSPS)). These appear in the Code of Federal Regulations (CFR), at 40 CFR 60. For example, boilers above a certain size built or modified after a certain date (as far back as the late 1970s or early 1980s) might be obliged to limit their NO_X emission rate (expressed in terms of lb/MMBTU).

These have been established over time to represent reasonably available control technology (RACT) without being directly driven by achieving a specific ozone air quality goal.

2.1.1.3 New or Modified Sources in Ozone Attainment Areas

The construction or modification of sources of ozone precursors would be subject to Federal New Source Review (NSR) requirements (though implemented by the States) in areas meeting the ozone NAAQS under what is referred to as the Prevention of Significant Deterioration (PSD) program.

These Regulations are documented at 40 CFR 52.21 and 40 CFR 51.166. The PSD program is complicated in its implementation, but the concept is simple. As evidenced by its name, the purpose is to make sure that air quality in areas meeting the ambient standards does not “significantly deteriorate” all the way up to the NAAQS concentration levels.

The PSD program is applicable to any facility that in aggregate has potential emissions of any one pollutant (whether particulate matter, sulfur dioxide, NO_X, etc.) above 250 (US) tons/year, or 100 tons/year for certain specified industries (such as petroleum refineries, fossil fuel fired power plants, metal smelters, cement plants, etc.). These facilities are called “major sources.”

If a major source wishes to add a unit or make modifications that would result in a “significant increase” in ozone precursors (defined as more than 40 tons/year of increase in either NO_X or VOC), the PSD requirements would have to be met. These include installation of Best Available Control Technology (BACT) for pollutants being “significantly” increased.

A summary of the NO_X and VOC emissions that define a major source, as well as the definition of a major modification to a source, is provided within **Table 4**.

Table 4: NO_X and VOC Emissions Defining Major Sources and Major Modifications under the PSD Program

Industry	NO_X / VOC Emission Rate (US) tons/year
Major Source	
Fossil fuel-fired steam electric plants of more than 250 million British thermal units per hour heat input, coal cleaning plants (with thermal dryers), kraft pulp mills, portland cement plants, primary zinc smelters, iron and steel mill plants, primary aluminum ore reduction plants (with thermal dryers), primary copper smelters, municipal incinerators capable of charging more than 250 tons of refuse per day, hydrofluoric, sulfuric, and nitric acid plants, petroleum refineries, lime plants, phosphate rock processing plants, coke oven batteries, sulfur recovery plants, carbon black plants (furnace process), primary lead smelters, fuel conversion plants, sintering plants, secondary metal production plants, chemical process plants (which does not include ethanol production facilities that produce ethanol by natural fermentation included in NAICS codes 325193 or 312140), fossil-fuel boilers (or combinations thereof) totalling more than 250 million British thermal units per hour heat input, petroleum storage and transfer units with a total storage capacity exceeding 300,000 barrels, taconite ore processing plants, glass fibre processing plants, and charcoal production plants	>100
All Other Industries	>250

Table 4: NO_X and VOC Emissions Defining Major Sources and Major Modifications under the PSD Program

Industry	NO_X / VOC Emission Rate
Major Modification	
All Industries	>40

Source: 40 CFR 52.21 http://frwebgate.access.gpo.gov/cgi-bin/get-cfr.cgi?TITLE=40&PART=52&SECTION=21&TYPE=PDF

In general, there is no requirement to model the photochemical transformations from ozone precursors in the PSD process, but a general demonstration would have to be made that, after the installation of BACT, the ambient air quality in the area can bear the increase in emissions.

A PSD increment is the maximum allowable increase in concentration that is allowed to occur above a baseline concentration for a given pollutant. The baseline concentration is defined for each pollutant and, in general, is the ambient concentration existing at the time that the first complete PSD permit application affecting the area is submitted. Significant deterioration is said to occur when the amount of new pollution would exceed the applicable PSD increment.

The relationships between NAAQS values (the maximum allowable concentration "ceiling") and their corresponding PSD increments are shown in **Table 5**.

The PSD Area Classes shown in **Table 5** are defined within the Clean Air Act. Class I Areas are defined as national parks (over 6,000 acres), wilderness areas (over 5,000 acres), national memorial parks (over 5,000 acres), and international parks that were in existence as of August 1977. Class I PSD areas have increments of permissible deterioration so low as to effectively preclude growth. Class II PSD areas are designated to allow moderate, controlled growth. This includes virtually all non-Class I areas. Currently, there are no Class III areas that allow a large amount of degradation to the air quality (http://www.nature.nps.gov/air/regs/psd.cfm).

Table 5: Relationship between NAAQS Values and PSD Increments

Pollutant	Averaging Period	NAAQS Value (µg/m^3)	PSD Increment by Area Class			PSD Increment as % of NAAQS		
			Class I	Class II	Class III	Class I	Class II	Class III
$PM_{2.5}$	Annual	15	1	4	8	7%	27%	53%
	24-hour	35	2	9	18	6%	26%	51%
PM_{10}	Annual	N/A	4	17	34	N/A	N/A	N/A
	24-hour	150	8	30	60	5%	20%	40%
SO_2	Annual	92	2	20	40	2%	22%	43%
	24-hour	367	5	91	182	1%	25%	50%
	3-hour	N/A	25	512	700	N/A	N/A	N/A
NO_2	Annual	100	2.5	25	50	3%	25%	50%

The information in **Table 5** is instructive as it shows the amount of pollution an area is allowed to increase (i.e. the PSD increment) as a percentage of the corresponding NAAQS "ceiling". While PSD increments are not used for ozone concentrations, such a relationship may be used as a guide for developing ozone increments deemed to have a significant impact.

It is acknowledged, however, that PSD is designed to manage individual impacts when ambient concentrations remain below national ambient air quality standards. If a standard is currently exceeded, there is no margin available and a new source must purchase emission offsets.

In California, there is a requirement for local air quality management districts / air pollution control districts to collect information about the cost of offset transactions from stationary source owners who purchase offsets as required by district New Source Review programs. State law also requires districts to adopt emission reduction credit banking programs. Districts are required to collect specific information about offset transactions including the price paid in dollars per ton, the pollutant traded, the amount traded and the year of the transaction.

The Air Resources Board (ARB) has compiled the information regarding offset transactions from all 35 districts to assemble a statewide report summarising the emission reduction offset transactions in California from 1993 through the present (CARB, 2011).

2.1.1.4 Existing Sources in Ozone Non-Attainment Areas

When an area is designated to be "non-attainment" with respect to the ozone NAAQS, the State is required to develop and implement a State Implementation Plan (SIP, http://www.epa.gov/reg5oair/sips/), to bring the area back into "attainment". Regulations governing SIP development are located at 40 CFR 51.

The State will generally select and implement a mix of measures to impose on both mobile and stationary sources. This selection is informed by photochemical dispersion modelling considering the NO_X and VOC emissions from all man-made and natural sources in the area as well as potentially from regions upwind of the area.

In general, mobile source emission standards are outside State jurisdiction and SIP measures are limited to requirements for regular vehicle emission inspections, incentive programs to replace or retrofit older vehicles/equipment, or transportation planning measures such as addition of carpool lanes on major highways. The effects of those measures are evaluated in the modelling and determinations are made about how much additional emission reduction is needed from existing stationary sources.

The State then issues emission standards constituting Reasonably Available Control Technology (RACT) on existing stationary sources in the non-attainment area. RACT measures are less stringent in nature than BACT measures. Typical measures include limiting the VOC content of paint used in production processes, requiring covers on mixing tanks, emissions limits on NO_X from combustion processes consistent with good combustion performance, etc. Sources in the non-attainment area would then have to comply with those RACT emission limits and standards.

RACT rules are issued on a state-by-state basis, and can apply to existing sources and may be specific down to a county basis. For example, the South Coast Air Quality Management District (SCAQMD, the air pollution control agency for all of Orange County and the urban portions of Los Angeles, Riverside and San Bernardino counties) specifies Regulation XI. This provides the SIP-approved rules for existing sources in Southern California (the highest ozone concentrations in the US). Individual regulations exist for a variety of ozone precursor sources. For example, Rule 1125 gives standards for VOC limitation from coil coating operations, while Rule 1195 specifies requirements for replacement of school buses with alternative-fuelled vehicles (SCAQMD, 2011a). Additionally, air quality rules for the State of Georgia specify rules (e.g. for VOC emissions from bulk mixing tanks / offset lithography) which apply only in specific counties (Georgia DNR, 2010). Those counties are in the Atlanta metropolitan area and are ozone non-attainment areas.

2.1.1.5 New or Modified Sources in Ozone Non-Attainment Areas

The most stringent requirements apply to those seeking to build new sources or increase emissions of ozone precursors in "non-attainment areas". Much like the PSD program, Federal requirements for "non-attainment" New Source Review (NSR) apply to major sources (those emitting more than 100 (US) tons/year of any one pollutant) seeking a significant increase (more than 40 tons/year of NO_X or VOC) in ozone precursors in an ozone non-attainment area (Rules at 40 CFR 51.165). Lower emission thresholds may apply in areas depending on the level of severity of the existing ozone concentrations.

A summary of the NO_X and VOC emission thresholds within different ozone non-attainment areas that define major sources / modifications is provided within **Table 6**.

Table 6: NO_X and VOC Emissions Defining Major Sources and Major Modifications within the Non-Attainment New Source Review [1]

Ozone Non-attainment Area	NO_X / VOC Emission Rate (US) tons/year
Major Stationary Source	
Serious Ozone Non-attainment Area (Area has a 1-hour ozone design value [2] of 0.160 up to 0.180 ppm [3])	>50
Area within an Ozone Transport Region (except for any Severe or Extreme Ozone Non-attainment Area)	>50
Severe Ozone Non-attainment Area (Area has a 1-hour ozone design value [2] of 0.180 up to 0.280 ppm [3])	>25
Extreme Ozone Non-attainment Area (Area has a 1-hour ozone design value [2] of 0.280 ppm and above [3])	>10
All Other Areas	>100
Major Modification	
Serious or Severe Ozone Non-attainment Area	>25
Extreme Ozone Non-attainment Area	Any Increase
All Other Areas	>40

Note 1: Source: 40 CFR 51.165 http://frwebgate.access.gpo.gov/cgi-bin/get-cfr.cgi?TITLE=40&PART=51&SECTION=165&TYPE=PDF
Note 2: For definition, refer **Section 2.1.1.7**.
Note 3: Source: http://www.epa.gov/oar/oaqps/greenbk/define.html#OzoneClassifications

If non-attainment NSR is triggered, the proposed sources must install emission controls consistent with Lowest Achievable Emission Rate (LAER – refer **Section 2.1.1.6**) performance and then find offsetting emission reductions from other existing sources in the area, often at a ratio greater than 1:1 on a mass basis (40 CFR 51.165 http://frwebgate.access.gpo.gov/cgi-bin/get-cfr.cgi?TITLE=40&PART=51&SECTION=165&TYPE=PDF).

Examples of specific rules implementing such a non-attainment NSR program can be found in the SCAQMD Regulation XIII (SCAQMD, 2011b). An example of how emissions trading can be implemented to allow sources to offset proposed emission growth can be found for the Georgia program for the Atlanta area (Georgia DNR, 2011) at: http://www.georgiaair.org/airpermit/html/erc/erc.htm

2.1.1.6 RACT/BACT/LAER Clearinghouse

Since 1977, US state and local air pollution control agencies have gradually assumed primary responsibility for implementing BACT and LAER. As this authority was decentralised, it became important that information be made available to control agencies to assist them in making control technology determinations in a nationally consistent manner.

The RACT/BACT/LAER Clearinghouse (RBLC, http://cfpub.epa.gov/RBLC/) is the primary vehicle for sharing control technology information in the form of a database of case-specific information on the best available air pollution technologies that have been required to reduce the emission of air pollutants from stationary sources. This information has been provided by state and local permitting agencies. The RBLC information system permits on-line querying of the database. It also supports direct submittals of control technology determinations by permitting agencies.

2.1.1.7 Use of Models to Demonstrate Attainment of Ozone Air Quality Goals

The USEPA has produced a key piece of documentation relevant to the present study, *Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, $PM_{2.5}$ and Regional Haze* (USEPA, 2007).

The purpose of this document is to provide guidance to air quality management authorities on how to prepare ozone (and $PM_{2.5}$) attainment demonstrations for the purposes of a State Implementation Plan (SIP) using air quality models and other technical analyses.

Key concepts of relevance to this study are:

- USEPA recommend that model estimates are used in a “relative” rather than an “absolute” sense. That is, the ratio of the model’s future to current (baseline) predictions at monitors is used. Such ratios are referred to as Relative Response Factors (RRFs).

- Future ozone concentrations are estimated at existing monitoring sites by multiplying a modelled RRF at locations “near” (approximately within 15 km) each monitor by the observation-based, monitor-specific “baseline” design value.

- The 8-hour ozone design value is calculated as the 3 year average of the fourth highest monitored daily 8-hour maximum value at each monitoring site.

- In unmonitored areas, interpolated spatial fields of ambient data are combined with gridded model outputs to create “gradient adjusted spatial fields”. USEPA has developed a software package called “Modeled Attainment Test Software” (MATS, Abt Associates, 2010) which will spatially interpolate monitoring data, adjust the spatial fields based on model output gradients, and multiply the fields by model calculated RRFs to determine “future concentrations” in unmonitored areas.

- Resulting predicted “future concentrations” are then compared to the NAAQS for 8-hour ozone.

2.1.1.8 State Based Permitting Guidance

Historically, the Scheffe Point Source Screening Tables (Scheffe Tables, discussed in more detail in **Section 2.2**) have been referenced by several US states in their guidance for ozone impact assessment. Previously, the Scheffe Tables were used to evaluate ozone impacts from sources emitting in excess of 100 (Imperial) tons of VOC annually (Oklahoma DEQ, 2008). Alternatively, other jurisdictions (City of Albuquerque, 2010) have required the Scheffe Tables to be used for facilities emitting up to 500 (US) tons per year.

The state of Oklahoma currently advises that until further guidance is published by USEPA, large sources of ozone precursors should be included in available photochemical modelling datasets and should be modelled using the Comprehensive Air Quality Model with extensions (CAMx) to assess impacts and demonstrate compliance with ozone standards. Permit applicants may be required to conduct extensive modelling using either CAMx, or the Community Multiscale Air Quality Modelling System (CMAQ) (Oklahoma DEQ, 2008). The use of these two gridded modelling systems is also referenced in other jurisdictions (City of Albuquerque, 2010).

2.1.2 European Union

The following summarises licence requirements pertaining to ozone precursors in European Union (EU) member countries.

2.1.2.1 Introduction

Industrial emissions in the 27 European Union (EU) Member States are controlled in an integrated manner, to prevent emissions into air, water or soil, wherever this is practicable, taking into account waste management, and, where it is not, to minimise them in order to achieve a high level of protection for the environment as a whole. It is integrated to ensure that measures to reduce emission to one medium do not adversely impact on another.

At the end of 2010 a new directive was adopted, the Industrial Emissions Directive (IED; 2010/75/EU; EPCEU, 2010), which came into force in January 2011. It consolidates seven existing Directives:

- Waste from the titanium dioxide industry (78/176/EEC; CEC 1978, 82/883/EEC; CEC 1982 and 92/112/EEC; CEC 1992);

- Solvents directive (1999/13/EC; CEU, 1999);

- Waste incineration directive (2000/76/EC; EPCEU, 2000);

- Large combustion plant directive (2001/80/EC; EPCEU, 2001); and
- Integrated pollution prevention and control (2008/1/EC; EPCEU, 2008).

The IED has to be transcribed into national legislation by January 2013, and will be reviewed every three years. The main reason for the new directive was that regulators were not applying Best Available Techniques (BAT) consistently across the EU. The IED regulates around 50,000 installations in the EU dealing with a wide range of industrial and agricultural activities.

The directive is divided into a series of chapters.

- Chapter 1 contains common provisions;
- Chapter 2 covers the activities previously in the IPPC Directives;
- Chapter 3 covers combustion plants;
- Chapter 4 covers waste incineration;
- Chapter 5 deals with the control of volatile organic compounds (VOC) from the use of organic solvents;
- Chapter 6 covers titanium dioxide; and
- Chapter 7 describes transitional arrangements.

The main text is supported by a series of Annexes:

Annex I	Sets out the industrial and agricultural activities to which IPPC applies. It covers energy, production and processing of metals, mineral industry, chemical industry, waste management, pulp production, and paper and board production, pre-treatment of dyeing of fibres, tanning, slaughterhouses, and disposal of animal carcasses, various food processes and intensive poultry and pig rearing installations.
Annex II	Provides a list of polluting substances for each media.
Annex III	Provides criteria for determining BAT.
Annex IV	Discusses the requirement for public involvement in the decision making.
Annexes V and VI	Give the technical specifications for combustion plants and waste incineration, respectively, including emission limits and monitoring requirements.
Annex VII	Gives technical specifications for installations producing titanium dioxide.

Annex VII	Lists the activities to which the control of organic solvents applies, and includes thresholds for the use of the materials and emission limits.

2.1.2.2 BAT Requirements

Member states have been using the EU BAT Reference documents (BREFs) (http://eippcb.jrc.ec.europa.eu/reference/) in different ways, often as guidance rather than a requirement. The IED makes their use effectively mandatory. If they are not used, the regulator needs to justify why not to the public.

The BREFs provide information on the emissions achievable with BAT, often as a range of emissions, and the Industrial Emissions Directive requires these should be used to set emission limits in the facility operating permit.

The IED requires the Commission to aim to update the BREFs every eight years.

The competent authority may set emission limits that differ from the BAT emission levels in terms of the values, periods of time and reference conditions applied, so long as it can be demonstrated, through the results of emission monitoring, that emissions have not exceeded the BAT emission levels. The competent authority shall, at least annually, assess the results of emission monitoring.

Where the application of BAT emission levels would lead to disproportionately high costs compared to the environmental benefits, competent authorities should be able to set emission limit values deviating from those levels. In any event, no significant pollution should be caused and a high level of protection of the environment taken as a whole should be achieved. The competent authority shall document in an annex to the permit conditions the reasons for the application of the first subparagraph including the result of the assessment and the justification for the conditions imposed.

However, with the exception of black carbon, emission limit values set must not exceed the emission limit values set out in the Annexes to the IED (i.e. for combustion plants, waste incineration, titanium dioxide production and organic solvent use).

The competent authority may set stricter permit conditions than those achievable by the use of BAT. Member States may establish rules under which the competent authority may set such stricter conditions.

Where an environmental quality standard requires stricter conditions than those achievable by BAT, additional measures shall be included in the permit.

Within 4 years of publication of a new BREF, the competent authority shall ensure that permit conditions for the installation concerned are reconsidered and, if necessary, updated and that the installation complies with those permit conditions. The reconsideration shall take into account all the new or updated BAT conclusions since the permit was granted or last reconsidered.

Member States must ensure that the public has access to a review procedure before a court of law or another independent and impartial body, to challenge the substantive or procedural legality of decisions, acts or omissions subject to a number of conditions.

Organic solvent use thresholds are applicable for different industries and process to assess whether the emission are controlled or not, and are applied to a wide range of activities from dry cleaners upwards. They apply to the cleaning of equipment but not the cleaning of products. Limits are set in the IED for emissions from point sources for each activity (mg C/Nm^3) and fugitive emissions (% of solvent input) and total emission limit values (g/kg or % of solvent input).

Alternatively, industry can use a reduction scheme, that is, use substitute products with no or minimal organic solvents content. Operators are required to supply the competent authority with data to verify compliance with the requirements which may be in the form of a solvent management plan. This is essentially a mass balance approach.

Member States are required to ensure that each installation complies with either of the following:

a. The emission of volatile organic compounds from installations shall not exceed the emission limit values in waste gases and the fugitive emission limit values, or the total emission limit values, and other requirements laid down in Parts 2 and 3 of Annex VII (EPCEU, 2010) are complied with; or

b. The requirements of the reduction scheme set out in Part 5 of Annex VII (EPCEU, 2010) provided that an equivalent emission reduction is achieved compared to that achieved through the application of the emission limit values referred to in point (a).

2.1.2.3 UK Air Quality Legislation

Industrial emissions of NO_X and VOC are controlled in England and Wales via the *Environmental Permitting (England and Wales) Regulations 2010* (HMSO, 2010).

An environmental permit is required for all installations covered by the IPPC Directive (now the IED) and waste operations and is regulated by the UK Environment Agency.

For major installations, emissions of NO_X and VOC are covered by the EU IED. For smaller installations, air emissions only are controlled by the local authority. The Environment Agency is increasingly issuing standard permits for specific industrial activities where operations are relatively straightforward. Bespoke permits are individually tailored to the operations and tend to be issued for higher risk operations.

The aim of UK Environmental Permitting Regulations is to provide a high level of environmental protection, by preventing, or if that is not practicable, reducing, emissions. Permits should include conditions on the use of BAT. As documented within the IED, the use of BAT can be balanced against the local conditions and the cost of implementing it.

2.1.3 Summary of Findings

The literature review of licence requirements for stationary sources of ozone precursors in OECD member countries concentrates on current licensing requirements within the US and EU, as the regulation of ozone precursors from stationary sources has been implemented principally in these jurisdictions.

In general, in the US, there are no Federal requirements specific to ozone that States would be obliged to impose on existing sources in ozone attainment areas.

The construction or modification of large sources of ozone precursors in ozone attainment areas would be subject to Federal New Source Review (NSR) obligations (though implemented by the States) in areas meeting the ozone NAAQS under what is referred to as the Prevention of Significant Deterioration (PSD) program.

The PSD program is applicable to any facility that in aggregate has potential emissions of NO_X and VOC detailed within **Table 7**.

Table 7: NO_X and VOC Emission Thresholds under the PSD Program

Industry	NO_X / VOC Emission Rate (US) tons/year
Major Source	
Fossil fuel-fired steam electric plants of more than 250 million British thermal units per hour heat input, coal cleaning plants (with thermal dryers), kraft pulp mills, portland cement plants, primary zinc smelters, iron and steel mill plants, primary aluminum ore reduction plants (with thermal dryers), primary copper smelters, municipal incinerators capable of charging more than 250 tons of refuse per day, hydrofluoric, sulfuric, and nitric acid plants, petroleum refineries, lime plants, phosphate rock processing plants, coke oven batteries, sulfur recovery plants, carbon black plants (furnace process), primary lead smelters, fuel conversion plants, sintering plants, secondary metal production plants, chemical process plants (which does not include ethanol production facilities that produce ethanol by natural fermentation included in NAICS codes 325193 or 312140), fossil-fuel boilers (or combinations thereof) totalling more than 250 million British thermal units per hour heat input, petroleum storage and transfer units with a total storage capacity exceeding 300,000 barrels, taconite ore processing plants, glass fibre processing plants, and charcoal production plants	>100
All Other Industries	>250
Major Modification	
All Industries	>40

Source: 40 CFR 52.21 http://frwebgate.access.gpo.gov/cgi-bin/get-cfr.cgi?TITLE=40&PART=52&SECTION=21&TYPE=PDF

In general, there is no requirement to model the photochemical transformations from ozone precursors in the PSD process, but a general demonstration would have to be made that, after the installation of Best Available Control Technologies (BACT), the ambient air quality in the area can bear the increase in emissions.

When an area is designated to be non-attainment with respect to the ozone NAAQS, a State is required to develop and implement a State Implementation Plan to bring the area back into attainment.

The State will generally select and implement a mix of measures to impose on both mobile and stationary sources. This selection is informed by photochemical dispersion modelling considering the NO_X and VOC emissions from all man-made and natural sources in the area as well as potentially from regions upwind of the area.

In general, mobile source emission standards are outside State jurisdiction and SIP measures are limited to requirements for regular vehicle emission inspections, incentive programs to replace or retrofit older vehicles/equipment, or transportation planning measures such as addition of carpool lanes on major highways. The effects of those measures are evaluated in the modelling and determinations are made about how much additional emission reduction is needed from existing stationary sources.

The State then issues emission standards constituting Reasonably Available Control Technology (RACT) on existing stationary sources in the non-attainment area. RACT measures are less stringent in nature than BACT measures. Typical measures are things like limiting the VOC content of paint used in production processes, requiring covers on mixing tanks, emissions limits on NO_X from combustion processes consistent with good combustion performance, etc. Sources in the non-attainment area would then have to comply with those RACT emission limits and standards.

The most stringent requirements apply to those seeking to build new sources or increase emissions of ozone precursors in non-attainment areas. Much like the PSD program, Federal requirements for non-attainment New Source Review (NSR) apply to major sources seeking a significant increase in ozone precursor emissions in an ozone non-attainment area, as summarised in **Table 8**.

Table 8: NO_X and VOC Emission Thresholds within the Non-Attainment New Source Review [1]

Ozone Non-attainment Area	**NO_X / VOC Emission Rate (US) tons/year**
Major Stationary Source	
Serious Ozone Non-attainment Area (Area has a 1-hour ozone design value [2] of 0.160 up to 0.180 ppm [3])	>50
Area within an Ozone Transport Region (except for any Severe or Extreme Ozone Non-attainment Area)	>50
Severe Ozone Non-attainment Area (Area has a 1-hour ozone design value [2] of 0.180 up to 0.280 ppm [3])	>25
Extreme Ozone Non-attainment Area (Area has a 1-hour ozone design value [2] of 0.280 ppm and above [3])	>10
All Other Areas	>100
Major Modification	
Serious or Severe Ozone Non-attainment Area	>25

Table 8: NO_X and VOC Emission Thresholds within the Non-Attainment New Source Review [1]

Ozone Non-attainment Area	NO_X / VOC Emission Rate
Extreme Ozone Non-attainment Area	Any Increase
All Other Areas	>40

Note 1: Source: 40 CFR 51.165 http://frwebgate.access.gpo.gov/cgi-bin/get-cfr.cgi?TITLE=40&PART=51&SECTION=165&TYPE=PDF
Note 2: For definition, refer **Section 2.1.1.7**.
Note 3: Source: http://www.epa.gov/oar/oaqps/greenbk/define.html#OzoneClassifications

If non-attainment NSR is triggered, the proposed sources must install emission controls consistent with Lowest Achievable Emission Rate (LAER) performance and then find offsetting emission reductions from other existing sources in the area, often at a ratio greater than 1:1 on a mass basis.

A database of control technology information falling into the above definitions is located within the USEPA RACT/BACT/LAER Clearinghouse (RBLC, http://cfpub.epa.gov/RBLC/).

Given the emphasis on demonstrating best practice control technologies within the permitting process, there is generally no requirement to model the photochemical transformations from ozone precursors, but a general demonstration would have to be made that after the installation of control technologies, the ambient air quality in the area can bear the increase in emissions.

In this sense, the EU has a similar approach to the permitting of major sources of ozone precursors. This requires that facilities demonstrate the adoption of Best Available Techniques (BAT). BAT is prescribed within the EU BAT Reference documents (BREFs) (http://eippcb.jrc.ec.europa.eu/reference/). The recent EU Industrial Emissions Directive (IED; EPCEU, 2010) makes the use of BREFs effectively mandatory.

The BREFs provide information on the emissions achievable with BAT, often as a range of emissions, and the IED requires that these should be used to set the emission limits in the operating permit for the normal operation of the facility.

Organic solvent thresholds are referenced for different industries and processes to assess whether additional control of VOC is required. Limits are set in the IED for emissions from point sources for each activity (mg C/Nm^3) and fugitive emissions (% of solvent input) and total emission limit values (g/kg or % of solvent input). Each installation has to comply with these emission limit values or alternatively, industry can use a reduction scheme, i.e. use substitute products with no or little organic solvents content.

The literature review has not identified ozone concentration increments for the evaluation of impacts associated with new or modified stationary sources.

While ozone concentration increments (i.e. Prevention of Significant Deterioration (PSD) increments) are not used in the US, the relationship between PSD increments and national ambient air quality standards (NAAQS) for other air pollutants may be used as a guide for developing them. For short-term (i.e. 24-hour or less) averaging periods, the PSD increment for a given pollutant is generally between 1% and 6% of the NAAQS. If this relationship is applied to *National Environment Protection (Ambient Air Quality) Measure* (Air NEPM) standards for ground-level ozone (NEPC 2003), PSD increments of between 1 and 6 ppb (expressed as a 1-hour average) and between 1 and 5 ppb (expressed as a 4-hour average) would apply.

The ground-level ozone PSD increments of between 1 and 6 ppb are consistent with US modelling practice. When the USEPA evaluated ozone transport between States for the Clean Air Interstate Rule (USEPA, 2004), ozone transport contributions associated with a 2 ppb increment in daily maximum 8-hour ozone were considered insignificant.

In this study, an incremental increase of greater than or equal to 1 ppb ozone (expressed as either a 1-hour or 4-hour average) has been selected as the level which represents a significant increase in ground-level ozone. This metric has been selected on the basis of the rationale detailed above, combined with the 1 ppb concentration representing a measurable change using conventional ambient monitoring instrumentation.

2.2 Literature Review of Ozone Screening Procedures

2.2.1 Introduction

Screening methods for primary pollutants (e.g. SO_2 and primary PM) have been successful because the relationship between emissions and ambient concentration can be parameterised in terms of easily measured meteorological parameters. However, screening methods for ozone are much more difficult to develop, and in most cases, ozone assessments are based on complex 3-D models. The challenge for ozone is the non-linear chemical relationships between secondary ozone and the primary ozone precursor emissions (Pandis and Seinfeld, 1998). Non-linear ozone chemistry has several consequences:

1. The ozone impact of a specific source depends upon emissions from neighbouring and upwind sources.
2. The ozone impact of a specific source has a complex dependence on meteorology.
3. NO_x and VOC emissions from a single source interact such that their ozone impacts are not simply additive.
4. The ozone impacts of VOC emissions depend upon the identity of the VOC (an effect called VOC reactivity).

The need to model interactions between multiple sources makes most plume or puff models (e.g. CALPUFF), which consider sources independently, inapplicable. One puff model (i.e. SCICHEM) can model ozone formation from VOC/NO_X plumes interacting with background air quality. USEPA has plans to explore the use of SCICHEM. However, at this time the body of work applying SCICHEM for ozone is very limited and we do not recommend attempting to develop a screening methodology based upon any plume or puff model.

2.2.2 Scheffe Tables

In 1988, Dr. Rich Scheffe of USEPA attempted to use a plume model to develop a screening methodology for ozone by making conservative assumptions. However, as documented by Dr. Scheffe, the resulting screening tables were technically unsound because the plume model could not overcome the challenges listed in **Section 2.2.1**. Dr. Scheffe has subsequently recommended against using the screening tables in the following words “the Scheffe method, which was deemed not adequate in 1989, would be even less adequate today.” US States have taken Dr. Scheffe’s advice. The state of Oklahoma advises that until further guidance is published by USEPA, large sources of ozone precursors should be included in available photochemical modelling datasets and should be modelled using the Comprehensive Air Quality Model with extensions (CAMx – refer **Section 2.5.2**) to assess impacts and demonstrate compliance with ozone standards. Permit applicants may be required to conduct extensive modelling using either CAMx, or the Community Multiscale Air Quality Modelling System (CMAQ – refer **Section 2.5.3**) (Oklahoma DEQ, 2008).

2.2.3 Maximum Incremental Reactivity (MIR) Factors

The fourth issue listed in **Section 2.2.1** (VOC reactivity) has been partially addressed by using photochemical models to develop reactivity weighting factors for VOC (Carter and Atkinson, 1989; Derwent et al., 1998). VOC reactivity scales provide a quantitative assessment of the relative reactivity of different VOC which is valuable, for example, when reformulating VOC mixtures (e.g. fuels, solvents and surface coatings) to reduce their ozone forming tendency. Maximum Incremental Reactivity (MIR) factors developed by Carter are used in US regulations that limit the ozone forming potential of VOC mixtures. However, VOC reactivity factors are not used in the US to assess what ozone concentration will result from emitting a specific mass of emissions. Therefore, VOC reactivity factors do not appear adequate for the type of screening assessment sought in this study.

2.2.4 Summary of Findings

The use of the Scheffe Tables represents the only known applicable screening procedure used for the evaluation of ozone impacts from stationary sources.

However, the Scheffe Tables have been deemed by their author as technically unsound because the plume model used to derive these tables could not adequately resolve the non-linear chemical relationships between secondary ozone and the primary ozone precursor emissions.

2.3 Literature Review of Photochemical Mechanisms

2.3.1 Introduction

Photochemical mechanisms are a critical component in ozone air quality planning because they are the bridge between precursor (i.e. CO, CH_4, NO_X and VOC) emission rates and ozone concentration impacts. Mechanisms are developed from laboratory measurements of kinetic data (i.e. rate constants for individual reactions) and mechanistic data (i.e. products formed by individual reactions). However, since mechanistic and kinetic data are incomplete and uncertain, photochemical mechanisms also are evaluated by comparing mechanism predictions to the results of smog chamber experiments. Smog chamber experiments expose captive mixtures of NO_X, VOC and air to sunlight or UV light and measure the ozone produced.

Kinetic data relevant to ozone chemistry are periodically reviewed and evaluated by two international committees comprised of experts in the field:

- IUPAC (http://www.iupac-kinetic.ch.cam.ac.uk/; Atkinson et al., 2010); and
- NASA-JPL (http://jpldataeval.jpl.nasa.gov/; Sander et al., 2006).

Reviews of mechanistic data also are available, for example, Calvert et al. (2000, 2002). Mechanism developers rely upon these data sources to periodically update mechanisms. Data for important reactions are still changing after decades of research (e.g. the rate constant for the important reaction of OH with NO_2 was recently revised by Mollner et al., 2010) making mechanism updates a necessity.

The following represents a review and comparison between several photochemical mechanisms used in Australia, the US and Europe. The review documents mechanisms in widespread use and provides a basis for OEH to decide which mechanisms are appropriate for use in NSW. The review documents important mechanism attributes including:

- Number of reactions;
- Number of chemical species;
- Classes of VOC compounds;
- Date when the main kinetic data were revised;
- Whether evaluated using smog chamber data; and
- References.

In addition to documenting the date of revision for the main kinetic data, the values for several of the most critical rate constants present in every mechanism (e.g. OH + NO_2, NO_2 photolysis and O_3 photolysis) are compared to check whether they are up to date.

The following mechanisms have been considered for inclusion in the review:

- Carbon Bond versions CB4 and CB05;
- Lurmann, Carter and Coyner (LCC);
- SAPRC versions S99, S07B and CS07A;
- Common Representative Intermediates (CRI) version 2-R5; and
- MELCHIOR2.

Documentation for the LCC mechanism (Lurmann et al., 1987) was not available so the LCC mechanism has not been reviewed. The LCC mechanism is a predecessor to the SAPRC mechanisms that are reviewed.

Key attributes of the chemical mechanisms are summarised in **Table 9** to **Table 11** and discussed below.

Table 9: Chemical Mechanisms: Reactions and Species

Mechanism	Reactions			Chemical Species		
	Inorganic	Organic	Total	Inorganic	Organic	Total
CB4	38	58	96	14	23	37
CB05	54	102	156	17	51	68
S99	45	176	221	17	58	75
S07B	45	230	275	17	87	104
CS07A	45	95	140	17	30	47
CRI v2-R5	47	508	555	19	177	196
MELCHIOR2	26	107	133	13	35	48

Table 10: Chemical Mechanisms: Organic Precursors

Mechanism	Alkane	Anthro-pogenic Alkene	Biogenic Alkene	Aromatic	Aldehyde	Other Oxygenate
CB4	2	2	1	2	2	2
CB05	3	3	2	2	3	2
S99	6	3	2	2	3	2
S07B	6	3	2	3	3	3
CS07A	3	3	2	2	3	0
CRI v2-R5	4	3	3	3	3	4
MELCHIOR2	3	2	7	1	2	0

Table 11: Chemical Mechanisms: Rate constant for OH + NO_2

Mechanism	k_{298} (cm^{-3} molecule^{-1} s^{-1})	Citation
CB4	11.4×10^{-12}	JPL (1985)
CB05	10.6×10^{-12}	Sander et al. (2006)
S99	8.9×10^{-12}	Personal communication from D. Golden, cited in Carter (2000)
S07B	10.6×10^{-12}	Sander et al. (2006)
CS07A	10.6×10^{-12}	Sander et al. (2006)
CRI v2-R5	11.9×10^{-12}	Atkinson et al. (2004)
MELCHIOR2	9.9×10^{-12}	Donahue et al.(1997)
Most recent recommendation	9.2×10^{-12}	Mollner et al. (2010)

2.3.2 History and Documentation

The Carbon Bond mechanism was developed in the 1980s and the first version to be used widely was CB4 (Gery et al., 1989). The CB4 mechanism received several updates (revised temperature dependence for PAN formation; revised reactions of organic RO_2 radicals; and revised isoprene mechanism based on Carter, 1996) and was used in the CMAQ and CAMx models from about 1997 onwards. This revised version of CB4, as documented in the CAMx User's Guide (ENVIRON, 2010) is the basis for this review. A more comprehensive update to CB4 was performed in 2005 leading to the CB05 mechanism (Yarwood et al., 2005) which is now used for most ozone and secondary particulate matter modelling within the US. CB4 and CB05 were both evaluated against smog chamber data and both have been used in multiple photochemical models (e.g. CAMx and CMAQ). CB6 is currently being developed and tested.

The SAPRC mechanism was developed in the early 1990s and the most widely used version has been the 1999 version (Carter, 2000) called SAPRC99 or simply S99. A comprehensive mechanism update was performed for SAPRC 2007 (Carter, 2010a) leading to several versions as described in Carter (2010b). The two versions summarised here are S07B and CS07A where the letters "A" and "B" designate alternate schemes for representing reactions of organic RO_2 radicals, with scheme "A" being more condensed than scheme "B". The prefix "C" in CS07A designates a mechanism that is more highly condensed by reducing the number of species included. S07B and CS07A were both evaluated against smog chamber data. The S07B mechanism has been implemented in the CMAQ model, but not yet released for general use.

The CRI v2-R5 mechanism is a condensation of the Master Chemical Mechanism (MCM; Saunders et al., 2003; Jenkin et al., 1997). The MCM is widely regarded as a comprehensive repository of current knowledge of atmospheric chemical reactions. The condensation of the MCM for version 2 of the CRI was achieved by using computer algorithms to combine chemical species with similar attributes (Jenkin et al., 2008). Several levels of condensation were developed with reduction 5 (CRI v2-R5) being the most highly condensed. The CRI v2-R5 mechanism has been applied in a global 3-D photochemical model (Utembe et al., 2010). The MCM is available via the website http://mcm.leeds.ac.uk/MCM/ which provides an interface to browse the mechanism and extract portions of the mechanism for use in modelling. There are plans to make CRI v2 mechanisms available via a similar website but, at this time, no mechanism listing is available for CRI v2-R5. This review is based on information provided by Watson et al. (2008). Portions of MCM have been evaluated against smog chamber data but CRI v2-R5 has not.

The MELCHIOR2 chemical mechanism was developed for use in the CHIMERE model. The mechanism MELCHIOR2 (Derognat, 2003) is a condensation of the MELCHIOR1 mechanism (Lattuati, 1997). A reaction listing for MELCHIOR2 is given in the CHIMERE User's Guide (IPSL, 2009) and is the basis for this review. MELCHIOR2 has not been evaluated against smog chamber data.

2.3.3 Numbers of Reactions and Species

The size of a chemical mechanism can be characterised by the numbers of reactions and chemical species included (**Table 9**). Mechanism size provides some indication of the amount of detail provided by a mechanism and has a very direct impact on the computational resources required when the mechanism is implemented in a 3-D model. The mechanisms reviewed here may be ordered from most to least compact as follows: CB4, MELCHIOR2, CS07A, CB05, S99, S07B and CRI v2-R5.

The inorganic reactions that are important for tropospheric oxidant chemistry are well understood (Atkinson et al., 2005; Sandet et al., 2006) leading to consistency in the inorganic species and reactions that mechanisms include. Most of the mechanisms reviewed here include 17 inorganic species (**Table 9**), namely O_3, $O(^3P)$, $O(^1D)$, OH, HO_2, H_2O_2, NO, NO_2, NO_3, N_2O_5, HONO, HNO_3, HNO_4, SO_2, H_2SO_4, H_2 and CO.

CB4 has 14 inorganic species because H_2, SO_2, H_2SO_4 are omitted (although modellers have added SO_2, H_2SO_4 to CB4 when needed). MELCHIOR2 has 14 inorganic species because H_2 and HNO_4 are omitted and oxygen atoms ($O(^3P)$ and $O(^1D)$) are eliminated as explicit species by building their concentrations into reaction rates. The number of inorganic species included in CRI v2-R5 was assumed to be the same as for MCM which is 19 because SO_3, HSO_3 are added to the 17 species listed above.

The number of inorganic reactions included in the mechanisms ranges from 26 (i.e. MELCHIOR2) to 54 (i.e. CB05) with most mechanisms having about 45 inorganic reactions. The CB05 mechanism includes more inorganic reactions than other mechanisms to better represent unpolluted conditions such as remote regions and the upper troposphere. MELCHIOR2 includes fewer inorganic reactions than other mechanisms by omitting chemistry that tends to be important only for unpolluted conditions.

Most of the variation in mechanism size results from differences in how organic reactions are represented. The approaches adopted by these mechanisms for representing the organic chemistry are discussed in the next section. The size of the organic chemistry included in these mechanisms may be ordered from smallest to largest as follows: CB4, CS07A, MELCHIOR2, CB05, S99, S07B and CRI v2-R5.

2.3.4 Organic Precursors

Organic compounds exhibit different tendencies to form ozone and other oxidants – a characteristic often referred to as VOC reactivity (Carter and Atkinson, 1989). For example, alkenes (e.g. ethene, propene and isoprene) are sometimes referred to as highly reactive VOC (HRVOC) because they react rapidly in the atmosphere and form degradation products that photolyse rapidly (Murphy and Allen, 2005). Reactivities of individual VOC have been characterised using reactivity scales based on computer modelling such as MIR (Carter, 1994) and POCP (Derwent et al., 1998).

Chemical mechanisms should be able to represent differences in VOC reactivity and the types and numbers of VOC included in a mechanism are indicators of this capability. **Table 10** summarises the number of VOC of different types included in each mechanism reviewed. For purposes of **Table 10** and the discussion below, attention is restricted to VOC that are expected to be present in emissions at more than trivial amounts. For example, when considering aldehydes, dicarbonyls such as glyoxal and methylglyoxal are not counted as emitted aldehydes because they are predominantly formed in the atmosphere by degradation of alkenes and aromatics (i.e. they are secondary rather than primary species).

All of the mechanisms use a “surrogate species” approach to represent hundreds of emitted VOC using a handful of model species. The use of surrogate species is also called lumping because several VOC are lumped together into a single model species. For example, all of the mechanisms include a lumped 1-alkene model species to represent all members of the sequence of compounds propene, 1-butene, 1-pentene, etc. This approach works well for 1-alkenes because the C=C double bond dominates the atmospheric reactions and reactivity of 1-alkenes.

All of the mechanisms also include some explicit VOC (e.g. isoprene and ethene) that represent a single compound.

2.3.4.1 Alkanes

All of the mechanisms treat methane explicitly and several (i.e. CB05, MELCHIOR2 and CRI v2-R5) also treat ethane explicitly. Mechanisms treat the lightest one or two alkanes explicitly because they are less reactive than other alkanes and often have large emissions. Alkanes that are not treated explicitly are represented by between one (i.e. CB4 and CB05) and five (i.e. S99 and S07B) lumped alkane species, depending upon the mechanism. Alkanes present a challenge for lumping because their reactivity increases with molecular size. The solution adopted by the carbon bond mechanisms (i.e. CB4 and CB05) is to use a single lumped alkane (i.e. PAR) to represent alkanes in proportion to their number of carbon atoms, e.g. n-butane = 4 PAR, n-hexane = 5 PAR, etc. Consequently, carbon bond mechanisms representing alkane reactivity increase monotonically with carbon number.

The solution adopted by the S99 and S07B mechanisms is to assign alkanes to one of five lumped alkanes (i.e. ALK1 through ALK5) with different numbers of carbon atoms (i.e. 2, 3, 4, 5 and 8 in S07B) (e.g. n-butane = ALK3 and n-hexane = ALK4). Consequently, alkane reactivity is represented as increasing in 5 discrete steps by the S99 and S07B mechanisms. The compact SAPRC mechanism CS07A uses only two lumped alkanes resulting in two “reactivity steps” for lumped alkanes. The MELCHIOR2 and CRI v2-R5 mechanisms represent all lumped alkanes as n-butane.

2.3.4.2 Anthropogenic alkenes

Most mechanisms include three anthropogenic alkenes: ethene, a class for 1-alkenes exemplified by propene and a class for n-alkenes (with n≠1) exemplified by 2-butene. CB4 and MELCHIOR omit the n-alkene class and have only two anthropogenic alkenes.

2.3.4.3 Biogenic alkenes

Most mechanisms include two biogenic alkenes: isoprene and a class for terpenes. CB4 omits the terpene class. CRI v2-R5 replaces the terpene class by two explicit terpenes, α- and β-pinene. MELCHIOR2 replaces the terpene class with 3 explicit terpenes, (i.e. α- and β-pinene and limonene) and three lumped terpenes (i.e. ocimene, humulene and terpenes).

2.3.4.4 Aromatics

Most mechanisms include two aromatics: a class for mono-substituted aromatics exemplified by toluene and a class for poly-substituted aromatics exemplified by xylene. S07B and CRI v2-R5 add benzene explicitly as a third aromatic. MELCHIOR2 has only a single aromatic class based on xylene, which is a limitation because mono-substituted aromatics have substantial emissions and lower reactivity than xylenes by about a factor of two (Carter and Atkinson, 1989; Derwent et al., 1998).

2.3.4.5 Aldehydes

Most mechanisms include three aldehydes: formaldehyde, acetaldehyde and a class for higher aldehydes exemplified by propionaldehyde. CB4 and MELCHIOR2 combine higher aldehydes with acetaldehyde.

2.3.4.6 Other oxygenates

The mechanisms reviewed differ widely in how they include oxygenates other than aldehydes. The carbon bond mechanisms (i.e. CB4 and CB05) include two alcohols (i.e. methanol and ethanol) whereas the SAPRC mechanisms (i.e. S99 and S07B) includes two ketones (i.e. acetone and butanone) and CRI v2-R5 includes all four of these oxygenates. MELCHIOR2 and CS07A include no oxygenates other than aldehydes.

2.3.5 Kinetic Data

All of the mechanisms reviewed rely upon evaluated kinetic data from the IUPAC and/or NASA review panels, discussed above, supplemented by other sources. The rate constant for the OH + NO_2 reaction (**Table 11**) provides a good indication of when kinetic data were updated for each mechanism. The CB4 mechanism dates from the 1980s, MELCHIOR2 and S99 date from the late 1990s, CB05, S07B, CS07A and CRI v2-R5 date from the mid 2000s.

The reaction of OH with NO_2 is one of the most important reactions in tropospheric smog chemistry because it strongly influences both the atmospheric lifetime of NO_X and the abundance of hydroxyl (OH). The OH + NO_2 rate constant depends upon both temperature and pressure and has proven difficult to measure (as discussed by Sander et al., 2006). **Table 11** shows that the mechanisms reviewed use values for the OH + NO_2 rate constant ranging from 8.9 to 11.9 x 10^{-12} cm^{-3} $molecule^{-1}$ s^{-1}. The study by Mollner et al. (2010) is likely to reduce uncertainty in this rate constant and cause mechanisms to adopt a value of 9.2 x 10^{-12} cm^{-3} $molecule^{-1}$ s^{-1} near the low end of the range in use. Lowering the OH + NO_2 rate constant tends to increase modelled ozone concentrations (Mollner et al., 2010) and make ozone more responsive to NO_X emission reductions and less responsive to VOC emission reductions.

2.3.6 Summary of Findings

Seven chemical mechanisms for modelling tropospheric ozone and smog have been reviewed, namely: CB4, CB05, S99, S07B, CS07A, CRI v2-R5 and MELCHIOR2. Key attributes of each mechanism have been documented. Use of any of these mechanisms for modelling tropospheric ozone in Australia is justified because all mechanisms have been peer-reviewed and/or used in peer-reviewed ozone modelling studies.

- The mechanisms reviewed may be ordered from most compact to least compact as follows: CB4, MELCHIOR2, CS07A, CB05, S99, S07B and CRI v2-R5.

- The CB4 mechanism has been superseded, and largely replaced, by CB05. CB05 should be used rather than CB4 whenever possible.

- The S07B mechanism has superseded S99 but has yet to be used in regional modelling studies. In addition, S07B is a larger mechanism than S99 and will demand more computational resources than S99. Continued use of S99 is appropriate until the impacts of changing to S07B have been tested and evaluated.

- The CS07A and CRI v2-R5 mechanisms have not yet been used in urban/regional ozone modelling studies and, if used, they should be compared to other mechanisms.

- The MELCHIOR2 mechanism is expected to be computationally efficient and it has been used extensively in one air quality model (i.e. CHIMERE). Using MELCHIOR2 is reasonable but comparison with other current mechanisms (e.g. CB05 and S99) would be useful.

- The LCC mechanism was not reviewed because documentation is not available. LCC dates from the 1980s and it is a predecessor to the SAPRC mechanisms (i.e. S99, S07B and CS07A). If the LCC mechanism is used, it should be compared to more current mechanisms (e.g. CB05 and S99) and if results are different a scientifically defensible explanation should be developed.

2.4 Literature Review of Photochemical Models

2.4.1 Introduction

This section briefly summarises the main features of several photochemical models that are widely used in Australia, the US and Europe. The purpose is to document model attributes that could be considered by OEH in determining which models are suitable for use in NSW.

The number of photochemical models developed for ozone probably now exceeds one hundred. The European Topic Centre on Air and Climate Change has developed a Model Documentation System (MDS) to catalogue air quality models and provide a central repository for information submitted by model developers (http://air-climate.eionet.europa.eu/databases/MDS/)

However, to focus the evaluation of suitable photochemical models, the following criteria are considered:

- The model can be used with input databases available for the OEH screening analysis;

- Includes state-of-the-science treatment of the governing processes;

- Is publicly available with adequate user documentation and supported by the model developers;

- Has a large user community and a user forum;

- Is well-documented in peer-reviewed literature and accepted as a credible model;

- Is extensively applied and evaluated over several geographical regions and modelling periods;

- Is used for policy decisions; and
- Is maintained and updated to reflect advances in the state-of-the-science.

A comprehensive review of photochemical models would be infeasible for this project and probably not useful. Thus, our review focuses on models that are widely used in Australia, the US and EU to provide OEH with relevant information for models of most interest. The following models have been reviewed:

- CAMx;
- CMAQ;
- CHIMERE;
- TAPM/TAPM-CTM; and
- CIT.

The CAMx and CMAQ models account for virtually all of the ozone assessment modelling currently performed in the US. The CIT and TAPM models are relevant because they are used in Australia. The CHIMERE model is probably the most widely used photochemical model that has been developed in Europe. Although, there are some important differences among the models listed above, they also share some common features. For example, all these models are source-oriented, Eulerian models that represent the atmosphere as a three-dimensional fixed grid, and simulate the transport, transformation and removal of air pollutants by solving the conservation of mass equation for this grid.

All the models incorporate atmospheric chemistry modules to describe the conversion of emitted pollutants to secondary pollutants such as ozone. The models are also referred to as “third-generation” (e.g. Peters et al., 1995) chemical transport models (CTMs), reflecting the large scientific and computational advances made from the first photochemical models developed in the early 1970s to those that are widely used today.

Because of the wide range in characteristic times of the various terms (i.e. transport terms, source terms, chemistry terms and sink terms) in the conservation equation, all the models employ a technique referred to as operator-splitting (e.g. McRae et al., 1982a; Lanser and Verwer, 1999; Sportisse, 2000; 2007; Odman and Hu, 2010), in which the different terms are solved sequentially using solvers and time scales appropriate for each term. This simplifies the solution and reduces computational requirements but also introduces numerical artifacts.

The differences among the models lie in their:

- Representation of the governing processes, such as transport, chemistry, and removal;
- Numerical solution of the transport and chemistry equations;
- Meteorological inputs;

- Grid configurations; and
- Ancillary capabilities such as source attribution, grid-nesting, and resolution of point source plumes.

The following sections provide brief background information on each model, followed by a comparison of the treatment of the key governing processes in the different models. **Appendix 2** provides a list of references for each model not explicitly cited within this report, which include additional information on the development, applications and testing of the model.

2.4.2 CAMx

The Comprehensive Air quality Model with extensions (CAMx), developed by ENVIRON International (ENVIRON, 2010), is an Eulerian photochemical dispersion model that allows for integrated "one-atmosphere" assessments of gaseous and particulate air pollution (e.g. ozone, $PM_{2.5}$, PM_{10} and air toxics) over many scales ranging from sub-urban to continental. It is a publicly available open-source computer modelling system that can be downloaded from the CAMx home page at http://www.camx.com/. This site also provides a comprehensive User's Guide and other technical documentation (including journal publications), as well as pre- and post-processing utilities. The model is actively maintained and updated by ENVIRON, and the latest version of the model (Version 5.3) was released in December 2010.

CAMx is written in Fortran and is designed for platforms running Unix/Linux, including Apple Mac OS X. The model is highly flexible and computationally efficient; it can take advantage of multi-core and multi-processor machines and workstation clusters by using Open-MP (OMP) on shared-memory systems and the Message Passing Interface (MPI) on distributed-memory systems (based on the MPICH implementation of MPI). CAMx is one of two multi-scale photochemical CTMs that are used extensively in the US for ozone, PM and visibility policy decisions. CAMx has a large user community, both in the US and world-wide, and the CAMx users group provides a forum for users to obtain and share information and to receive technical support from the model developers.

2.4.3 CMAQ

The Community Multiscale Air Quality (CMAQ) model (Byun and Schere, 2006), developed by the USEPA, is an Eulerian modelling system designed to approach air quality as a whole by including state-of-the-science capabilities for modelling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation. CMAQ is a publicly available open-source modelling system. Although it is developed by the USEPA (http://www.cmaq-model.org/), it is distributed by the Community Modelling and Analysis System (CMAS) centre, which is also responsible for providing user training and support and maintaining a users group for information sharing and bug reports.

The CMAS centre is also responsible for organizing an annual workshop that is primarily devoted to CMAQ and CMAQ-related development and application topics. The CMAQ modelling system (including science codes, meteorology and emissions processors, technical documentation and User's Guide) can be downloaded from http://www.cmascenter.org/.

CMAQ is continuously maintained and updated through US-EPA/CMAS and contributions from the user community. The latest version (4.7.1) was released in June 2010 and the next version (5.0) is slated for release around the time of the annual CMAS workshop (October 2011).

The CMAQ science code is written in Fortran and its multi-processing capability uses the publicly available MPICH2 implementation of MPI from Argonne National Laboratory. CMAQ is used extensively in the US and around the world and has a large and active user community. In addition to traditional regulatory and research applications, CMAQ is also being used in the US and Europe to provide real time air quality forecasts.

2.4.4 CHIMERE

The CHIMERE multi-scale model (IPSL, 2009) is primarily designed to produce daily forecasts of ozone, aerosols and other pollutants and to make long-term simulations for emission control scenarios.

CHIMERE is one of the leading air quality models in Europe and has been collaboratively developed by a number of French organizations: IPSL/LMD (Institut Pierre-Simon Laplace/Laboratoire de Météorologie Dynamique), INERIS (Institut National de l'Environnement Industriel et des Risques or the French National Institute for Industrial Environment and Risks), and LISA (Laboratoire Interuniversitaire des Systèmes Atmosphériques).

The code is supported and maintained by the model developers and training courses are provided twice a year at IPSL/LMD. The code is publicly available and distributed under the GNU General Public Licence. Information on downloading the code and User's Guide is provided on the official CHIMERE website at http://www.lmd.polytechnique.fr/chimere/.

The latest version of CHIMERE, referred to as CHIMERE2008c, was released in July 2009. The CHIMERE science code is written in Fortran (Fortran 90 and 95), and its parallel processing capability is based on the Open MPI or LAM/MPI implementation of the MPI specification. A CHIMERE user's mailing list is available for users to exchange and receive information from the model developers and other users. More than 120 users, from 30 institutes, are registered on the model email list.

2.4.5 TAPM/TAPM-CTM

The Air Pollution Model (TAPM; Hurley, 2008) differs from the other models reviewed here in that it is an integrated prognostic meteorological/air quality model. The other models are all driven by externally generated meteorological fields from meteorological models such as MM5, WRF, ECMWF or RAMS.

TAPM was developed in Australia by CSIRO Marine & Atmospheric Research and copies of the TAPM software can be purchased from CSIRO along with synoptic meteorological analyses for various regions. Information on licence purchases and user documentation can be found at http://www.csiro.au/products/TAPM.html. The latest version of the model is

Version 4, released in October 2008. The model is used widely in Australia and also has been used and evaluated in other regions, such as New Zealand, Thailand, Europe and the United States. It has been distributed under licence to more than 190 national and international users in 25 countries. The base version of TAPM offers a simplified photochemical mechanism, referred to as the Generic Reaction Set (GRS). For urban airshed applications requiring more complex chemistry (such as the LCC or CB04 mechanisms), a version of TAPM, referred to as TAPM-CTM (Cope et al., 2009), is available for an additional cost. The code is supported and maintained by CSIRO and TAPM training is available through the Clean Air Society of Australia & New Zealand (CASANZ).

2.4.6 CIT

The California Institute of Technology (CIT or Caltech) photochemical airshed model was initially developed as a “second-generation” model in the early 1980s (McRae et al., 1982b; 1983), with subsequent development and refinement over the years (e.g. Harley et al., 1992; 1993; Meng et al., 1998; Nguyen and Dabdub, 2001; Griffin et al., 2002a; Martien et al., 2006).

Unlike the other models reviewed here, which have a single point of contact for model access, various versions of the model exist at a number of Universities (e.g. Caltech, University of California, Berkeley (UCB); University of California, Davis (UCD); and University of California, Irvine (UCI)). Additionally, a version of CIT adapted for Australian conditions has been developed by CSIRO (Cope and Ischtwan, 1996) before the TAPM-CTM alternative configuration (**Section 2.5.5**) became available. Currently, the model is under continuous revision and development at UCI, in collaboration with researchers from the other institutions mentioned previously.

Another difference between CIT and the other models is the lack of up-to-date documentation for model users and lack of user support and user training. The last available User’s Guide is dated 1992 (McRae et al., 1992). Thus, while the model has a strong pedigree and incorporates state-of-the-science treatments of the governing processes, it has primarily been used in academic settings for research applications that lead to model improvements and doctoral dissertations. Furthermore, a large number of the CIT model applications have been confined to Southern California, while the other models have been applied in a variety of settings.

2.4.7 Model Background Information

Table 12 summarises the background information for each model documented above.

Table 12: Photochemical Air Quality Models - Background

Model	Full Name/Developer	Latest Model Version	Model Access, Documentation, Support
CAMx	Comprehensive Air quality Model with extensions (developed and distributed by ENVIRON at http://www.camx.com/; ask-camx@environ.org)	Version 5.30, December 2010	Publicly available open-source model; current User's Guide; users group and mailing list; training available
CMAQ	Community Multiscale Air Quality model (developed by the U.S. EPA and distributed by the CMAS centre at http://www.cmascenter.org/; cmas@unc.edu)	Version 4.7.1, June 2010	Publicly available open-source model; current User's Guide; users group and mailing list; annual training at CMAS
CHIMERE	CHIMERE (developed by IPSL/LMD, INERIS and LISA and distributed by IPSL/LMD at http://www.lmd.polytechnique.fr/chimere/ ; chimere@lmd.polytechnique.fr)	Version 2008c, July 2009	Publicly available and open-source model; current User's Guide; users mailing list; twice-yearly training at IPSL/LMD
TAPM / TAPM-CTM	The Air Pollution Model-Chemical Transport Model (developed and sold by CSIRO at http://www.csiro.au/products/TAPM.html ; Simon.Torok@csiro.au)	Version 4, October 2008	Available under licence from CSIRO; current User's Guide; training available
CIT	California Institute of Technology model (Caltech, UCB, UCD, UCI)	Different versions available from various developers	User's guide dated 1992; information on user support or training not available

2.4.8 Model Characteristics

All the models reviewed are three-dimensional Eulerian grid models. However, there are important differences among the models in their formulation, input requirements, treatment of the various atmospheric processes governing pollutant transport, transformation and removal and some ancillary capabilities. These differences are summarised in a series of tables, with each table focusing on a key set of model attributes.

Table 13 compares the grid configurations of the different models and their sources of meteorological data inputs.

Table 13: Model Attributes - Configuration

Model	Scale/Coordinate System	Nesting / Plume-in-grid	Meteorology
CAMx	• Multiscale (urban to continental) • Horizontal projection: Lambert Conformal, Polar Stereographic, Universal Transverse Mercator, Lat-Lon • Vertical grid structure: height-based terrain-following coordinate system	• Two-way grid nesting, flexi-nesting • Vertical nesting available but not recommended • Optional plume-in-grid for point source plumes	• Externally generated • Processors available for MM5, WRF, RAMS, TAPM
CMAQ	• Multiscale (urban to continental) • Horizontal projection: Lambert Conformal, Polar	• One-way grid nesting (coarse grid simulation provides boundary conditions	• Externally generated • Processors available for

Table 13: Model Attributes - Configuration

Model	Scale/Coordinate System	Nesting / Plume-in-grid	Meteorology
	Stereographic, Mercator (projection and resolution tied to meteorological data) • Vertical grid structure: terrain-following normalised pressure coordinate system	for inner grid) • Optional plume-in-grid for point source plumes (Karamchandani et al., 2010a; 2010b)	MM5, WRF
CHIMERE	• Multiscale (urban to continental) • Horizontal projection: Lambert Conformal, Polar Stereographic, Mercator, Lat-Lon • Vertical grid structure: hybrid normalised pressure coordinate system	• One-way grid nesting (coarse grid simulation provides boundary conditions for inner grid)	• Externally-generated • Processors available for MM5, WRF, IFS/ECMWF
TAPM / TAPM-CTM	• Urban scale • Horizontal projection: local Cartesian • Vertical grid structure: height-based terrain-following coordinate system	• One-way grid nesting (coarse grid simulation provides boundary conditions for inner grid)	• Internally generated by TAPM run in meteorological mode
CIT	• Urban scale • Horizontal projection: Universal Transverse Mercator • Vertical grid structure: height-based terrain-following coordinate system	• One-way grid nesting possible but typically applied for single grids	• Externally-generated (MM5, WRF)

The first three models (i.e. CAMx, CMAQ and CHIMERE) can be applied to scales ranging from urban (i.e. typical grid resolution of 1 to 5 km) to regional (i.e. typical resolution of 12 km) to continental (i.e. typical resolution of 36 km), while TAPM-CTM and CIT are urban scale models. With the exception of TAPM/TAPM-CTM, all the models use off-line meteorology (i.e. outputs of prognostic or diagnostic meteorological models).

Table 14 compares the chemistry capabilities of the different models.

Table 14: Model Attributes - Chemistry

Model	Gas-Phase Chemistry Mechanism/Solver	Aerosol Treatment	Other
CAMx	• Mechanisms: two versions of CB4; CB05; SAPRC-99 • Solvers: Euler Backward Iterative (EBI; Hertel et al., 1993); Implicit-Explicit Hybrid (IEH; Sun et al., 1994); LSODE (Hindmarsh, 1983)	• ISORROPIA inorganic aerosol partitioning • Secondary organic aerosol (SOA) formation and partitioning • Multi-section or static 2-mode size distribution	• Heterogeneous chemistry on particle surfaces • Aqueous sulfur chemistry • Mercury chemistry

Table 14: Model Attributes - Chemistry

Model	Gas-Phase Chemistry Mechanism/Solver	Aerosol Treatment	Other
CMAQ	• Mechanisms: CB05; CB05 with chlorine extensions; SAPRC-99 • Solvers: EBI; SMVGEAR (Jacobson and Turco, 1994); Rosenbrock (Sandu et al., 1997)	• ISORROPIA inorganic aerosol partitioning • SOA formation and partitioning • 3-mode size distribution (2 interacting fine particle modes and 1 coarse mode)	• Heterogeneous chemistry on particle surfaces • Aqueous sulfur chemistry and 2 organic oxidation reactions • Mercury chemistry
CHIMERE	• Mechanisms: MELCHIOR1; MELCHIOR2 • Solver: TWOSTEP (Verwer, 1994; Verwer et al., 1996)	• ISORROPIA inorganic aerosol partitioning • SOA formation and partitioning • Multi-section size distribution	• Heterogeneous chemistry on particle surfaces • Aqueous sulfur chemistry
TAPM / TAPM-CTM	• Mechanisms: Generic Reaction Set (GRS); Lurmann-Carter-Coyner (LCC); CB05 • Solver: Modified version of hybrid predictor-corrector scheme of Young and Boris (1977)	• MARS or ISORROPIA inorganic aerosol partitioning (MARS only for commercial version) • SOA formation and partitioning • 2-section size distribution	• Aqueous sulfur chemistry
CIT	• Mechanisms: Extended LCC; CACM; GRS (for Australia) • Solver: Hybrid predictor-corrector scheme of Young and Boris (1977)	• SCAPE2 inorganic aerosol partitioning • SOA formation and partitioning • Multi-section size distribution	• No information available

As shown in **Table 14**, all the models include fairly comprehensive and well documented gas-phase photochemical mechanisms, such as CB4 (Gery et al., 1989), CB05 (Yarwood et al., 2005), SAPRC99 (Carter, 2000), MELCHIOR1 and MELCHIOR2 (Latuatti, 1997), LCC (Lurmann et al., 1987) and the Caltech Atmospheric Chemistry Mechanism (CACM; Griffin et al., 2002b). TAPM/TAPM-CTM and the version of CIT used in Australia (Cope and Ischtwan, 1996) also offer the option of a simplified semi-empirical photochemical mechanism, the Generic Reaction Set (GRS; Azzi et al., 1992).

All the models include treatments for both inorganic aerosols and secondary organic aerosols. Three of the models (i.e. CAMx, CMAQ and CHIMERE) use the ISORROPIA model of Nenes et al. (1998; 1999) for the inorganic aerosol thermodynamics calculations.

ISORROPIA is also used in TAPM-CTM, but only in the research version that is used internally at CSIRO. The commercial version of TAPM-CTM uses the Model for an Aerosol Reacting System (MARS; Saxena et al., 1986). The CIT module uses the Simulating Composition of Atmospheric Particles at Equilibrium, Version 2 (SCAPE2; Meng et al., 1998) for its inorganic aerosol partitioning calculations. For the aerosol dynamics and size distribution, CAMx offers both a multi-section and a static bi-model option, CMAQ uses a modal representation, CHIMERE and CIT have multi-section size distributions, and TAPM-CTM uses a 2-section representation.

Additionally, **Table 14** shows that CAMx, CMAQ, CHIMERE and TAPM-CTM have some treatment of aqueous-phase reactions, primarily for the oxidation of SO_2 to sulphate in cloud droplets. However, there is no information available on aqueous-phase chemistry in the CIT model. As mentioned previously, there are several versions of the CIT model, and detailed documentation on the model formulation is both dated and sparse. All documented applications of the model make no mention of aqueous-phase chemistry or wet deposition.

Table 15 compares the model treatments for horizontal and vertical transport by the mean winds (advection) and parameterisations of sub-grid turbulent transport.

Table 15: Model Attributes - Transport and Mixing

Model	Transport	Mixing
CAMx	• Horizontal advection: Bott (1989); PPM (Colella and Woodward, 1984) • Vertical advection: Implicit backward-Euler (time) hybrid centred/upstream (space)	• Horizontal diffusion: K-theory 1st order closure (Smagorinsky, 1963) • Vertical diffusion: K-theory 1st order closure (K fields externally supplied via several options) or ACM2 non-local convection/diffusion (Pleim, 2007)
CMAQ	• Horizontal advection: PPM • Vertical advection: PPM with iterative Yamartino flux adjustments to maintain mass conservation	• Horizontal diffusion: K-theory 1st order closure (variant on Smagorinsky (1963)) • Vertical diffusion: K-theory 1st order closure (Byun and Ching, 1999) or ACM2 non-local convection/diffusion
CHIMERE	• Horizontal advection: simple first order upwind scheme; first order van Leer (1984) scheme; PPM • Vertical advection: first order upwind scheme	• Horizontal diffusion: N/A • Vertical diffusion: K-theory 1st order closure (Troen and Mahrt, 1986),deep convection (Tiedtke, 1989)
TAPM / TAPM-CTM	• Horizontal and vertical advection: Blackman constrained cubic scheme of Yamartino (1993)	• Horizontal diffusion: K-theory 1st order closure (Smagorinsky, 1963; Hess, 1989) • Vertical diffusion: K-theory (Draxler and Hess, 1997)
CIT	• Horizontal and vertical advection: Smolarkiewicz (1983); Galerkin (McRae et al., 1982); Quintic Spline Taylor-Series Expansion (QSTSE;	• Horizontal and vertical diffusion: K-theory 1st order closure

Table 15: Model Attributes - Transport and Mixing

Model	Transport	Mixing
	Nguyen and Dabdub, 2001) in UCI-CIT version	

Table 16 compares the removal processes (dry and wet deposition) in the various models. As mentioned above, it is not clear from the available documentation if the CIT model includes a treatment of wet deposition.

Table 16: Model Attributes - Removal Processes

Model	Dry Deposition	Wet Deposition
CAMx	Resistance model: 1) for gases: Wesely (1989) or Zhang et al. (2003) 2) for particles: Slinn and Slinn (1980) or Zhang et al. (2001)	In-cloud and below-cloud scavenging for gases and particles based on Seinfeld and Pandis (1998). Particle scavenging assumes complete absorption by cloud and rain water, gas scavenging depends on species solubility and rates of diffusive transfer
CMAQ	Resistance model, Pleim et al. (2001)	Scavenging coefficients for particles assuming complete absorption by cloud and rain water; wet deposition of gases calculated in aqueous chemistry module if they participate in the chemistry, otherwise in a separate scavenging module
CHIMERE	Resistance model: 1) for gases: Wesely (1989) 2) for particles: Giorgi (1986); Peters and Eiden (1992); Seinfeld and Pandis (1998); Zhang et al. (2001)	In-cloud and below-cloud scavenging for gases and particles based on Seinfeld and Pandis (1998); Mircea and Stefan (1998); Guelle et al. (1998); Loosmore and Cederwall (2004)
TAPM / TAPM-CTM	Resistance model based on Wesely (1989)	Scavenging coefficients (Seinfeld and Pandis, 1998; Draxler and Hess, 1977) with option of explicit calculation for species participating in aqueous chemistry
CIT	Resistance model (Russell et al., 1993)	No information available

Finally, **Table 17** compares advanced tools available in most current third-generation models that provide insights into model results, derive estimates of model sensitivity, and report source attribution.

Table 17: Model attributes - Probing and Analysis Tools

Model	Process Analysis	Sensitivity Analysis and Source Attribution
CAMx	• Integrated Processes Rate (IPR) analysis (Wang et al., 1995) • Integrated Reaction Rate (IRR) analysis (Jeffries and Tonnesen, 1994) • Chemical Process Analysis	• Ozone Source Apportionment Technology (OSAT); Yarwood et al. (1996) • Anthropogenic Precursor Culpability Assessment (APCA) • Particulate Source Apportionment Technology (PSAT); Wagstrom et al.

Table 17: Model attributes - Probing and Analysis Tools

Model	Process Analysis	Sensitivity Analysis and Source Attribution
	(CPA); Tonnesen and Dennis, 2000)	(2008) • Decoupled Direct Method (DDM); Dunker et al. (2002); Koo et al. (2007) • Higher-Order DDM (HDDM); Hakami et al. (2003); Cohan et al. (2005) • Reactive Tracer (RTRAC) Source Apportionment
CMAQ	• IPR analysis and IRR analysis (Jeffries and Tonnesen, 1994; Jang et al., 1995)	• HDDM-3D (Napelenok et al., 2006; 2008) • CMAQ-Adjoint (Hakami et al., 2007) • Sulfur Tracking • Primary Carbon Apportionment (Bhave et al., 2004) • Tagged Species Source Apportionment (TSSA; Wang et al., 2009)
CHIMERE	N/A	• CHIMERE-Adjoint (Menut, 2003; Menut et al., 2007)
TAPM / TAPM-CTM	N/A	N/A
CIT	N/A	• DDM-3D (Yang et al., 1997) • CIT-Adjoint (Martien et al., 2006)

2.4.9 Summary of Findings

A summary of the key features of the following models is provided below:

- CAMx;
- CMAQ;
- CHIMERE;
- TAPM/TAPM-CTM; and
- CIT.

The CAMx and CMAQ models account for virtually all of the ozone assessment modelling currently performed in the US. The CIT and TAPM models are relevant because they are used in Australia. The CHIMERE model is probably the most widely used photochemical model which has been developed in Europe.

Although, there are some important differences among the models listed above, they also share some common features. For example, all these models are source-oriented, Eulerian models that represent the atmosphere as a three-dimensional fixed grid, and simulate the transport, transformation and removal of air pollutants by solving the conservation of mass equation for this grid.

All the models incorporate atmospheric chemistry modules to describe the conversion of emitted pollutants to secondary pollutants such as ozone. The above models are also referred to as “third-generation” chemical transport models.

The differences among the models lie in their:

- Representation of the governing processes, such as transport, chemistry and removal;
- Numerical solution of the transport and chemistry equations;
- Meteorological inputs;
- Grid configurations; and
- Ancillary capabilities such as source attribution, grid-nesting, and resolution of point source plumes.

3. Development and Analysis of Level 1 Screening Procedure

3.1 Introduction

This section documents the development and analysis of the Level 1 screening procedure for estimating ground-level ozone impacts from stationary sources of CO, CH_4, NO_X and VOC.

As summarised in **Section 2.5**, the only tools now in widespread use for estimating ozone impacts are photochemical grid models (PGMs). Thus, the methodology for the Level 1 screening procedure is based on PGM simulations conducted specifically for the GMR. As discussed in **Section 2.2**, simplified modelling approaches based on plume or box models, such as the Scheffe Tables, have serious technical limitations which caused USEPA to retract these tools.

To develop a robust modelling approach that can be implemented in a simple to use format such as a spreadsheet or database, ENVIRON has elected to use the decoupled direct method (DDM) for sensitivity analysis to achieve this goal. When DDM is applied to compute higher order sensitivities, as in the development of the Level 1 screening procedure, it is abbreviated as HDDM.

3.2 Model and Input Data

3.2.1 Model Selection

The CAMx model (ENVIRON, 2010) was selected because it can be applied to the GMR airshed using data available for this study and includes features essential to the proposed methodology (i.e. HDDM).

A detailed overview of CAMx is provided in **Section 2.5.2**. CAMx is an Eulerian photochemical dispersion model that allows for integrated “one-atmosphere” assessments of gaseous and particulate air pollution and can be applied to scales ranging from urban to continental. A “third-generation” chemical transport model, CAMx incorporates atmospheric chemistry modules to describe the conversion of emitted pollutants to secondary pollutants such as ozone. It has treatments for both inorganic aerosols and secondary organic aerosols and additionally can treat aqueous-phase reactions, primarily for the oxidation of SO_2 to sulphate in cloud droplets.

CAMx is one of two multi-scale photochemical CTMs that are used extensively in the US for ozone, visibility and PM policy decisions. A publicly available open-source computer modelling system, CAMx has a current User’s Guide and training is available for this model.

3.2.2 Chemical Mechanism

The 2005 version of the Carbon Bond chemical mechanism (CB05) was selected. CB05 supersedes the CB4 mechanism and should be used rather than CB4. CB05 has been evaluated against smog chamber data and has been used in multiple photochemical models (e.g. CAMx and CMAQ). Key attributes of CB05 are discussed in **Section 2.4**. The application of CB05 for modelling tropospheric ozone in Australia is justified given that it has been peer-reviewed and used in peer-reviewed ozone modelling studies.

The Air Emission Inventory for the Greater Metropolitan Region in NSW (DECC, 2007a) has been compiled for the CB4 mechanism. However, CB4 emission inventories can be used with CB05 without causing any problems because CB05 is backwards compatible with CB4. When new sources were added to develop the screening tool, their VOC emissions were speciated for the CB05 mechanism.

3.2.3 Geographical Extent of Modelling Domain

The CAMx modelling domain is compatible with the gridded emission inventory (DECC, 2007a) and meteorological input data provided by OEH, which are discussed below. The CAMx domain corresponds to the GMR.

The GMR is defined as an area covering 57,330 km^2, which includes the greater Sydney, Newcastle and Wollongong regions. **Figure 2** shows the GMR and Sydney, Newcastle and Wollongong regions. Approximately 76% of the NSW population resides in the GMR.

Although the GMR inventory is based on a 1 km by 1 km grid resolution, a computational grid resolution of 3 km by 3 km has been adopted within CAMx. This represents the resolution typically used for urban scale modelling. A 3 km by 3 km grid resolution is also consistent with the resolution of the meteorological input data.

Source: DECC, 2007a

Figure 2: GMR Modelling Domain and the Sydney, Newcastle and Wollongong regions

3.2.4 Meteorological Data

Meteorological input data has been developed by OEH using TAPM as summarised in **Table 18** and reformatted for input to CAMx.

Meteorological data was provided for the GMR, at a grid resolution of 3 km by 3 km, with 25 vertical levels extending up to 8,000 m aloft.

TAPM was run in data assimilation mode, referencing local observations from OEH meteorological monitoring sites within the modelling domain (refer **Figure 11**, **Figure 12** and **Figure 13**).

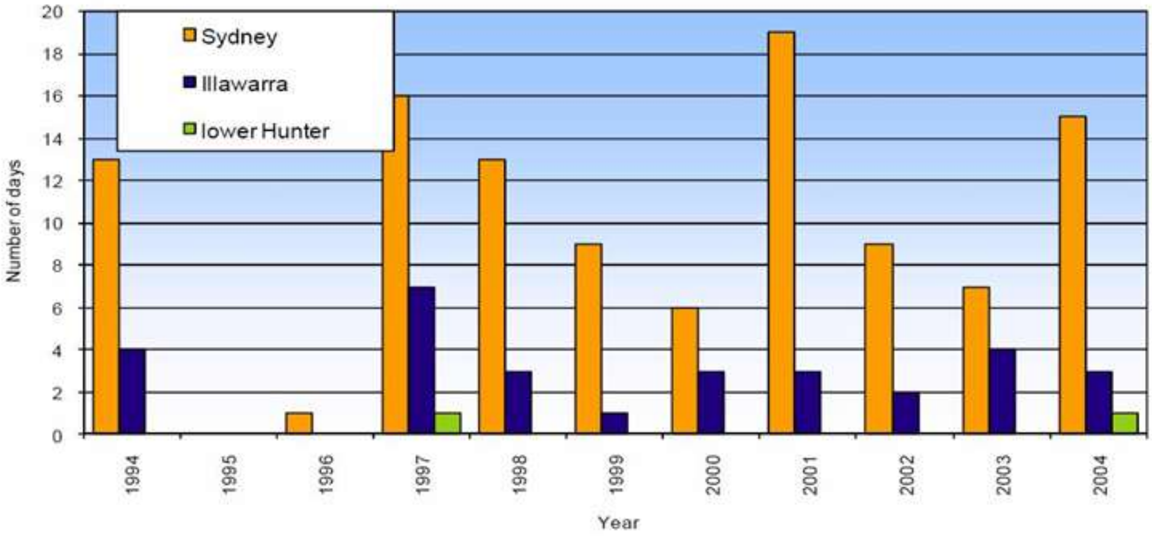
Table 18: Model Inputs – Meteorology

	TAPM (v 4)
Number of grids (spacing)	3 (4 km, 3 km, 2 km)
Number of grid points	70 x 90 x 25
Vertical Levels	10m, 25m, 50m, 100m, 150m, 200m, 250m, 300m, 400m, 500m, 750m, 1000m, 1250m, 1500m, 1750m, 2000m, 2500m, 3000m, 3500m, 4000m, 5000m, 6000m, 7000m, 8000m
Time Periods	December 2003 – January 2004, December 2004 - January 2005,
Centre of analysis	315000 E, 6295500 S (UTM, WGS84 Projection, Zone 56S)
Data assimilation	All OEH meteorological monitoring sites within the modelling domain.

For computational efficiency, two ozone seasons (i.e. December – January; 2003-4 – 2004-5) have been selected as inputs within the development of the procedures. The rationale for the selection of these ozone seasons is provided below.

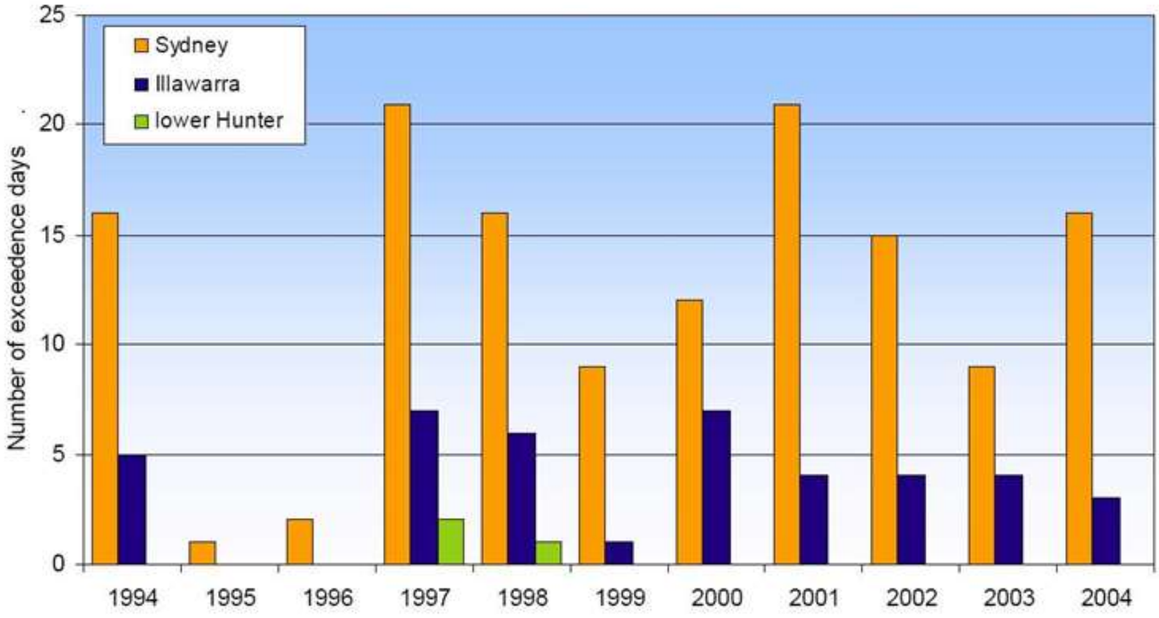
The December 2003 – January 2004 ozone season was selected to capture those meteorological conditions where significant transport of ozone precursors was known to occur between the Sydney and Illawarra airsheds. During this period, four exceedances of the 1-hour Air NEPM ozone standard were observed (DECCW, 2010b).

The December 2004 – January 2005 ozone season was selected based on an evaluation of ambient ozone monitoring trends by year, as shown in **Figure 3** and **Figure 4**.



Source: DECCW, 2010b.

Figure 3: Number of Days Exceeding the NEPM 1-hour Ozone Concentration by Year



Source: DECCW, 2010b.

Figure 4: Number of Days Exceeding the NEPM 4-hour Ozone Concentration by Year

Figure 3 and **Figure 4** indicate that, to capture the meteorology likely to cause exceedances of the Air NEPM ozone standards, the December 2001 – January 2002 and December 2004 – January 2005 ozone seasons are good candidates for development of the procedures.

However, the 2001-2002 ozone season is known to have been influenced by additional precursors associated with bushfire events. It is anticipated that bushfires near Sydney in the summer of 2001-2002 contributed to five of the 19 exceedances of the 1-hour Air NEPM ozone standard in that year (DECCW, 2010b). Thus, the December 2004 to January 2005 ozone season was selected for input, as this has the next highest number of ozone exceedance days, and is not anticipated to be significantly impacted by bushfire events.

3.2.5 Emission Inventory Data

Emission inventory data for anthropogenic sources was provided by OEH based on the 2003 Air Emission Inventory for the NSW GMR (DECC, 2007a). The emissions inventory data are summarised in **Table 19**. The gridded area and point source emissions provided by OEH have been reformatted for input to CAMx. Biogenic emissions (i.e. soil NO_x and tree canopy and pasture VOC) have been developed separately and merged with the anthropogenic emissions provided by OEH.

Table 19: Model Inputs – Emissions Inventory

2003 Air Emission Inventory for the GMR (DECC, 2007a)	
Domain	GMR (refer **Figure 2**)
Photochemical Mechanism Lumping	CBIV
Months	December, January
Scenario Days	Weekday, Weekend
Grid Resolution	1 km x 1 km
Point Source File	All point source emissions from commercial and industrial sources
Vehicle Emission File	All area source emissions from on-road mobile sources
Area Source File	All area source emissions and fugitive emissions from biogenic (with exclusions), commercial, domestic, industrial and off-road mobile sources
Exclusions	Bushfires / prescribed burning and biogenic (i.e. soil NO_x and tree canopy and pasture VOC) – refer **Section 3.2.6**.

3.2.6 Biogenic Emissions

The biogenic emission data available from OEH represents diurnal emission profiles for each 1 km by 1 km grid cell, averaged by month. However, for the current application, date specific (temperature driven) biogenic emissions have been used.

ENVIRON used MEGAN (Model of Emissions of Gases and Aerosols from Nature) to calculate biogenic emissions within the GMR. MEGAN computes emissions for plant functional types as a function of temperature, solar radiation, leaf area index and leaf age. Fractional coverage for each plant functional type and vegetation-specific emission factors are based on the MEGAN 1 km by 1 km land cover data, informed by satellite imagery

(Sakulyanontvittaya, 2008; Guenther et al., 2006). Temperature and total solar radiation data for MEGAN have been obtained from TAPM.

Biogenic emission estimates from MEGAN and the Air Emission Inventory for the NSW GMR have been compared as documented in **Appendix 3**. On the basis of this comparison, it was decided to use MEGAN with isoprene emissions reduced by 50%.

It is noted that ozone precursor emissions from bushfire events and prescribed burns have not been included in the CAMx modelling. Although the Air Emissions Inventory for the NSW GMR includes emissions from bushfires and prescribed burns, ozone precursor emissions from such events have not been included in the assessment so that model performance was not confounded on days when such events greatly influenced air quality in the GMR. However, in comparing predicted concentrations to ambient measurements, model performance may be confounded for days when fires influence air quality in the GMR.

3.2.7 Model Boundary Conditions

Boundary conditions are needed to specify background concentrations of ozone, CO, NO_X and VOC at the extremes of the GMR modelling domain. Boundary concentrations are most influential for species with long atmospheric lifetimes and significant background concentrations (i.e. ozone and CO). Background concentrations for the GMR have been assessed from ambient data (Cope et al, 2008, Duc and Azzi, 2009, Vingarzan, 2004). OEH (Pers. Comm. Hiep Duc) advised that ozone background concentration should be 20-30 ppb and noted that in Sydney the average ozone background level is about 20 ppb but is increasing.

Date specific boundary conditions have been obtained from the global model MOZART (Model for Ozone and Related chemical Tracers; Emmons et al., 2010) available from the (US) National Center for Atmospheric Research (NCAR). The ozone boundary conditions from MOZART are consistent with the 20-30 ppb concentration recommended by OEH.

3.3 Decoupled Direct Method (DDM)

The DDM is an efficient and accurate method for computing sensitivity coefficients that can be applied within a PGM (Dunker, 1981; Dunker et al, 2002). The sensitivity coefficients are partial derivatives between model output (O) and input (I) parameters ($\partial O/\partial I$) and may, for example, describe the relationship between ozone and emissions from a single source ($\partial O_3/\partial E$) which is applicable to this project.

A first order sensitivity coefficient ($\partial O_3/\partial E$) describes a linear relationship between ozone and emissions, but ozone formation is known to be a non-linear process. Therefore, higher order sensitivity coefficients (e.g. $\partial^2 O_3/\partial E^2$) are useful for describing this relationship more accurately (Hakami et al., 2003). When DDM is applied to compute higher order sensitivities, it is abbreviated as HDDM. Both DDM and HDDM are available in CAMx.

Operationally, DDM (and HDDM) can calculate multiple sensitivity coefficients within a single PGM simulation. This means that a single run of the CAMx model can compute all of the sensitivity coefficients that are needed for the Level 1 screening procedure.

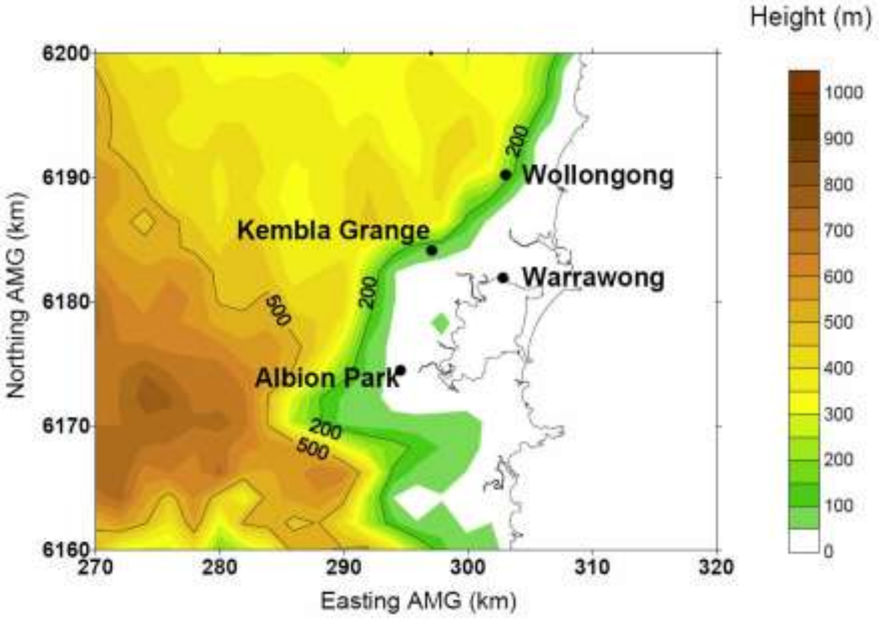
3.4 New Source Locations

Based on the spatial distribution of NO_x and VOC sources within the GMR air shed, five potential new source locations have been determined as part of the Level 1 screening procedure.

These comprise one source location within the Illawarra air region (**Figure 5**), one source location within the Lower Hunter air region (**Figure 6**), and three locations within the Sydney air region, including:

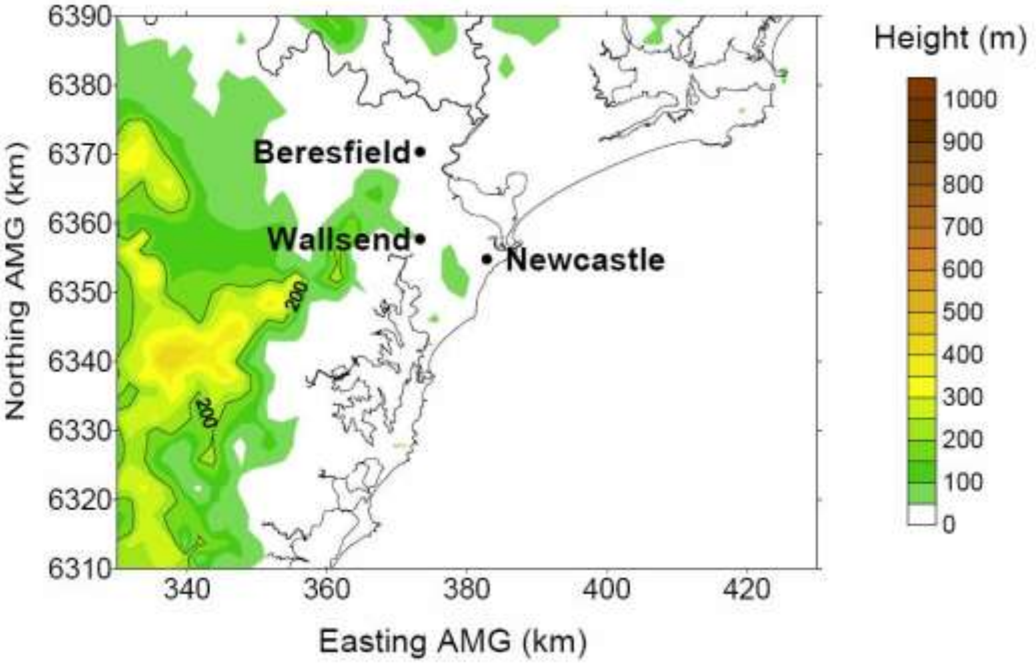
- Sydney West;
- Sydney Central; and
- Sydney East

The regional boundaries of these locations are consistent with those used by OEH for the evaluation of how far towards the NO_X-limited regime photochemistry has progressed (DECCW, 2010b), as reproduced in **Figure 7**.



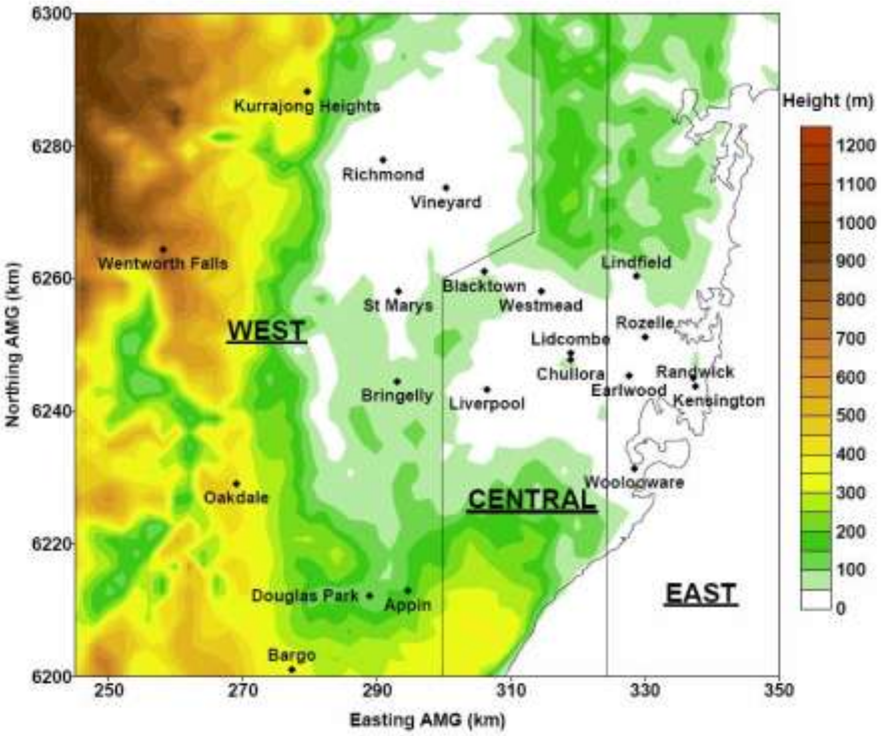
Source: DECCW, 2010b.

Figure 5: Illawarra Air Region



Source: DECCW, 2010b.

Figure 6: Lower Hunter Air Region



Source: DECCW, 2010b.

Figure 7: Regional Boundaries Defined by OEH for Photochemical Regime Analysis

The five locations have been determined by finding the Weighted Mean Centre (WMC) for all fugitive/point industrial sources of NO_x and VOC within each of the five air regions.

The equation to determine the coordinates of the WMC for each region is as follows:

$$\bar{X}_w = \frac{\sum_{i=1}^{n} w_i x_i}{\sum_{i=1}^{n} w_i}, \bar{Y}_w = \frac{\sum_{i=1}^{n} w_i y_i}{\sum_{i=1}^{n} w_i}$$

Where,

$\bar{X}_w$ = WMC Easting Coordinate

$\bar{Y}_w$ = WMC Northing Coordinate

W_i = Emissions (kg/year) for pollutant/source type i

X_i = Easting coordinate for pollutant/source type i

Y_i = Northing coordinate for pollutant/source type i

In this manner, a probabilistic approach has been used to derive the likely location of any future source of ozone precursors within each of the above regions.

The coordinates for the five calculated WMC locations and the (weighted) sum of annual ozone precursor (NO_x and VOC) emissions is presented within **Table 20**.

Table 20: Calculated WMC Locations for Major GMR Air Regions

GMR Air Region	Location (m, MGA56)		Annual Emissions - NO_x and VOC (tpa)
	Easting	Northing	
Sydney East	334328	6237782	9,834
Sydney Central	315087	6248465	11,386
Sydney West	288217	6232623	6,840
Newcastle	382452	6359948	3,002
Wollongong	305546	6183844	8,716

Figure 8 illustrates the location and weighted magnitude of emission of each of the five calculated locations.

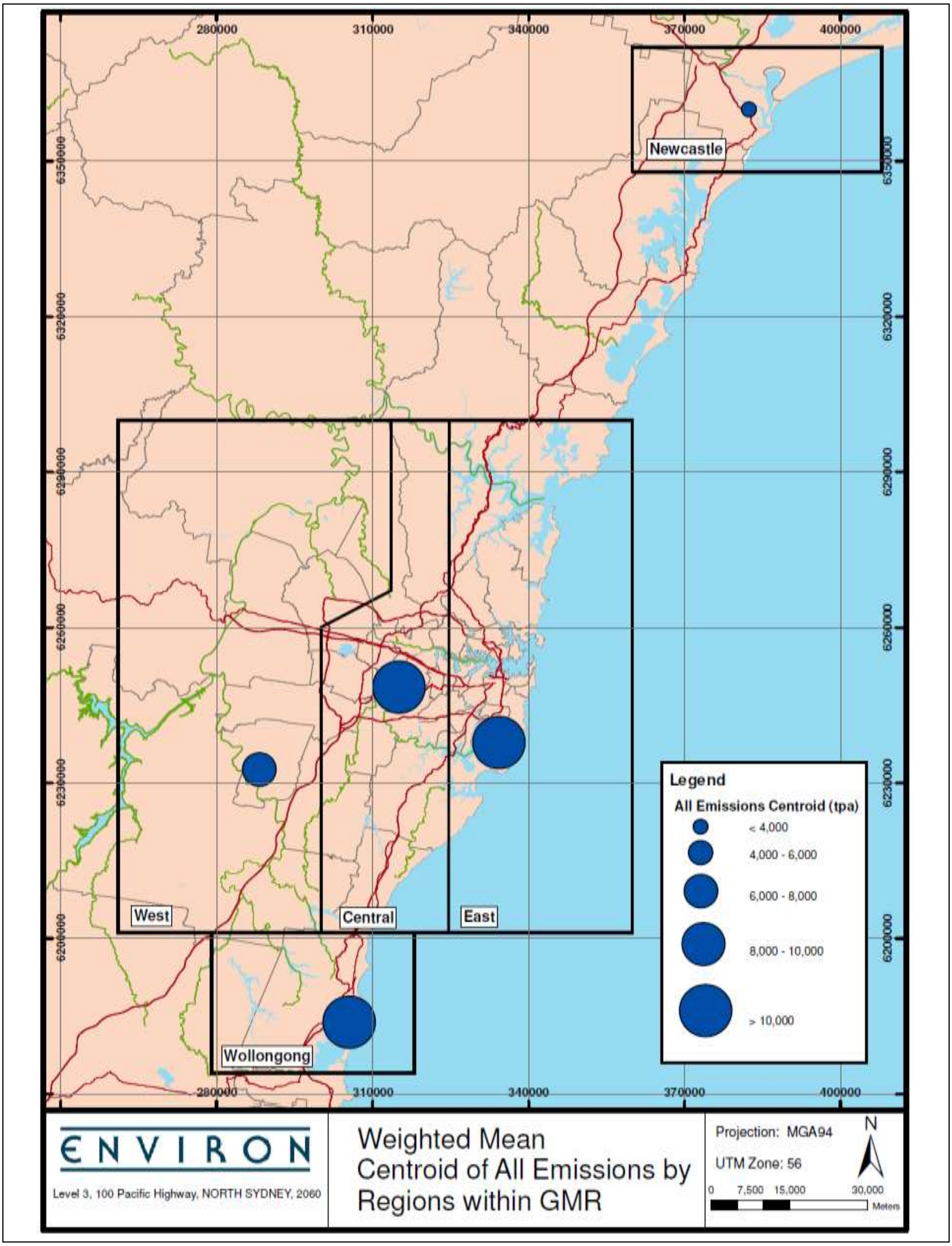


Figure 8: Weighted Mean Centroids of Emissions by Region within the GMR

Within the Sydney air region, the WMC coordinates do not fall within appropriate land use zones. The Sydney East WMC is located within Botany Bay, while the Sydney Central and West WMCs fall within residential and rural areas respectively.

Since the Sydney WMC coordinates do not fall within an existing industrial zone, coordinates have been adjusted so that each simulated new source is located within the closest significant industrial area. In the case of the Newcastle and Wollongong air regions, these locations fall within existing industrial zones and therefore do not need to be adjusted. The derived new source locations, along with their respective industrial areas and distances from the original WMC locations are presented within **Table 21**.

Table 21: Derived New Source Locations and Corresponding Industrial Area Regions

GMR Air Region	Location (m, MGA56)		Distance Between Source Location and WMC	Industrial Area
	Easting	Northing		
Sydney East	336000	6239500	2.4km	Port Botany
Sydney Central	311000	6252000	5.4km	Yennora/Smithfield
Sydney West	288217	6232623	10.2km	Appin
Newcastle	382452	6359948	N/A [1]	Mayfield
Wollongong	305546	6183844	N/A [1]	Port Kembla

Note 1: Unadjusted from original WMC coordinates

Figure 9 shows the location of the WMC points within the Sydney air region relative to their final new source location, adjusted for land use.

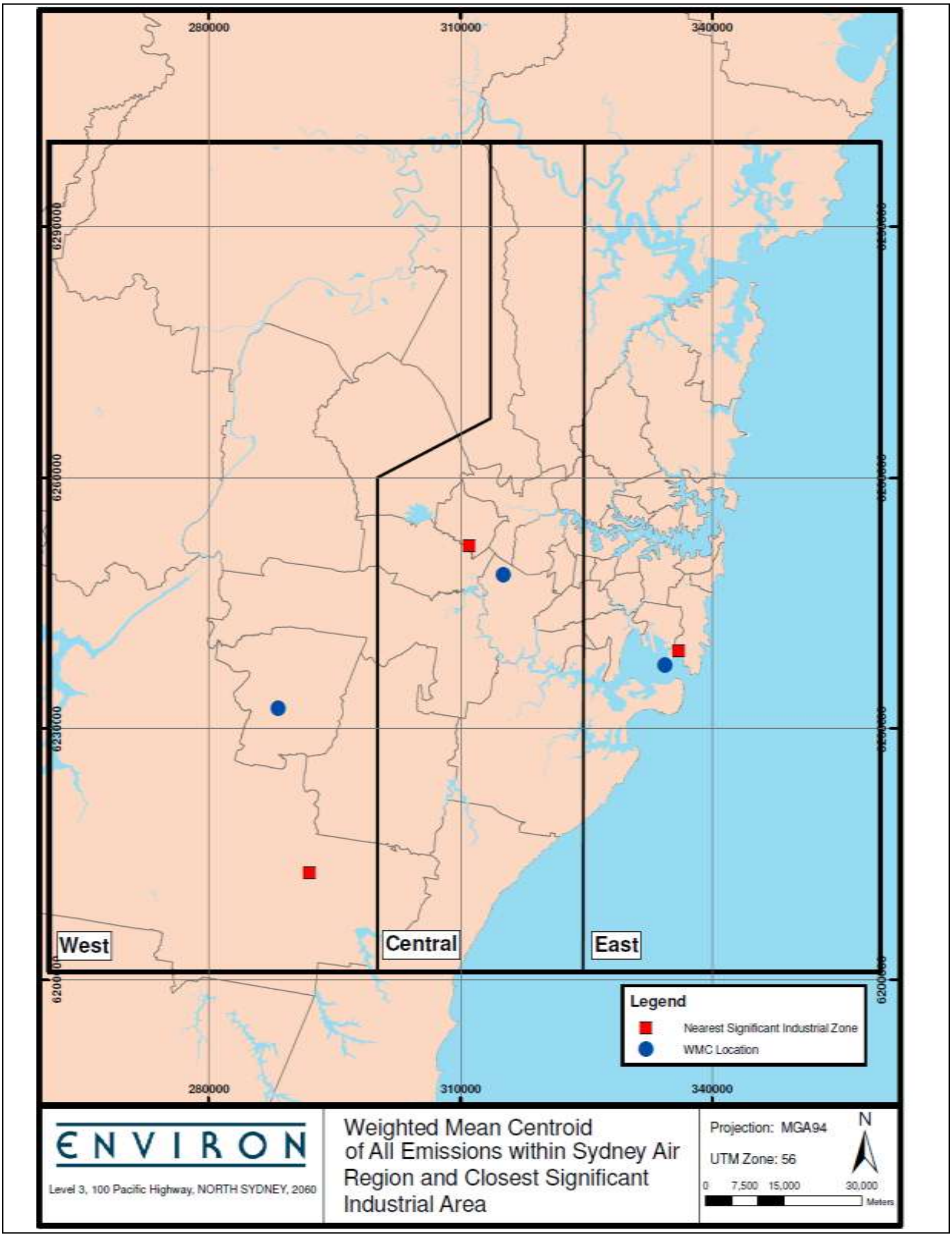


Figure 9: Location of Weighted Mean Centres and Final (Land Use Adjusted) Locations within Sydney Air Region

In terms of characterising the likely make up of any new source of ozone precursors, it is instructive to examine the relative contribution to total (weighted) annual emissions of ozone precursors.

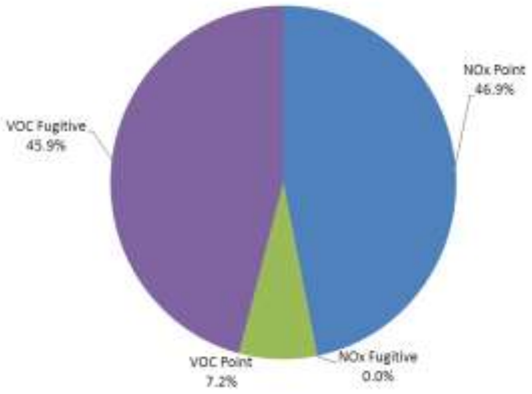
A summary of the weighted contributions of ozone precursors (i.e. point and fugitive NO_x and VOC) for each of the five WMC locations are presented within **Figure 10**.

Figure 10 indicates that point sources of NO_x are routinely the dominant contributor to annual emissions from industrial sources across all five air regions, ranging from 34% in Sydney Central to 91% in Wollongong.

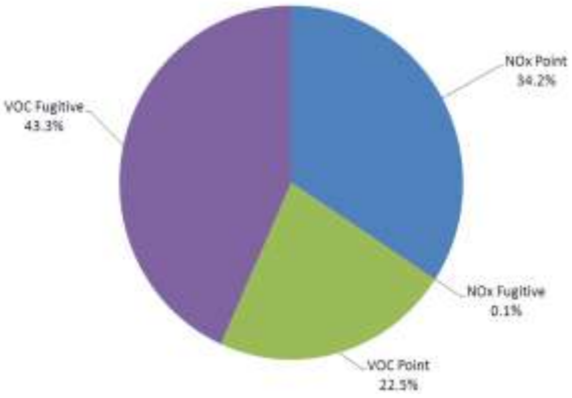
Fugitive sources of VOC are significant in the Sydney East, Sydney Central and Newcastle air regions, contributing to 46%, 43% and 23% respectively. The contribution of point sources of VOC varies across all regions, ranging from 7% in Sydney East to 23% in Sydney Central. Sources of fugitive NO_x emissions are comparatively insignificant in the five air regions of the GMR air shed.

The mass ratio of VOC to NO_x emissions in the overall GMR inventory is 0.68 whereas for point sources alone the ratio is 0.22. Point sources have a lower VOC to NO_x ratio than the overall inventory because of large NO_x emissions from a small number of point sources. Focussing just on point sources with emissions (VOC + NO_x) less than 500 tonnes/year, the mass ratio of VOC to NO_x emissions is 1.24 which on a molar basis is equivalent to a VOC to NO_x ratio of 3.9 (mole C/mole NO_x).

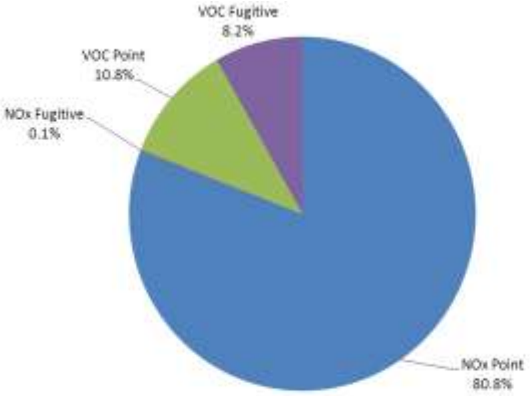
Sydney East



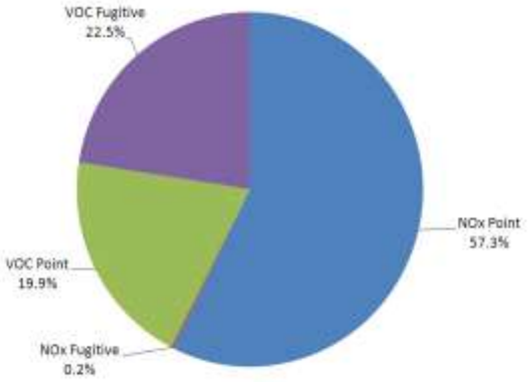
Sydney Central



Sydney West



Newcastle



Wollongong

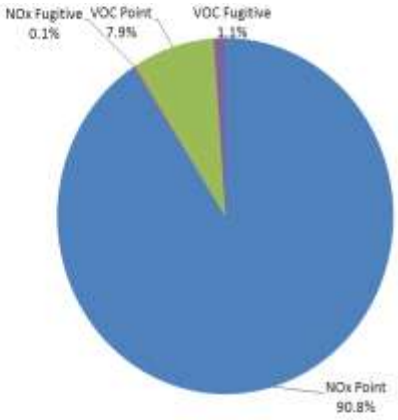
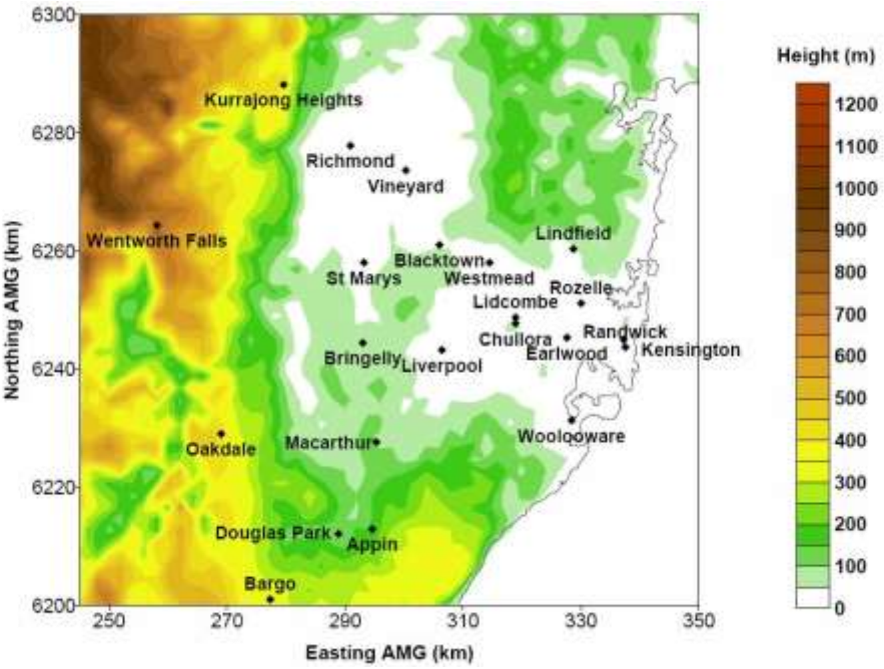


Figure 10: Relative Contribution to Emissions of Ozone Precursors at Derived WMC Locations

3.5 Ambient Monitoring Data

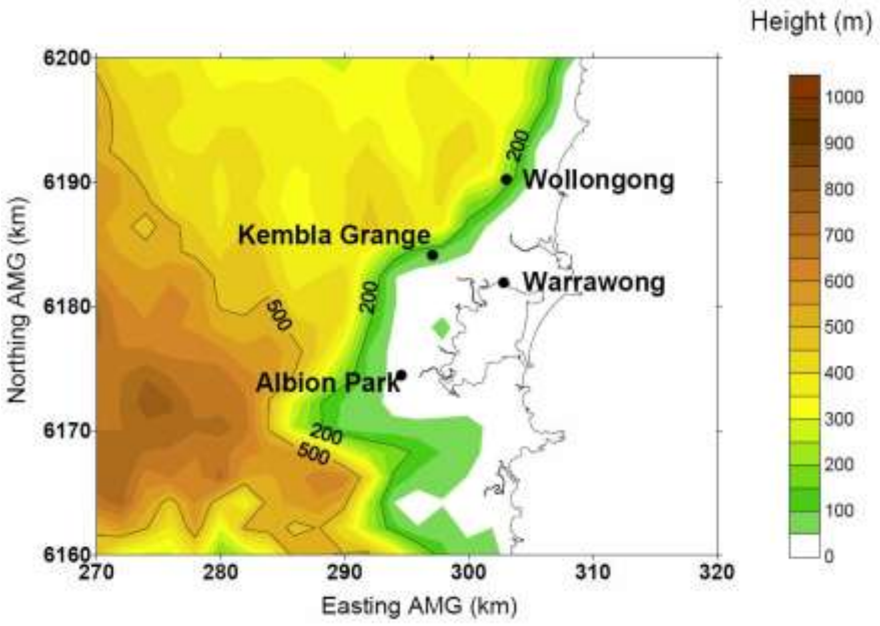
Ambient ozone monitoring data for all locations within the GMR are referenced within the Level 1 screening procedure tool. Locations of monitoring sites are shown within **Figure 11**, **Figure 12** and **Figure 13**.

Ambient ozone monitoring data provide the basis for assessing the overall ozone impact due to additional sources using data from the closest ambient monitoring site.



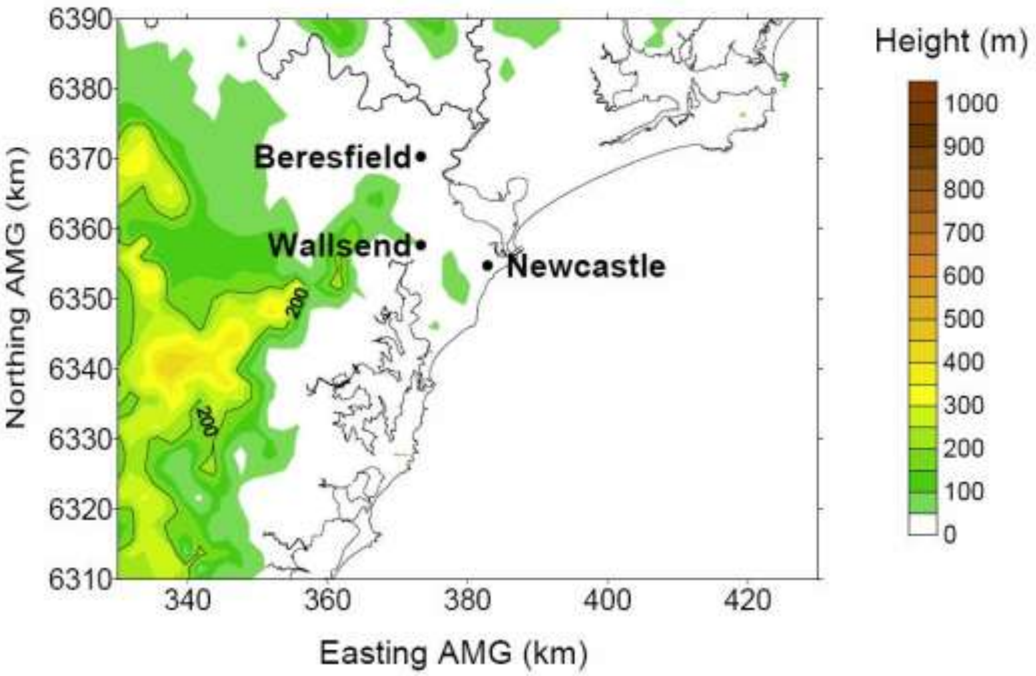
Source: DECCW, 2010b.

Figure 11: OEH Ambient Monitoring Stations within the Sydney Air Region



Source: DECCW, 2010b.

Figure 12: OEH Ambient Monitoring Stations within the Illawarra Air Region



Source: DECCW, 2010b.

Figure 13: OEH Ambient Monitoring Stations within the Lower Hunter Air Region

3.6 Level 1 Screening Procedure Overview

The Level 1 screening procedure has been developed from CAMx simulations for the NSW GMR airshed. Simulations have been performed for two ozone seasons (2003/4 and 2004/5) with and without new sources added to identify days on which the new sources have high ozone impacts. The days have been selected on the basis of enhanced ozone in the GMR (DECCW, 2010b) and a demonstration of acceptable model performance. The selected high ozone impact days have then been used for CAMx simulations, with the higher order Decoupled Direct Method (HDDM) used to calculate sensitivity coefficients of ozone to the additional NO_X and/or VOC emissions from a new source. .

The sensitivity coefficients have been embedded in the Level 1 screening procedure tool that can estimate ozone impacts for sources with different emissions of NO_X and/or VOC This screening procedure approximates to second order accuracy the result of running CAMx to assess the source impact.

An advantage of the Level 1 screening procedure is its close correspondence to the Level 2 refined procedure discussed in **Section** 4. If a source fails to pass the Level 1 assessment, a new CAMx (or other PGM) model run may be performed to assess the ozone impact of the source emissions. The new PGM run can use the modelling databases already developed for the Level 1 assessment.

3.6.1 Source Characteristics

Representative sources have been used to develop the Level 1 screening procedure tool. Five locations have been selected as discussed in **Section 3.4**, and as shown in **Table 22**.

Table 22: Derived New Source Locations and Corresponding Industrial Area Regions

GMR Air Region	Location (m, MGA56)		Industrial Area
	Easting	Northing	
Sydney East	336000	6239500	Port Botany
Sydney Central	311000	6252000	Yennora/Smithfield
Sydney West	288217	6232623	Appin
Newcastle	382452	6359948	Mayfield
Wollongong	305546	6183844	Port Kembla

The source type was selected conservatively (i.e. to obtain the greatest ozone impact) by choosing a ground-level release rather than an elevated source, and by releasing both NO_X and VOC together. Additional source characteristics are detailed in **Table 23.**

Table 23: New Source Characteristics

Parameter	Characteristic
Source Type	Ground-level point source
Combined VOC-NO_X Emission Rate	500 tonnes/annum
VOC/NO_x ratio	1.24 [1]
VOC Speciation Profile	USEPA SPECIATE Profile Number 0000, normalised after removing methane, unreactive, unknown or non-volatile compounds [2]

Note 1: Average for point sources in the GMR inventory with less that 500 tonnes/year of emissions. Resulting emission rates are 0.61 tonne/day for NO_X and 0.76 tonne/day for VOC.

Note 2: Refer to **Section 3.6.4.1**.

3.6.2 Sensitivity Coefficients for the Level 1 Screening Procedure Tool

The procedure for computing sensitivity coefficients for the Level 1 screening procedure is as follows:

1. CAMx was run for two recent ozone seasons (i.e. December and January; 2003/4 and 2004/5) in the GMR with and without the five new sources.

2. For each new source, the days when the new source caused high ozone impacts have been identified, considering both 1-hour and 4-hour ozone averages. The selected days had enhanced ozone in the GMR (DECCW, 2010b) and acceptable model performance.

3. For each new source on each of the selected high ozone days, up to 100 grid cells downwind of the new source with the greatest increase in daily maximum ozone have been identified. From this pool, the 300 grid cells with the largest ozone increases have been selected. Grid cells located over the Pacific Ocean have been excluded from the 300 (**Table 24**).

4. CAMx was run again with HDDM applied to each new source to calculate first and second order ozone sensitivities to NO_X and VOC emissions from each source. This produced sets of 5 first and second-order sensitivity coefficients for each new source:

$$
\begin{aligned}
S^1_{NOx} &= \partial O_3/\partial NO_x \\
S^1_{VOC} &= \partial O_3/\partial VOC \\
S^2_{NOx} &= \partial^2 O_3/\partial NO_x^2 \\
S^2_{VOC} &= \partial^2 O_3/\partial VOC^2 \\
S^2_{NOxVOC} &= \partial^2 O_3/\partial NO_x \cdot \partial VOC
\end{aligned}
$$

These coefficients have been saved for each of the 300 grid cells for each source (300 grid cells x 5 sources x 5 coefficients = 7,500 coefficients in total). The number of sensitivity coefficients doubled to 15,000 since both 1-hour and 4-hour ozone averages have been included.

5. CAMx was run again with HDDM applied to each new source to calculate first order ozone sensitivities to emissions of individual CB05 VOC and CO. For each source, this produced sets of 15 first-order sensitivity coefficients:
   $dO_3/dALD2$
   $dO_3/dALDX$
   $dO_3/dETH$
   $dO_3/dETHA$
   $dO_3/dETOH$
   $dO_3/dFORM$
   $dO_3/dIOLE$
   $dO_3/dISOP$
   $dO_3/dMEOH$
   $dO_3/dOLE$
   $dO_3/dPAR$
   $dO_3/dTERP$
   $dO_3/dTOL$
   $dO_3/dXYL$
   dO_3/dCO

   These coefficients have been saved (45,000 for 1-hour and 4-hour ozone averages) for use in the VOC reactivity adjustment discussed below.

Table 24: Dates contributing to the 300 grid cells selected for each source

Source/Date	Number of grid cells used for 1-hr ozone	Number of grid cells used for 4-hr ozone
Sydney East		
27-Jan-04	69	33
28-Jan-04	89	70
3-Jan-05	100	100
14-Jan-05	42	97
Sydney Central		
1-Jan-04	97	82
27-Jan-04	29	41
28-Jan-04	65	77
3-Jan-05	85	24
14-Jan-05	24	76
Sydney West		
1-Jan-04	100	100
28-Jan-04	49	10
3-Jan-05	100	60
14-Jan-05	51	69
Newcastle		
11-Dec-03	68	19
5-Jan-04	22	66
11-Jan-04	86	99
27-Jan-04	84	78
28-Jan-04	40	38

Table 24: Dates contributing to the 300 grid cells selected for each source

Source/Date	Number of grid cells used for 1-hr ozone	Number of grid cells used for 4-hr ozone
Wollongong		
1-Jan-04	96	98
10-Jan-04	70	49
27-Jan-04	47	47
28-Jan-04	59	52
1-Jan-05	28	54

3.6.3 Negative Reactivities

The first order sensitivities $dO_3/dVOC$ for each source location are summarized in **Figure 14** for both 1-hr and 4-hr average ozone. The reactivities shown are averages for the 300 grid cells included in the Level 1 screening procedure.

Alkenes (represented in CB05 by model species ETH, OLE, IOLE and ISOP) consistently have the highest reactivity ($dO_3/dVOC$) because they react rapidly and form reactive products such as radicals and formaldehyde.

Formaldehyde (FORM) also has consistently high reactivity because it photolyzes to produce radicals. Alkanes (i.e. PAR and ETHA) and alcohols (i.e. MEOH and ETOH) consistently have low reactivity because they react slowly. The reactivity of aromatics (i.e. TOL and XYL) and higher aldehydes (i.e. ALD2 and ALDX) varies by location and can be either positive or negative.

Negative reactivities occur when VOC degradation reactions tend to sequester NO_x and ozone formation is limited by the availability of NO_x. Higher aldehydes sequester NO_x by forming peroxy acyl nitrate (PAN) compounds. Aromatics, in particular toluene, sequester NO_x by forming organic nitrates such as nitrocresols (Calvert et al., 2002). Negative reactivities are most prevalent for the Sydney West source which is located downwind of Sydney.

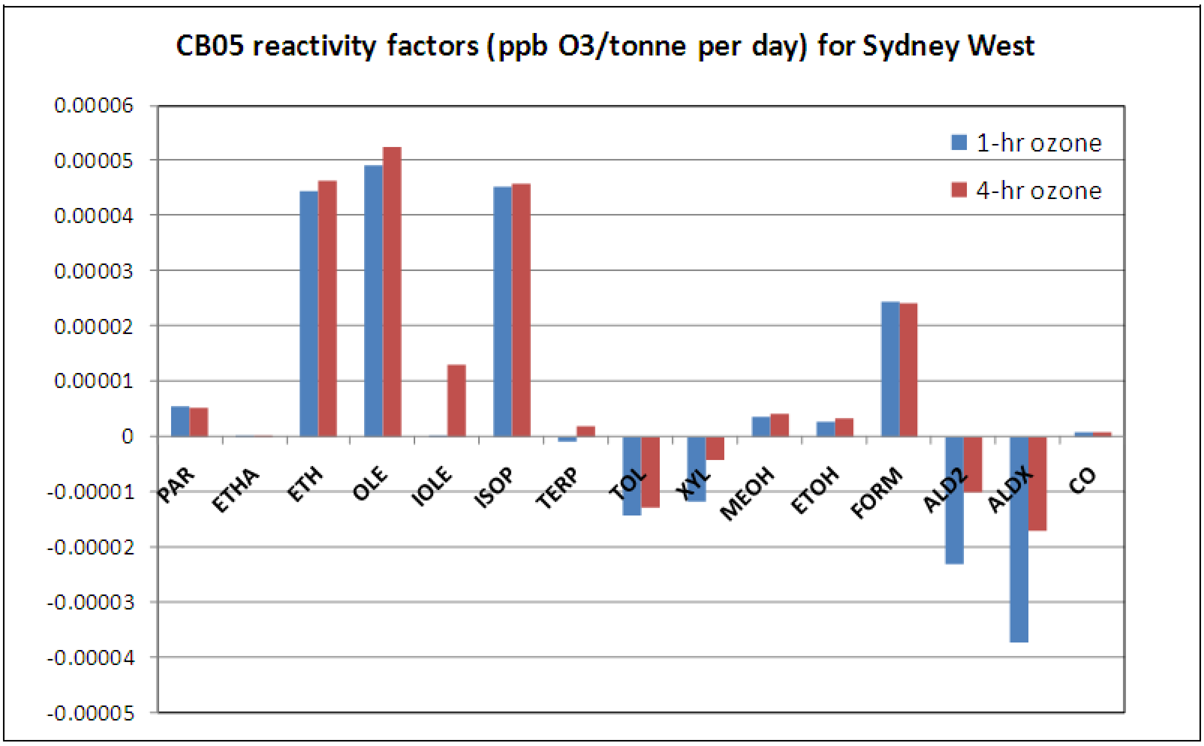


Figure 14 (a): First order sensitivities $dO_3/dVOC$ for Sydney West for both 1-hr and 4-hr average ozone

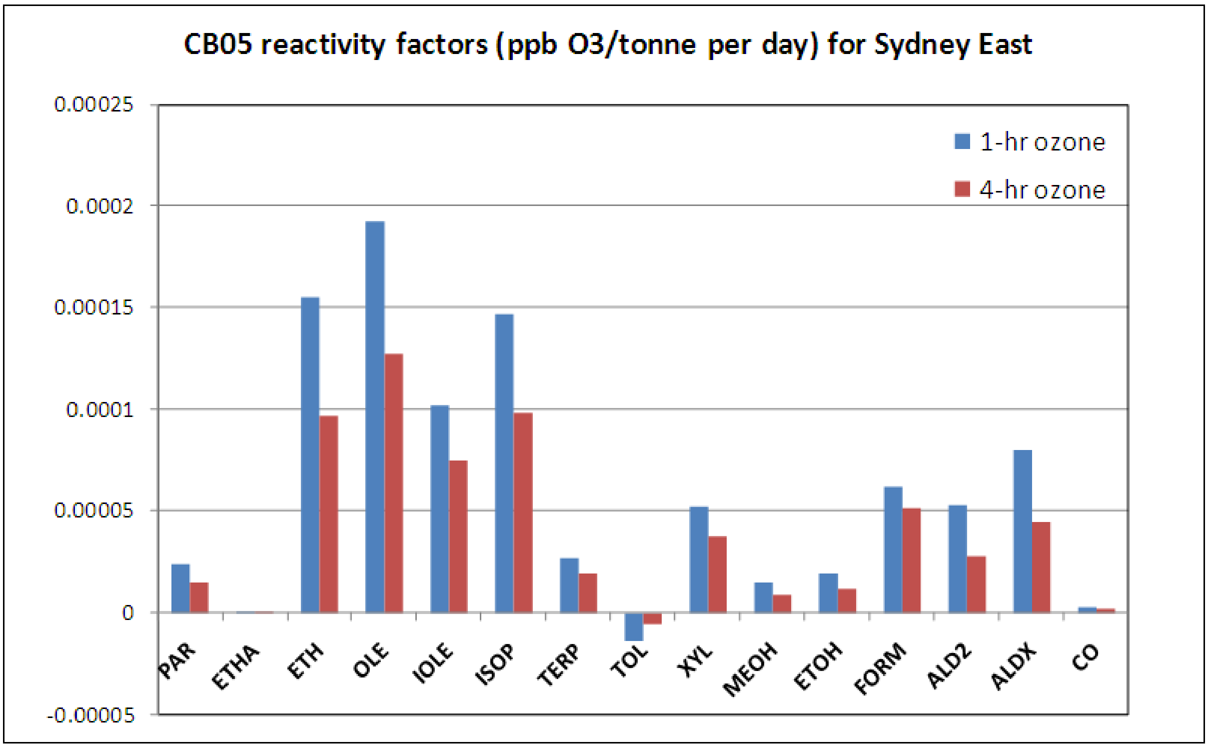


Figure 14 (b): First order sensitivities $dO_3/dVOC$ for Sydney East for both 1-hr and 4-hr average ozone

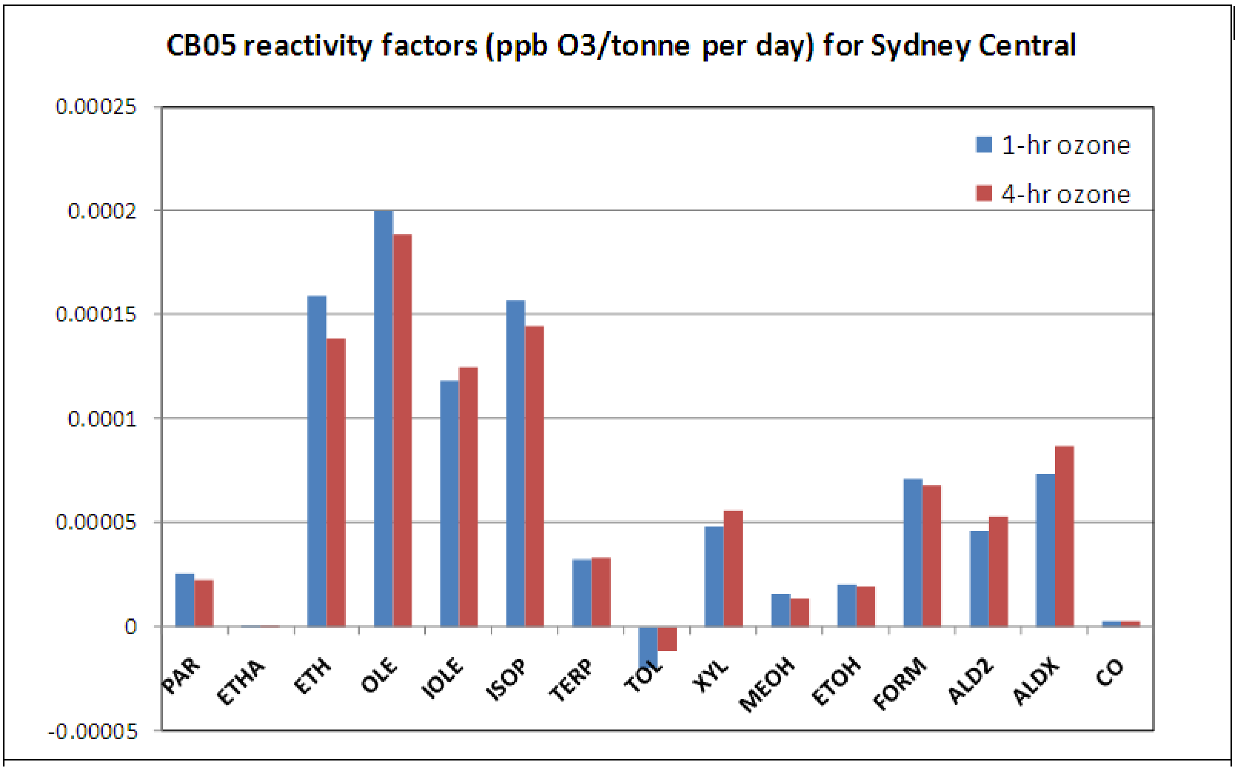


Figure 14 (c): First order sensitivities $dO_3/dVOC$ for Sydney Central for both 1-hr and 4-hr average ozone

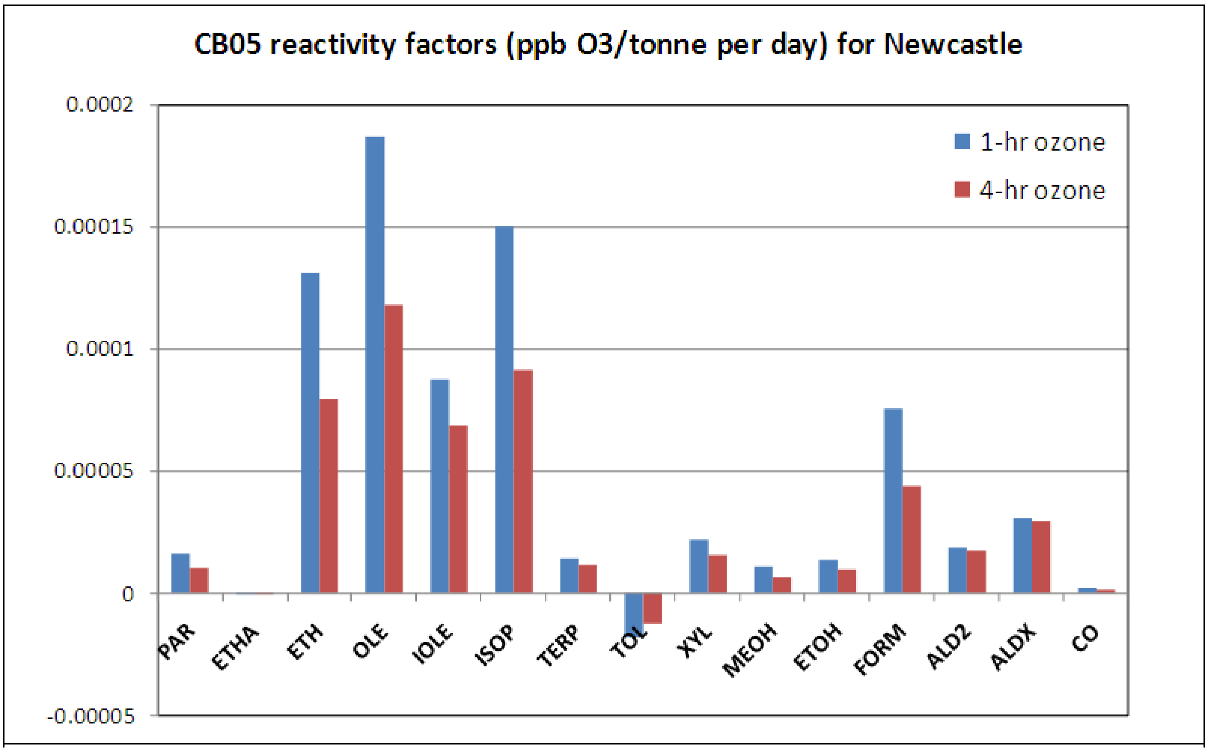


Figure 14 (d): First order sensitivities $dO_3/dVOC$ for Newcastle for both 1-hr and 4-hr average ozone

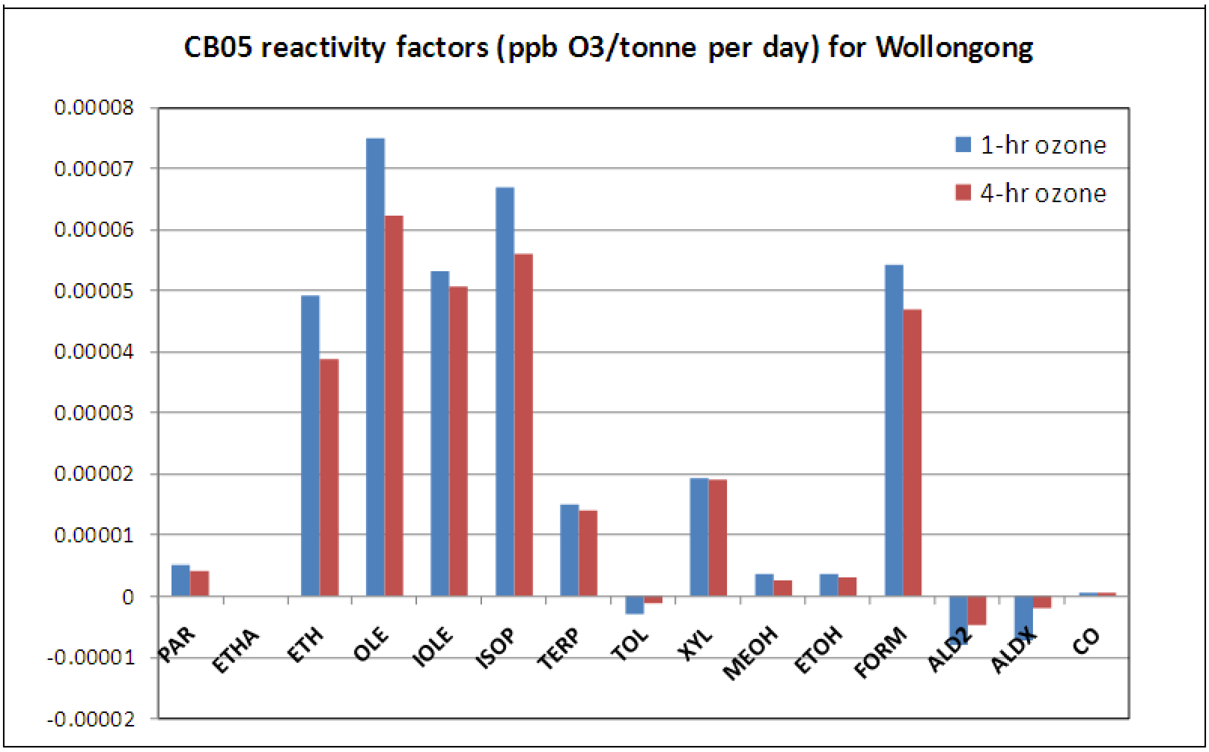


Figure 14 (e): First order sensitivities $dO_3/dVOC$ for Wollongong for both 1-hr and 4-hr average ozone

3.6.4 VOC Speciation and Reactivity

VOC have differing tendencies to form ozone as described by reactivity factors such as MIR (Carter and Atkinson, 1989). The Level 1 screening procedure tool has two options for dealing with VOC reactivity, namely:

- Use a source-specific VOC emission rate combined with a default VOC speciation profile; or
- Use a source-specific VOC emission rate combined with a source-specific VOC speciation profile.

The simpler option requires only the total VOC emission rate (tonnes/day) to be input and applies the default VOC composition, as documented in **Section 3.6.4.1**, in which case no reactivity adjustment is needed.

Alternatively, emission rates can be specified for different types of VOC in which case a reactivity adjustment (RA) is performed (Refer to **Section 3.6.4.2**).

Note: Although the Level 1 Screening Procedure Tool may be run with the default VOC speciation profile for trial runs, source-specific emissions and speciation data should be used.

3.6.4.1 Default VOC Speciation Profile

The default VOC profile included in the Level 1 screening procedure tool is based on VOC Profile Number 0000 based on the average of all profiles in SPECIATE, the USEPA's repository of total organic compound (TOC) and particulate matter (PM) speciation profiles of air pollution sources (USEPA, 2008).

Profile Number 0000 within SPECIATE(2) has been converted into the CB05 chemical mechanism lumped groups (refer **Section 2.4**) as shown in **Table 25**.

Table 25: SPECIATE Profile Number 0000 Converted to CB05 Chemical Mechanism on a Weight Percent Basis

CB05 Lumped Group	Weight %	
	Original Profile	Re-Normalised Values for Assessment Purposes
ALD2	1.78	2.40
ALDX	2.10	2.84
CH4	7.36	0.00
ETH	3.71	5.01
ETHA	1.39	1.88
ETOH	1.38	1.86
FORM	1.57	2.12
IOLE	0.67	0.90
ISOP	0.40	0.54
MEOH	1.40	1.89
NVOL	0.39	0.53
OLE	5.57	7.53
PAR	42.63	57.59
TERP	0.68	0.92
TOL	6.23	8.42
UNK	0.02	0.00
UNR	18.60	0.00
XYL	4.12	5.57

Inspection of the second column in **Table 25** shows that there are several groups that will not make a contribution to ozone formation, namely;

- CH4 (methane);
- NVOL (non-volatile compounds);
- UNK (unknown species); and
- UNR (unreactive compounds).

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2 http://cfpub.epa.gov/si/speciate/ehpa_speciate_browse_details.cfm?ptype=G&pnumber=0000

Collectively, these groups comprise approximately 26% of the weight percentage of Profile Number 0000. To make the ozone assessment process more conservative, these groups have been removed from the speciation profile, with the remaining lumped group weight percents normalised as detailed in the third column of **Table 25**.

3.6.4.2 Source-specific VOC Speciation

Source-specific emission rates can be specified for different types of VOC (Refer to **Appendix 4**) in which case a reactivity adjustment (RA) is performed as described below.

Speciated VOC emissions should be derived using either site specific or site representative source emission test results. If such data are not available then VOC emission estimates should be based on emission estimation techniques from credible sources such as:

- United States Environmental Protection Agency (USEPA) - Air Pollutant Emission Factors AP-42(3).
- USEPA - Emissions Inventory Improvement Programme(4).
- European Monitoring and Evaluation Programme (EMEP) / European Environment Agency (EEA) Air Pollution Emissions Inventory Guidebook(5).

VOC emissions may be speciated using source type-specific profiles derived from credible sources such as:

- USEPA Speciate V4.2(6).
- California Air Resources Board (CARB) California Emission Inventory Development and Reporting System (CEIDARS) Organic Gas Profile Data(7).

Reactivity factors (RFs) for each source have been developed specifically for the GMR airshed using HDDM in CAMx, as described above. These RFs have units “ppb O_3 per mass of VOC emitted.” The reactivity weighted VOC (VOC_{RW}) is calculated as:

$$VOC_{RW} = \sum VOC_i \cdot RF_i$$

For reference, the reactivity weighted VOC with default VOC reactivity (VOC_{avgRW}) is also calculated as:

$$VOC_{avgRW} = RF_{avg} \sum VOC_i$$

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3 http://www.epa.gov/ttnchie1/ap42/

4 http://www.epa.gov/ttn/chief/eiip

5 http://reports.eea.europa.eu/EMEPCORINAIR/en; http://tfeip-secretariat.org/emep-eea-guidebook/

6 http://www.epa.gov/ttnchie1/software/speciate/

7 http://www.arb.ca.gov/ei/drei/maintain/database.htm

The reactivity adjustment (RA) is then:

$$RA = VOC_{RW}/VOC_{avgRW}$$

The reactivity adjusted VOC emissions ($EVOC_{RA}$) are then:

$$EVOC_{RA} = EVOC \times RA$$

For example, if the source VOC has twice the reactivity of the default VOC (RA = 2), then the mass of VOC emissions from the source will be doubled ($EVOC_{RA} = 2 \times EVOC$).

Emissions of CO are similarly accounted for by multiplying the CO emissions by the RF calculated for CO and adding the reactivity adjusted CO emissions to the VOC emissions.

3.6.5 Application of the Level 1 Screening Procedure Tool

The Level 1 screening procedure tool is applied as follows for a source with X tonnes/day of NO_X, Y tonnes/day of VOC and Z tonnes/day of CO. The mass of VOC emissions is adjusted for reactivity, if necessary, as described above. Emissions of CO and CH_4 are adjusted for reactivity and added to the VOC emissions. In the discussion below, VOC refers to reactivity adjusted mass of VOC plus CO and CH_4.

1. Select the region containing the source (i.e. from the GMR air regions detailed in **Table 22**) and use the sensitivity coefficients computed for the source located in that region.

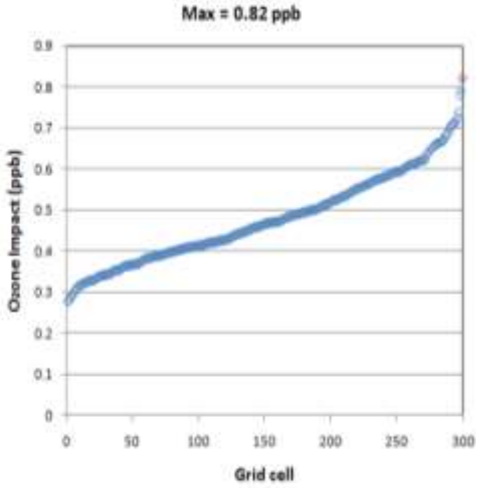
2. The Level 1 screening procedure tool computes the ozone impact in each of the 300 screening grid cells (ΔO_3) using the following Taylor series expansion:

$$\Delta O_3 \text{ (ppb)} = X \cdot S^1_{NOx} + Y \cdot S^1_{VOC} + (X^2 \cdot S^2_{NOx} /2) + (Y^2 \cdot S^2_{VOC} /2) + (X \cdot Y \cdot S^2_{NOxVOC} /2)$$

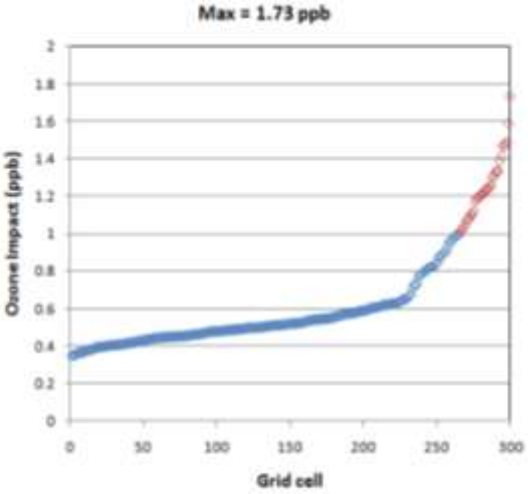
3. The ozone impacts for the 300 grid cells are rank ordered from lowest to highest showing the maximum impact. Given that the region is an “ozone non-attainment area” the fraction of the 300 grid cells (if any) which exceed the maximum allowable increment of 1 ppb ozone is noted (Refer to **Section 3.7.1** and **Section 3.7.5**). Examples results are shown for 1-hour ozone in **Figure 19** and 4-hour ozone in **Figure 20**.

4. Criteria for passing the Level 1 assessment are then established based on maximum impact as discussed in **Section 3.7**.

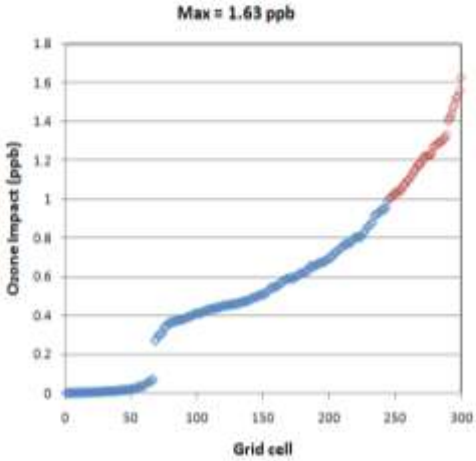
Sydney West



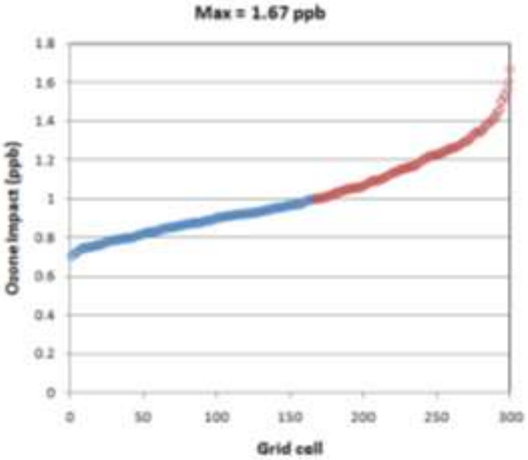
Sydney Central



Sydney East



Newcastle



Wollongong

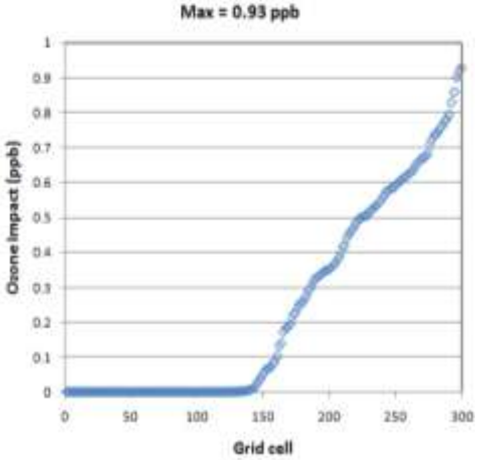
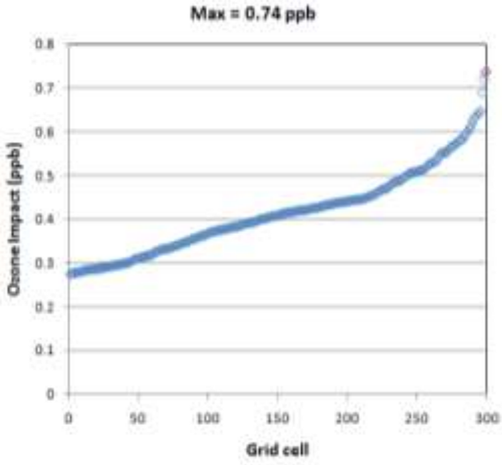
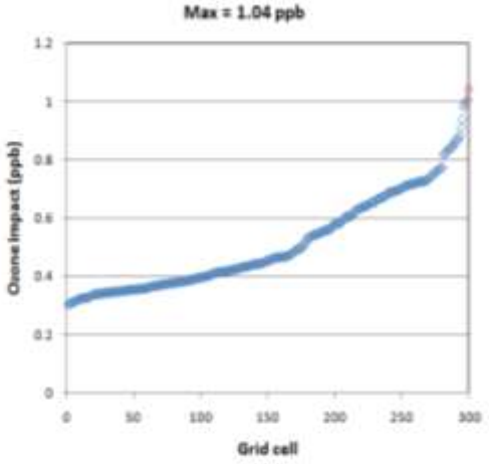


Figure 15: Level 1 screening procedure assessments for 1-hour ozone for sources emitting 2 tonnes/day of NO_x and 5 tonnes/day of VOC

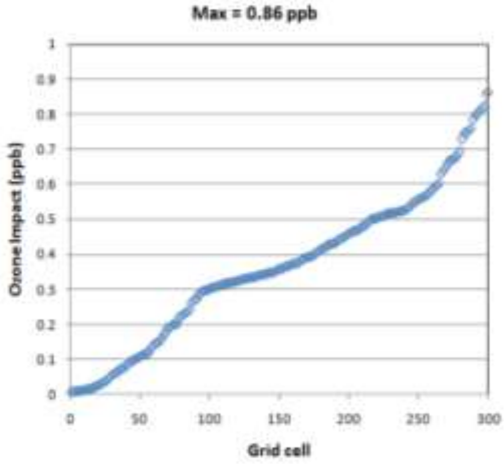
Sydney West



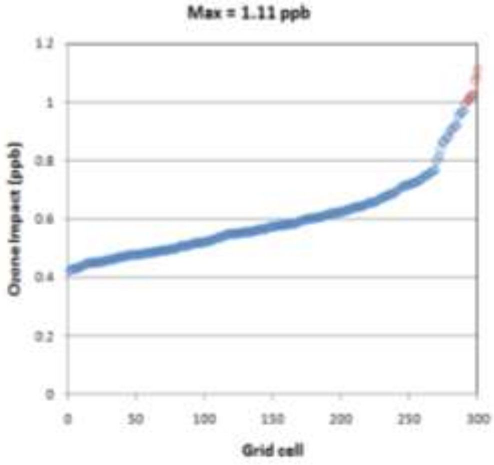
Sydney Central



Sydney East



Newcastle



Wollongong

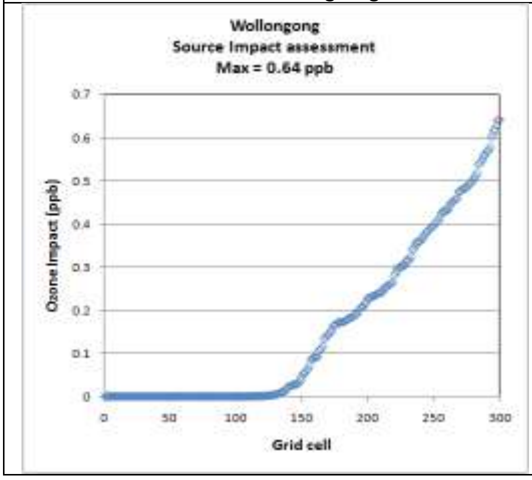


Figure 16: Level 1 screening procedure assessments for 4-hour ozone for sources emitting 2 tonnes/day of NO_x and 5 tonnes/day of VOC

3.6.6 Testing the Level 1 Screening Procedure Tool

The accuracy of ozone changes predicted by the Level 1 screening procedure tool was evaluated by comparison with results of “brute force” CAMx simulations, where brute force refers to the ozone difference between two CAMx simulations one with and one without adding a new source. The new sources have been added at the Central Sydney location with source parameters specified in **Table 22** and **Table 23**, except that the emissions have been scaled by factors of 0, 1, 10 and/or 25 as shown in **Table 26**.

Table 26: New Source Emissions used for Bruce Force Tests of the Level 1 Screening Procedure Tool

Brute Force Case	NO_x Tonnes/day	VOC Tonnes/day
Base source	0.611	0.759
1 x NO_x only	0.611	0
1 x VOC only	0	0.759
10 x base	6.11	7.59
10 x NO_x only	6.11	0
10 x VOC only	0	7.59
25 x base	15.3	19.0
25 x NO_x only	15.3	0
25 x VOC only	0	19.0

Ozone differences due to emissions from the new sources added in the brute force tests have been compared to ozone differences estimated by the screening tool using HDDM sensitivity coefficients, as described in **Section 3.6.5**. Scatter plots are shown in **Figure 21** and **Figure 22** for the top 100 grid cells on January 1, 2004 and January 3, 2005. Spatial plots of ozone plume differences throughout the entire modelling domain are shown in **Figure 23**. **Figure 23** shows that the location and magnitude of the ozone plume predicted by the screening tool is almost identical to the brute force result with emissions of 1, 10 and 25 times the base source emissions, respectively.

For the scatter plots shown in **Figure 21** and **Figure 22**, the reported precision for the brute force ozone changes was restricted to 0.01 ppb and this is apparent in tests that produced small ozone changes (e.g. 1 x VOC only). In many cases, because the analysis was for the 100 grid cells with the largest ozone changes, linear regression for 2 parameters resulted in non-zero intercepts and in these cases a second regression is shown with the intercept forced to zero.

The following findings derive from the brute force testing shown in **Figure 21** and **Figure 22**:

- The screening tool slightly under-predicted ozone changes for the 1 x the base emission tests with responses in the range 91% to 97% (as determined from regressions with zero intercept). This under-prediction bias is not a concern because the ozone changes for the 1 x base emissions tests are smaller than 0.2 ppb.

The screening tool accuracy improved for 10 x base emission tests with responses ranging from 97% to 100% (as determined from regressions with zero intercept).

The screening tool accuracy degraded slightly for 25 x base emission tests with responses ranging from 95% to 105% (as determined from regressions with zero intercept).

The screening tool predicted ozone changes with less scatter for VOC sources (excepting 1 x VOC which caused very small changes) than NO_X sources which is consistent with ozone chemistry exhibiting greater non-linearity with respect to changes in NO_X than VOC.

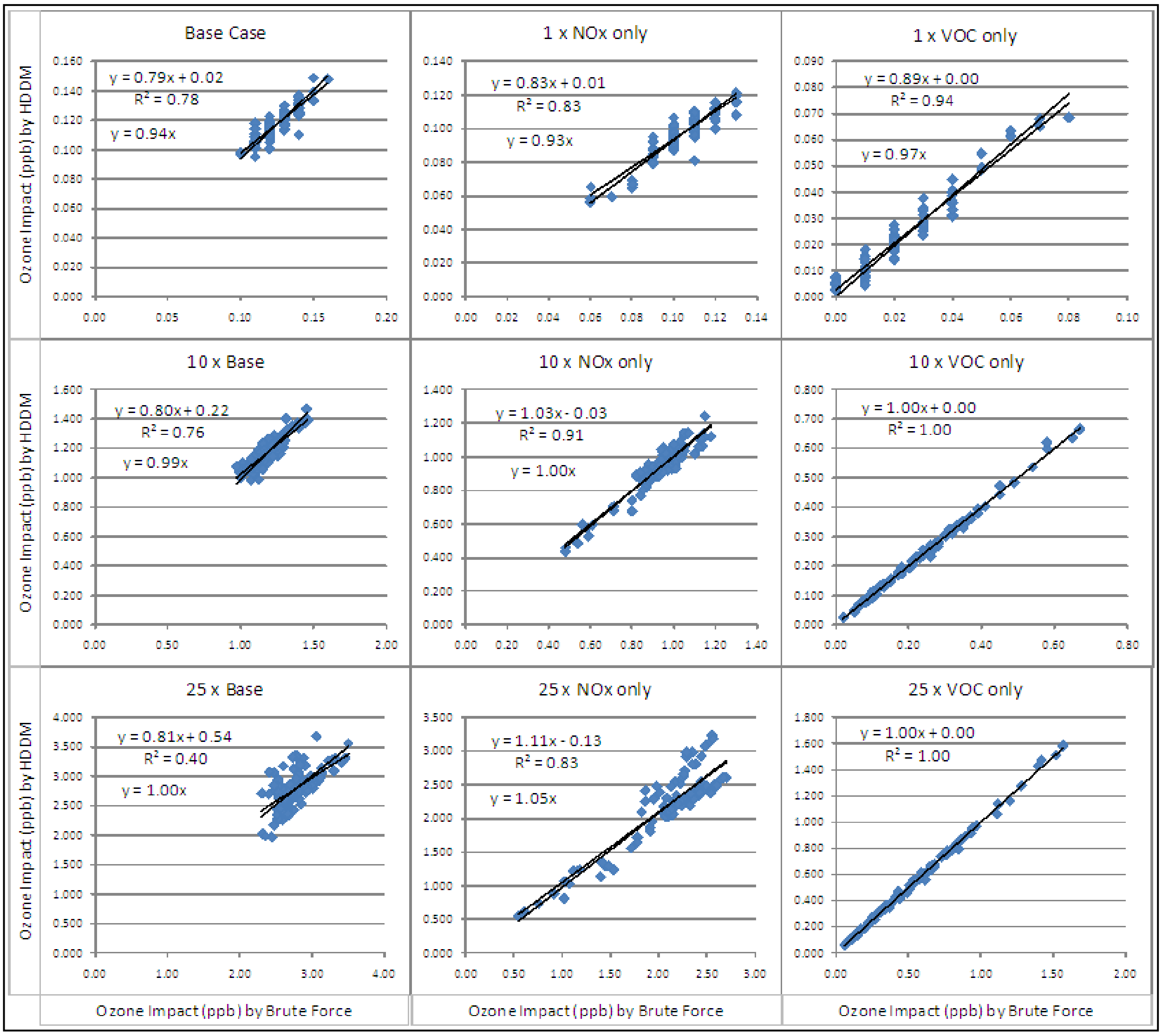


Figure 17: Comparison of Level 1 Screening Procedure Tool results to Brute Force CAMx results for 1-hour ozone on January 1, 2004 for sources in Central Sydney

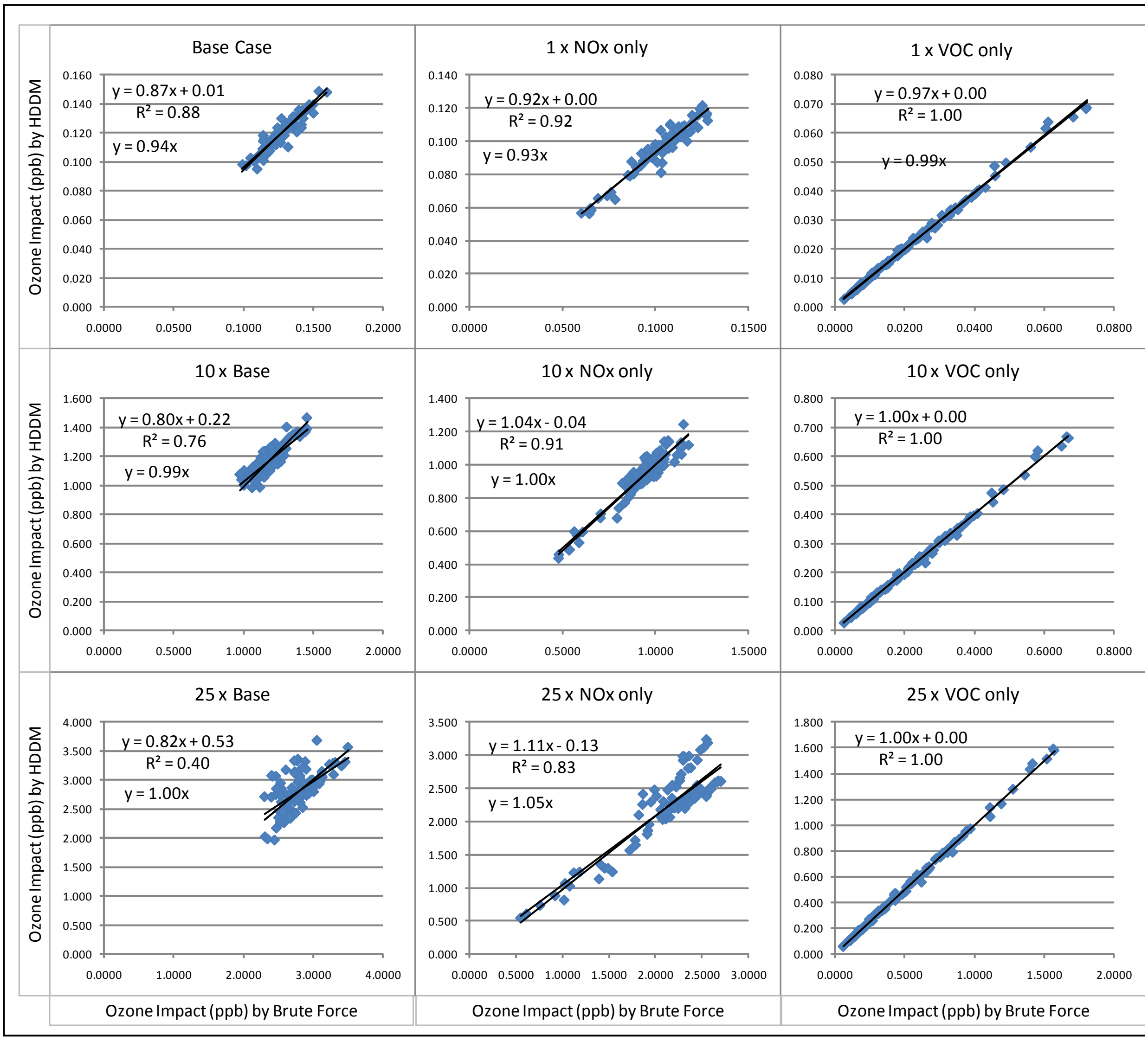


Figure 18: Comparison of Level 1 Screening Procedure Tool results to Brute Force CAMx results for 1-hour ozone on January 3, 2005 for sources in Central Sydney

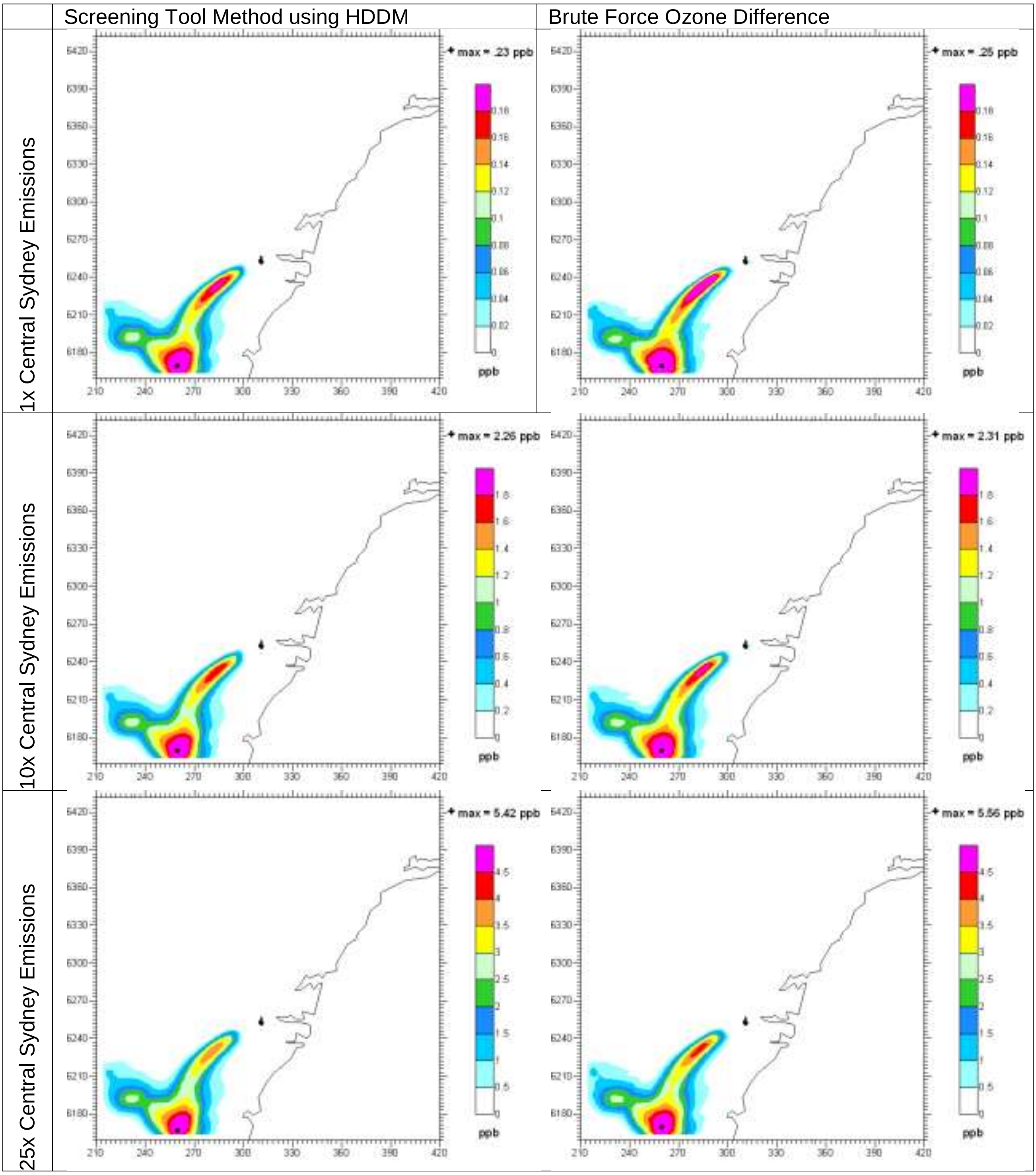


Figure 19 (a): Comparison of Screening Tool results to Brute Force CAMx results for 1-hour ozone at 13:00 on January 1, 2004 for sources in Central Sydney

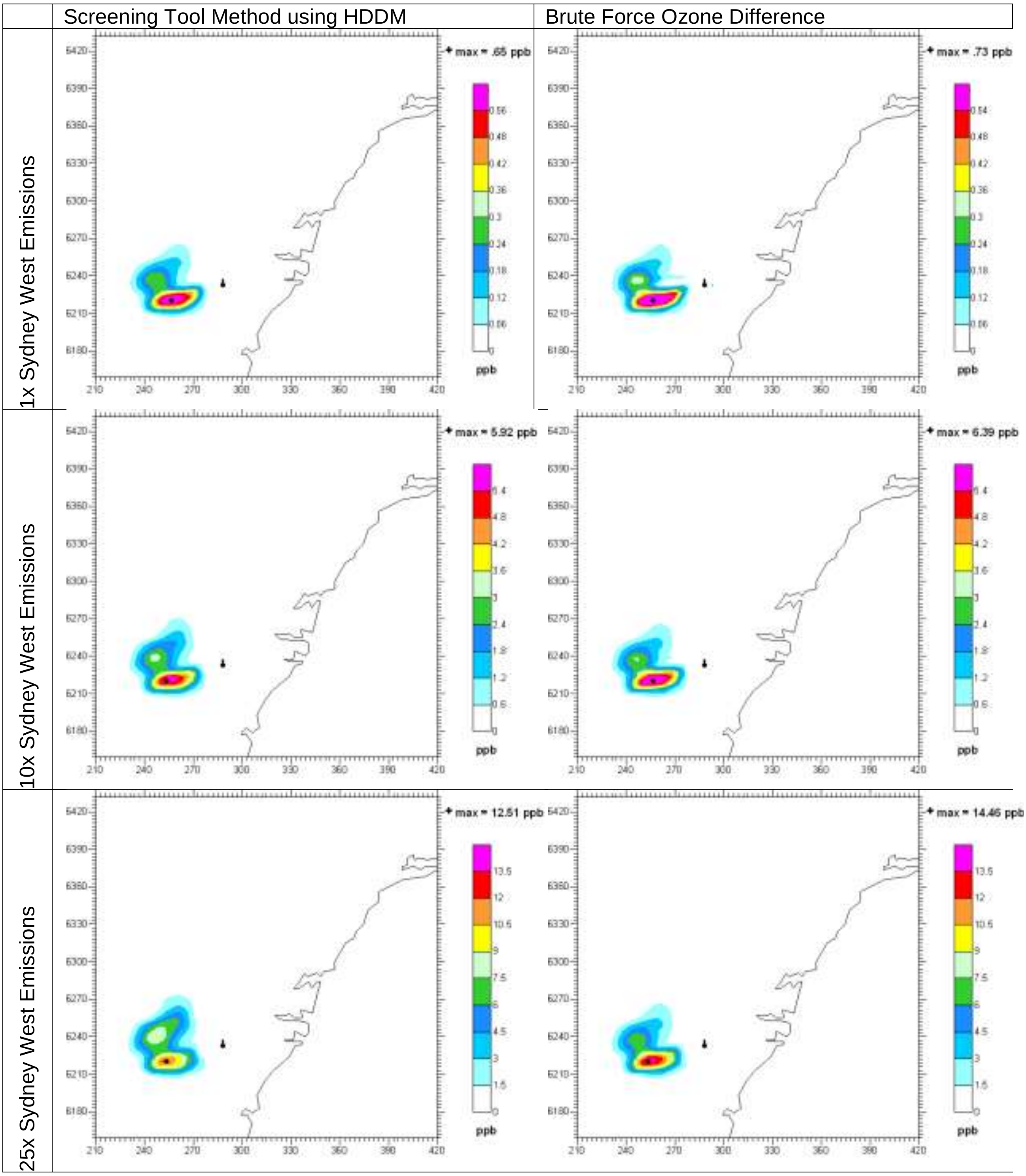


Figure 19 (b): Figure Comparison of Screening Tool results to Brute Force CAMx results for 1-hour ozone at 13:00 on January 28, 2004 for sources in Sydney West

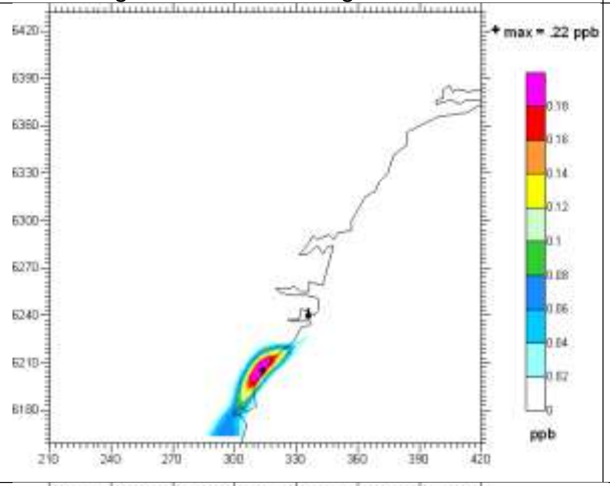
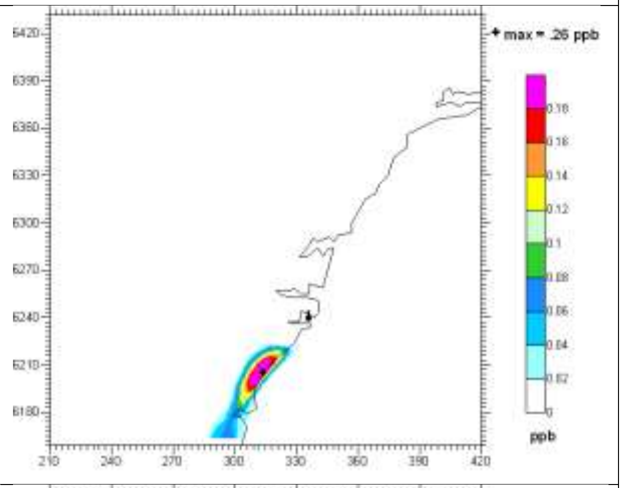
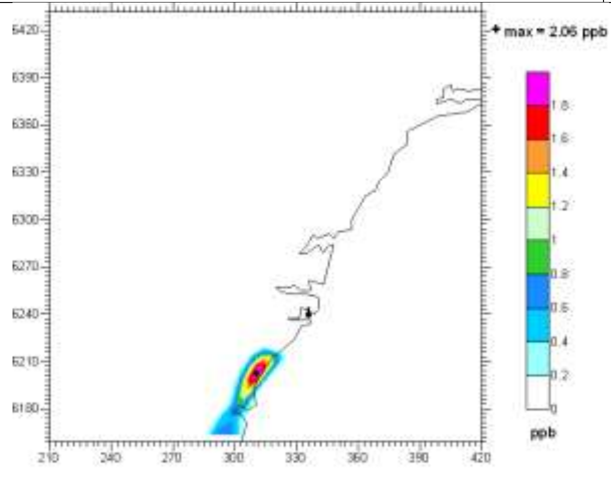
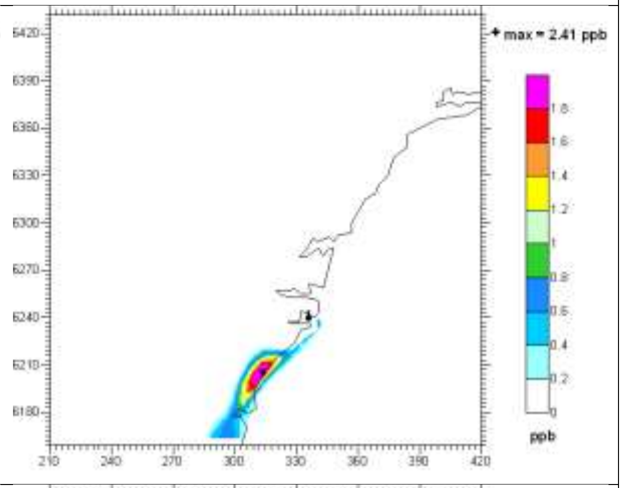
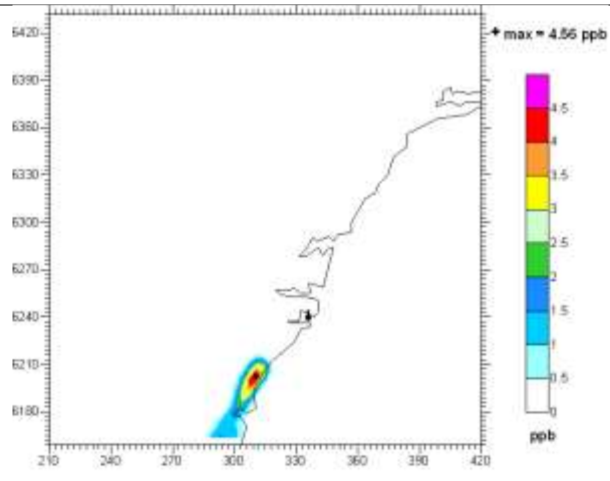
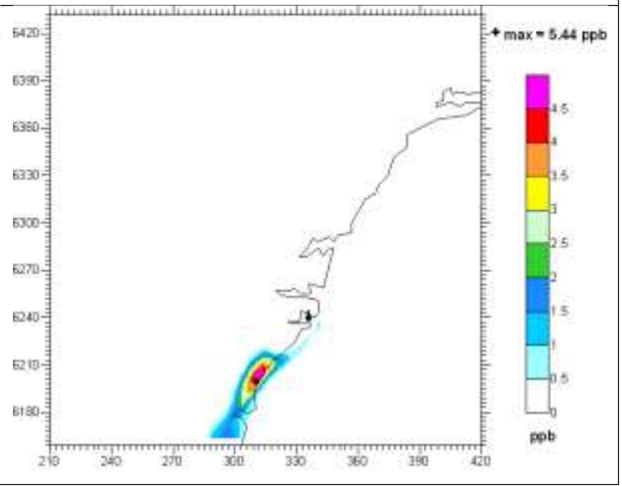
	Screening Tool Method using HDDM	Brute Force Ozone Difference
1x Sydney East Emissions		
10x Sydney East Emissions		
25x Sydney East Emissions		

Figure 19 (c): Comparison of Screening Tool results to Brute Force CAMx results for 1-hour ozone at 13:00 on January 14, 2005 for sources in Sydney East

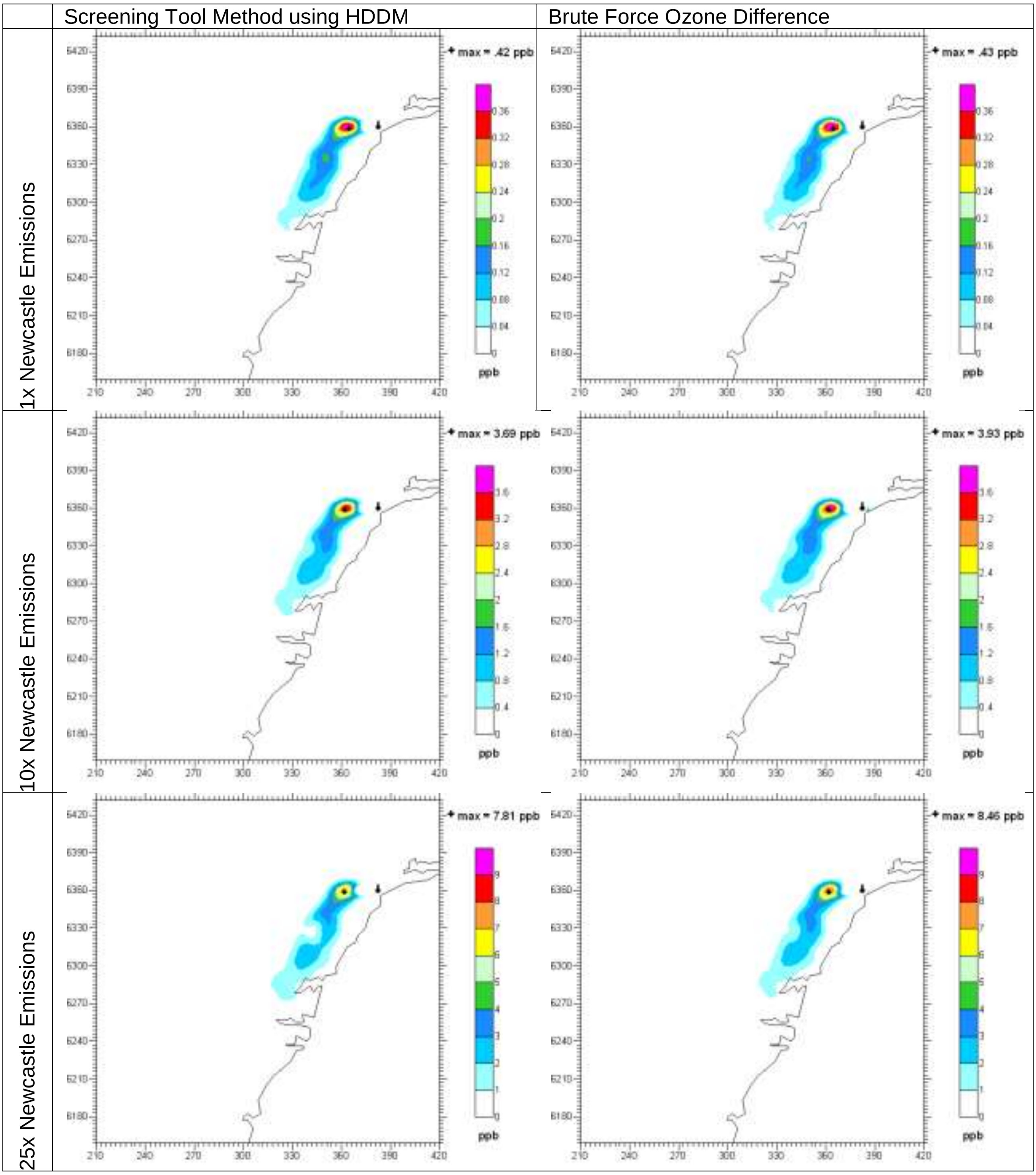


Figure 19 (d): Comparison of Screening Tool results to Brute Force CAMx results for 1-hour ozone at 13:00 on January 28, 2004 for sources in Newcastle

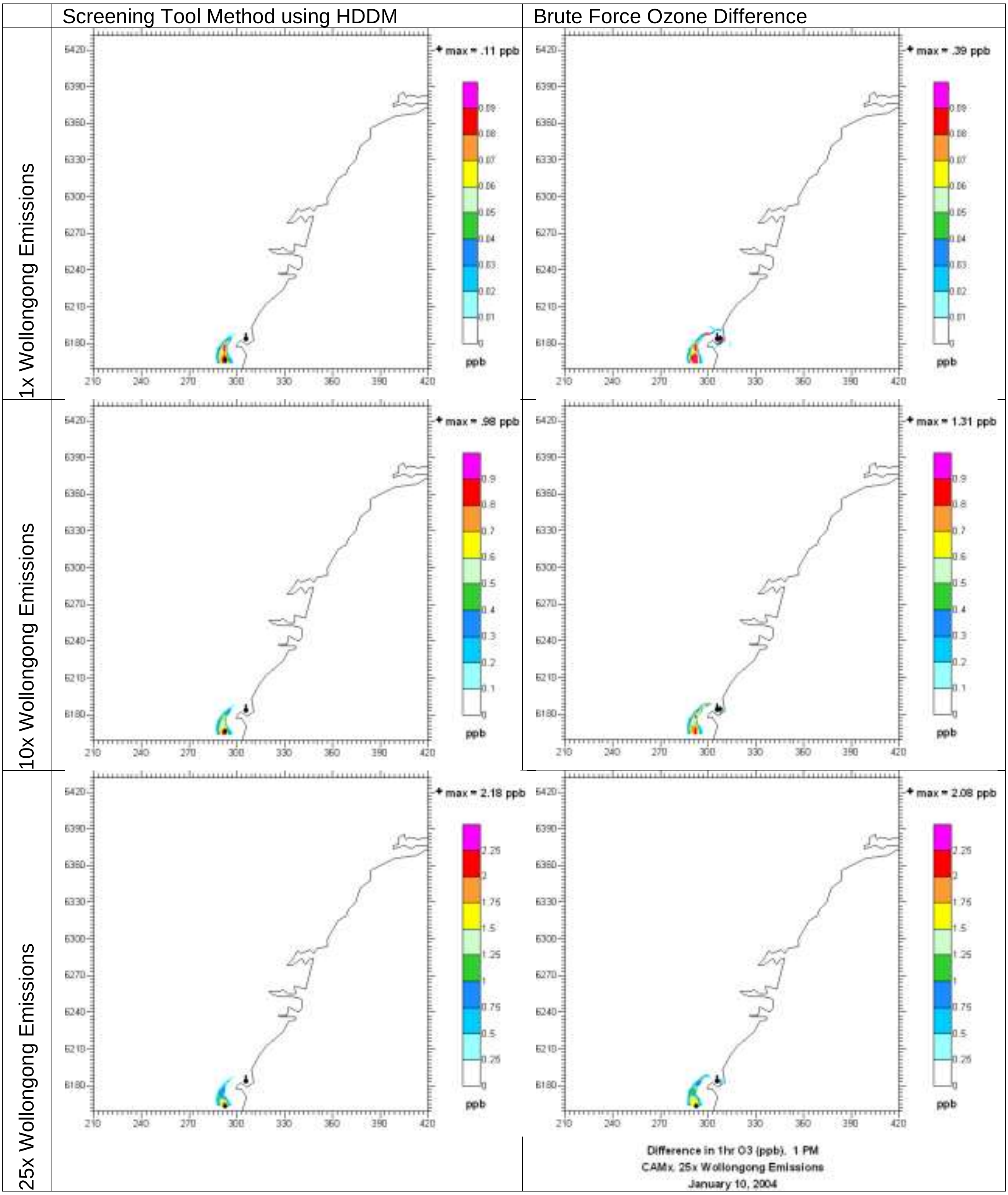


Figure 19 (e): Comparison of Screening Tool results to Brute Force CAMx results for 1-hour ozone at 13:00 on January 10, 2004 for sources in Wollongong

The conclusions drawn from testing the screening tool are as follows:

- The methodology implemented in the Level 1 screening procedure tool can accurately predict the ozone changes that would be obtained by directly modelling the source using CAMx.
- The Level 1 screening procedure tool appears to have a low-bias (smaller than 10% bias) for sources with small emissions (i.e. sources that result in ozone changes less than 0.2 ppb) but this is not of concern because the Level 1 screening procedure tool correctly predicts that these sources produce small ozone changes.
- The Level 1 screening procedure tool shows some degradation in accuracy for large sources (i.e. sources 25 times larger than have been used to develop the tool) suggesting that an upper limit should be placed on the emissions input to the screening tool.
- The accuracy of the screening tool over wide variations in NO_X and VOC emission inputs derives from including second-order sensitivity coefficients to account for non-linearity in ozone formation.

3.7 Application of Level 1 Screening Procedure to Assess Source Significance

3.7.1 Ozone Attainment and Non-attainment Areas

In evaluating the significance of Level 1 screening procedure results a distinction should be made between sources within ozone attainment areas and those within ozone non-attainment areas.

In determining whether an area is classified as either ozone attainment or non-attainment, reference should be made to measured ambient ozone concentrations from OEH ambient air quality monitoring stations recorded over the past 5 years.

The maximum 1-hour and 4-hour average ozone concentrations recorded over the most current 5 year period should be averaged to obtain the 5-year average 1-hour and 4-hour maximum ozone concentrations for each monitoring station. Reference should then be made to the highest 5-year average maximums recorded across monitoring stations in the region where the source is located. The Level 1 screening procedure tool contains measured ozone concentrations for three regions, including Sydney, Illawarra and Lower Hunter for the 2006-2010 period (**Table 27, Table 28**).

The 5-year average 1-hour and 4-hour maximum ozone concentrations for the source region should be compared to the screening procedure acceptance limits for ozone, expressed as 82% of the Air NEPM Standard(8).

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8 *NEPC (Ambient Air Quality) Measure Technical Paper No. 4, Revision 1 – January 2007, Screening Procedures.*

Areas where the 5-year average 1-hour maximum ozone concentration is greater than 0.082 ppm, and/or where the 5-year average 4-hour maximum ozone concentration is greater than 0.0656 ppm, are classified as non-attainment areas. Similarly, areas where the 5-year average 1-hour maximum ozone concentration is less than 0.082 ppm, and/or where the 5-year average 4-hour maximum ozone concentration is less than 0.0656 ppm, are classified as attainment areas. Based on the 5-year average maximums recorded in Sydney, the Illawarra and the Lower Hunter during the 2006-2010 period (**Table 27, Table 28**), all three regions are classifiable as ozone non-attainment areas (**Table 29**).

Table 27: Measured highest 1-hour ozone concentrations in ppm (2006-2010)

Station	2006	2007	2008	2009	2010	Average
Sydney						0.117
Bargo	0.121	0.117	0.091	0.122	0.110	0.112
Bringelly	0.119	0.111	0.093	0.120	0.104	0.109
Chullora	0.117	0.088	0.080	0.154	0.083	0.104
Earlwood	0.111	0.083	0.063	0.138	0.085	0.096
Lindfield	ND	ND	0.075	0.109	0.082	0.089
Liverpool	0.128	0.116	0.098	0.151	0.091	0.117
Macarthur	0.128	0.121	0.085	0.116	0.119	0.114
Oakdale	0.109	0.142	0.093	0.128	0.099	0.114
Prospect	ND	0.089	0.107	0.126	0.104	0.107
Randwick	0.083	0.090	0.061	0.078	0.084	0.079
Richmond	0.108	0.134	0.078	0.102	0.089	0.102
Rozelle	0.093	0.088	0.056	0.083	0.073	0.079
St Marys	0.124	0.123	0.096	0.132	0.095	0.114
Vineyard	0.104	0.127	0.081	0.100	0.090	0.100
Illawarra						0.089
Albion Park Sth	0.096	0.092	0.062	0.102	0.093	0.089
Kembla Grange	0.093	0.093	0.072	0.103	0.081	0.088
Wollongong	0.096	0.077	0.067	0.083	0.082	0.081
Lower Hunter						0.078
Beresfield	0.088	0.080	0.064	0.072	0.088	0.078
Newcastle	0.068	0.053	0.064	0.073	0.086	0.069
Wallsend	0.086	0.070	0.057	0.086	0.067	0.073

Table 28: Measured highest 4-hour ozone concentrations in ppm (2006-2010)

Station	2006	2007	2008	2009	2010	Average
Sydney						0.098
Bargo	0.103	0.105	0.074	0.111	0.086	0.096
Bringelly	0.110	0.095	0.078	0.108	0.089	0.096
Chullora	0.104	0.074	0.074	0.112	0.072	0.087
Earlwood	0.095	0.071	0.056	0.104	0.074	0.080
Lindfield	ND	ND	0.064	0.097	0.079	0.080
Liverpool	0.124	0.094	0.089	0.103	0.081	0.098

Table 28: Measured highest 4-hour ozone concentrations in ppm (2006-2010)

Station	2006	2007	2008	2009	2010	Average
Macarthur	0.117	0.101	0.070	0.097	0.103	0.098
Oakdale	0.086	0.116	0.075	0.108	0.088	0.095
Prospect	ND	0.085	0.096	0.100	0.097	0.095
Randwick	0.079	0.084	0.057	0.073	0.077	0.074
Richmond	0.095	0.121	0.067	0.090	0.082	0.091
Rozelle	0.082	0.075	0.048	0.073	0.067	0.069
St Marys	0.109	0.105	0.082	0.106	0.083	0.097
Vineyard	0.085	0.116	0.065	0.088	0.079	0.087
Illawarra						0.079
Albion Park Sth	0.078	0.080	0.055	0.083	0.073	0.074
Kembla Grange	0.081	0.082	0.066	0.090	0.078	0.079
Wollongong	0.086	0.073	0.063	0.074	0.073	0.074
Lower Hunter						0.072
Beresfield	0.074	0.075	0.062	0.065	0.082	0.072
Newcastle	0.064	0.047	0.058	0.067	0.076	0.062
Wallsend	0.066	0.068	0.054	0.076	0.063	0.065

3.7.2 Assessing Level 1 Screening Procedure Tool Applicability

The Level 1 screening procedure tool has been tested by comparison with nine CAMx simulations in which different size sources have been added at the Central Sydney location. The Level 1 screening procedure tool provided accurate results over a wide range of source sizes with NO_X varied from zero to 5,578 tonnes/annum and VOC varied from zero to 6,921 tonnes/annum. The upper ends of these emission ranges are 25 times larger than the source emissions used to develop the tool. The accurate performance of the tool over wide variations in NO_X and VOC emission inputs derives from including second-order sensitivity coefficients to account for non-linearity in ozone formation.

Based on the default VOC speciation, the tool is considered to be applicable for sources with emission ranges of up to 5,500 tonnes/annum of NO_X and 7,000 tonnes/annum of VOC. In the event that these emission ranges are exceeded, the Level 2 refined procedure is required.

For source-specific VOC speciation, the Reactivity Factors (RFs) developed for the GMR airshed are applied, and the reactivity-weighted emission rates are compared by the tool to the relative reactivity-weighted upper VOC emission range based on the default VOC speciation. In the event that the upper range is exceeded, the tool is not applicable and a Level 2 refined procedure is required.

3.7.3 Level 1 Screening Procedure Tool Outputs

The Level 1 screening procedure tool outputs the following:

- Maximum 1-hour and 4-hour average ozone concentrations due to the source's emissions (i.e. incremental ozone concentrations).

- Cumulative ozone concentration levels, with the maximum 1-hour and 4-hour increment being added to the 5-year average 1-hour and 4-hour maximum for the region (**Table 27, Table 28**). The screening tool provides an upper bound estimate since the maximum source impact is added to the maximum ambient measurement, regardless of space and time.

Note: To evaluate the significance of emissions from a source and its impact on ground-level ozone in the GMR, the ozone impacts calculated using the Level 1 screening procedure tool should be compared to the most recent ambient monitoring data for ozone in the GMR. Comparisons should not be restricted to the ozone monitor nearest to the source because ozone impacts occur downwind of the source at locations that vary from day to day. Comparisons within the subregion (i.e. Sydney, Illawarra/Wollongong and Lower Hunter/Newcastle) containing the source are appropriate. Comparing the source impacts to ozone in other subregions would be appropriate if that subregion is considered to be downwind of the source on high ozone days.

3.7.4 Evaluation of Sources within Ozone Attainment Areas

Maximum 1-hour and 4-hour average ozone concentration increments calculated for the source using the Level 1 screening procedure tool should be compared to the significant impact level (SIL) for ozone attainment areas, specified as 0.5 ppb. Where incremental concentrations are below this SIL, no further ozone impact assessment is required but further requirements may be triggered (Refer to **Section 5**).

Where the maximum 1-hour or 4-hour average ozone concentration increment is equivalent to or above the SIL (0.5 ppb), the calculated increment should be evaluated against the maximum allowable ozone increments calculated for the region.

The maximum allowable ozone increments are defined as 25% of the difference between the 5-year average 1-hour and 4-hour maximums for the region and the relevant Air NEPM Standard(9)(**Table 29**).

Screening procedure acceptance limits for ozone are expressed as 82% of the Air NEPM Standard(10). Given the application of an acceptable level of 82%, the difference between the 5-year average maximums and the relevant standard will be greater than or equivalent to 18 ppb for an 1-hour averaging period and greater than or equivalent to 14.4 ppb for a 4-hour averaging period.

Where the maximum 1-hour and 4-hour increment is below the relevant maximum allowable increment, no further ozone impact assessment is required, but further requirements may be triggered (Refer to **Section 5**). In other cases, a Level 2 refined assessment should be undertaken.

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9 The maximum allowable ozone increment reflects the maximum increase in ozone concentrations allowed above the existing baseline ozone concentration. An increment comprising 25% of the residual was selected in line with US PSD increments defined for Class 2 areas, which are designated to allow moderate, controlled growth. (Refer to **Section 2.1.1.3**).

10 *NEPC (Ambient Air Quality) Measure Technical Paper No. 4, Revision 1 – January 2007, Screening Procedures.*

3.7.5 Evaluation of Sources within Ozone Non-attainment Areas

For sources within ozone non-attainment areas, the need for further assessment is initially determined based on the comparison of the maximum 1-hour and 4-hour increments with the relevant SIL (0.5 ppb).

Maximum 1-hour and 4-hour increments are subsequently evaluated against the maximum allowable increment specified as 1 ppb for ozone non-attainment areas (**Table 29**).

Where the incremental concentrations are below 1 ppb, no further ozone impact assessment is required but other requirements may be triggered (Refer to **Section 5**).

Where the maximum 1-hour or 4-hour average ozone concentration increment is equivalent to or above 1 ppb, a Level 2 refined assessment should be undertaken.

The rationale for the SIL and maximum allowable increment applied in the ozone impact assessment procedure is provided in **Section 5.1.7**.

Table 29: Classification of Regions based on Maximum 5-year average Ozone Concentrations recorded at OEH Stations during 2006-2010

Station	Maximum 5-year average 1-hour Ozone Concentration (ppb)	Air NEPM Ozone Standard (ppb)	Difference between Standard and Ambient (ppb)	25% of Residual	Region Classification
Sydney	116.8	100	-16.8	NA(a)	Non-attainment
Illawarra	89.0	100	11.0	NA(a)	Non-attainment
Lower Hunter	78.4	100	21.6	5.4	Attainment
Station	**Maximum 5-year average 4-hour Ozone Concentration (ppb)**	**Air NEPM Ozone Standard (ppb)**	**Difference between Standard and Ambient (ppb)**	**25% of Residual**	**Region Classification**
Sydney	98.2	80	-18.2	NA(a)	Non-attainment
Illawarra	79.4	80	0.6	NA(a)	Non-attainment
Lower Hunter	71.6	80	8.4	NA(a)	Non-attainment

(a) Maximum allowable increment specified as 1 ppb for ozone non-attainment areas.

3.8 Findings and Recommendations

The Level 1 screening procedure tool has been developed from CAMx simulations for the NSW Greater Metropolitan Region (GMR) airshed. Simulations have been performed for two ozone seasons (i.e. December and January; 2003/4 and 2004/5) with and without new sources added to identify days on which the new sources would have high ozone impacts. Days have been selected with enhanced ozone in the GMR and acceptable model performance. The selected high ozone impact days have then been used for CAMx simulations with the higher order Decoupled Direct Method (HDDM) used to calculate sensitivity coefficients of ozone to the additional NO_X and/or VOC emissions from a new source. These ozone sensitivity coefficients enable estimation of ozone impacts for new sources with different NO_X and/or VOC emissions than were used to develop the Level 1 screening procedure tool.

The sensitivity coefficients have been embedded in the Level 1 screening procedure tool that can estimate ozone impacts for sources with different emissions of CO, CH_4, NO_X and/or VOC. Five source locations are included within the tool: West Sydney, Central Sydney, East Sydney, Newcastle and Wollongong. VOC emissions can be specified either as total VOC, in which case default VOC composition is assumed, or as emissions of source-specific types of VOC.

Source-specific VOC emissions data is required to meet OEH ozone impact assessment requirements (Refer to **Section 5**). If non-default VOC emissions are provided, ozone impacts are adjusted for VOC reactivity using reactivity factors calculated specifically for each source location.

The Level 1 screening procedure tool has been tested by comparison with nine CAMx simulations in which different size sources have been added at the Central Sydney location. The Level 1 screening procedure tool provided accurate results over a wide range of source sizes with NO_X varied from zero to 5,578 tonnes/annum and VOC varied from zero to 6,921 tonnes/annum. The upper ends of these emission ranges are 25 times larger than the source emissions used to develop the tool. The accurate performance of the tool over wide variations in NO_X and VOC emission inputs derives from including second-order sensitivity coefficients to account for non-linearity in ozone formation.

The following recommendations are given for use of the Level 1 screening procedure tool:

- Source-specific VOC emissions and speciation are required when applying the Level 1 screening procedure tool to meet OEH ozone impact assessment requirements. Documentation should be provided describing the basis for the VOC emissions and speciation and why it is appropriate for the type of source.

- The Level 1 screening procedure tool is applicable for the assessment of sources with emissions up to 5,500 tonnes/annum of NO_X and 7,000 tonnes/annum of VOC (given default VOC composition). In the event that source-specific VOC compositions are used, the tool estimates the reactivity-weighted VOC emissions and compares these emissions to the reactivity-weighted VOC emissions using the default speciation. In the event that source emissions exceed the upper bound emission rates of the tool, a Level 2 refined procedure should be conducted.

- Criteria for determining the significance of predicted incremental ozone concentrations due to sources are presented within **Section 3.7**, and comprise primarily the following:

  - Evaluation of sources located within ozone attainment areas against a screening impact level (SIL) of 0.5 ppb, and against the maximum allowable increment calculated for each region.

- Evaluation of sources located within ozone non-attainment areas against a SIL of 0.5 ppb, and against a maximum allowable increment for non-attainment areas specified as 1 ppb.

4. Development and Analysis of Level 2 Refined Procedure

The Level 1 screening and Level 2 refined procedures should be closely related to provide consistent evaluations of new source ozone impacts. In short, if a source fails the Level 1 assessment, new CAMx (or other PGM) runs should be performed to directly assess the ozone impact of the new source. The intent of directly modelling the source using a Level 2 assessment is to eliminate uncertainties attributable to the parameterisation of model results within the Level 1 screening procedure tool. This section of the report provides an example Level 2 refined procedure.

A Level 2 assessment permits more precise specification of the source characteristics (location, stack parameters) compared to the use of a representative source in the Level 1 assessment.

The modelling performed for a Level 2 assessment should not be less detailed than the modelling used to develop the Level 1 screening procedure tool. One option is that the Level 2 assessment can use the modelling databases used to develop the Level 1 screening procedure tool.

Exactly the same criteria should be used to evaluate the significance of source ozone impacts for the Level 1 screening and Level 2 refined procedures.

4.1 Documenting a Level 2 Refined Procedure

The following elements should be included in the documentation for a Level 2 assessment:

- Photochemical model used
- Chemical mechanism used
- Modelling domain
- Source of input data
  - Emissions
  - Meteorology
  - Boundary conditions
- Modelling period(s)
- Procedures for evaluating base case model performance
  - Source(s) of ambient data
  - Statistical evaluation methods
  - Graphical evaluation methods

- Characteristics of new source
  - Location
  - Stack parameters
  - Emission rates for NO_X, VOC and CO
  - VOC speciation
- Procedures for selecting days to evaluate new source ozone impacts
- Ozone increases from new source emissions on each evaluation day
  - Results for 1-hour and 4-hour ozone
  - Maximum ozone increase
  - Base case ozone at location of maximum increase
- Significance assessment of new source ozone increases against 1-hour and 4-hour average incremental ozone criterion
- Ozone impact (i.e. increase plus background) due to new source emissions on each evaluation day
  - Results for 1-hour and 4-hour ozone
- Significance assessment of new source ozone impact against 1-hour and 4-hour average Air NEPM ozone standards

The model selection, chemical mechanism, domain, sources of input data, modelling periods and source characteristics for the Level 2 assessment have been documented in **Section 3.2**.

The source selected for the Level 2 assessment was the Central Sydney source located in Yennora/Smithfield (**Table 22**) with 500 tonnes/annum of ozone precursor emissions (**Table 23**).

4.2 Level 2 Refined Procedure Case Study

The purpose of this case study is to illustrate the steps required to undertake such an assessment. In this way, the Level 2 assessment is non-prescriptive, but provides a demonstration of OEH expectations for this form of assessment.

Two model runs have been performed, with and without including the emissions for the new source. The ozone impacts of the new source have been determined from the difference between the two model runs. The significance of the ozone impacts was evaluated against the same criteria used for the Level 1 screening procedure (**Section 3.7**).

4.2.1 Base Case Model Performance Evaluation

Ambient ozone data for the model performance evaluation have been obtained from OEH and had been quality assured. Model performance evaluation focused on 1-hour ozone since 4-hour averaging allows errors in different hours to be offset and therefore is considered a less stringent basis for evaluation.

Statistical evaluation metrics included a comparison of spatially-paired daily maximum ozone, normalised mean bias (NMB) and normalised mean error (NME) for spatially and temporally paired ozone:

$$NMB = \frac{\sum_{i=1}^{N}\left(C_m - C_o\right)}{\sum_{i=1}^{N} C_o} \qquad NME = \frac{\sum_{i=1}^{N}\left|C_m - C_o\right|}{\sum_{i=1}^{N} C_o}$$

where C_o is the observed concentration, C_m is the paired model prediction and N is the number of data pairs (C_o, C_m). NMB and NME have been calculated for data pairs with observed ozone greater than 50 ppb to focus on periods of photochemical ozone production within the GMR.

Graphical evaluation methods employed include spatial plots of daily maximum 1-hour ozone with observations superimposed and time-series plots comparing model predictions and observations.

Figure 28 to **Figure 31** provide an overview for the four months modelled (December 2003, January 2004, December 2004, January 2005) showing for each day: (1) the range of daily maximum ozone observed; (2) a comparison of the peak observed and the modelled maximum at the same location; (3) the NMB; and (4) the NME. These statistics are also in **Table 30** and **Table 31**. These figures have been reviewed to identify dates which are potentially suitable for evaluating the impact of the new source added in Central Sydney. Ideally, suitable dates had high modelled ozone combined with low model bias and error. Dates listed in red have been selected for further evaluation. Time series plots (examples in **Figure 32**) and spatial plots (examples in **Figure 33**) have also been reviewed to understand model performance on dates of interest.

In this study, there was no opportunity to improve the model performance by undertaking diagnostic and/or sensitive tests and revising important model input parameters.

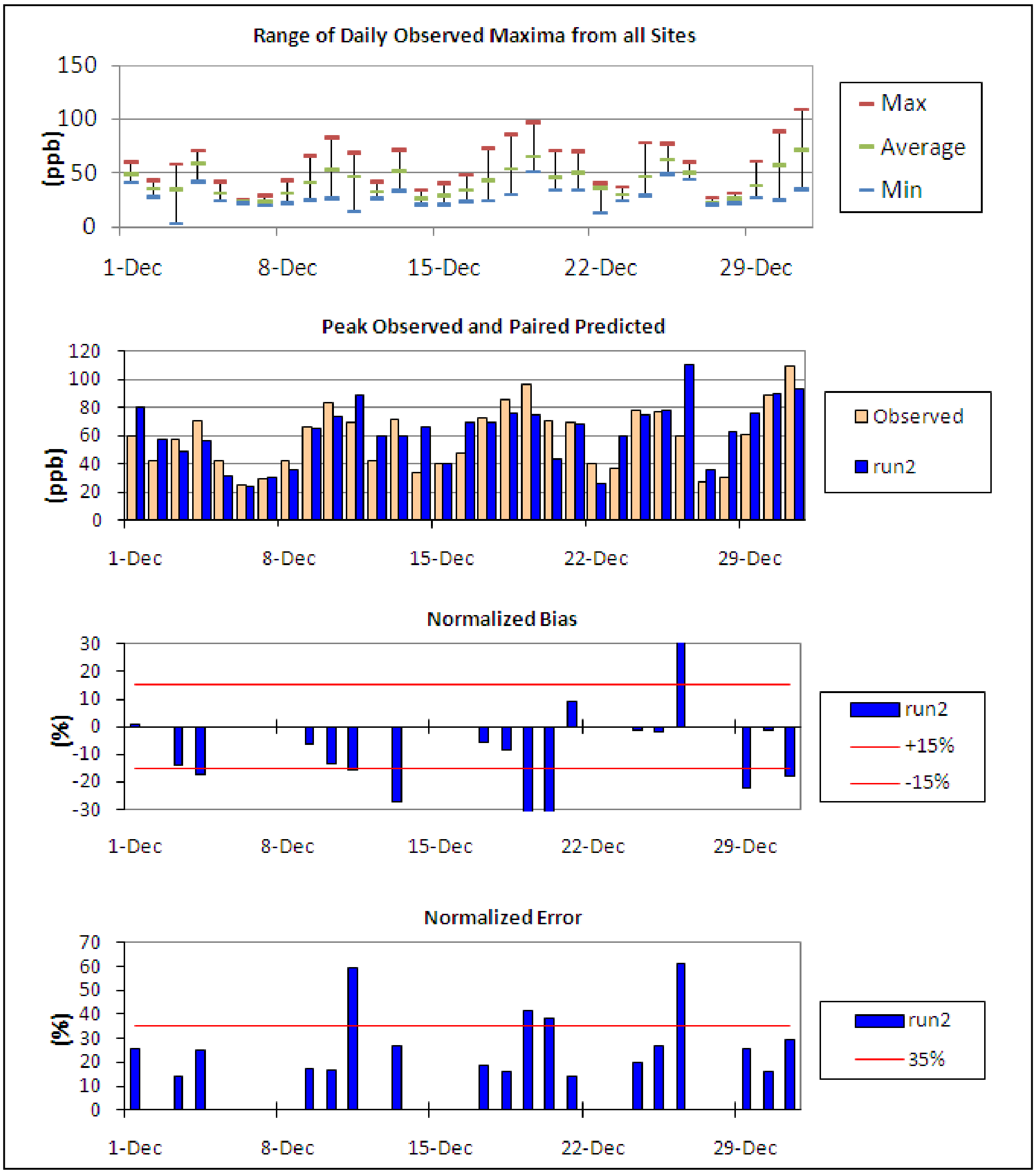


Figure 20: Daily maximum 1-hour ozone and statistical evaluation metrics for Sydney monitoring stations in December, 2003

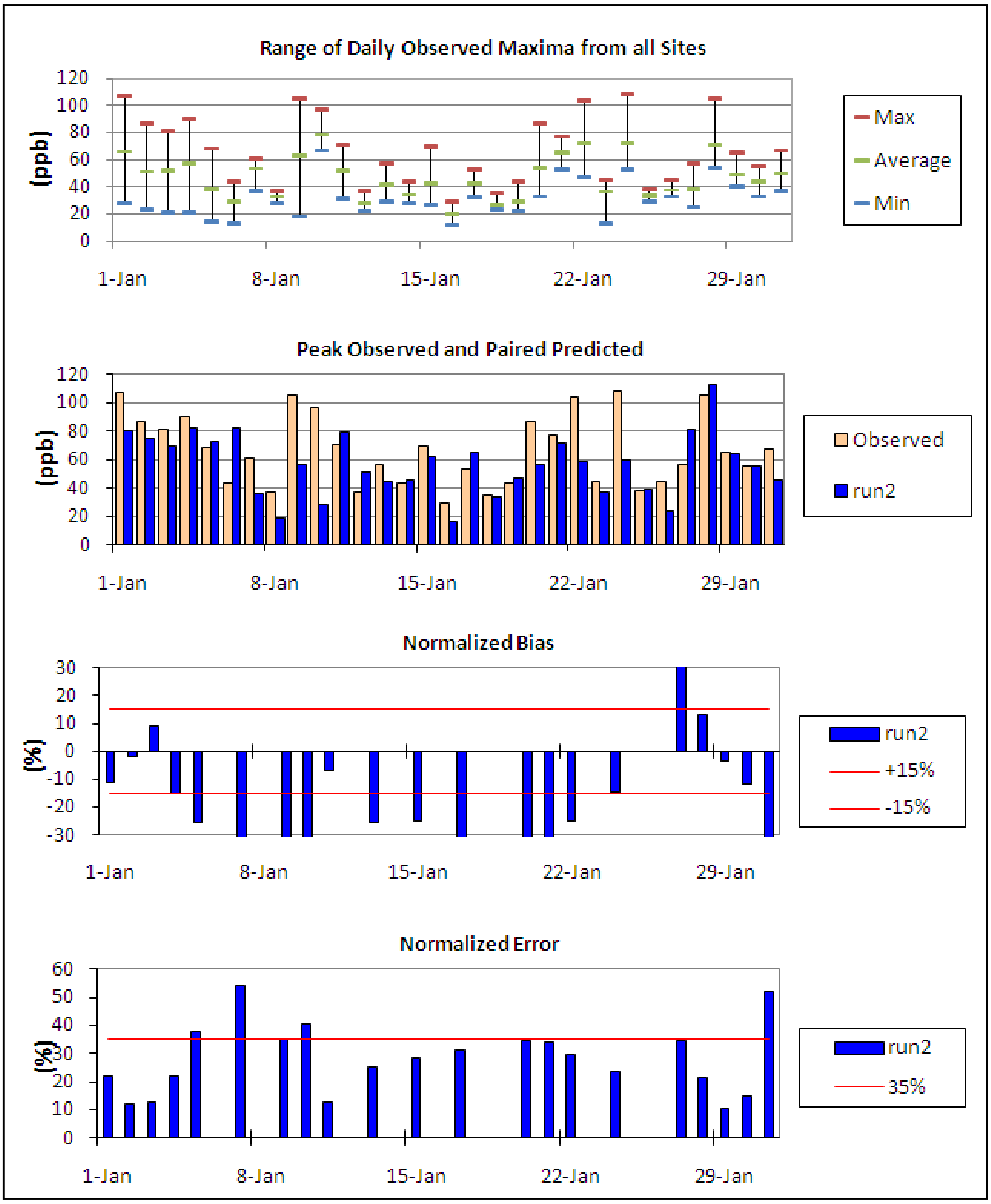


Figure 21: Daily maximum 1-hour ozone and statistical evaluation metrics for Sydney monitoring stations in January, 2004

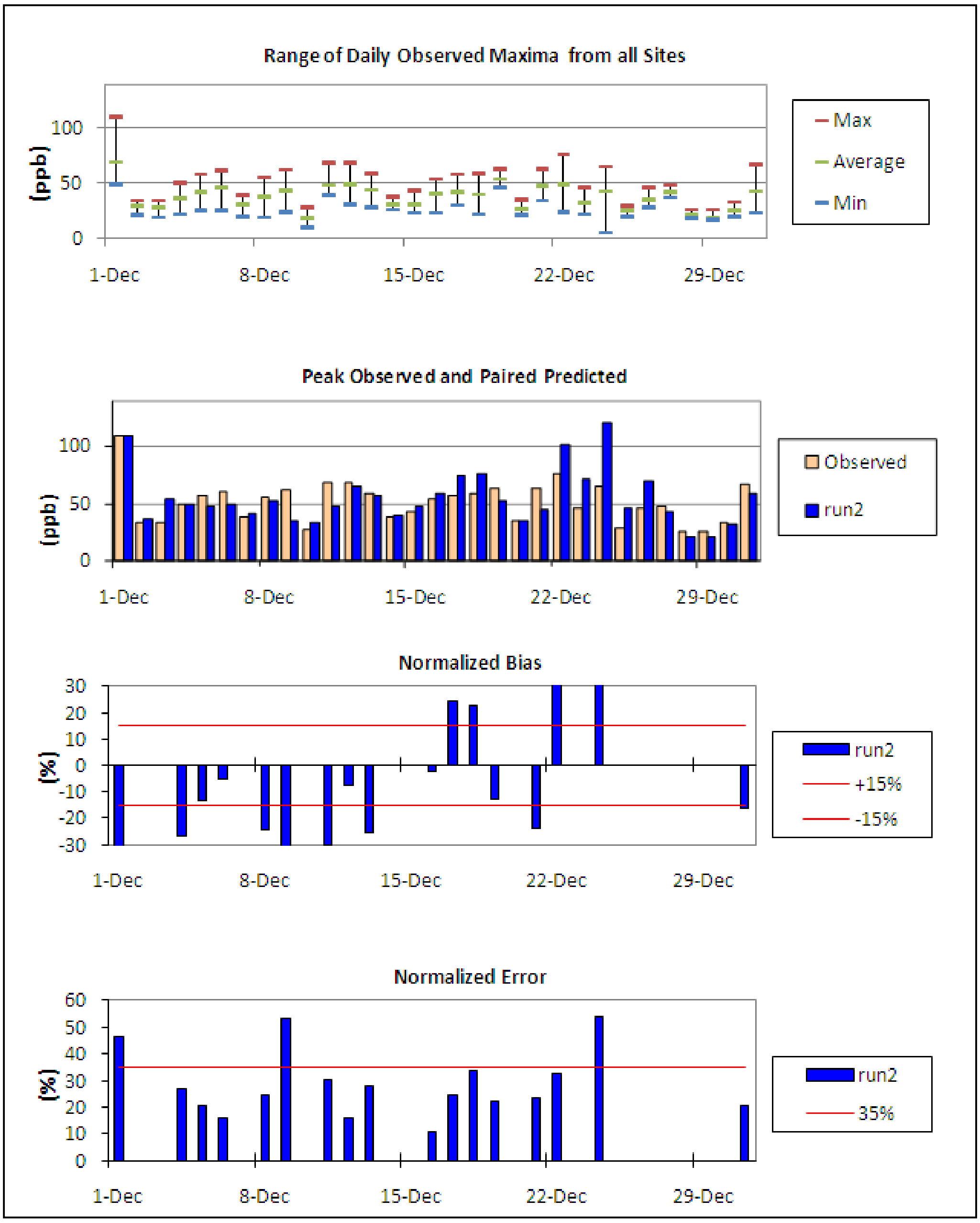


Figure 22: Daily maximum 1-hour ozone and statistical evaluation metrics for Sydney monitoring stations in December, 2004

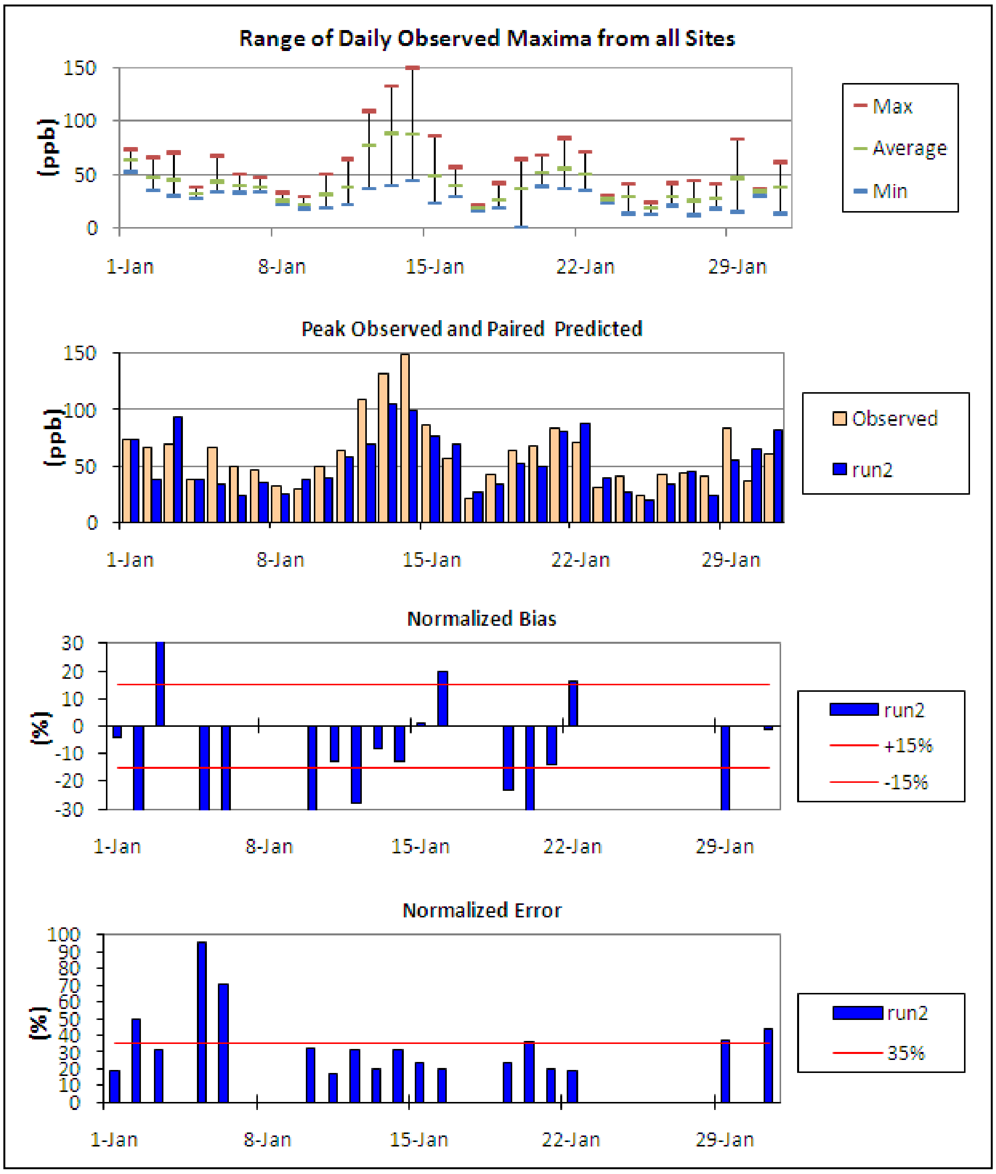


Figure 23: Daily maximum 1-hour ozone and statistical evaluation metrics for Sydney monitoring stations in January 2005

Table 30: Daily 1-hour ozone model performance statistics at Sydney monitoring stations in the 2003-2004 episode

Date	Peak Observed (ppb)	Paired Predicted (ppb)	Norm. Bias (%)	Norm. Error (%)	Date	Peak Observed (ppb)	Paired Predicted (ppb)	Norm. Bias (%)	Norm. Error (%)
1-Dec-03	60	80	1	26	1-Jan-04	107	80	-11	22
2-Dec-03	43	58			2-Jan-04	87	75	-2	12
3-Dec-03	58	49	-14	14	3-Jan-04	81	70	9	13
4-Dec-03	71	57	-17	25	4-Jan-04	90	82	-15	22
5-Dec-03	42	32			5-Jan-04	68	73	-26	38
6-Dec-03	25	24			6-Jan-04	44	82		
7-Dec-03	29	30			7-Jan-04	61	36	-54	54

Table 30: Daily 1-hour ozone model performance statistics at Sydney monitoring stations in the 2003-2004 episode

Date	Peak Observed (ppb)	Paired Predicted (ppb)	Norm. Bias (%)	Norm. Error (%)	Date	Peak Observed (ppb)	Paired Predicted (ppb)	Norm. Bias (%)	Norm. Error (%)
8-Dec-03	43	36			8-Jan-04	37	18		
9-Dec-03	66	65	-6	17	9-Jan-04	105	57	-35	35
10-Dec-03	83	74	-14	17	10-Jan-04	97	28	-37	41
11-Dec-03	69	88	-16	59	11-Jan-04	71	80	-7	13
12-Dec-03	42	60			12-Jan-04	37	52		
13-Dec-03	72	60	-27	27	13-Jan-04	57	45	-26	26
14-Dec-03	34	67			14-Jan-04	44	45		
15-Dec-03	40	41			15-Jan-04	70	62	-25	28
16-Dec-03	48	69			16-Jan-04	29	17		
17-Dec-03	73	69	-6	19	17-Jan-04	53	65	-31	31
18-Dec-03	86	76	-9	16	18-Jan-04	35	33		
19-Dec-03	97	75	-36	42	19-Jan-04	44	47		
20-Dec-03	71	43	-38	38	20-Jan-04	87	56	-34	34
21-Dec-03	70	69	9	14	21-Jan-04	77	71	-33	34
22-Dec-03	40	26			22-Jan-04	104	59	-25	30
23-Dec-03	37	60			23-Jan-04	45	38		
24-Dec-03	78	75	-1	20	24-Jan-04	108	60	-14	24
25-Dec-03	77	78	-2	27	25-Jan-04	38	40		
26-Dec-03	60	110	43	62	26-Jan-04	45	25		
27-Dec-03	27	36			27-Jan-04	57	81	32	35
28-Dec-03	31	63			28-Jan-04	105	113	13	21
29-Dec-03	61	76	-22	26	29-Jan-04	65	65	-3	11
30-Dec-03	89	90	-1	16	30-Jan-04	55	55	-12	15
31-Dec-03	109	94	-18	30	31-Jan-04	67	46	-52	52

Table 31: Daily 1-hour ozone model performance statistics at Sydney monitoring stations in the 2004-2005 episode

Date	Peak Observed (ppb)	Paired Predicted (ppb)	Norm. Bias (%)	Norm. Error (%)	Date	Peak Observed (ppb)	Paired Predicted (ppb)	Norm. Bias (%)	Norm. Error (%)
1-Dec-04	110	110	-43	47	1-Jan-05	73	73	-4	19
2-Dec-04	34	37			2-Jan-05	66	38	-42	49
3-Dec-04	34	53			3-Jan-05	70	93	32	32
4-Dec-04	50	49	-27	27	4-Jan-05	38	38		
5-Dec-04	58	48	-13	21	5-Jan-05	67	34	-95	95
6-Dec-04	61	50	-5	16	6-Jan-05	50	24	-71	71
7-Dec-04	39	41			7-Jan-05	47	36		
8-Dec-04	55	53	-24	25	8-Jan-05	33	26		
9-Dec-04	62	35	-53	53	9-Jan-05	29	38		
10-Dec-04	28	34			10-Jan-05	50	40	-32	32
11-Dec-04	68	47	-30	30	11-Jan-05	64	58	-13	17
12-Dec-04	68	65	-8	16	12-Jan-05	109	69	-28	31

Table 31: Daily 1-hour ozone model performance statistics at Sydney monitoring stations in the 2004-2005 episode

Date	Peak Observed (ppb)	Paired Predicted (ppb)	Norm. Bias (%)	Norm. Error (%)	Date	Peak Observed (ppb)	Paired Predicted (ppb)	Norm. Bias (%)	Norm. Error (%)
13-Dec-04	59	57	-26	28	13-Jan-05	132	105	-8	20
14-Dec-04	38	40			14-Jan-05	149	99	-13	31
15-Dec-04	43	48			15-Jan-05	86	77	1	24
16-Dec-04	54	59	-2	11	16-Jan-05	57	70	20	20
17-Dec-04	58	74	24	24	17-Jan-05	21	26		
18-Dec-04	59	77	23	34	18-Jan-05	42	34		
19-Dec-04	63	53	-13	22	19-Jan-05	64	52	-23	24
20-Dec-04	35	35			20-Jan-05	68	49	-36	36
21-Dec-04	63	45	-24	24	21-Jan-05	84	81	-14	20
22-Dec-04	76	101	32	32	22-Jan-05	71	87	16	19
23-Dec-04	46	71			23-Jan-05	31	40		
24-Dec-04	65	120	54	54	24-Jan-05	41	27		
25-Dec-04	29	47			25-Jan-05	24	19		
26-Dec-04	46	70			26-Jan-05	42	33		
27-Dec-04	48	43			27-Jan-05	44	46		
28-Dec-04	26	20			28-Jan-05	41	23		
29-Dec-04	26	21			29-Jan-05	83	56	-32	37
30-Dec-04	33	32			30-Jan-05	37	65		
31-Dec-04	67	59	-16	20	31-Jan-05	61	82	-1	44

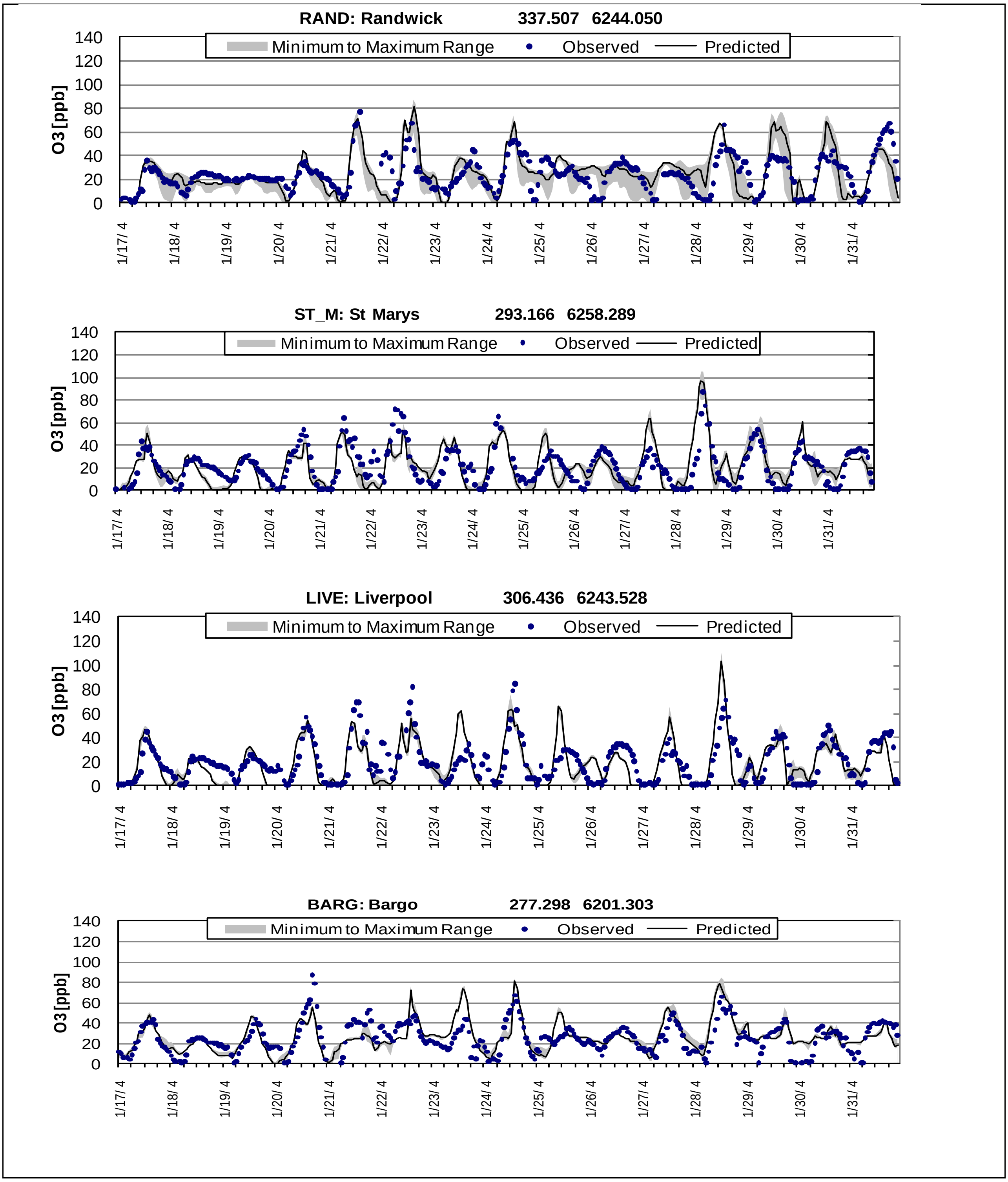
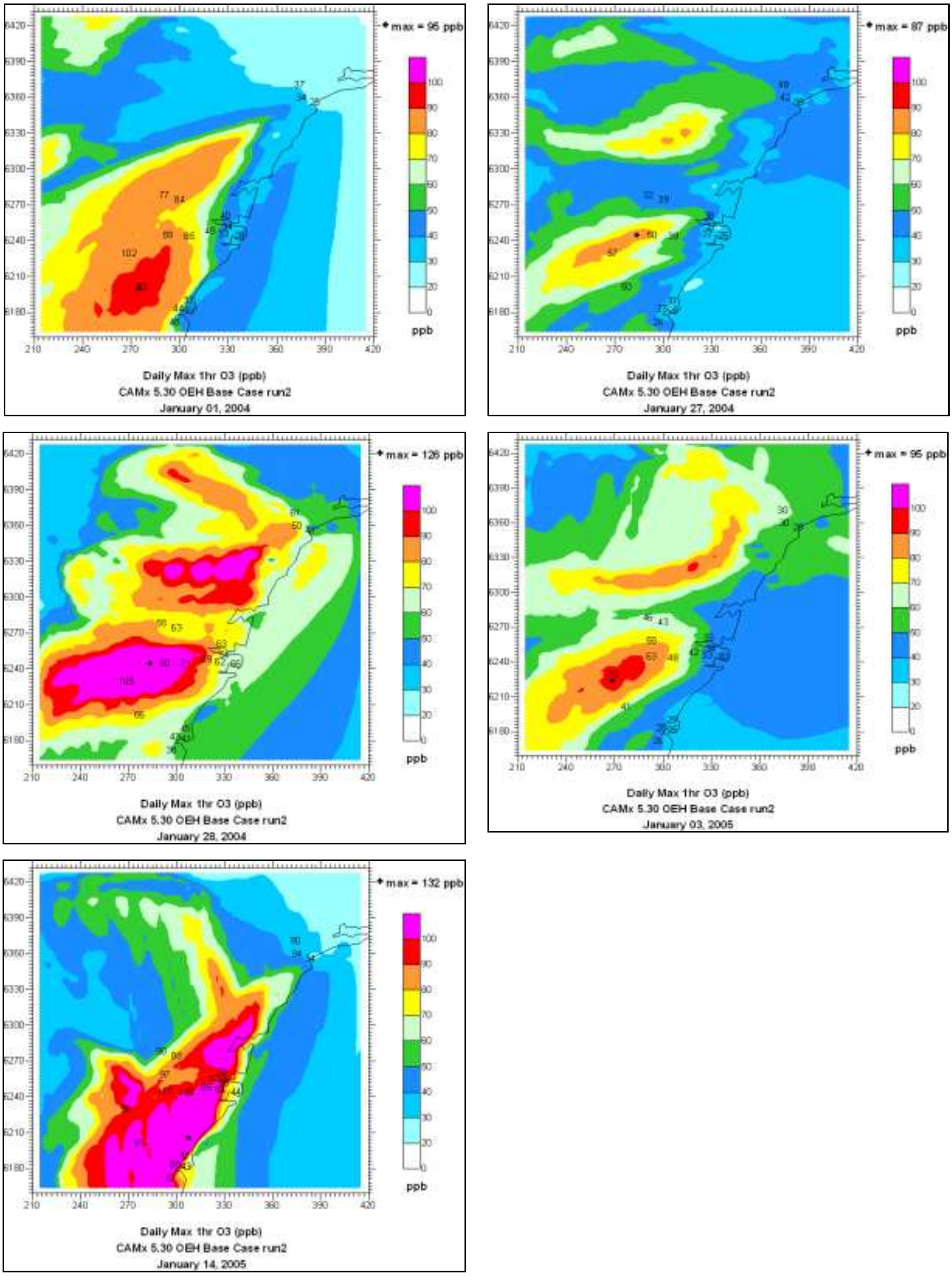


Figure 24: Time series plots for 4 Sydney monitors on January 17-31, 2004

4.2.2 Selection of Dates for the Level 2 Refined Procedure Assessment

Criteria to be considered in selecting dates for the Level 2 assessment are as follows. The maximum modelled ozone should be comparable to the Air NEPM standards to ensure that the conditions are relevant to non-attainment of the standards. The model should have acceptable performance, meaning low bias and error statistics, to gain confidence that the simulation provides a realistic representation of conditions on the high ozone day. The impacts of the new source should occur primarily over land, rather than over the ocean, for relevance to non-attainment of the Air NEPM standard. Several days should be selected, and as a minimum at least three, to enable comparison of source impacts across multiple high ozone days.

The following dates have been selected for the Level 2 assessment: 1-Jan-04, 27-Jan-04, 28-Jan-04, 3-Jan-05 and 14-Jan-05. Spatial plots of modelled and observed daily maximum 1-hour ozone for these dates are shown in **Figure 33**. Spatial plots of the impacts from the new Central Sydney source to the daily maximum 1-hour and 4-hour ozone are displayed in **Figure 34** and **Figure 35**, respectively.



Daily Max 1hr O3 (ppb)
CAMx 5.30 OEH Base Case run2
January 01, 2004

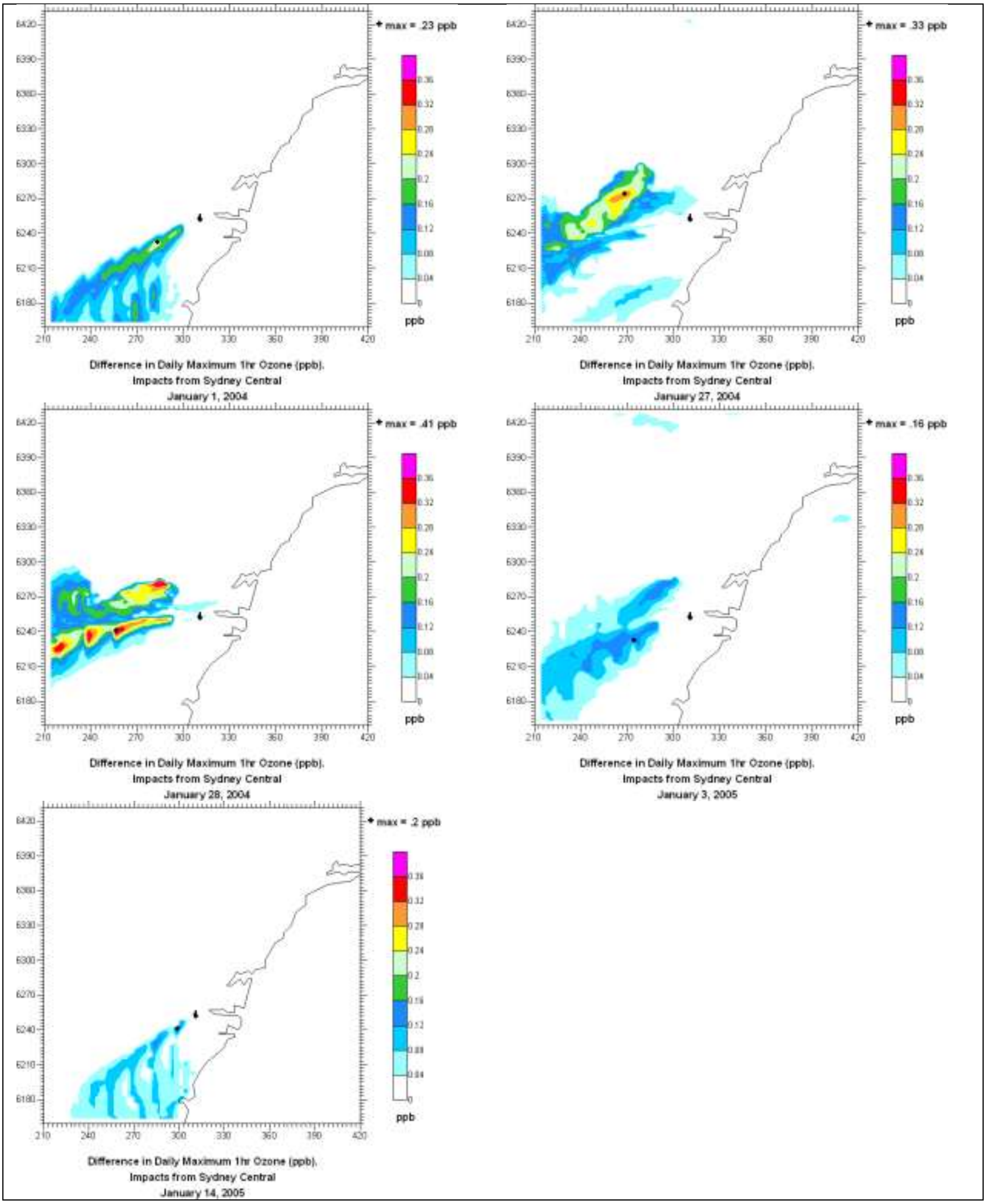
Daily Max 1hr O3 (ppb)
CAMx 5.30 OEH Base Case run2
January 27, 2004

Daily Max 1hr O3 (ppb)
CAMx 5.30 OEH Base Case run2
January 28, 2004

Daily Max 1hr O3 (ppb)
CAMx 5.30 OEH Base Case run2
January 03, 2005

Daily Max 1hr O3 (ppb)
CAMx 5.30 OEH Base Case run2
January 14, 2005

Figure 25: Spatial plots of modelled and observed daily maximum 1-hour ozone on the dates selected for the Level 2 refined procedure



Difference in Daily Maximum 1hr Ozone (ppb).
Impacts from Sydney Central
January 1, 2004

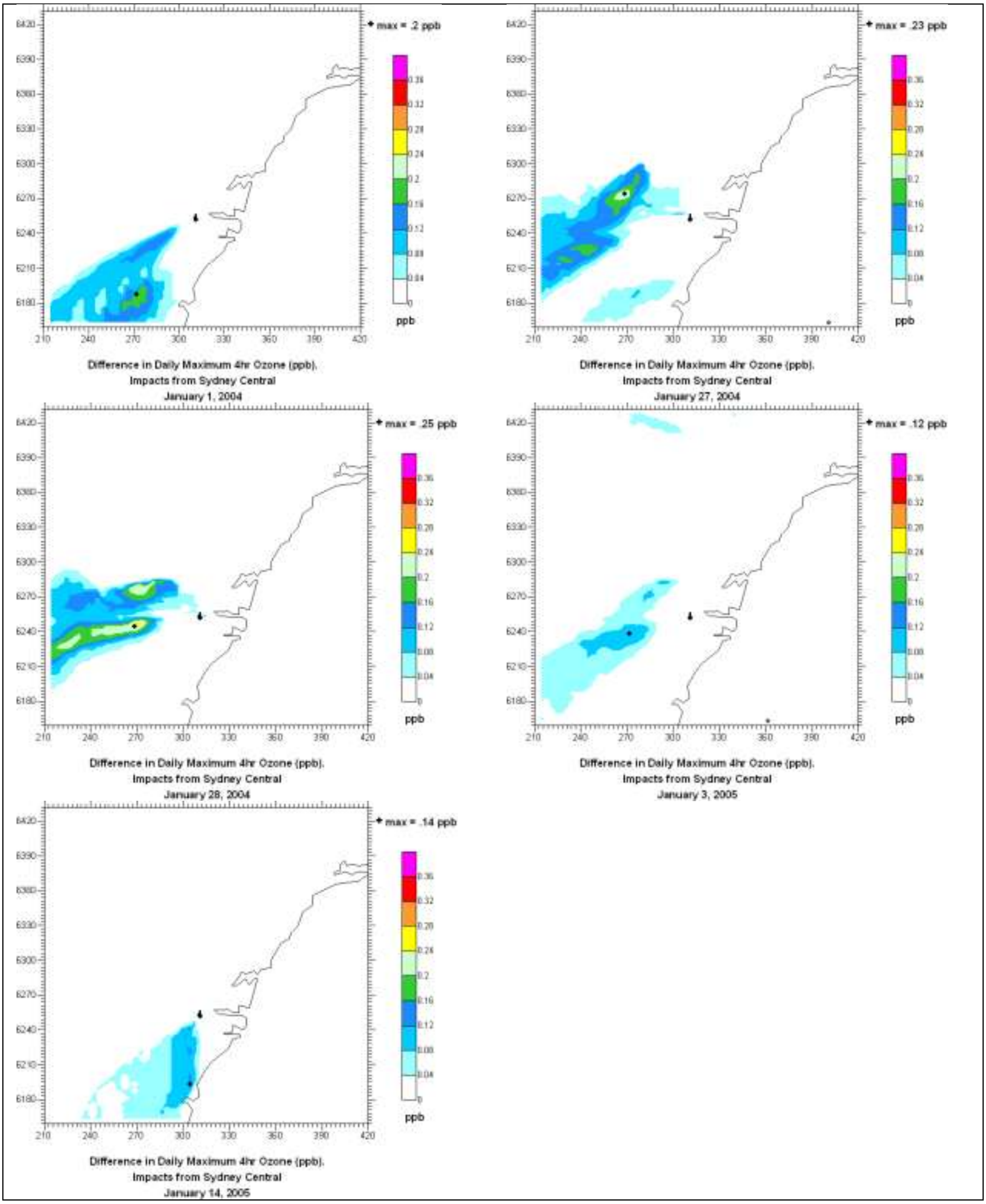
Difference in Daily Maximum 1hr Ozone (ppb).
Impacts from Sydney Central
January 27, 2004

Difference in Daily Maximum 1hr Ozone (ppb).
Impacts from Sydney Central
January 28, 2004

Difference in Daily Maximum 1hr Ozone (ppb).
Impacts from Sydney Central
January 3, 2005

Difference in Daily Maximum 1hr Ozone (ppb).
Impacts from Sydney Central
January 14, 2005

Figure 26: Spatial plots of modelled impacts from the new Central Sydney source to daily maximum 1-hour ozone on the dates selected for the Level 2 refined procedure



Difference in Daily Maximum 4hr Ozone (ppb).
Impacts from Sydney Central
January 1, 2004

Difference in Daily Maximum 4hr Ozone (ppb).
Impacts from Sydney Central
January 27, 2004

Difference in Daily Maximum 4hr Ozone (ppb).
Impacts from Sydney Central
January 28, 2004

Difference in Daily Maximum 4hr Ozone (ppb).
Impacts from Sydney Central
January 3, 2005

Difference in Daily Maximum 4hr Ozone (ppb).
Impacts from Sydney Central
January 14, 2005

Figure 27: Spatial plots of modelled impacts from the new Central Sydney source to the daily maximum 4-hour ozone on dates selected for the Level 2 refined procedure

4.2.3 Level 2 Refined Procedure Results

The maximum increase in 1-hour ozone (ppb) due to the new Central Sydney source is shown in **Table 32** for the five dates considered in the Level 2 assessment. The maximum increases ranged from 0.16 ppb to 0.4 ppb. Also shown in **Table 32** is the base case 1-hour ozone concentration at the same location and time as each maximum concentration increment, ranging from 65.4 ppb to 114.2 ppb. The maximum increase of 0.4 ppb coincided with the base case ozone concentration of 114.2 ppb.

Table 32: Maximum increase in 1-hour ozone (ppb) due to the new Central Sydney source on five dates considered in the Level 2 refined procedure

Date	Maximum Increase in 1-hr Ozone due to Source (ppb)	Base Case 1-hr Ozone at the Same Location and Time
1-Jan-04	0.23	85.6
27-Jan-04	0.23 (0.33)	65.4 (51.5)
28-Jan-04	0.41	114.2
3-Jan-05	0.16	90.3
14-Jan-05	0.20	94.2

The maximum increase in 4-hour ozone (ppb) due to the new Central Sydney source is shown in **Table 33**.

Table 33: Maximum increase in 4-hour ozone (ppb) due to the new Central Sydney source on five dates considered in the Level 2 refined procedure

Date	Maximum Increase in 4-hr Ozone due to Source (ppb)	Base Case 4-hr Ozone at the Same Location and Time
1-Jan-04	0.20	85.8
27-Jan-04	0.23	48.5
28-Jan-04	0.25	105.6
3-Jan-05	0.12	81.4
14-Jan-05	0.14	112.0

4.2.4 Evaluation of Level 2 Refined Procedure Results

The ozone increases due to the new Central Sydney source presented in **Section 4.2.3** have been compared to the significance criteria discussed in **Section 3.7**. Given that the maximum increase (0.4 ppb) is less than 0.5 ppb, the new source is considered to have no impact on compliance with the Air NEPM Standards.

4.3 Findings and Recommendations

An example Level 2 refined procedure has been performed to provide a demonstration of OEH expectations for this form of assessment, while not being prescriptive in approach. The Level 2 assessment used the model inputs developed for the Level 1 assessment. In short, two CAMx runs have been performed, with and without the new source emissions, to directly assess the ozone impact of the new source.

The Level 2 refined assessment is closely related to the Level 1 screening assessment to provide consistent evaluations of new source ozone impacts. The intent of directly modelling the source for using a Level 2 refined assessment is to eliminate any uncertainties attributable to the parameterisation of model results within the Level 1 screening procedure tool.

The modelling performed using a Level 2 refined assessment should not be less detailed than the modelling used to develop the level 1 screening procedure tool. One option is that the Level 2 refined assessment can use the modelling databases used to develop the Level 1 screening procedure tool.

Exactly the same criteria should be used to evaluate the significance of new source ozone impacts for the Level 1 screening and Level 2 refined procedures as documented in **Section 5**.

5. Guidance for Ozone Impact Assessment

The legislative and regulatory context underpinning ozone impact assessment and management is documented in **Section 5.1**.

The framework for ozone impact assessment and management is outlined in **Section 5.2**.

Specific guidance is provided on the application of the Level 1 screening procedure in **Section 5.3** and the Level 2 refined procedure in **Section 5.4**.

5.1 Legislative and Regulatory Context for Ozone Impact Assessment

5.1.1 Provision for Scheduled Activities

The *Protection of the Environment Operations Act 1997* (POEO Act) is the key piece of environment protection legislation administered by the Environment Protection Authority (EPA), which is part of the Office of Environment and Heritage (OEH).

The POEO Act establishes a system of environment protection licensing for “scheduled” activities with the potential to have a significant impact on the environment. Schedule 1 of the POEO Act lists those scheduled activities, which are licensed by the EPA. Most “non-scheduled” activities are regulated by local councils.

5.1.2 Requirement for Proper and Efficient Operation of Plant

Part 5.4 (sections 124-135) of the POEO Act deals specifically with air pollution. This includes the general obligation that the occupiers of non-residential premises do not cause air pollution by failing to operate or maintain plant, carry out work or deal with materials in a proper and efficient manner (sections 124-126).

5.1.3 Air Emission Standards

Section 128 (1) of the POEO Act requires occupiers of non-residential premises to comply with any air emission standards prescribed by regulations. These standards are contained in Part 5 and Part 6 of the *Protection of the Environment Operations (Clean Air) Regulation 2010*. The standards are in-stack emission limits and are the maximum emissions permissible for an industrial source anywhere in NSW. Section 128 (2) of the POEO Act requires that all necessary practicable means are used to prevent or minimise air pollution, where emission standards are not prescribed by regulations, which is essentially a requirement to use best management practice.

As a secondary pollutant, ozone is not the subject of air emission standards. However precursors of ozone, notably oxides of nitrogen and volatile organic compounds, are regulated within Part 5 and Part 6 of the Clean Air Regulation.

5.1.4 Air Quality Assessment

The emission limits in Part 5 and Part 6 of the Clean Air Regulation do not take into account site-specific features such as meteorology and background air quality, and therefore do not necessarily protect against adverse air quality impacts in the areas surrounding the premises. These site-specific features are accounted for in an air quality impact assessment.

The *Approved Methods for the Modelling and Assessment of Air Pollutants in NSW* lists the statutory methods that are to be used to model and assess emissions of air pollutants from stationary sources in NSW. The purpose of an air quality impact assessment is to demonstrate acceptable impacts at the sensitive receptors surrounding the premises.

The Approved Methods for Modelling is referred to in Part 5: Air impurities from emitted activities and plant of the Clean Air Regulation. This document may also be referred to in conditions attached to statutory instruments, such as licences or notices issued under the Protection of the Environment Operations Act 1997; and OEH Chief Executive's requirements under the Environmental Planning and Assessment Act 1979.

The Approved Methods for Modelling does not currently contain a documented procedure for predicting impacts associated with the release of precursors of ozone, primarily NO_X and/or VOC. The tiered approach to ozone impact assessment for stationary sources of NO_X and/or VOC developed in this study could be incorporated in the Approved Methods for Modelling.

5.1.5 Air Quality Standards for Ozone

The *National Environment Protection (Ambient Air Quality) Measure* (Air NEPM) 2003 establishes ambient air quality standards and monitoring and reporting protocols for common air pollutants, including photochemical oxidants (measured as ozone) (**Table 34**). These standards are referenced within the Approved Methods for Modelling.

Table 34: National Ambient Air Quality Standards and Goals (Air Quality NEPM)

Pollutant	Averaging Period	Maximum Concentration	Maximum Allowable Exceedences (Goal to be Met by 2008)
Photochemical oxidants (as ozone)	1 hour 4 hours	0.10 ppm 0.08 ppm	1 day a year 1 day a year

Notes:

- The averaging periods are defined as follows: 1 hour (clock hour average), 4 hour (rolling 4 hour average based on 1 hour averages).
- Maximum allowable exceedance time periods are defined as follows:
  - day: calendar day during which the associated standard is exceeded
  - year: calendar year.
- All averaging periods of 8 hours or less must be referenced by the end time of the averaging period. This determines the calendar day to which the averaging periods are assigned.
- For the purposes of calculating and reporting 4 and 8 hour averages, the first rolling average in a calendar day ends at 1.00 am, and includes hours from the previous calendar day.
- Maximum concentrations are the arithmetic mean concentrations.

Ozone standards have been selected on the basis of providing health protection for the majority of the population including susceptible groups (e.g. the elderly and asthmatics), being technically achievable, and providing comparable costs and benefits within the limitations of the analysis. No threshold exposure level has been identified for ozone, so it is not possible to define either a No Observable Adverse Effect Level (NOAEL) or a Lowest Observed Adverse Effect Level (LOAEL). The Air NEPM review concludes there are significant health effects observed at levels below the current ozone standards (NEPC 2010).

5.1.6 Definition of Ozone Attainment and Non-attainment Areas

The ozone impact assessment procedure makes reference to ozone “attainment areas” and ozone “non-attainment areas”.

In determining whether an area is classified as an ozone attainment or non-attainment area, reference is made to measured ambient ozone concentrations from OEH ambient air quality monitoring stations recorded over the past 5 years.

The maximum 1-hour and 4-hour average ozone concentrations recorded over the most current 5 year period should be averaged to obtain the 5-year average 1-hour and 4-hour maximum ozone concentrations for each monitoring station. Reference should then be made to the highest 5-year average maximum recorded across monitoring stations in the region within which the source is located.

The 5-year average 1-hour and 4-hour maximums for the source region are compared to the screening procedure acceptance limits for ozone, expressed as 82% of the Air NEPM Standard(11).

Areas where the 5-year average 1-hour maximum ozone concentration is greater than 0.082 ppm, and/or where the 5-year average 4-hour maximum ozone concentration is greater than 0.0656 ppm, are classified as non-attainment areas. Remaining areas are classified as attainment areas.

Based on the 5-year average maximums recorded in Sydney, the Illawarra and the Lower Hunter during the 2006-2010 period (**Table 35, Table 36**), all three regions are classifiable as ozone non-attainment areas (**Table 37**).

Table 35: Measured highest 1-hour ozone concentrations in ppm (2006-2010)

Station	2006	2007	2008	2009	2010	Average
Sydney						0.117
Bargo	0.121	0.117	0.091	0.122	0.110	0.112
Bringelly	0.119	0.111	0.093	0.120	0.104	0.109
Chullora	0.117	0.088	0.080	0.154	0.083	0.104
Earlwood	0.111	0.083	0.063	0.138	0.085	0.096
Lindfield	ND	ND	0.075	0.109	0.082	0.089
Liverpool	0.128	0.116	0.098	0.151	0.091	0.117
Macarthur	0.128	0.121	0.085	0.116	0.119	0.114
Oakdale	0.109	0.142	0.093	0.128	0.099	0.114
Prospect	ND	0.089	0.107	0.126	0.104	0.107
Randwick	0.083	0.090	0.061	0.078	0.084	0.079
Richmond	0.108	0.134	0.078	0.102	0.089	0.102
Rozelle	0.093	0.088	0.056	0.083	0.073	0.079
St Marys	0.124	0.123	0.096	0.132	0.095	0.114

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11 *NEPC (Ambient Air Quality) Measure Technical Paper No. 4, Revision 1 – January 2007, Screening Procedures.*

Table 35: Measured highest 1-hour ozone concentrations in ppm (2006-2010)

Station	2006	2007	2008	2009	2010	Average
Vineyard	0.104	0.127	0.081	0.100	0.090	0.100
Illawarra						0.089
Albion Park Sth	0.096	0.092	0.062	0.102	0.093	0.089
Kembla Grange	0.093	0.093	0.072	0.103	0.081	0.088
Wollongong	0.096	0.077	0.067	0.083	0.082	0.081
Lower Hunter						0.078
Beresfield	0.088	0.080	0.064	0.072	0.088	0.078
Newcastle	0.068	0.053	0.064	0.073	0.086	0.069
Wallsend	0.086	0.070	0.057	0.086	0.067	0.073

Table 36: Measured highest 4-hour ozone concentrations in ppm (2006-2010)

Station	2006	2007	2008	2009	2010	Average
Sydney						0.098
Bargo	0.103	0.105	0.074	0.111	0.086	0.096
Bringelly	0.110	0.095	0.078	0.108	0.089	0.096
Chullora	0.104	0.074	0.074	0.112	0.072	0.087
Earlwood	0.095	0.071	0.056	0.104	0.074	0.080
Lindfield	ND	ND	0.064	0.097	0.079	0.080
Liverpool	0.124	0.094	0.089	0.103	0.081	0.098
Macarthur	0.117	0.101	0.070	0.097	0.103	0.098
Oakdale	0.086	0.116	0.075	0.108	0.088	0.095
Prospect	ND	0.085	0.096	0.100	0.097	0.095
Randwick	0.079	0.084	0.057	0.073	0.077	0.074
Richmond	0.095	0.121	0.067	0.090	0.082	0.091
Rozelle	0.082	0.075	0.048	0.073	0.067	0.069
St Marys	0.109	0.105	0.082	0.106	0.083	0.097
Vineyard	0.085	0.116	0.065	0.088	0.079	0.087
Illawarra						0.079
Albion Park Sth	0.078	0.080	0.055	0.083	0.073	0.074
Kembla Grange	0.081	0.082	0.066	0.090	0.078	0.079
Wollongong	0.086	0.073	0.063	0.074	0.073	0.074
Lower Hunter						0.072
Beresfield	0.074	0.075	0.062	0.065	0.082	0.072
Newcastle	0.064	0.047	0.058	0.067	0.076	0.062
Wallsend	0.066	0.068	0.054	0.076	0.063	0.065

Table 37: Classification of Regions based on Maximum 5-year average Ozone Concentrations recorded at OEH Stations during 2006-2010

Station	Maximum 5-year average 1-hour Ozone Concentration (ppb)	Air NEPM Ozone Standard (ppb)	Difference between Standard and Ambient (ppb)	25% of Residual	Region Classification
Sydney	116.8	100	-16.8	NA(a)	Non-attainment
Illawarra	89.0	100	11.0	NA(a)	Non-attainment
Lower Hunter	78.4	100	21.6	5.4	Attainment
Station	**Maximum 5-year average 4-hour Ozone Concentration (ppb)**	**Air NEPM Ozone Standard (ppb)**	**Difference between Standard and Ambient (ppb)**	**25% of Residual**	**Region Classification**
Sydney	98.2	80	-18.2	NA(a)	Non-attainment
Illawarra	79.4	80	0.6	NA(a)	Non-attainment
Lower Hunter	71.6	80	8.4	NA(a)	Non-attainment

(a) Maximum allowable increment specified as 1 ppb for ozone non-attainment areas.

5.1.7 Screening Impact Levels and Maximum Allowable Increments

In determining whether or not the ambient ozone impacts of a source warrant further assessment, a screening impact level (SIL) of 0.5 ppb is applied. Sources giving rise to maximum 1-hour average or 4-hour average ozone increments equal to or above 0.5 ppb are required to undertake further analysis. The limit of 0.5 ppb is specified taking into consideration ambient ozone measurement and reporting limits.

While ozone concentration increments (i.e. Prevention of Significant Deterioration (PSD) increments) are not used in the US, the relationship between PSD increments and national ambient air quality standards (NAAQS) for other air pollutants may be used as a guide for developing them. For short-term (i.e. 24-hour or less) averaging periods, the PSD increment for a given pollutant is generally between 1% and 6% of the NAAQS. If this relationship is applied to *National Environment Protection (Ambient Air Quality) Measure* (Air NEPM) standards for ground-level ozone (NEPC 2003), PSD increments of between 1 and 6 ppb (expressed as a 1-hour average) and between 1 and 5 ppb (expressed as a 4-hour average) would apply.

The ground-level ozone PSD increments of between 1 and 6 ppb are consistent with US modelling practice. When the USEPA evaluated ozone transport between States for the Clean Air Interstate Rule, ozone transport contributions associated with a 2 ppb increment in daily maximum 8-hour ozone were considered insignificant.

An incremental increase in excess of 1 ppb ozone (expressed as either a 1-hour or 4-hour average) has been selected as an unacceptable level within an ozone non-attainment area. This metric is selected based on the above considerations, combined with the 1 ppb value being a “measurable” change using conventional ambient monitoring instrumentation.

For ozone attainment areas, the maximum allowable increment is calculated as a function of the difference between ambient ozone concentrations and air quality standards (**Table 37**). Further details on this approach are provided in **Section 5.1.2**.

5.1.8 Best Management Practice as a Guiding Principle

For a pollutant such as ozone with no safe level of exposure, best management practice (BMP) is the guiding principle in meeting an objective of the POEO Act, which is to reduce the risks to human health by reducing emissions to harmless levels (Chapter 1, Section 3).

Best management practice is also the guiding principle for non-residential premises in meeting the requirements of the POEO Act. Sections 124 to 126 of the POEO Act require that air pollution related activities be conducted in a proper and efficient manner, while section 128 requires that all necessary practicable means be used to prevent or minimise air pollution.

In undertaking BMP determinations for sources to be located within an ozone attainment area, consideration should be given to reasonably available techniques (RAT) for point and fugitive sources (Refer **Section 5.1.9**).

BMP determinations for sources proposed for location within ozone non-attainment areas should consider best available techniques (BAT) and/or emission offsets for point and fugitive sources (Refer **Section 5.1.10** and **Section 5.1.11** respectively).

5.1.9 Reasonably Available Techniques

New or modified facilities to be located within ozone attainment areas should consider RAT for point and fugitive sources when undertaking BMP determinations, as specified within the ozone impact assessment procedure.

RAT refers to control technology that is both reasonably available, and technologically and economically feasible. Reasonable relates to the application of judgement in arriving at a decision, taking into account: mitigation benefits, cost of mitigation versus benefits provided, community views and the nature and extent of potential improvements. Feasible relates to engineering considerations and what is practical to build(12).

5.1.10 Best Available Techniques

New or modified facilities to be located within ozone non-attainment areas should consider BAT and/or emission offsets for point and fugitive sources when undertaking BMP determinations, as specified within the ozone impact assessment procedure. Emission offsets are addressed in **Section 5.1.11**, with BAT explained in this subsection.

In defining BAT, OEH makes reference to the European Directive on Integrated Pollution Prevention and Control(13).

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12 http://caselaw.lawlink.nsw.gov.au/isysquery/42abed99-b8ad-4c1d-bc9e-c4bf3a1ffd14/91-100/list/

13 http://www.environment.nsw.gov.au/air/cogentrigen.htm

BAT covers all aspects of a proposal including fuel source, technology selection and controls. As outlined in the European Union Directive on Integrated Pollution Prevention and Control, the following definitions apply(14):

Best available techniques shall mean the most effective and advanced stage in the development of activities and their methods of operation which indicate the practical suitability of particular techniques for providing in principle the basis for emission limit values designed to prevent and, where that is not practicable, generally to reduce emissions and the impact on the environment as a whole:

Best shall mean most effective in achieving a high general level of protection of the environment as a whole.

Available techniques shall mean those developed on a scale which allows implementation in the relevant industrial sector, under economically and technically viable conditions, taking into consideration the costs and advantages, whether or not the techniques are used or produced inside the Member State in question, as long as they are reasonably accessible to the operator.

Techniques shall include both the technology used and the way in which the installation is designed, built, maintained, operated and decommissioned.

5.1.11 Emission Offsetting

New or modified facilities to be located within ozone non-attainment areas should consider BAT and/or emission offsets for point and fugitive sources when undertaking BMP determinations, as specified within the ozone impact assessment procedure. BAT is addressed in **Section 5.1.10**, with the concept of emission offsetting explained in this subsection.

A framework for NO_X offsets is provided within the *Interim OEH Nitrogen Oxide Policy for Cogeneration in Sydney and the Illawarra.* A concise description of this framework is provided below.

The objective of offsets is to provide a cost-effective way of addressing environmental issues while at the same time allowing economic development to occur. The main economic principle underpinning offsets is the reduction of environmental impact as least cost.

Offsets recognise that it is not always practical to achieve zero environmental impact from a single source. Where cost-effective mitigation and prevention measures have been exhausted, offsets can achieve environmental improvement at a greatly reduced cost by offsetting the remaining impacts elsewhere.

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14 *DIRECTIVE 2008/1/EC OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 15 January 2008 concerning integrated pollution prevention and control*

The central principles that are proposed to guide development of pollution offsets in NSW are as follows(15):

- Environmental impacts must be avoided first by using all cost-effective prevention and mitigation measures on-site. Offsets are then only used to address the remaining loads of pollutants.
- All standard regulatory requirements must still be met.
- Offsets must never reward ongoing poor environmental performance.
- Offsets will complement other government programs.
- Offsets must result in no net increase of target pollutants.

The general offset principles outlined above provide the basis for the ozone precursor emission offset requirement for new sources that choose to offset their ozone precursor emissions instead of, or in addition to, implementing Best Available Techniques.

The criteria to be used by OEH to assess whether proposed offsets meet the objectives of reducing current NO_x or VOC emission are as follows:

- Technical infeasibility of the control technology
- Operating schedule and project length — if the equipment will operate much fewer hours per year than what is typical, or for a much shorter project length, it can affect what is considered “achieved in practice”.
- Availability of fuel. By example, unavailability of natural gas for cogeneration projects.
- Local air quality issues. By example, high NO_2 levels within the CBD may require lower NO_X limits than BAT on a similar project located elsewhere.
- Supplementary requirement. The offsets must be beyond existing requirements and not already being funded under another scheme. An offset proposal cannot include pollution abatement actions if they are already required under federal, state or council legislation, or any other legal requirements, or if Government funds them. This includes actions required by an environment protection licence condition (including pollution reduction programs, although this may be subject to negotiation). Credit will not be given for work that would have happened anyway (e.g. decommissioning a plant that was already scheduled for closure).
- Enforceability. The requirement to offset all new ozone precursor emissions must be clearly stated in the development consent conditions and will become implemented as licence conditions. Conditions relating to green offset schemes or works are permitted

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15 www.environment.nsw.gov.au/greenoffsets/principles.htm.

under section 69 of the POEO Act. Penalties for non-compliance with licence conditions are up to $1 million for a corporation (section 64).

5.2 Framework for Ozone Impact Assessment and Management

5.2.1 Applicability of the Procedure

The ozone impact assessment is intended for those “scheduled” activities listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* which emit ozone precursors and are located or proposed to be located within the Greater Metropolitan Area (GMA) as defined within the *Protection of the Environment Operations (Clean Air) Regulation 2010*.

A stationary source refers to a premises undertaking “scheduled” activities listed in Schedule 1 of the *Protection of the Environment Operations Act 1997*, and may comprise one or more emission units. As defined within the *Protection of the Environment Operations (Clean Air) Regulation* 2010, an emission unit means an item of plant that forms part of, or is attached to, some larger plant, being an item of plant that emits, treats or processes air impurities or controls the discharge of air impurities into the atmosphere.

5.2.2 Ozone Impact Assessment Procedure

The ozone impact assessment procedure is illustrated by means of a flowchart in **Figure 36**, with steps to be followed described in this subsection.

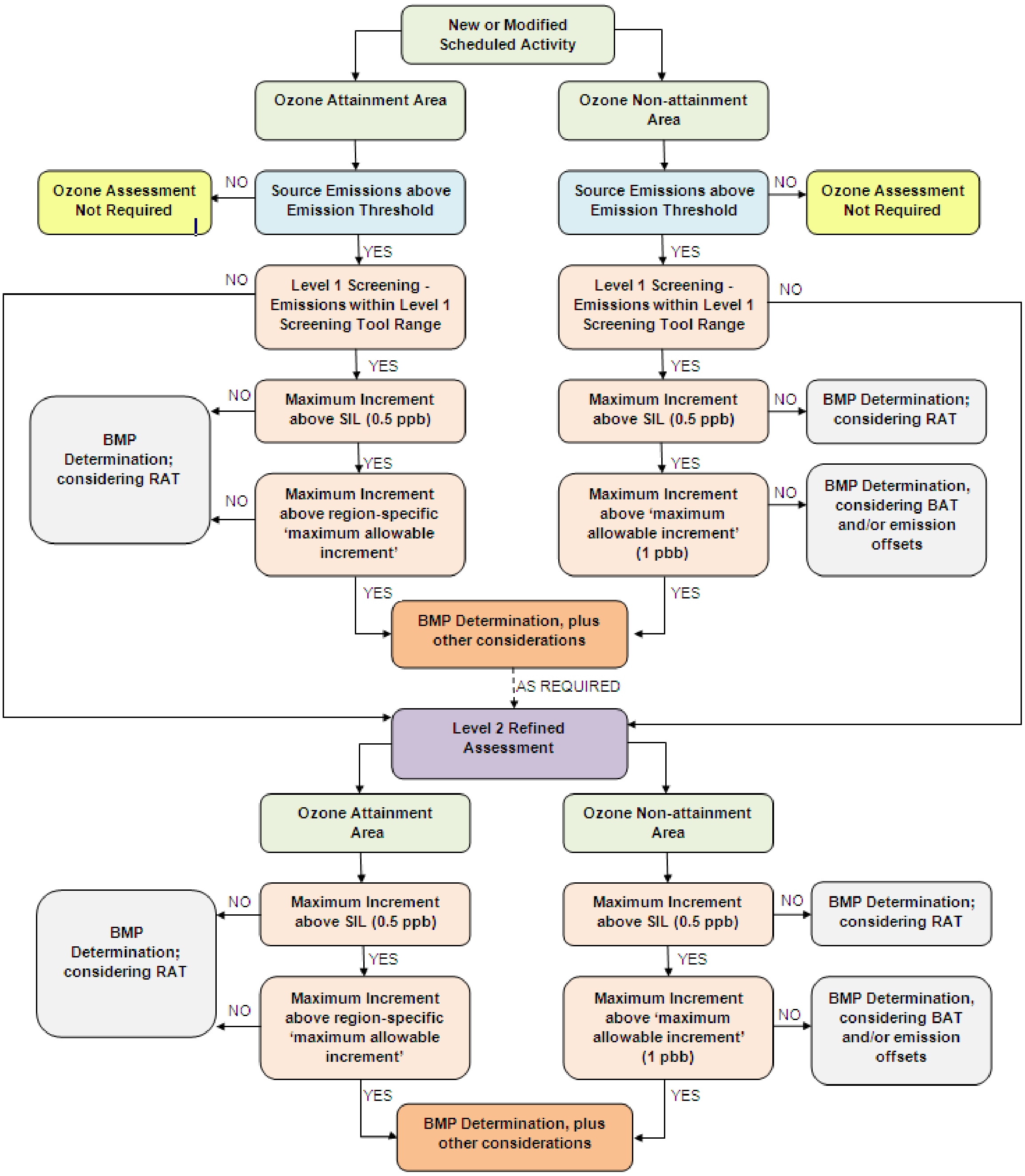

Figure 28: Ozone impact assessment procedure for new or modified scheduled activities located within the NSW GMA

The ozone impact assessment and management procedure comprises the following key steps:

(1) Check whether the proposed source is located in an area of ozone attainment or non-attainment.

In determining whether an area is classifiable as an ozone attainment or non-attainment area, reference should be made to measured ambient ozone concentrations from OEH ambient air quality monitoring stations recorded over the past 5 years.

The maximum 1-hour and 4-hour average ozone concentrations recorded over the most current 5 year period should be averaged to obtain the 5-year average 1-hour and 4-hour maximum ozone concentrations for each monitoring station. Reference should then be made to the highest 5-year average maximums recorded across monitoring stations in the region within which the source is located. The Level 1 screening procedure tool contains measured ozone concentrations for the 2006-2010 period for three regions, including Sydney, Illawarra and Lower Hunter (**Table 38** and **Table 39**).

Table 38: Measured highest 1-hour ozone concentrations in ppm (2006-2010)

Station	2006	2007	2008	2009	2010	Average
Sydney						0.117
Bargo	0.121	0.117	0.091	0.122	0.110	0.112
Bringelly	0.119	0.111	0.093	0.120	0.104	0.109
Chullora	0.117	0.088	0.080	0.154	0.083	0.104
Earlwood	0.111	0.083	0.063	0.138	0.085	0.096
Lindfield	ND	ND	0.075	0.109	0.082	0.089
Liverpool	0.128	0.116	0.098	0.151	0.091	0.117
Macarthur	0.128	0.121	0.085	0.116	0.119	0.114
Oakdale	0.109	0.142	0.093	0.128	0.099	0.114
Prospect	ND	0.089	0.107	0.126	0.104	0.107
Randwick	0.083	0.090	0.061	0.078	0.084	0.079
Richmond	0.108	0.134	0.078	0.102	0.089	0.102
Rozelle	0.093	0.088	0.056	0.083	0.073	0.079
St Marys	0.124	0.123	0.096	0.132	0.095	0.114
Vineyard	0.104	0.127	0.081	0.100	0.090	0.100
Illawarra						0.089
Albion Park Sth	0.096	0.092	0.062	0.102	0.093	0.089
Kembla Grange	0.093	0.093	0.072	0.103	0.081	0.088
Wollongong	0.096	0.077	0.067	0.083	0.082	0.081
Lower Hunter						0.078
Beresfield	0.088	0.080	0.064	0.072	0.088	0.078
Newcastle	0.068	0.053	0.064	0.073	0.086	0.069
Wallsend	0.086	0.070	0.057	0.086	0.067	0.073

Table 39: Measured highest 4-hour ozone concentrations in ppm (2006-2010)

Station	2006	2007	2008	2009	2010	Average
Sydney						0.098
Bargo	0.103	0.105	0.074	0.111	0.086	0.096
Bringelly	0.110	0.095	0.078	0.108	0.089	0.096
Chullora	0.104	0.074	0.074	0.112	0.072	0.087
Earlwood	0.095	0.071	0.056	0.104	0.074	0.080
Lindfield	ND	ND	0.064	0.097	0.079	0.080
Liverpool	0.124	0.094	0.089	0.103	0.081	0.098
Macarthur	0.117	0.101	0.070	0.097	0.103	0.098
Oakdale	0.086	0.116	0.075	0.108	0.088	0.095
Prospect	ND	0.085	0.096	0.100	0.097	0.095
Randwick	0.079	0.084	0.057	0.073	0.077	0.074
Richmond	0.095	0.121	0.067	0.090	0.082	0.091
Rozelle	0.082	0.075	0.048	0.073	0.067	0.069
St Marys	0.109	0.105	0.082	0.106	0.083	0.097
Vineyard	0.085	0.116	0.065	0.088	0.079	0.087
Illawarra						0.079
Albion Park Sth	0.078	0.080	0.055	0.083	0.073	0.074
Kembla Grange	0.081	0.082	0.066	0.090	0.078	0.079
Wollongong	0.086	0.073	0.063	0.074	0.073	0.074
Lower Hunter						0.072
Beresfield	0.074	0.075	0.062	0.065	0.082	0.072
Newcastle	0.064	0.047	0.058	0.067	0.076	0.062
Wallsend	0.066	0.068	0.054	0.076	0.063	0.065

The 5-year average 1-hour and 4-hour maximums for the source region should be compared to the screening procedure acceptance limits for ozone, expressed as 82% of the Air NEPM Standard(16).

Areas where the 5-year average 1-hour maximum ozone concentration is greater than 0.082 ppm, and/or where the 5-year average 4-hour maximum ozone concentration is greater than 0.0656 ppm, are classified as non-attainment areas. Similarly, areas where the 5-year average 1-hour maximum ozone concentration is less than 0.082 ppm, and/or where the 5-year average 4-hour maximum ozone concentration is less than 0.0656 ppm, are classified as attainment areas.

Each region is classified as an ozone attainment or non-attainment area using the Air NEPM screening procedure acceptance limits (**Table 40**).

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16 *NEPC (Ambient Air Quality) Measure Technical Paper No. 4, Revision 1 – January 2007, Screening Procedures.*

Table 40: Classification of Regions based on Maximum 5-year average Ozone Concentrations recorded at OEH Stations during 2006-2010

Station	Maximum 5-year average 1-hour Ozone Concentration (ppb)	Air NEPM Ozone Standard (ppb)	Difference between Standard and Ambient (ppb)	25% of Residual	Region Classification
Sydney	116.8	100	-16.8	NA(a)	Non-attainment
Illawarra	89.0	100	11.0	NA(a)	Non-attainment
Lower Hunter	78.4	100	21.6	5.4	Attainment
Station	**Maximum 5-year average 4-hour Ozone Concentration (ppb)**	**Air NEPM Ozone Standard (ppb)**	**Difference between Standard and Ambient (ppb)**	**25% of Residual**	**Region Classification**
Sydney	98.2	80	-18.2	NA(a)	Non-attainment
Illawarra	79.4	80	0.6	NA(a)	Non-attainment
Lower Hunter	71.6	80	8.4	NA(a)	Non-attainment

(a) Maximum allowable increment specified as 1 ppb for ozone non-attainment areas.

(2) For sources within ozone attainment areas:

a. Evaluate the source's emissions against the new or modified source thresholds for NO_x and VOC emissions specified in **Table 41**(17). Total emissions from the new or modified source, from all individual emission units, should be compared to the emission thresholds.

Table 41: NO_X and VOC Emission Thresholds for New or Modified Sources within Ozone Attainment Areas

Source Type	NO_X / VOC Emission Rate tonnes/year
New Source	
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997*	>90
Modified Source	
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997*	>35

For a source with emissions below the relevant emission threshold, an ozone impact assessment is not required but the source should assess air quality impacts for other air pollutants as required by the *Approved Methods for the Modelling and Assessment of Air Pollutants in NSW* (DEC, 2005).

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17 The thresholds reference the US New Source Review (NSR) emission thresholds for new or modified sources located within areas that meet the ozone NAAQS under the Prevention of Significant Deterioration (PSD) program (refer to **Section 2.1.1.3**)

For cases where source emissions are above the relevant emission threshold, a Level 1 assessment should be undertaken using the Level 1 screening procedure tool (Refer to **Section 5.3**). In the event the source emissions exceed the upper range of the tool, the licensee should consult with the EPA. The EPA may require that a Level 2 refined assessment be undertaken for the source (Refer to **Section 5.4**). Results from the Level 2 refined assessment should be compared to the relevant SIL and maximum allowable increment as defined for the Level 1 screening assessment.

b. Maximum 1-hour and 4-hour average ozone concentration increments calculated for the source using the Level 1 screening procedure should be compared to the significant impact level (SIL) for ozone attainment areas, specified as 0.5 ppb.

Where incremental concentrations are below the SIL, no further ozone impact assessment is required but a BMP determination, considering reasonably available techniques (RAT) should be undertaken.

Where the maximum 1-hour or 4-hour average ozone concentration increment is above the SIL, the calculated increment should be evaluated against the maximum allowable ozone increments for the region.

c. The maximum allowable ozone increments are defined as 25% of the difference between the 5-year average 1-hour and 4-hour maximums for the region and the relevant Air NEPM Standard(18). Screening procedure acceptance limits for ozone are expressed as 82% of the Air NEPM Standard(19). Given the application of an acceptable level of 82%, the difference between the 5-year average maximums and the relevant standard will be greater than or equivalent to 18 ppb for an 1-hour averaging period and greater than or equivalent to 14.4 ppb for a 4-hour averaging period.

Where the maximum 1-hour and 4-hour increment is below the relevant maximum allowable increment, no further ozone impact assessment is required, but a BMP determination considering RAT should be undertaken. In the event the impacts are greater than the maximum allowable increment, the EPA may consider the impact of the source on local and regional air quality having regard to the following matters:

i. The outcomes of the BMP determination;

ii. The frequency and duration of ground-level ozone impacts;

iii. Any pollution reduction programs established or agreed to;

iv. Any control equipment installed or agreed to;

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18 The maximum allowable ozone increment reflects the maximum increase in ozone concentrations allowed above the existing baseline ozone concentration. An increment comprising 25% of the residual was selected in line with US PSD increments defined for Class 2 areas, which are designated to allow moderate, controlled growth. (Refer to **Section 2.1.1.3**).

19 *NEPC (Ambient Air Quality) Measure Technical Paper No. 4, Revision 1 – January 2007, Screening Procedures.*

v. Any load reduction agreement entered; and

vi. The principles of ecologically sustainable development.

The EPA may require that a Level 2 refined assessment be undertaken for the source (Refer to **Section 5.4**). Results from the Level 2 refined assessment should be compared to the relevant SIL and maximum allowable increment as defined for the Level 1 screening assessment, and the procedure outlined in **Figure 36** followed.

(3) For sources within ozone non-attainment areas:

a. Evaluate the source's emissions against the new or modified source thresholds for NO_x, VOC and CO emissions specified in **Table 42**(20). Total emissions from the new or modified source, from all individual emission units, should be compared to the emission thresholds.

Table 42: NO_X and VOC Emission Thresholds for New or Modified Sources within Ozone Non-attainment Areas

Source Type	NO_X / VOC Emission Rate tonnes/year
New Source	
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in all Other Areas	>90
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in Serious Ozone Non-attainment Area (Area has a 5-year average 1-hour maximum ozone concentration in the range of 0.13 to 0.15 ppm, and/or a 5-year average 4-hour maximum ozone concentration in the range of 0.11 to 0.12 ppm.)	>45
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in Severe Ozone Non-attainment Area (Area has a 5-year average 1-hour maximum ozone concentration in the range of 0.15 to 0.23 ppm, and/or a 5-year average 4-hour maximum ozone concentration in the range of 0.12 to 0.19 ppm.)	>25
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in Extreme Ozone Non-attainment Area (Area has a 5-year average 1-hour maximum ozone concentration in the range of 0.23 ppm and above, and/or a 5-year average 4-hour maximum ozone concentration in the range of 0.19 ppm and above.)	>10
Modified Source	
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in all Other Areas	>35
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in Serious or Severe Ozone Non-attainment Area	>25
Any scheduled activity listed in Schedule 1 of the *Protection of the Environment Operations Act 1997* located in Extreme Ozone Non-attainment Area	Any Increase

For a source with emissions below the relevant emission threshold, an ozone impact assessment is not required but the source should assess air quality impacts for other air

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20 Thresholds reference the US New Source Review (NSR) emission thresholds for new or modified sources located in areas that exceed the ozone NAAQS, i.e. non-attainment areas (refer to **Section 2.1.1.5**)

pollutants as required by the *Approved Methods for the Modelling and Assessment of Air Pollutants in NSW* (DEC, 2005).

For cases where source emissions are above the relevant emission threshold, a Level 1 assessment should be undertaken using the Level 1 screening procedure tool (Refer to **Section 5.3**). In the event the source emissions exceed the upper range of the tool, the licensee should consult with the EPA. The EPA may require that a Level 2 refined assessment be undertaken for the source (Refer to **Section 5.4**). Results from the Level 2 refined assessment should be compared to the relevant SIL and maximum allowable increment as defined for the Level 1 screening assessment.

b. Maximum 1-hour and 4-hour average ozone concentration increments calculated for the source using the Level 1 screening procedure should be compared to the significant impact level (SIL) specified as 0.5 ppb.

Where incremental concentrations are below the SIL, no further ozone impact assessment is required but a BMP determination, considering reasonably available techniques (RAT) should be undertaken. Where the incremental concentrations are above the SIL further assessment is required.

c. Maximum 1-hour and 4-hour average increments calculated for the source using the Level 1 screening procedure tool should be evaluated against the maximum allowable ozone increment of 1 ppb specified for ozone non-attainment areas.

Where incremental concentrations are below 1 ppb, no further ozone impact assessment is required but a BMP determination should be undertaken including a cost-benefit analysis of BAT and/or consideration of emission offsets. Where either the maximum 1-hour increment or the maximum 4-hour increment exceeds 1 ppb, the EPA may consider the impact of the source on local and regional air quality having regard to the following matters:

i. The outcomes of the BMP determination;

ii. The frequency and duration of ground-level ozone impacts;

iii. Any pollution reduction programs established or agreed to;

iv. Any control equipment installed or agreed to;

v. Any load reduction agreement entered; and

vi. The principles of ecologically sustainable development.

The EPA may require that a Level 2 refined assessment be undertaken for the source (Refer to **Section 5.4**). In this event, results from the Level 2 refined assessment should be compared to the relevant SIL and maximum allowable increment as defined for the Level 1 screening assessment.

5.3 Guidance for Level 1 Screening Procedure

The Level 1 screening assessment should be conducted using the Level 1 screening procedure tool as provided by OEH.

The Level 1 screening procedure tool is based on first and second-order sensitivity coefficients calculated using the higher order Decoupled Direct Method (HDDM) in the CAMx photochemical model. This tool provides a Level 1 assessment of the impact of a new or modified source's NO_x and/or VOC emissions on downwind ozone concentrations.

The tool is applicable for sources located within the following regions within the GMR: West Sydney, Central Sydney, East Sydney, Newcastle and Wollongong.

The tool can estimate increases in 1-hour and 4-hour ground-level ozone concentrations for sources with different emissions of CO, CH_4, NO_x and/or VOC.

Prior to the use of the tool for a Level 1 assessment, it should be determined whether the source emissions are within the range of the tool's applicability. Following the specification of the source emission rates, the tool will indicate whether or not the reactivity-weighted total emissions attributable to the source are within the tool's range.). In the event the source emissions exceed the upper range of the tool, the licensee should consult with the EPA. The EPA may require that a Level 2 refined assessment be undertaken for the source.

Procedure to be followed in applying the Level 1 screening procedure tool:

1) Select the location of the new source from the 5 source regions provided for.

2) Specify the CO emissions, if any, for this source (in tonnes/day)

3) Specify the CH_4 emissions, if any, for this source (in tonnes/day)

4) Specify the NO_x emissions, if any, for this source (in tonnes/day)

5) Specify the VOC emissions, if any, for this source for each species or species group (in tonnes/day).

   Consistent with the requirements of the Clean Air Regulation, VOC means any chemical that: is based on carbon chains or rings, and contains hydrogen, and has a vapour pressure greater than 0.27 kPa at 25°C and 101.3 kPa. VOC include any such compound containing oxygen, nitrogen or other elements, but does not include methane, carbon monoxide, carbon dioxide, carbonic acid, metallic carbides and carbonate salts.

Speciated VOC emissions should be derived using either site specific or site representative source emission test results. If such data are not available then VOC emission estimates should be based on emission estimation techniques from credible sources such as:

- United States Environmental Protection Agency (USEPA) - Air Pollutant Emission Factors AP-42[21].
- USEPA - Emissions Inventory Improvement Program[22].
- European Monitoring and Evaluation Program (EMEP) / European Environment Agency (EEA) Air Pollution Emissions Inventory Guidebook[23].

VOC emissions may be speciated using source type-specific profiles derived from credible sources such as:

- USEPA Speciate V4.2[24]
- California Air Resources Board (CARB) California Emission Inventory Development and Reporting System (CEIDARS) Organic Gas Profile Data[25].

Note: The Level 1 screening procedure tool includes a “default VOC speciation” option. When this option is selected, a default VOC composition based on USEPA SPECIATE Profile Number 0000 is used. This has been normalised after removing methane plus unreactive, unknown and non-volatile compounds. Although the user may use the default VOC speciation option in trial runs, source-specific speciation data should be used in the tool to comply with the ozone impact assessment procedure.

6) Input the maximum 1-hour and 4-hour average ozone concentrations recorded over the past 5 years at each of the OEH air quality monitoring stations within the region.

7) Calculate the maximum allowable increment for the region selected, for use in Level 1 assessments for sources within ozone attainment areas.

   The tool calculates the maximum allowable ozone increments for 1-hour and 4-hour averages, with these limits equivalent to 25% of the difference between the 5-year average 1-hour and 4-hour maximums for the region and the relevant Air NEPM Standard.

8) Calculate the 1-hour and 4-hour maximum ozone levels. The tool outputs the following results:

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[21] http://www.epa.gov/ttnchie1/ap42/

[22] http://www.epa.gov/ttn/chief/eiip

[23] http://reports.eea.europa.eu/EMEPCORINAIR/en; http://tfeip-secretariat.org/emep-eea-guidebook/

[24] http://www.epa.gov/ttnchie1/software/speciate/

[25] http://www.arb.ca.gov/ei/drei/maintain/database.htm

- Maximum 1-hour and 4-hour average ozone concentrations due to the source's emissions (i.e. incremental ozone concentrations) for comparison with the relevant screening impact level (SIL).

- Cumulative ozone concentration levels, with the maximum 1-hour and 4-hour average increment being added to the 5-year average 1-hour and 4-hour average maximum for the region. The tool provides an upper bound estimate by adding the maximum source impact to the maximum ambient measurement, regardless of space and time.

9) For sources within ozone attainment areas, evaluate the need for further assessment based on the comparison of the maximum 1-hour and 4-hour average increments with the relevant SIL (0.5 ppb), and with the maximum allowable increment calculated by the tool (Refer to **Section 5.2**).

10) For sources within ozone non-attainment areas, evaluate the need for further assessment based on the comparison of the maximum 1-hour and 4-hour average increments with the relevant SIL (0.5 ppb) and the maximum allowable increment for ozone non-attainment areas (1 ppb) (Refer to **Section 5.2**).

5.4 Guidance for Level 2 Refined Assessment Procedure

5.4.1 Photochemical Model and Chemical Mechanism Selection

The Level 2 refined assessment should be conducted with a suitable photochemical model and appropriate photochemical mechanisms.

The following "third-generation" chemical transport models are considered suitable for application within a Level 2 refined assessment:

- CAMx
- CMAQ
- CHIMERE
- TAPM(26)/TAPM-CTM
- CIT

These models are source-oriented, Eulerian models that represent the atmosphere as a three-dimensional fixed grid, and simulate the transport, transformation and removal of air pollutants by solving the conservation of mass equation for this grid. Atmospheric chemistry modules are incorporated to describe the conversion of emitted pollutants to secondary pollutants such as ozone.

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26 Application of TAPM with the Generic Reaction Set (*GRS*) photochemistry module is not permissible.

The following atmospheric chemical mechanisms are considered suitable for application within the photochemical modelling conducted for a Level 2 refined assessment:

- CB4(27)
- CB05
- S99(28)
- S07B
- CS07A(29)
- CRI v2-R5(30)
- MELCHIOR2(31)

Each of these chemical mechanisms have been peer-reviewed and/or used in peer-reviewed ozone modelling studies.

The LCC mechanism dates from the 1980s and it is a predecessor to the SAPRC mechanisms (i.e. S99, S07B and CS07A) listed above. If the LCC mechanism is used, it should be compared to more current mechanisms (e.g. CB05 and S99) and if results are different a scientifically defensible explanation should be developed for the use of this mechanism.

5.4.2 Model Application

The photochemical grid model (PGM) selected should be used to conduct base case (without the new source) and sensitivity case (with the new source) simulations to calculate the impacts of the new source on 1-hour and 4-hour average ozone concentrations.

The steps to be followed in conducting the Level 2 refined assessment are described in **Section** 4, where a Level 2 refined procedure is presented. These steps include:

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27 The CB4 mechanism has been superseded, and largely replaced, by CB05. CB05 should be used rather than CB4 whenever possible.

28 S99 has been superseded by the S07B mechanism. However the S07B mechanism has yet to be used in regional modelling studies. In addition, S07B is a larger mechanism than S99 and will demand more computational resources than S99. Continued use of S99 is appropriate until the impacts of changing to S07B have been tested and evaluated.

29 CS07A has not yet been used in urban/regional ozone modelling studies and, if used, should be compared to other mechanisms.

30 CRI v2-R5 has not yet been used in urban/regional ozone modelling studies and, if used, should be compared to other mechanisms.

31 The MELCHIOR2 mechanism is expected to be computationally efficient and it has been used extensively in one air quality model (CHIMERE). Using MELCHIOR2 is reasonable but comparison with other current mechanisms (e.g., CB05, S99) would be useful.

- Preparation of base case modelling protocol document addressing: selection of PGM, chemical mechanism, modelling domain, model inputs, and model performance evaluation protocol.

- Evaluation of base case model performance and documentation of results.

- Selection of dates for the Level 2 assessment of the new source.

- Preparation of new source modelling protocol document addressing:

    - Source description and characteristics;

    - Days to be selected for impact calculations as determined from base case results, with a minimum of four to five days to be selected for use; and

    - Method to combine predicted changes in ozone concentrations with ambient measurements (e.g. adding maximum ozone increments to the 5-year average maximum 1-hourly and 4-hourly average measurements as in the Level 1 screening procedure, or apply relative changes in predicted concentrations to the measured values, similar to the relative reduction factor (RRF) approach).

- Conduct emissions sensitivity study with the new source and evaluate the impacts using the protocol document from the previous step.

Additional guidance with respect to the modelling domain and model inputs for a Level 2 refined assessment is as follows:

- The geographical extent of the modelling domain should be defined to be compatible with the gridded OEH GMR Emissions Inventory.

- The meteorological input data should be generated using a prognostic meteorological model such as TAPM, MM5 or WRF, or alternatively should be approved for use by OEH.

- The Air Emission Inventory for the NSW GMR will be provided for use in the study to characterise baseline anthropogenic emissions.

- A minimum of four to five days should be selected, based on the base case results, for use in the new source modelling. Day-specific biogenic emission data are to be derived for the selected days through the application of MEGAN (Model of Emissions of Gases and Aerosols from Nature)(32).

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32 http://acd.ucar.edu/~guenther/MEGAN/MEGAN.htm

6. Glossary of Acronyms And Symbols

Approved Methods	Approved Methods for the Modelling and Assessment of Air Pollutants in NSW
BACT	Best Available Control Technology
BAT	Best Available Techniques
BoM	Australian Bureau of Meteorology
BREF	EU BAT Reference document
CAMx	Comprehensive Air quality Model with extensions
CB	Carbon Bond
CFR	(US) Code of Federal Regulations
Clean Air Regulation	Protection of the Environment Operations (Clean Air) Regulation 2002
CMAQ	Community Multiscale Air Quality model
CMAS	Community Modelling and Analysis System
CO	Carbon Monoxide
CSIRO	Commonwealth Scientific and Industrial Research Organisation
CTM	Chemical Transport Model
ENVIRON	ENVIRON Australia Pty Ltd
EPA	Environmental Protection Authority, NSW
EU	European Union
IED	(EU) Industrial Emissions Directive
LAER	Lowest Achievable Emission Rate
MATS	Modelled Attainment Test Software
mg	Milligram (g x 10^{-3})
µg	Microgram (g x 10^{-6})
µm	Micrometre or micron (metre x 10^{-6})
m^3	Cubic metre

NAAQS	(US) National Ambient Air Quality Standards
NO_x	Oxides of Nitrogen
NO_2	Nitrogen Dioxide
NPI	National Pollutant Inventory
NSPS	New Source Performance Standards
NSR	New Source Review
NSW	New South Wales
OEH	Office of Environment and Heritage
POEO Act	Protection of the Environment Operations Act 1997
PM_{10}	Particulate matter less than 10microns in aerodynamic diameter
ppb	Parts per billion by volume
ppm	parts per million by volume
PSD	Potential for Significant Deterioration
RACT	Reasonably Available Control Technology
RAT	Reasonably Available Techniques
RBLC	RACT/BACT/LAER Clearinghouse
RRF	Relative Response Factor
SCAQMD	South Coast Air Quality Management District
SIL	Screening Impact Level
SIP	State Implementation Plan
SO_2	Sulfur Dioxide
TAPM	“The Air Pollution Model”
US	United States
USEPA	United States Environmental Protection Agency
VOC	Volatile Organic Compound

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Appendix 1

Technical Brief – Ozone Impact Assessment: Tiered procedure for estimating ground-level ozone impacts from stationary sources

New South Wales Department of Environment, Climate Change & Water

OZONE IMPACT ASSESSMENT: Tiered procedure for estimating ground-level ozone impacts from stationary sources

TECHNICAL BRIEF

1. Objective

The overall objective of the study is to develop a tiered ozone impact assessment procedure for estimating ground-level ozone impacts from stationary sources of oxides of nitrogen (NO_x) and/or volatile organic compounds (VOCs).

2. Background information

Historical data show that Sydney exceeds the *National Environment Protection (Ambient Air Quality) Measure* (*Air NEPM*)33 ozone standards up to 19 days per year[34].

In 1998 the NSW Government released *Action for Air*[35], its 25-year air quality management plan for the NSW Greater Metropolitan Region (GMR), which covers the Sydney, Lower Hunter and Illawarra regions. *Action for Air* focuses on regional air pollution and includes strategies that represent a comprehensive attack on the two pollutants of primary concern: photochemical smog (ground-level ozone); and fine particle pollution.

The State Plan – Investing in a Better Future[36] sets targets to improve outcomes and services for the people of NSW. *The State Plan* commits the NSW Government to meeting the goals of the *Air NEPM*. These national health-based goals apply to six air pollutants: carbon monoxide; lead; sulfur dioxide; nitrogen dioxide; ozone and fine particles.

EPA-licenced premises and commercial businesses make a significant contribution to anthropogenic ozone precursors (i.e. oxides of nitrogen (NO_x) and volatile organic compounds (VOCs)) in the NSW GMR. On an annual basis, EPA-licenced premises and commercial businesses contribute ~61% and ~19% of NO_x and VOC emissions, respectively[37].

Any future review of the *Protection of the Environment Operations (Clean Air) Regulation*

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33 http://www.ephc.gov.au/taxonomy/term/23
34 http://www.environment.nsw.gov.au/air/cpairqual.htm
35 http://www.environment.nsw.gov.au/air/actionforair/index.htm
36 http://more.nsw.gov.au/stateplan
37 http://www.environment.nsw.gov.au/air/airinventory.htm

2010[38] (*Clean Air Regulation*) and *Approved Methods for Modelling and Assessment of Air Pollutants in NSW*[39] (*Approved Methods for Modelling*) is likely to continue the focus on emissions of NO_x and VOCs.

The minimum performance standards for NO_x and VOCs in the *Clean Air Regulation* are generic and do not focus on the sensitivity of the receiving environment and the management of cumulative impacts.

The *Approved Methods for Modelling* defines the environmental outcomes for a broad suite of air pollutants and outlines the methods to be followed for assessing air quality impacts on a site-specific basis. The assessment may conclude that emission limits more stringent than those prescribed in the *Clean Air Regulation* may be necessary in certain circumstances to ensure acceptable impacts on human health and the environment.

While the *Approved Methods for Modelling* presently defines environmental outcomes for ground-level ozone, a procedure for predicting the impacts associated with ozone precursors is not available, unlike other air pollutants.

To support effective regulation of air pollution, DECCW proposes to develop a tiered ozone impact assessment procedure for estimating ground-level ozone impacts from stationary sources of NO_x and VOCs, which is consistent with the Level 1 and 2 philosophy in the *Approved Methods for Modelling*.

The USEPA has developed a screening procedure[40] for predicting ground-level ozone from stationary sources although it cannot be directly applied in NSW due to differences in emission sources, location, topography and meteorology, among other reasons. Nevertheless, the USEPA screening procedure may provide a useful starting point for the development of an ozone impact assessment procedure that is suitable for NSW.

W. P. L Carter[41] has developed and/or documented a number of photochemical mechanisms and reactivity scales for NO_x and VOCs. Other photochemical mechanisms developed by CSIRO[42] include IER and GRS.

The USEPA[43] lists a suite of photochemical models and provides guidance for predicting the air quality impacts from stationary sources. TAPM and TAPM-CTM[44] and CALPUFF[45] are the most popular photochemical models for predicting the air quality impacts from stationary sources in NSW, although they are mainly used for larger sources of NO_x but rarely for VOCs.

This *Technical Brief* identifies the problem which needs to be solved, that is, to develop a tiered ozone impact assessment procedure for estimating ground-level ozone impacts from stationary sources of NO_x and/or VOCs. Any suggestions for fulfilling the scope of work and/or references included in this *Technical Brief* have been provided for illustrative purposes only and should not be interpreted as exhaustive requirements.

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[38] http://www.environment.nsw.gov.au/air/poeocleanair.htm
[39] http://www.environment.nsw.gov.au/air/appmethods.htm
[40] http://ndep.nv.gov/bapc/permitting/download/model/scheffe.doc
[41] http://www.cert.ucr.edu/~carter/
[42] http://www.cmar.csiro.au/airquality/ier_calc/description.html
[43] http://www.epa.gov/ttn/scram/
[44] http://www.cmar.csiro.au/research/tapm/
[45] http://www.src.com/calpuff/calpuff1.htm

3. Scope of Work

The scope of work includes three key components:

Part 1: Develop analysis methodology

1. Conduct a literature review of licence requirements for stationary sources of ozone precursors with particular emphasis on best available technology and air quality impact assessment definitions and requirements in OECD member countries[46], new source review (NSR) requirements implemented by USEPA[47] and permitting guidance developed in various states in the US[48,49,50,51,52] .

2. Conduct a literature review of screening procedures for estimating ground-level ozone impacts from stationary sources of ozone precursors. Discuss the merits and drawbacks of each procedure, data requirements, its ease of use and any practical limitations of applying it in NSW.

3. Conduct a literature review of photochemical mechanisms for estimating ground-level ozone impacts from stationary sources of ozone precursors. Discuss the merits and drawbacks of each mechanism, data requirements, its ease of use and any practical limitations of applying it in NSW.

4. Conduct a literature review of photochemical models for estimating ground-level ozone impacts from stationary sources of ozone precursors. Discuss the merits and drawbacks of each model, data requirements, its ease of use and any practical limitations of applying it in NSW.

5. Using the outcomes of the literature review, document the methodology for developing a Level 1 – screening procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors, including the photochemical mechanism and photochemical model that will be used.

- The Level 1 – screening procedure should typically account for:
    - Emission quantities and ratios of ozone precursors (i.e. NO_x, VOCs and CO)
    - Reactivity adjustment of ozone precursor emissions (e.g. MIR[53])
    - Source type (i.e. stack, area or volume)
    - Release parameters including; height, velocity, diameter and temperature (i.e. momentum and buoyancy induced plume rise)
    - Location (e.g. urban/rural, NO_x limited/light (VOC) limited or any other suitable classification)
    - Meteorology
    - Background air quality
    - Any other factors which may influence ground-level ozone formation

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[46] http://www.oecd.org/home/0,2987,en_2649_201185_1_1_1_1_1,00.html
[47] http://www.epa.gov/nsr/index.html
[48] http://www.deq.state.ok.us/aqdnew/permitting/Modeling_Guide_0108.pdf
[49] http://www.cabq.gov/airquality/pdf/aqd_model_guidelines.pdf
[50] http://ndep.nv.gov/bapc/permitting/qa/Model_Guide.pdf
[51] http://www.doeal.gov/SWEIS/OtherDocuments/397%20NMAQB%202003%20dispersion%20modeling%20guidelines.pdf
[52] http://www.blm.gov/pgdata/etc/medialib/blm/wy/information/NEPA/pfodocs/anticline/rd-seis/tsd.Par.67355.File.dat/02appA.pdf
[53] http://www.cert.ucr.edu/~carter/SAPRC/

- The Level 1 - screening procedure should ideally be contained within a Microsoft Excel Workbook or Microsoft Access Database and typically contain:
    - Forms for entering all site-specific parameters
    - All underlying calculations for estimating the incremental increase in ground-level ozone
    - Hourly average background ozone concentrations for each of the DECCW ambient monitoring stations in NSW[54]
    - Analysis tools for calculating the total ground-level ozone impact (i.e. background plus incremental increase) by hour for a year
    - Analysis tools for calculating the frequency distribution of existing background plus total ground-level ozone impact by hour for a year
    - Graphical tools for presenting the total ground-level ozone impact by hour for a year
    - Graphical tools for presenting the frequency distribution of existing background plus total ground-level ozone impact by hour for a year
    - Analysis and graphical tools for 1-hour and 4-hour average ground-level ozone
    - Any other features necessary to conduct analysis and graphically present the results
- The Microsoft Excel Workbook or Microsoft Access Database and instructions could potentially form a supplement to the *Approved Methods for Modelling* and be made available on the DECCW web site[55].
- The Level 1 – screening procedure should include sufficiently detailed guidance for inclusion in the *Approved Methods for Modelling*.

6. Using the outcomes of the literature review, document the methodology for developing a Level 2 – refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors, including the photochemical mechanism(s) and photochemical model(s) that will be used.

- The Level 2 - refined procedure should account for all site-specific parameters that may affect plume release, dispersion, transport and photochemical transformation and include sufficiently detailed guidance for inclusion in the *Approved Methods for Modelling*.

Part 2: Conduct analysis and develop analysis tools

1. Conduct analysis and develop a Level 1 – screening procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors.

- The Level 1 – screening procedure should typically account for the considerations listed in Part 1, Section 5 as a minimum and any other factors as necessary.
- The Level 1 - screening procedure should ideally be contained within a Microsoft Excel Workbook or Microsoft Access Database and typically contain the functionalities listed in Part 1, Section 5 as a minimum and any other features as necessary.
    - **Note 1**: To demonstrate your appreciation of the technical brief, your proposal will need to provide details about the nature and number of model scenarios that will be run to develop the Level 1 - screening procedure.
    - **Note 2**: DECCW can provide CIT, TAPM and TAPM-CTM format emissions

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[54] http://www.environment.nsw.gov.au/AQMS/sitesyd.htm, http://www.environment.nsw.gov.au/AQMS/sitesill.htm http://www.environment.nsw.gov.au/AQMS/sitesuh.htm, http://www.environment.nsw.gov.au/AQMS/siteslh.htm http://www.environment.nsw.gov.au/aqms/sitesrural.htm

[55] http://www.environment.nsw.gov.au/air/appmethods.htm

input data files for the analysis, so your proposal will need to provide details if this information is required. Please refer to DECCW's EDMS User's Manual[56] for specific details.

- Instructions should be developed for the Microsoft Excel Workbook or Microsoft Access Database analysis tool.

2. Conduct analysis and develop a Level 2 – refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors.

- The Level 2 - refined procedure should account for all site-specific parameters that may affect plume release, dispersion, transport and photochemical transformation.
- The level 2 – refined procedure will need to be demonstrated on a suitable suite of scenarios considered in Part 2, Section 1.
    - **Note 1**: To demonstrate your appreciation of the technical brief, your proposal will need to provide details about the nature and number of model scenarios that will be run to develop the Level 2 - refined procedure.
    - **Note 2**: DECCW can provide CIT, TAPM and TAPM-CTM format emissions input data files for the analysis, so your proposal will need to provide details if this information is required. Please refer to DECCW's EDMS User's Manual for specific details.

Part 3: Document tiered procedure

1. Develop detailed guidance for inclusion in the *Approved Methods for Modelling* for Level 1 – screening procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors.

2. Develop detailed guidance for inclusion in the *Approved Methods for Modelling* for Level 2 – refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors.

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[56] http://www.environment.nsw.gov.au/resources/air/tr9aei08181.pdf

4. Tasks for the Applicant

The applicant is to provide DECCW with the deliverables that address the tasks outlined in Table 1.

Table 1: Tasks for the applicant

Part	Task	Deliverable
1	1.1 Conduct a literature review of licence requirements for stationary sources of ozone precursors with particular emphasis on best available technology and air quality impact assessment requirements in OECD member countries , new source review (NSR) requirements implemented by USEPA and permitting guidance developed in various states in the US.	Interim Report 1: Analysis methodology for Level 1 – screening procedure and Level 2 – refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors.
1	1.2 Conduct a literature review of screening procedures for estimating ground-level ozone impacts from stationary sources of ozone precursors. Discuss the merits and drawbacks of each procedure, data requirements, its ease of use and any practical limitations of applying it in NSW.	
1	1.3 Conduct a literature review of photochemical mechanisms for estimating ground-level ozone impacts from stationary sources of ozone precursors. Discuss the merits and drawbacks of each mechanism, data requirements, its ease of use and any practical limitations of applying it in NSW.	
1	1.4 Conduct a literature review of photochemical models for estimating ground-level ozone impacts from stationary sources of ozone precursors. Discuss the merits and drawbacks of each model, data requirements, its ease of use and any practical limitations of applying it in NSW.	
1	1.5 Using the outcomes of the literature review, document the methodology for developing a Level 1 – screening procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors, including the photochemical mechanism and photochemical model.	
1	1.6 Using the outcomes of the literature review, document the methodology for developing a Level 2 – refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors, including the photochemical mechanism(s) and photochemical model(s).	
2	2.1 Conduct analysis and develop a Level 1 – screening procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors.	Interim Report 2: Analysis results for Level 1 – screening procedure and Level 2 – refined procedure for estimating ground-level ozone impacts from
2	2.2 Conduct analysis and develop a Level 2 – refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors.	

Part	Task	Deliverable
		stationary sources of ozone precursors; Instructions for Level 1 - screening procedure e contained within a Microsoft Excel Workbook or Microsoft Access Database; and Analysis tool for Level 1 - screening procedure e contained within a Microsoft Excel Workbook or Microsoft Access Database.
3	3.1 Develop detailed guidance for inclusion in the Approved Methods for Modelling for Level 1 – screening procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors.	Final Report 3: Consolidate Interim Reports 1 and 2; and Guidance for Level 1 – screening procedure and Level 2 – refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors.
3	3.2 Develop detailed guidance for inclusion in the Approved Methods for Modelling for Level 2 – refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors.	

5. Deliverables

- Progress reports to the DECCW project manager.

- Interim Report 1:
  - “Analysis methodology for Level 1 – screening procedure and Level 2 – refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors”, including tasks 1.1 to 1.6 outlined in Section 4 to the satisfaction of DECCW.

- Interim Report 2:
  - “Analysis results for Level 1 – screening procedure and Level 2 – refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors” and “Instructions for Level 1 - screening procedure contained within a Microsoft Excel Workbook or Microsoft Access Database”, including tasks 2.1 and 2.2 outlined in Section 4 to the satisfaction of DECCW; and
  - “Analysis tool for Level 1 - screening procedure contained within a Microsoft Excel Workbook or Microsoft Access Database”, including tasks 2.1 and 2.2 outlined in Section 4 to the satisfaction of DECCW.

- Draft Report 3:
    - Interim Report 1, including tasks 1.1 to 1.6 outlined in Section 4 to the satisfaction of DECCW;
    - Interim Report 2, including tasks 2.1 to 2.2 outlined in Section 4 to the satisfaction of DECCW; and
    - Guidance for Level 1 – screening procedure and Level 2 – refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors, including tasks 3.1 to 3.2 outlined in Section 4 to the satisfaction of DECCW.

- Final Report 3:
    - Interim Report 1, including tasks 1.1 to 1.6 outlined in Section 4 to the satisfaction of DECCW;
    - Interim Report 2, including tasks 2.1 to 2.2 outlined in Section 4 to the satisfaction of DECCW; and
    - Guidance for Level 1 – screening procedure and Level 2 – refined procedure for estimating ground-level ozone impacts from stationary sources of ozone precursors, including tasks 3.1 to 3.2 outlined in Section 4 to the satisfaction of DECCW.

Note 1: All reports must be submitted in Microsoft Word 2003 and .pdf formats. All spreadsheets and databases must be submitted in Microsoft Excel 2003 and Microsoft Access 2003 formats, respectively.

6. Project Management

6.1 Timeframe and Milestones

Milestones and progress payments are outlined in Table 2.

Table 2: Milestones and progress payments

Milestone	Deliverable	Progress Payment	Timing
1	Agreement of terms and conditions and commencement of study	20% progress payment - $16,000 (excluding GST)	Project commencement
2	Delivery of interim report 1	20% progress payment - $16,000 (excluding GST)	6 weeks after commencement
3	Delivery of interim report 2	20% progress payment - $16,000 (excluding GST)	14 weeks after commencement
4	Delivery of draft report 3	20% progress payment - $16,000 (excluding GST)	16 weeks after commencement
5	Delivery of final report 3	20% progress payment - $16,000 (excluding GST) [a]	2 weeks following submission of DECCW comments

[a] Allows two weeks for DECCW to provide comments.

6.2 Progress Reports

Brief progress reports are required to be submitted to the DECCW project officer by C.O.B. on Friday every fortnight. The progress reports must be emailed to the project officer and include the following details:

- Tasks undertaken in the last fortnight and personnel responsible for the task.
- Tasks planned for the next fortnight and personnel responsible for the task.
- Any outstanding information/new issues.
- Meetings held / planned (inc. dates) (External / Internal).
- Budgetary issues / changes to scope / schedule issues.

The DECCW project officer will supply a progress report template to the successful applicant.

6.3 Contract

The successful applicant will be required to sign a standard DECCW contract (“the Agreement”). All major changes in direction of the project need to be confirmed in writing by the successful applicant keeping a running log of all changes requested and confirmed.

7. Project Budget

The indicative budget for this work is $80,000 (exclusive of GST).

8. Submission of Tenders

8.1 Information Required at Tender

In providing a tender for this work, please provide a submission including:

- a detailed summary of your relevant experience in this area;
- a detailed discussion of the approach to the study and methods that will be used;
- CVs for the applicant(s) who would conduct the work;
- detailed work plans including timetables for delivering outputs;
- demonstrated understanding of the requirements of the consultancy (including any proposed variations or innovations);
- proposed timetable (including the availability of key personnel);
- proposed budget;
- documentation of previous relevant experience;
- names of relevant referees; and
- declaration of any conflict of interest or risk of conflict of interest.

8.2 Tender Evaluation Criteria

The selection criteria used to award this tender will be:

- quality of the proposed method and approach to the project;
- experience in similar tasks and/or demonstrated capacity to undertake the work;
- the relevant expertise of the applicant(s);
- ability to perform the work within the timeframe;
- value for money; and
- high level of report writing and communication skills.

Note 1: Except where specific reference is being made to meeting the requirements contained within this *Technical Brief*, any reproduction of the *Technical Brief* verbatim will be viewed unfavourably by the tender evaluation panel.

8.3 Lodgement of Tender

Tenders should be lodged via email to Nick.Agapides@environment.nsw.gov.au and in hard copy format in quadruplicate to:
The Tender Box
Department of Environment, Climate Change and Water
Level 14, 59 Goulburn Street
Sydney, NSW 2000

All tenders should be marked to the attention of:
Mr Nick Agapides
Manager Major Air Projects
Air Major Projects Unit
Climate Change, Policy and Programs Group
Department of Environment, Climate Change and Water

Tenders must be received by DECCW by 4.00 pm, Friday 28 January 2011.

8.4 Further Information

Mr Nick Agapides
Manager Major Air Projects
Air Major Projects Unit
Climate Change, Policy and Programs Group
Department of Environment, Climate Change and Water
Phone: 02 9995 6047
Fax: 02 9995 5938
Email: Nick.Agapides@environment.nsw.gov.au

Appendix 2
Photochemical Model Review References

The following is a list of references for each model reviewed in the study that provides additional information on the development, applications and testing of the model.

CAMx References

Andreani-Aksoyoglu, S., A.S.H. Prévôt, U. Baltensperger, J. Keller, and J. Dommen, 2004. Modeling of formation and distribution of secondary aerosols in the Milan area (Italy), *J. Geophys. Res.*, **109**, D05306.

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Gaydos, T.M., R. Pinder, B. Koo, K.M. Fahey, G. Yarwood, and S.N. Pandis, 2007. Development and application of a three-dimensional aerosol chemical transport model, PMCAMx, *Atmos. Environ.*, **41**, 2594-2611.

Jorquera, H. and J. Castro, 2010. Analysis of urban pollution episodes by inverse modeling, *Atmos. Environ.*, **44**, 42-54.

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Appendix 3
Comparison of Isoprene Emissions from GMR Atmospheric Emissions Inventory and MEGAN

Estimated isoprene emissions provided within the OEH's GMR Air Emissions Inventory are hourly-specific but do not vary from day to day for a given month. OEH has estimated biogenic emissions using TAPM derived meteorological data inputs coupled with the CSIRO canopy and pasture model (Azzi et. al., 2004; Huber, 2005).

The Model of Emissions of Gases and Aerosol from Nature (MEGAN) is widely used for regional and global scale air quality modelling. MEGAN, developed by the Biosphere-Atmosphere Interactions (BAI) group of the Atmospheric Chemistry Division (ACD) at the National Center for Atmospheric Research (NCAR), is a modelling system for estimating the net emission of gases and aerosols from terrestrial ecosystems into the atmosphere (Sakulyanontvittaya, 2008; Guenther et al., 2006). MEGAN computes emissions for plant functional types as a function of temperature, solar radiation, leaf area index, and leaf age. Fractional coverage for each plant functional type and vegetation-specific emission factors are based on the MEGAN 1km X 1km land cover data, informed by satellite imagery. The current official release of the MEGAN model is version 2.04 and it is available from http://acd.ucar.edu/~guenther/MEGAN/MEGAN.htm.

MEGAN isoprene emissions are hourly-specific and so vary from day to day. For comparison with the GMR Emission Inventory emissions (based on TAPM-CTM), ENVIRON calculated average emissions for a January day by averaging over all the days in the month. The daily MEGAN emissions have been based on temperature and solar radiation predictions from TAPM.

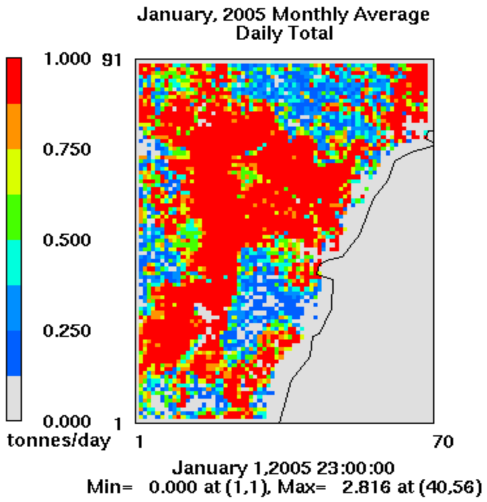
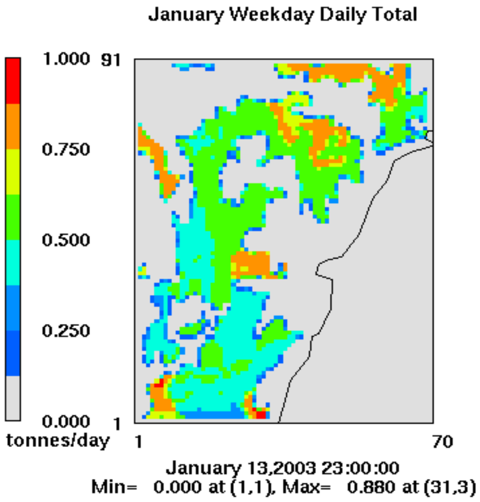
The comparison between MEGAN and GMR Emission Inventory emissions shows isoprene emissions at noon for a typical January weekday.

Similarly, the GMR emissions inventory (DECC, 2007b) predicts soil NOx emission rates across the GMR of 1,051 tonnes/month and 1,035 tonnes/month for December and January respectively. Equivalent emission estimations using MEGAN indicate soil NOx emissions of the order of 285 kg/month and 265 kg/month.

Findings

1. On average MEGAN soil NO_X emissions are about 4 times lower than those within the GMR Emissions Inventory.

2. On average, MEGAN isoprene emissions are about 3 times higher than those within the GMR Emissions Inventory.

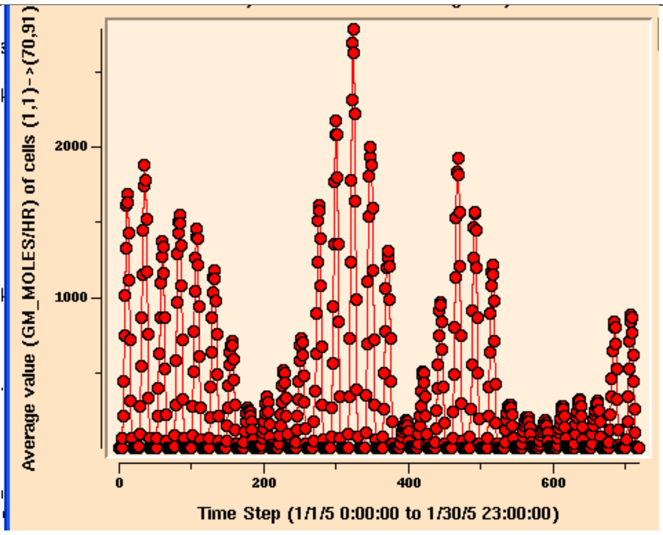
MEGAN Isoprene Inventory (3,831 tonnes/day)	**GMR Isoprene Inventory (1,274 tonnes/day)**
	

3. The GMR Emissions Inventory isoprene emission rates vary discretely in space – they rise/fall in steps. MEGAN isoprene emissions have more complex spatial variation resulting from the satellite characterization of leaf-area index (LAI) and plan functional type (PFT). MEGAN does correctly recognize areas with zero emissions such as Lake Burragorang.

4. There are broad similarities in where the high isoprene emission areas are located.

5. MEGAN shows more infiltration into urban areas of isoprene emissions (most likely urban forest).

6. MEGAN emissions vary by an order of magnitude from day to day due to meteorology (they are lower on cool and/or cloudy days).

Time series of domain-wide average MEGAN isoprene for January Lowest daily maximums occur on cloudy days (Jan 23-28). Other dates can be ~10x larger.	

Recommendations

1. Use date-specific MEGAN emissions because day-to-day variation in isoprene emissions is likely to be important, and isoprene emissions in urban areas are likely to be important.

2. Similarly, MEGAN soil NO_X emissions are variable day-to-day and should be used.

3. Consider scaling back MEGAN isoprene emissions to reduce the difference from OEH data. We recommend that the MEGAN predicted isoprene emissions be divided by 2. A comparison of MEGAN isoprene against aircraft-based measurements in the US has suggested that MEGAN over-estimated isoprene by up to a factor of 2 (Warneke et al., 2010).

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Appendix 4
VOC Species included in the Level 1 Screening Tool

Description	**Mwt**	**C**	**H**	**O**	**CAS**
(1-METHYLPROPYL)BENZENE (SEC-BUTYL BENZENE)	134.22	10	14		135-98-8
(1S)-(-)-ALPHA-PINENE	136.23	10	16		7785-26-4
(2-METHYLBUTYL)CYCLOHEXANE	154.29	11	22		54105-77-0
(2-METHYLPROPYL)BENZENE	134.22	10	14		538-93-2
1-(BUTOXYETHOXY)-2-PROPANOL	176.25	9	20	3	124-16-3
1,1,2,2-TETRAMETHYLCYCLOPENTANE	126.24	9	18		52688-89-8
1,1,2,3-TETRAMETHYL CYCLOHEXANE	140.27	10	20		6783-92-2
1,1,2,3-TETRAMETHYLCYCLOHEXANE	140.27	10	20		
1,1,2-TRIMETHYLCYCLOHEXANE	126.24	9	18		7094-26-0
1,1,2-TRIMETHYLCYCLOPENTANE	112.21	8	16		4259-00-1
1,1,3,3-TETRAMETHYL CYCLOPENTANE	126.24	9	18		50876-33-0
1,1,3,4-TETRAMETHYL CYCLOPENTANE	126.24	9	18		53907-60-1
1,1,3,4-TETRAMETHYLCYCLOHEXANE	140.27	10	20		24612-75-7
1,1,3,5-TETRAMETHYLCYCLOHEXANE	140.27	10	20		4306-65-4
1,1,3-TRIMETHYLCYCLOHEXANE	126.24	9	18		3073-66-3
1,1,3-TRIMETHYLCYCLOPENTANE	112.21	8	16		4516-69-2
1,1,4-TRIMETHYLCYCLOHEXANE	126.24	9	18		7094-27-1
1,1-DIMETHYL-2-PROPYLCYCLOHEXANE	154.29	11	22		
1,1-DIMETHYLCYCLOHEXANE	112.21	8	16		590-66-9
1,1-DIMETHYLCYCLOPENTANE	98.19	7	14		1638-26-2
1,1-METHYLETHYLCYCLOPENTANE	112.21	8	16		16747-50-5
1,2,3,4-TETRAMETHYLBENZENE	134.22	10	14		488-23-3
1,2,3,5-TETRAMETHYLBENZENE	134.22	10	14		527-53-7
1,2,3-TRIMETHOXYBENZENE	168.19	9	12	3	634-36-6
1,2,3-TRIMETHYL-4-ETHYLBENZENE	148.24	11	16		61827-86-9
1,2,3-TRIMETHYL-5-ETHYL BENZENE	148.24	11	16		31366-00-4
1,2,3-TRIMETHYLBENZENE	120.19	9	12		526-73-8
1,2,3-TRIMETHYLCYCLOHEXANE	126.24	9	18		1678-97-3
1,2,3-TRIMETHYLCYCLOPENTANE	112.21	8	16		
1,2,4,5-TETRAMETHYLBENZENE	134.22	10	14		95-93-2
1,2,4-TRIMETHYL CYCLOHEXANE	126.24	9	18		2234-75-5
1,2,4-TRIMETHYLBENZENE	120.19	9	12		95-63-6
1,2,4-TRIMETHYLCYCLOPENTANE	112.21	8	16		
1,2,4-TRIMETHYLCYCLOPENTENE	110.20	8	14		2815-58-9
1,2-BENZENEDIOL	110.11	6	6	2	120-80-9
1,2-BUTADIENE {METHYLALLENE}	54.09	4	6		590-19-2
1,2-BUTANEDIOL	90.12	4	10	2	584-03-2
1,2-DIACETYL BENZENE	162.19	10	10	2	704-00-7
1,2-DIETHYL-1-METHYLCYCLOHEXANE	154.29	11	22		
1,2-DIETHYL-3-METHYLBENZENE	148.24	11	16		
1,2-DIETHYL-4-METHYLBENZENE	148.24	11	16		13732-80-4
1,2-DIETHYL-4-METHYLBENZENE	148.24	11	16		
1,2-DIETHYLBENZENE (ORTHO)	134.22	10	14		135-01-3
1,2-DIHYDRONAPHTHALENE	130.19	10	10		447-53-0
1,2-DIHYDROXY HEXANE	118.17	6	14	2	6920-22-5
1,2-DIMETHOXY-4-METHYL BENZENE	152.19	9	12	2	494-99-5

Description	Mwt	C	H	O	CAS
1,2-DIMETHYL CYCLOHEXENE	110.20	8	14		1674-10-8
1,2-DIMETHYL-3-ETHYLBENZENE	134.22	10	14		933-98-2
1,2-DIMETHYL-3-ETHYLCYCLOHEXANE	140.27	10	20		
1,2-DIMETHYL-3-PROPYL BENZENE	148.24	11	16		17059-44-8
1,2-DIMETHYL-4-ETHENYL BENZENE	132.20	10	12		27831-13-6
1,2-DIMETHYL-4-ETHYLBENZENE	134.22	10	14		934-80-5
1,2-DIMETHYL-4-PROPYL BENZENE	148.24	11	16		3982-66-9
1,2-DIMETHYLCYCLOPENTANE	98.19	7	14		2452-99-5
1,2-DIMETHYLCYCLOPENTENE	96.17	7	12		765-47-9
1,2-DIMETHYLINDENE	144.21	11	12		70063-93-3
1,2-EPOXYBUTANE	72.11	4	8	1	106-88-7
1,2-PENTADIENE	68.12	5	8		
1,2-PROPADIENE	40.06	3	4		463-49-0
1,2-PROPYLENE GLYCOL DIACETATE	160.17	7	12	4	623-84-7
1,3,5-OCTATRIENE	108.18	8	12		
1,3,5-TRIMETHYLBENZENE	120.19	9	12		108-67-8
1,3,5-TRIMETHYLCYCLOHEXANE	126.24	9	18		1839-63-0
1,3-BUTADIENE	54.09	4	6		106-99-0
1,3-BUTADIYNE	50.06	4	2		460-12-8
1,3-BUTANEDIOL	90.12	4	10	2	107-88-0
1,3-CYCLOPENTADIENE	66.10	5	6		542-92-7
1,3-DIETHYL, TRANS CYCLOPENTANE	126.24	9	18		62016-60-8
1,3-DIETHYL-2-METHYL BENZENE	148.24	11	16		13632-95-6
1,3-DIETHYL-4-METHYL BENZENE	148.24	11	16		1758-85-6
1,3-DIETHYL-5-METHYL BENZENE	148.24	11	16		2050-24-0
1,3-DIETHYL-5-METHYL CYCLOHEXANE	154.29	11	22		164259-42-1
1,3-DIETHYLBENZENE (META)	134.22	10	14		141-93-5
1,3-DIETHYL-CYCLOHEXANE	140.27	10	20		1678-99-5
1,3-DIMETHYL-2-ETHYLBENZENE	134.22	10	14		2870-04-4
1,3-DIMETHYL-2-PROPYL BENZENE	148.24	11	16		17059-45-9
1,3-DIMETHYL-4-ETHYLBENZENE	134.22	10	14		874-41-9
1,3-DIMETHYL-4-ISOPROPYLBENZENE	148.24	11	16		4706-89-2
1,3-DIMETHYL-5-ETHYLBENZENE	134.22	10	14		934-74-7
1,3-DIMETHYL-5-PROPYLBENZENE	148.24	11	16		3982-64-7
1,3-DIOXOLANE	74.08	3	6	2	646-06-0
1,3-HEXADIENE	82.14	6	10		592-48-3
1,3-OCTADIENE	110.20	8	14		1002-33-1
1,4-BUTANEDIOL	90.12	4	10	2	110-63-4
1,4-BUTANEDIOL DIGLYCIDYL ETHER	202.25	10	18	4	2425-79-8
1,4-DIETHYLBENZENE (PARA)	134.22	10	14		105-05-5
1,4-DIETHYL-CYCLOHEXANE	140.27	10	20		1679-00-1
1,4-DIMETHYL-2-ETHENYL BENZENE	132.20	10	12		2039-89-6
1,4-DIMETHYL-2-ETHYLBENZENE	134.22	10	14		1758-88-9
1,4-DIMETHYL-2-PROPYL BENZENE	148.24	11	16		3042-50-0
1,4-DIOXANE	88.11	4	8	2	123-91-1
1,4-HEXADIENE	82.14	6	10		592-45-0
1,4-PENTADIENE	68.12	5	8		591-93-5

Description	Mwt	C	H	O	CAS
1,5-HEPTADIENE	96.17	7	12		1541-23-7
1,5-HEXADIENE	82.14	6	10		592-42-7
1,6-HEPTADIENE	96.17	7	12		3070-53-9
1-BUTENE	56.11	4	8		106-98-9
1-BUTYNE (ETHYLACETYLENE)	54.09	4	6		107-00-6
1-DECANOL	158.28	10	22	1	112-30-1
1-DECENE	140.27	10	20		872-05-9
1-DECYNE	138.25	10	18		764-93-2
1-ETHOXY-2-PROPANOL	104.15	5	12	2	1569-02-4
1-ETHYL CYCLOPENTENE	96.17	7	12		2146-38-5
1-ETHYL-1,2-DIMETHYLCYCLOHEXANE	140.27	10	20		
1-ETHYL-2,2,6-TRIMETHYLCYCLOHEXANE	154.29	11	22		
1-ETHYL-2,3,5-TRIMETHYL BENZENE	148.24	11	16		18262-85-6
1-ETHYL-2,3,6-TRIMETHYL BENZENE	148.24	11	16		41903-41-7
1-ETHYL-2,3-DIMETHYL CYCLOHEXANE	140.27	10	20		7058-05-1
1-ETHYL-2,4,5-TRIMETHYL BENZENE	148.24	11	16		17851-27-3
1-ETHYL-2,4-DIMETHYL CYCLOHEXANE	140.27	10	20		61142-69-6
1-ETHYL-2,4-DIMETHYLCYCLOHEXANE	140.27	10	20		
1-ETHYL-2-ISOPROPYLBENZENE	148.24	11	16		18970-44-0
1-ETHYL-2-PROPYL BENZENE	148.24	11	16		
1-ETHYL-2-PROPYL CYCLOHEXANE	154.29	11	22		62238-33-9
1-ETHYL-2-PROPYLBENZENE	148.24	11	16		16021-20-8
1-ETHYL-3-PROPYL BENZENE	148.24	11	16		
1-ETHYL-4-ISOPROPYLBENZENE	148.24	11	16		4218-48-8
1-ETHYL-4-PROPYL BENZENE	148.24	11	16		
1-ETHYLANTHRACENE	206.28	10	22	4	66291-35-8
1-HEPTANOL	116.20	7	16	1	111-70-6
1-HEPTENE	98.19	7	14		592-76-7
1-HEXANOL (N-HEXANOL)	102.17	6	14	1	111-27-3
1-HEXENE	84.16	6	12		592-41-6
1-HEXYNE	82.14	6	10		693-02-7
1-HYDROXY-2-METHOXY-4-METHYL BENZENE	138.16	8	10	2	
1-INDANONE	132.16	9	8	1	83-33-0
1-ISOPROPYL-2-METHYL CYCLOHEXANE	140.27	10	20		16580-23-7
1-METHYL CYCLOHEXENE	96.17	7	12		591-49-1
1-METHYL INDAN	132.20	10	12		767-58-8
1-METHYL NAPHTHALENE	142.20	11	10		90-12-0
1-METHYL-1-ETHYLCYCLOHEXANE	126.24	9	18		4926-90-3
1-METHYL-2-ISOPROPYLBENZENE	134.22	10	14		527-84-4
1-METHYL-2-ISOPROPYLCYCLOHEXANE	140.27	10	20		
1-METHYL-2-N-BUTYLBENZENE	148.24	11	16		1595-11-5
1-METHYL-2N-PROPYLBENZENE	134.22	10	14		1074-17-5
1-METHYL-2-PROPYL CYCLOPENTANE	126.24	9	18		3728-57-2
1-METHYL-2-TERT-BUTYLBENZENE	148.24	11	16		1074-92-6
1-METHYL-3-BUTYLBENZENE	148.24	11	16		1595-04-6
1-METHYL-3-ETHYLCYCLOPENTANE	112.21	8	16		

Description	Mwt	C	H	O	CAS
1-METHYL-3-ISOPROPYL CYCLOHEXANE	140.27	10	20		16580-24-8
1-METHYL-3-ISOPROPYLBENZENE	134.22	10	14		535-77-3
1-METHYL-3-ISOPROPYLCYCLOHEXANE	140.27	10	20		
1-METHYL-3N-PROPYLBENZENE	134.22	10	14		1074-43-7
1-METHYL-4-ISOBUTYLBENZENE	148.24	11	16		
1-METHYL-4-ISOPROPYLBENZENE	134.22	10	14		99-87-6
1-METHYL-4-ISOPROPYLCYCLOHEXANE	140.27	10	20		99-82-1
1-METHYL-4N-PROPYLBENZENE	134.22	10	14		1074-55-1
1-METHYL-4-T-BUTYLBENZENE	148.24	11	16		98-51-1
1-METHYLCYCLOPENTENE	82.14	6	10		693-89-0
1-NONENE	126.24	9	18		124-11-8
1-NONENE-4-ONE	140.22	9	16	1	61168-10-3
1-OCTANOL	130.23	8	18	1	111-87-5
1-OCTENE	112.21	8	16		111-66-0
1-PENTENE	70.13	5	10		109-67-1
1-PENTYNE	68.12	5	8		627-19-0
1-PHENOXY-2-PROPANOL	152.19	9	12	2	770-35-4
1-PHENYL-1,3-BUTADIENE	130.19	10	10		1515-78-2
1-PROPYNE	40.06	3	4		74-99-7
1-T-BUTYL-2-METHYLBENZENE	148.24	11	16		27138-21-2
1-UNDECENE	154.29	11	22		821-95-4
1-UNDECYNE	152.28	11	20		2243-98-3
2-(2-BUTOXYETHOXY)ETHANOL {BUTYL CARBITOL}	162.23	8	18	3	112-34-5
2-(2-ETHOXYETHOXY) ETHYL ACETATE	176.21	8	16	4	112-15-2
2-(2-ETHYLHEXYLOXY)ETHANOL (ETHYLENE GLYCOL MONO-2-ETHYLHEXYL ETHER)	174.28	10	22	2	1559-35-9
2-(2-HEXYLOXYETHOXY) ETHANOL	190.28	10	22	3	112-59-4
2-(2-METHOXYPROPOXY)-1-PROPANOL (DIPROPYLENE GLYCOL METHYL ETHER ISOMER)	148.20	7	16	3	13588-28-8
2-(2-PROPOXYETHOXY) ETHANOL	148.20	7	16	3	6881-94-3
2,2,3,3-TETRAMETHYL BUTANE	114.23	8	18		594-82-1
2,2,3,3-TETRAMETHYLPENTANE	128.26	9	20		7154-79-2
2,2,3,4-TETRAMETHYLPENTANE	128.26	9	20		1186-53-4
2,2,3,TRIMETHYLHEXANE	128.26	9	20		16747-25-4
2,2,3-TRIMETHYLBUTANE	100.20	7	16		464-06-2
2,2,3-TRIMETHYLPENTANE	114.23	8	18		564-02-3
2,2,4,4-TETRAMETHYL-3-PENTANONE	142.24	9	18	1	815-24-7
2,2,4-TRIMETHYL-1,3-PENTANEDIOL	146.23	8	18	2	144-19-4
2,2,4-TRIMETHYLHEPTANE	142.28	10	22		14720-74-2
2,2,4-TRIMETHYLHEXANE	128.26	9	20		16747-26-5
2,2,4-TRIMETHYLPENTANE	114.23	8	18		540-84-1
2,2,5-TRIMETHYLHEPTANE	142.28	10	22		20291-95-6
2,2,5-TRIMETHYLHEXANE	128.26	9	20		3522-94-9
2,2-DIMETHYL CYCLOBUTANONE	98.14	6	10	1	1192-14-9
2,2-DIMETHYLBUTANE	86.18	6	14		75-83-2
2,2-DIMETHYLHEPTANE	128.26	9	20		1071-26-7

Description	Mwt	C	H	O	CAS
2,2-DIMETHYLHEXANE	114.23	8	18		590-73-8
2,2-DIMETHYLOCTANE	142.28	10	22		15869-87-1
2,2-DIMETHYLPENTANE	100.20	7	16		590-35-2
2,2-DIMETHYLPROPANAL (PIVALDEHYDE)	86.13	5	10	1	630-19-3
2,2-DIMETHYLPROPANE	72.15	5	12		463-82-1
2,3,3-TRIMETHYL-1-BUTENE	98.19	7	14		594-56-9
2,3,3-TRIMETHYL-1-HEXENE	126.24	9	18		360769-33-1
2,3,3-TRIMETHYLPENTANE	114.23	8	18		560-21-4
2,3,4,6-TETRAMETHYL HEPTANE	156.31	11	24		61868-54-0
2,3,4,6-TETRAMETHYLPHENOL (ISODURENOL)	150.22	10	14	1	3238-38-8
2,3,4-TRIMETHYL 1,3-PENTADIENE	110.20	8	14		85893-67-0
2,3,4-TRIMETHYL HEPTANE	142.28	10	22		52896-95-4
2,3,4-TRIMETHYLCYCLOPENTANONE	126.20	8	14	1	85794-10-1
2,3,4-TRIMETHYLHEXANE	128.26	9	20		921-47-1
2,3,4-TRIMETHYLPENTANE	114.23	8	18		565-75-3
2,3,5-TEIMETHYLHEXYL ACETATE	186.29	11	22	2	
2,3,5-TRIMETHYL PHENOL	136.19	9	12	1	697-82-5
2,3,5-TRIMETHYLHEPTANE	142.28	10	22		20278-85-7
2,3,5-TRIMETHYLHEXANE	128.26	9	20		1069-53-0
2,3,6-TRIMETHYL PHENOL	136.19	9	12	1	2416-94-6
2,3,6-TRIMETHYLHEPTANE	142.28	10	22		4032-93-3
2,3-BENZOFURAN	118.13	8	6	1	271-89-6
2,3-BUTANEDIOL	90.12	4	10	2	513-85-9
2,3-DIHYDROFURAN	70.09	4	6	1	1191-99-7
2,3-DIMETHYL PHENOL	122.16	8	10	1	526-75-0
2,3-DIMETHYL-1-BUTENE	84.16	6	12		563-78-0
2,3-DIMETHYL-1-PENTENE	98.19	7	14		3404-72-6
2,3-DIMETHYL-2-BUTENE	84.16	6	12		563-79-1
2,3-DIMETHYL-2-HEPTENE	126.24	9	18		3074-64-4
2,3-DIMETHYL-2-HEXENE	112.21	8	16		7145-20-2
2,3-DIMETHYL-2-OCTENE	140.27	10	20		19781-18-1
2,3-DIMETHYL-2-PENTENE	98.19	7	14		10574-37-5
2,3-DIMETHYLBUTANE	86.18	6	14		79-29-8
2,3-DIMETHYLBUTYL ACETATE	144.21	8	16	2	
2,3-DIMETHYLHEPTANE	128.26	9	20		3074-71-3
2,3-DIMETHYLHEPTYL ACETATE	186.29	11	22	2	
2,3-DIMETHYLHEXANE	114.23	8	18		584-94-1
2,3-DIMETHYLOCTANE	142.28	10	22		7146-60-3
2,3-DIMETHYLPENTANE	100.20	7	16		565-59-3
2,4,4-TRIMETHYL-1-PENTENE	112.21	8	16		107-39-1
2,4,4-TRIMETHYL-2-PENTENE (BETA DIISOBUTYLENE)	112.21	8	16		107-40-4
2,4,4-TRIMETHYLHEPTANE	142.28	10	22		
2,4,4-TRIMETHYLHEXANE	128.26	9	20		16747-30-1
2,4,5-TRIMETHYLHEPTANE	142.28	10	22		20278-84-6
2,4,5-TRIMETHYLPHENOL	136.19	9	12	1	496-78-6

Description	Mwt	C	H	O	CAS
2,4,5-TRIMETHYLSTYRENE	146.23	11	14		3937-24-4
2,4,6-TRIMETHYL HEPTANE	142.28	10	22		2613-61-8
2,4,6-TRIMETHYLOCTANE	156.31	11	24		62016-37-9
2,4-DIMETHYL FURAN	96.13	6	8	1	3710-43-8
2,4-DIMETHYL HEXANE	114.23	8	18		116502-44-4
2,4-DIMETHYL PHENOL	122.16	8	10	1	105-67-9
2,4-DIMETHYL-1,3-HEXADIENE	110.20	8	14		
2,4-DIMETHYL-1-HEPTENE	126.24	9	18		19549-87-2
2,4-DIMETHYL-1-PENTENE	98.19	7	14		2213-32-3
2,4-DIMETHYL-1-PROPYL BENZENE	148.24	11	16		61827-85-8
2,4-DIMETHYL-2-PENTENE	98.19	7	14		625-65-0
2,4-DIMETHYLBENZALDEHYDE	134.18	9	10	1	15764-16-6
2,4-DIMETHYLHEPTANE	128.26	9	20		2213-23-2
2,4-DIMETHYLHEPTYL ACETATE	186.29	11	22	2	
2,4-DIMETHYLHEXANE	114.23	8	18		589-43-5
2,4-DIMETHYLHEXYL ACETATE	172.26	10	20	2	
2,4-DIMETHYLNONANE	156.31	11	24		17302-24-8
2,4-DIMETHYLOCTANE	142.28	10	22		4032-94-4
2,4-DIMETHYLPENTANE	100.20	7	16		108-08-7
2,4-DIMETHYLPENTYL ACETATE	158.24	9	18	2	
2,4-HEXADIENAL	96.13	6	8	1	142-83-6
2,4-PENTANEDIONE	100.12	5	8	2	123-54-6
2,5,5-TRIMETHYLHEPTANE	142.28	10	22		
2,5,8,11-TETRAOXATRIDECAN-13-OL	208.25	9	20	5	23783-42-8
2,5-DIMETHYL FURAN	96.13	6	8	1	625-86-5
2,5-DIMETHYL PHENOL	122.16	8	10	1	95-87-4
2,5-DIMETHYLBENZALDEHYDE	134.18	9	10	1	5779-94-2
2,5-DIMETHYLHEPTANE	128.26	9	20		2216-30-0
2,5-DIMETHYLHEPTYL ACETATE	186.29	11	22	2	
2,5-DIMETHYLHEX-2-ENE	112.21	8	16		3404-78-2
2,5-DIMETHYLHEXANE	114.23	8	18		592-13-2
2,5-DIMETHYLNONANE	156.31	11	24		17302-27-1
2,5-DIMETHYLOCTANE	142.28	10	22		15869-89-3
2,6-DIMETHYL-1-HEPTENE	126.24	9	18		3074-78-0
2,6-DIMETHYL-4-HEPTANOL	144.25	9	20	1	108-82-7
2,6-DIMETHYL-4-HEPTANONE (DIISOBUTYL KETONE)	142.24	9	18	1	108-83-8
2,6-DIMETHYLHEPTANE	128.26	9	20		1072-05-5
2,6-DIMETHYLNONANE	156.31	11	24		17302-28-2
2,6-DIMETHYLOCTANE	142.28	10	22		2051-30-1
2,7-DIHYDROXYNAPHTHALENE	160.17	10	8	2	582-17-2
2,7-DIMETHYLOCTANE	142.28	10	22		1072-16-8
2,9-DIMETHYL DECANE	156.31	11	24		1002-17-1
2-[2-(2-ETHOXYETHOXY) ETHOXY] ETHANOL	178.23	8	18	4	112-50-5
2-[2-(2-METHOXYETHOXY) ETHOXY] ETHANOL	164.20	7	16	4	112-35-6
2-[2-(2-PROPOXYETHOXY) ETHOXY] ETHANOL (TRIETHYLENE GLYCOL	192.25	9	20	4	23305-64-8

Description	Mwt	C	H	O	CAS
MONOPROPYL ETHER)					
2-BUTOXYETHYL ACETATE (ETHYLENE GLYCOL BUTYL ETHER ACETATE)	160.21	8	16	3	112-07-2
2-BUTYL CYCLOHEXANONE	154.25	10	18	1	1126-18-7
2-BUTYL-4-METHYL-PHENOL	164.24	11	16	1	6891-45-8
2-BUTYLTETRAHYDROFURAN	128.21	8	16	1	1004-29-1
2-BUTYNE	54.09	4	6		503-17-3
2-DECANONE	156.27	10	20	1	693-54-9
2-ETHOXYETHANOL {CELLOSOLVE} {EGEE}	90.12	4	10	2	110-80-5
2-ETHOXYETHYL ACETATE {CELLOSOLVE ACETATE}	132.16	6	12	3	111-15-9
2-ETHYL BICYCLO[3.2.0]HEPTANE	124.22	9	16		
2-ETHYL FURAN	96.13	6	8	1	3208-16-0
2-ETHYL HEXANAL	128.21	8	16	1	123-05-7
2-ETHYL HEXYL ACETATE	172.26	10	20	2	103-09-3
2-ETHYL-1,3,4-TRIMETHYL BENZENE	148.24	11	16		61827-87-0
2-ETHYL-1,3,5-TRIMETHYL BENZENE	148.24	11	16		3982-67-0
2-ETHYL-1,3-DIMETHYL CYCLOHEXANE	140.27	10	20		7045-67-2
2-ETHYL-1,3-DIMETHYLCYCLOHEXANE	140.27	10	20		
2-ETHYL-1,3-HEXANEDIOL	146.23	8	18	2	94-96-2
2-ETHYL-1-BUTENE	84.16	6	12		760-21-4
2-ETHYL-1-HEXANOL	130.23	8	18	1	104-76-7
2-ETHYL-1-HEXENE	112.21	8	16		1632-16-2
2-ETHYL-1-PENTENE	98.19	7	14		3404-71-5
2-ETHYL-3-METHYL-1-BUTENE	98.19	7	14		7357-93-9
2-ETHYLHEXANOIC ACID	144.21	8	16	2	149-57-5
2-ETHYL-HEXYL ACRYLATE	184.28	11	20	2	103-11-7
2-ETHYLINDAN	146.23	11	14		56147-63-8
2-ETHYLPHENOL	122.16	8	10	1	90-00-6
2-FURANCARBOXALDEHYDE, 5-(HYDROXYMETHYL)-	126.11	6	6	3	67-47-0
2-FURFURAL	96.08	5	4	2	98-01-1
2-HEPTENAL	112.17	7	12	1	2463-63-0
2-HEXANOL	102.17	6	14	1	626-93-7
2-HEXYLOXYETHANOL	146.23	8	18	2	112-25-4
2-METHOXY-1-(2-METHOXY-1-METHYLETHOXY)-PROPANE	162.23	8	18	3	89399-28-0
2-METHOXY-1-PROPANOL	90.12	4	10	2	1589-47-5
2-METHOXY-1-PROPANOL ACETATE	132.16	6	12	3	70657-70-4
2-METHOXYETHANOL {METHYL CELLOSOLVE} {EGME}	76.09	3	8	2	109-86-4
2-METHOXY-NAPHTHALENE	158.20	11	10	1	93-04-9
2-METHYL FURAN	82.10	5	6	1	534-22-5
2-METHYL-1,4-PENTADIENE	82.14	6	10		763-30-4
2-METHYL-1,5-HEXADIENE	96.17	7	12		4049-81-4
2-METHYL-1-BUTANOL	88.15	5	12	1	137-32-6
2-METHYL-1-BUTENE	70.13	5	10		563-46-2
2-METHYL-1-BUTYL ACETATE	130.18	7	14	2	624-41-9
2-METHYL-1-HEPTENE	112.21	8	16		15870-10-7

Description	**Mwt**	**C**	**H**	**O**	**CAS**
2-METHYL-1-HEXENE	98.19	7	14		6094-02-6
2-METHYL-1-OCTENE	126.24	9	18		4588-18-5
2-METHYL-1-PENTENE	84.16	6	12		763-29-1
2-METHYL-2-BUTENE	70.13	5	10		513-35-9
2-METHYL-2-HEPTENE	112.21	8	16		627-97-4
2-METHYL-2-HEXENE	98.19	7	14		2738-19-4
2-METHYL-2-OCTENE	126.24	9	18		16993-86-5
2-METHYL-2-PENTENE	84.16	6	12		625-27-4
2-METHYL-2-PROPENAL (METHACROLEIN)	70.09	4	6	1	78-85-3
2-METHYL-3-BUTEN-2-OL	86.13	5	10	1	115-18-4
2-METHYL-3-ETHYLPENTANE	114.23	8	18		609-26-7
2-METHYL-3-HEXANONE	114.19	7	14	1	7379-12-6
2-METHYL-4-ETHYLHEXANE	128.26	9	20		3074-75-7
2-METHYLBENZENE-1,4-DIOL	124.14	7	8	2	95-71-6
2-METHYLBENZOIC ACID	136.15	8	8	2	118-90-1
2-METHYL-BUTANE	72.15	5	12		78-78-4
2-METHYLBUTYRALDEHYDE	86.13	5	10	1	96-17-3
2-METHYL-CIS-3-HEXENE	98.19	7	14		15840-60-5
2-METHYLDECALIN	152.28	11	20		2958-76-1
2-METHYLDECANE	156.31	11	24		6975-98-0
2-METHYLFURALDEHYDE	110.11	6	6	2	
2-METHYLHEPTANE	114.23	8	18		592-27-8
2-METHYL-HEXANAL	114.19	7	14	1	925-54-2
2-METHYLHEXANE	100.20	7	16		591-76-4
2-METHYLHEXYL ACETATE	158.24	9	18	2	
2-METHYLINDAN	132.20	10	12		824-63-5
2-METHYLNAPHTHALENE	142.20	11	10		91-57-6
2-METHYLNONANE	142.28	10	22		871-83-0
2-METHYLOCTANE	128.26	9	20		3221-61-2
2-METHYLOCTYL ACETATE	186.29	11	22	2	
2-METHYLPENTANE	86.18	6	14		107-83-5
2-METHYLPENTYL ACETATE	144.21	8	16	2	
2-METHYLPROPANE; ISOBUTANE	58.12	4	10		75-28-5
2-METHYLPROPENE (ISOBUTENE)	56.11	4	8		115-11-7
2-METHYL-TRANS-3-HEXENE	98.19	7	14		692-24-0
2-NONANONE	142.24	9	18	1	821-55-6
2-OCTANOL	130.23	8	18	1	4128-31-8
2-OCTANONE	128.21	8	16	1	111-13-7
2-OXOBUTANAL; ETHYL GLYOXAL	86.09	4	6	2	
2-PENTANOL (SEC AMYL ALCOHOL)	88.15	5	12	1	6032-29-7
2-PHENOXYETHANOL	138.16	8	10	2	122-99-6
2-PROPYL CYCLOHEXANONE	140.22	9	16	1	94-65-5
2-TERT-BUTOXY-1-PROPANOL	132.20	7	16	2	94023-15-1
2-UNDECANONE	170.29	11	22	1	112-12-9
2-UNDECENAL	168.28	11	20	1	2463-77-6
3,3,5-TRIMETHYLHEPTANE	142.28	10	22		7154-80-5
3,3-DIETHYLPENTANE	128.26	9	20		1067-20-5

Description	Mwt	C	H	O	CAS
3,3-DIMETHYL-1-BUTENE	84.16	6	12		558-37-2
3,3-DIMETHYL-1-PENTENE	98.19	7	14		3404-73-7
3,3-DIMETHYLHEPTANE	128.26	9	20		4032-86-4
3,3-DIMETHYLHEXANE	114.23	8	18		563-16-6
3,3-DIMETHYLOCTANE	142.28	10	22		4110-44-5
3,3-DIMETHYLPENTANE	100.20	7	16		562-49-2
3,4-DIETHYL HEXANE	142.28	10	22		19398-77-7
3,4-DIETHYL-2-HEXENE (E)	140.27	10	20		59643-70-8
3,4-DIMETHOXYBENZOIC ACID	182.17	9	10	4	93-07-2
3,4-DIMETHYL PHENOL	122.16	8	10	1	95-65-8
3,4-DIMETHYL-1-OCTYNE-7,8-DIOL	170.25	10	18	2	
3,4-DIMETHYL-1-PENTENE	98.19	7	14		7385-78-6
3,4-DIMETHYL-2-PENTENE	98.19	7	14		24910-63-2
3,4-DIMETHYLBENZOIC ACID	150.17	9	10	2	619-04-5
3,4-DIMETHYL-CIS-2-PENTENE	98.19	7	14		4914-91-4
3,4-DIMETHYLHEPTANE	128.26	9	20		922-28-1
3,4-DIMETHYLHEXANE	114.23	8	18		583-48-2
3,4-DIMETHYLHEXYL ACETATE	172.26	10	20	2	
3,4-DIMETHYLOCTANE	142.28	10	22		15869-92-8
3,5,5-TRIMETHYL-1-HEXENE	126.24	9	18		4316-65-8
3,5-DIETHYL HEPTANE	156.31	11	24		61869-02-1
3,5-DIMETHYL-1-HEXYNE-3-OL	126.20	8	14	1	107-54-0
3,5-DIMETHYLBENZYL ALCOHOL	136.19	9	12	1	27129-87-9
3,5-DIMETHYLHEPTANE	128.26	9	20		926-82-9
3,5-DIMETHYLHEPTYL ACETATE	186.29	11	22	2	
3,5-DIMETHYLHEXYL ACETATE	172.26	10	20	2	
3,5-DIMETHYLNONANE	156.31	11	24		
3,5-DIMETHYLOCTANE	142.28	10	22		15869-93-9
3,6-DIMETHYLHEPTYL ACETATE	186.29	11	22	2	
3,6-DIMETHYLOCTANE	142.28	10	22		15869-94-0
3,7-DIMETHYL-1-OCTANOL	158.28	10	22	1	106-21-8
3,7-DIMETHYL-1-OCTENE	140.27	10	20		4984-01-4
3,7-DIMETHYLNONANE	156.31	11	24		17302-32-8
3-BUTOXY-1-BUTENE	128.21	8	16	1	37027-60-4
3-CARENE	136.23	10	16		13466-78-9
3-ETHOXY-1-PROPANOL (PROPYLENE GLYCOL, MONOETHYL ETHER)	104.15	5	12	2	111-35-3
3-ETHYL -1-HEPTENE	126.24	9	18		3525-27-7
3-ETHYL NONANE	156.31	11	24		17302-11-3
3-ETHYL-1-PENTENE	98.19	7	14		4038-04-4
3-ETHYL-2,2-DIMETHYL PENTANE	128.26	9	20		16747-32-3
3-ETHYL-2,4-DIMETHYL PENTANE	128.26	9	20		1068-87-7
3-ETHYL-2-METHYL-2-HEPTENE	140.27	10	20		19780-61-1
3-ETHYL-2-METHYLHEPTANE	142.28	10	22		14676-29-0
3-ETHYL-2-PENTENE	98.19	7	14		816-79-5
3-ETHYL-3-METHYL HEXANE	128.26	9	20		3074-76-8
3-ETHYL-3-METHYLOCTANE	156.31	11	24		

Description	Mwt	C	H	O	CAS
3-ETHYL-4-METHYLHEPTANE	142.28	10	22		52896-91-0
3-ETHYLCYCLOPENTENE	96.17	7	12		694-35-9
3-ETHYLHEPTANE	128.26	9	20		15869-80-4
3-ETHYLHEPTYL ACETATE	186.29	11	22	2	
3-ETHYLHEXANE	114.23	8	18		619-99-8
3-ETHYLHEXYL ACETATE	172.26	10	20	2	
3-ETHYLNONANE	156.31	11	24		
3-ETHYLOCTANE	142.28	10	22		5881-17-4
3-ETHYLPENTANE	100.20	7	16		617-78-7
3-ETHYLPENTYL ACETATE	158.24	9	18	2	
3-METHOXY-1-BUTANOL	104.15	5	12	2	2517-43-3
3-METHOXY-1-PROPANOL	90.12	4	10	2	1320-67-8
3-METHYL FURAN	82.10	5	6	1	930-27-8
3-METHYL-1,2-BUTADIENE	68.12	5	8		
3-METHYL-1-BUTENE	70.13	5	10		563-45-1
3-METHYL-1-DECENE	154.29	11	22		13151-28-5
3-METHYL-1-HEXENE	98.19	7	14		3404-61-3
3-METHYL-1-PENTENE	84.16	6	12		760-20-3
3-METHYL-2,4-HEXADIENE	96.17	7	12		28823-42-9
3-METHYL-2-HEXANONE	114.19	7	14	1	2550-21-2
3-METHYL-2-ISOPROPYL-1-BUTENE	112.21	8	16		111823-35-9
3-METHYL-3-ETHYLPENTANE	114.23	8	18		1067-08-9
3-METHYL-3-METHOXY-1-BUTANOL	118.17	6	14	2	56539-66-3
3-METHYL-5-ETHYLHEPTANE	142.28	10	22		
3-METHYLBENZOIC ACID	136.15	8	8	2	
3-METHYLBUTANOIC ACID	102.13	5	10	2	503-74-2
3-METHYL-CIS-2-HEXENE	98.19	7	14		10574-36-4
3-METHYL-CIS-2-PENTENE	84.16	6	12		922-62-3
3-METHYL-CIS-3-HEXENE	98.19	7	14		4914-89-0
3-METHYLCYCLOPENTENE	82.14	6	10		1120-62-3
3-METHYLDECANE	156.31	11	24		13151-34-3
3-METHYLHEPTANE	114.23	8	18		589-81-1
3-METHYLHEPTYL ACETATE	172.26	10	20	2	
3-METHYLHEXANE	100.20	7	16		589-34-4
3-METHYLHEXYL ACETATE	158.24	9	18	2	
3-METHYLNONANE	142.28	10	22		5911-04-6
3-METHYLOCTANE	128.26	9	20		2216-33-3
3-METHYLPENTANE	86.18	6	14		96-14-0
3-METHYLPENTYL ACETATE	144.21	8	16	2	
3-METHYL-TRANS-2-HEXENE	98.19	7	14		20710-38-7
3-METHYL-TRANS-2-PENTENE	84.16	6	12		616-12-6
3-METHYL-TRANS-3-HEXENE	98.19	7	14		3899-36-3
3-OCTANOL	130.23	8	18	1	20296-29-1
3-PENTANOL (DIETHYL CARBINOL)	88.15	5	12	1	584-02-1
3-PENTEN-1-YNE	66.10	5	6		2206-23-7
3-PHENYLPENTANE	148.24	11	16		1196-58-3
3-PROPYL-1-HEPTENE	140.27	10	20		35648-55-6

Description	Mwt	C	H	O	CAS
4,4-DIMETHYL-1-HEXENE	112.21	8	16		1647-08-1
4,4-DIMETHYL-1-PENTENE	126.24	9	18		762-62-9
4,4-DIMETHYL-2-PENTENE	98.19	7	14		26232-98-4
4,4-DIMETHYL-3-OXAHEXANE	116.20	7	16	1	919-94-8
4,4-DIMETHYL-CIS-2-PENTENE	98.19	7	14		762-63-0
4,4-DIMETHYLHEPTANE	128.26	9	20		1068-19-5
4,4-DIMETHYLOCTANE	142.28	10	22		15869-95-1
4,5-DIMETHYL-2,3,DIHYDRO-1-H-INDENES	146.23	11	14		1685-83-2
4,5-DIMETHYLHEPTYL ACETATE	186.29	11	22	2	
4,5-DIMETHYLHEXYL ACETATE	172.26	10	20	2	
4,5-DIMETHYLOCTANE	142.28	10	22		15869-96-2
4,6-DIMETHYL-2,3,DIHYDRO-1-H-INDENES	146.23	11	14		1685-82-1
4,6-DIMETHYL-2-OCTYNE	138.25	10	18		
4,6-DIMETHYLHEPTYL ACETATE	186.29	11	22	2	
4,7-DIMETHYL-2,3,DIHYDRO-1-H-INDENES	146.23	11	14		6682-71-9
4-ALLYL-GUAIACOL-TMS , ALSO NOTED AS "A4GUCL"	164.20	10	12	2	97-53-0
4-ETHYL NONANE	156.31	11	24		5911-05-7
4-ETHYL OCTANE	142.28	10	22		15869-86-0
4-ETHYL-1-OCTENE	140.27	10	20		19781-30-7
4-ETHYLHEPTANE	128.26	9	20		2216-32-2
4-ETHYLPHENANTHRENE	206.28	10	22	4	66291-36-9
4-ETHYLSYRINGOL	182.22	10	14	3	
4-HEPTEN-2-ONE	112.17	7	12	1	24332-22-7
4-HYDROXY BENZENEETHANOL	138.16	8	10	2	501-94-0
4-ME-GUAIACOL-TMS , ALSO NOTED AS "M4GUCL"	138.16	8	10	2	93-51-6
4-METHYL CYCLOHEXENE	96.17	7	12		591-47-9
4-METHYL-1-HEPTENE	112.21	8	16		13151-05-8
4-METHYL-1-HEXENE	98.19	7	14		3769-23-1
4-METHYL-1-NONENE	140.27	10	20		26741-20-8
4-METHYL-1-PENTENE	84.16	6	12		691-37-2
4-METHYL-2-HEPTENE	112.21	8	16		3404-56-6
4-METHYL-2-PENTANOL (METHYL ISOBUTYL CARBINOL)	102.17	6	14	1	108-11-2
4-METHYL-2-PROPYL-PHENOL	150.22	10	14	1	4074-46-8
4-METHYLBENZOIC ACID	136.15	8	8	2	
4-METHYL-CIS-2-PENTENE	84.16	6	12		691-38-3
4-METHYLCYCLOPENTENE	82.14	6	10		1759-81-5
4-METHYLDECANE	156.31	11	24		2847-72-5
4-METHYLHEPTANE	114.23	8	18		589-53-7
4-METHYLHEPTYL ACETATE	172.26	10	20	2	
4-METHYLHEXYL ACETATE	158.24	9	18	2	
4-METHYLINDAN	132.20	10	12		824-22-6
4-METHYLNONANE	142.28	10	22		17301-94-9
4-METHYLOCTANE	128.26	9	20		2216-34-4
4-METHYLOCTYL ACETATE	186.29	11	22	2	
4-METHYLPENTYL ACETATE	144.21	8	16	2	

Description	Mwt	C	H	O	CAS
4-METHYLSTYRENE	118.18	9	10		622-97-9
4-METHYL-SYRINGOL-TMS , ALSO NOTED AS "M4SYRG"	168.19	9	12	3	6638-05-7
4-METHYL-TRANS-2-HEXENE	98.19	7	14		3683-22-5
4-METHYL-TRANS-2-PENTENE	84.16	6	12		674-76-0
4-NONENE	126.24	9	18		2198-23-4
4-OCTANOL	130.23	8	18	1	589-62-8
4-PHENYL-1-BUTENE	132.20	10	12		768-56-9
4-PROPYL CYCLOHEXANONE	140.22	9	16	1	40649-36-3
4-PROPYL HEPTANE	142.28	10	22		3178-29-8
4-PROPYL-3-HEPTENE	140.27	10	20		4485-13-6
4-PROPYLSYRINGOL	196.24	11	16	3	
4-VINYLCYCLOHEXENE	108.18	8	12		100-40-3
4-VINYLPHENOL	120.15	8	8	1	2628-17-3
5,6-DIMETHYL-2,3,DIHYDRO-1-H-INDENES	146.23	11	14		1075-22-5
5,8-DIHYDROXY-1,4-NAPHTHALENEDIONE	190.15	10	6	4	475-38-7
5-BUTYLDIHYDRO-2(3H)-FURANONE	142.20	8	14	2	
5-ETHYL NONANE	156.31	11	24		17302-12-4
5-ETHYLDIHYDRO-2(3H)-FURANONE	114.14	6	10	2	
5-HEPTYLDIHYDRO-2(3H)-FURANONE	184.28	11	20	2	
5-HEXYLDIHYDRO-2(3H)-FURANONE	170.25	10	18	2	706-14-9
5-METHYL-1-HEPTANOL	130.23	8	18	1	7212-53-5
5-METHYL-1-HEXENE	98.19	7	14		3524-73-0
5-METHYL-CIS-2-HEXENE	98.19	7	14		3404-62-4
5-METHYLDECANE	156.31	11	24		13151-35-4
5-METHYLHEPTYL ACETATE	172.26	10	20	2	
5-METHYLHEXYL ACETATE	158.24	9	18	2	
5-METHYLINDAN	132.20	10	12		874-35-1
5-METHYLNONANE	142.28	10	22		15869-85-9
5-METHYLOCTYL ACETATE	186.29	11	22	2	
5-METHYL-TRANS-2-HEXENE	98.19	7	14		7385-82-2
5-PENTYLDIHYDRO-2(3H)-FURANONE	156.22	9	16	2	
5-PROPYLDIHYDRO-2(3H)-FURANONE	128.17	7	12	2	
6-ETHYL-2-METHYLOCTANE	156.31	11	24		
7-METHYL 1-NONENE	140.27	10	20		26741-23-1
8-METHYL-1-NONANOL (ISODECYL ALCOHOL)	158.28	10	22	1	25339-17-7
ACETAL (1,1-DIETHOXYETHANE)	118.17	6	14	2	105-57-7
ACETALDEHYDE	44.05	2	4	1	75-07-0
ACETIC ACID	60.05	2	4	2	64-19-7
ACETIC ANHYDRIDE	102.09	4	6	3	108-24-7
ACETONE	58.08	3	6	1	67-64-1
ACETOPHENONE (PHENYL METHYL KETONE)	120.15	8	8	1	98-86-2
ACETOVANILLONE-TMS , ALSO NOTED AS "ACETVA"	166.17	9	10	3	498-02-2
ACETYLENE	26.04	2	2		74-86-2
ACROLEIN (2-PROPENAL)	56.06	3	4	1	107-02-8
ACRYLIC ACID	72.06	3	4	2	79-10-7

Description	Mwt	C	H	O	CAS
ADIPIC ACID	146.14	6	10	4	124-04-9
ALLYLBENZENE	118.18	9	10		300-57-2
ALPHA-METHYLTETRAHYDROFURAN (2-METHYL TETRAHYDROFURAN)	86.13	5	10	1	96-47-9
ALPHA-PHELLANDRENE	136.23	10	16		99-83-2
A-METHYLSTYRENE	118.18	9	10		98-83-9
AMYL ACETATE	130.18	7	14	2	628-63-7
ANETHOL	148.20	10	12	1	104-46-1
A-PINENE	136.23	10	16		80-56-8
A-TERPINEOL	154.25	10	18	1	98-55-5
BENZALDEHYDE	106.12	7	6	1	100-52-7
BENZALDEHYDE, 3,4-DIMETHOXY-	166.17	9	10	3	120-14-9
BENZENE	78.11	6	6		71-43-2
BENZOIC ACID	122.12	7	6	2	65-85-0
BENZOIC ACID, 4-HYDROXY-3-METHOXY-, METHYL ESTER	182.17	9	10	4	3943-74-6
BENZYL ACETATE	150.17	9	10	2	140-11-4
BENZYL ALCOHOL	108.14	7	8	1	100-51-6
BENZYLCARBINYL PROPIONATE	178.23	11	14	2	122-70-3
BETA-NICOTYRINE	182.17	9	10	4	487-19-4
BETA-PHENETHYL ALCOHOL	122.16	8	10	1	60-12-8
BIACETYL	86.09	4	6	2	431-03-8
BICYCLO[3.2.1] OCTANE	110.20	8	14		6221-55-2
BICYCLO[3.3.1] NONANE	124.22	9	16		280-65-9
B-METHYLSTYRENE	118.18	9	10		637-50-3
BORNEOL	138.25	10	18		507-70-0
B-PHELLANDRENE {1(7)-2-P-MENTHADIENE}	136.23	10	16		555-10-2
B-PINENE	136.23	10	16		127-91-3
BUTANOIC ACID	88.11	4	8	2	107-92-6
BUTYL CELLOSOLVE {2-BUTOXYETHANOL} {EGBE}	118.17	6	14	2	111-76-2
BUTYL METHACRYLATE	142.20	8	14	2	97-88-1
BUTYL PROPIONATE	130.18	7	14	2	590-01-2
BUTYLCYCLOHEXANE	140.27	10	20		1678-93-9
BUTYRALDEHYDE	72.11	4	8	1	123-72-8
CAMPHENE	136.23	10	16		5794-03-6
CAMPHOR	152.23	10	16	1	76-22-2
CARBITOL {DEGEE} {2-(2-ETHOXYETHOXY)ETHANOL}	134.17	6	14	3	111-90-0
CARVOMENTHOL (2-P-MENTHANOL) (2-METHYL-5-(1-METHYLETHYL)-CYCLOHEXANOL)	156.27	10	20	1	499-69-4
CARVONE	150.22	10	14	1	99-49-0
CINNAMIC ALCOHOL	134.18	9	10	1	104-54-1
CINNAMIC ALDEHYDE	132.16	9	8	1	104-55-2
CIS 1,2-DIETHYL CYCLOHEXANE	140.27	10	20		824-43-1
CIS 1,3-DIETHYL CYCLOHEXANE	140.27	10	20		13991-43-0
CIS 1,3-PENTADIENE	68.12	5	8		1574-41-0
CIS 1,4-DIETHYL CYCLOHEXANE	140.27	10	20		13990-92-6

Description	Mwt	C	H	O	CAS
CIS 1-ETHYL-4-METHYL CYCLOHEXANE	126.24	9	18		4926-78-7
CIS 1-METHYL-2-PROPYL CYCLOHEXANE	140.27	10	20		4926-71-0
CIS 1-METHYL-3-PROPYL CYCLOHEXANE	140.27	10	20		42806-75-7
CIS 1-METHYL-4-PROPYL CYCLOHEXANE	140.27	10	20		28954-42-9
CIS,CIS,CIS-1,2,3-TRIMETHYL CYCLOHEXANE	126.24	9	18		1839-88-9
CIS,CIS,TRANS-1,2,3-TRIMETHYL, CCT CYCLOHEXANE	126.24	9	18		7667-55-2
CIS,CIS,TRANS-1,2,4-TRIMETHYL CYCLOHEXANE	126.24	9	18		7667-58-5
CIS,CIS-1,2,4-TRIMETHYLCYCLOHEXANE	126.24	9	18		
CIS,TRANS,CIS-1,2,3-TRIMETHYL CYCLOHEXANE	126.24	9	18		1678-81-5
CIS,TRANS,CIS-1,2,3-TRIMETHYL CYCLOPENTANE	112.21	8	16		19374-46-0
CIS,TRANS,CIS-1,2,4-TRIMETHYL CYCLOHEXANE	126.24	9	18		7667-59-6
CIS,TRANS,CIS-1,2,4-TRIMETHYL CYCLOPENTANE	112.21	8	16		18679-30-6
CIS,TRANS-1,2,3-TRIMETHYLCYCLOHEXANE	126.24	9	18		20348-72-5
CIS,TRANS-1,2,4-TRIMETHYLCYCLOHEXANE	126.24	9	18		
CIS-1,2-DIMETHYLCYCLOHEXANE	112.21	8	16		2207-01-4
CIS-1,3-DIMETHYLCYCLOHEXANE	112.21	8	16		638-04-0
CIS-1,3-DIMETHYLCYCLOPENTANE	98.19	7	14		2532-58-3
CIS-1,4-DIMETHYLCYCLOHEXANE	112.21	8	16		624-29-3
CIS-1,CIS-2,3-TRIMETHYLCYCLOPENTANE	112.21	8	16		2613-69-6
CIS-1,CIS-2,4-TRIMETHYLCYCLOPENTANE	112.21	8	16		
CIS-1,CIS-3,5-TRIMETHYLCYCLOHEXANE	126.24	9	18		1795-27-3
CIS-1,TRANS-2,3-TRIMETHYLCYCLOPENTANE	112.21	8	16		15890-40-1
CIS-1,TRANS-2,4-TRIMETHYLCYCLOPENTANE	112.21	8	16		
CIS-1,TRANS-2,CIS-4-TRIMETHYLCYCLOHEXANE	126.24	9	18		
CIS-1,TRANS-2,TRANS-4-TRIMETHYLCYCLOHEXANE	126.24	9	18		7667-60-9
CIS-1-2-DIMETHYLCYCLOPENTANE	98.19	7	14		1192-18-3
CIS-1-ETHYL-2-METHYLCYCLOHEXANE	126.24	9	18		4923-77-7
CIS-1-ETHYL-2-METHYLCYCLOPENTANE	112.21	8	16		930-89-2
CIS-1-ETHYL-3-METHYLCYCLOHEXANE	126.24	9	18		19489-10-2
CIS-1-METHYL-3-ETHYLCYCLOPENTANE	112.21	8	16		2613-66-3
CIS-2-BUTENE	56.11	4	8		590-18-1
CIS-2-HEPTENE	98.19	7	14		6443-92-1
CIS-2-HEXENE	84.16	6	12		7688-21-3
CIS-2-NONENE	126.24	9	18		6434-77-1
CIS-2-OCTENE	112.21	8	16		7642-04-8
CIS-2-PENTENE	70.13	5	10		627-20-3
CIS-3-HEPTENE	98.19	7	14		7642-10-6
CIS-3-HEXENE	84.16	6	12		7642-09-3
CIS-3-NONENE	126.24	9	18		20237-46-1
CIS-4-OCTENE	112.21	8	16		7642-15-1
CIS-5-DECENE	140.27	10	20		7433-78-5

Description	Mwt	C	H	O	CAS
CIS-BICYCLO[3.3.0]OCTANE	110.20	8	14		694-72-4
CIS-BICYCLO[4.3.0]NONANE	124.22	9	16		4551-51-3
CIS-DECALIN	138.25	10	18		493-01-6
CIS-ISO-EUGENOL	164.20	10	12	2	5912-86-7
CITRONELLOL (3,7-DIMETHY-6-OCTEN-1-OL)	154.25	10	18	1	106-22-9
CONIFERALDEHYDE	178.18	10	10	3	458-36-6
CROTONALDEHYDE	70.09	4	6	1	4170-30-3
CUMENE (ISOPROPYL BENZENE)	120.19	9	12		98-82-8
CUMENE HYDROPEROXIDE	152.19	9	12	2	80-15-9
CYCLOBUTANE	56.11	4	8		287-23-0
CYCLOBUTANONE	70.09	4	6	1	1191-95-3
CYCLOHEPTANE	98.19	7	14		291-64-5
CYCLOHEPTANONE	112.17	7	12	1	502-42-1
CYCLOHEXANE	84.16	6	12		110-82-7
CYCLOHEXANOL	100.16	6	12	1	108-93-0
CYCLOHEXANONE	98.14	6	10	1	108-94-1
CYCLOHEXENE	82.14	6	10		110-83-8
CYCLOOCTANE	112.21	8	16		292-64-8
CYCLOPENTANE	70.13	5	10		287-92-3
CYCLOPENTANOL	86.13	5	10	1	96-41-3
CYCLOPENTANONE	84.12	5	8	1	120-92-3
CYCLOPENTENE	68.12	5	8		142-29-0
CYCLOPENTYLCYCLOPENTANE	138.25	10	18		1636-39-1
CYCLOPROPANE	42.08	3	6		75-19-4
DECANAL	156.27	10	20	1	112-31-2
DECANEDIOIC ACID	202.25	10	18	4	111-20-6
DI N-PROPYL ETHER	102.17	6	14	1	111-43-3
DIACETONE ALCOHOL (4-HYDROXY-4-METHYL-2-PENTANONE)	116.16	6	12	2	123-42-2
DIBUTYL ETHER	130.23	8	18	1	142-96-1
DICYCLOPENTADIENE	132.20	10	12		77-73-6
DIETHYL CYCLOHEXANE	140.27	10	20		1331-43-7
DIETHYL KETONE	86.13	5	10	1	96-22-0
DIETHYLENE GLYCOL (2,2'-OXYBISETHANOL)	106.12	4	10	3	111-46-6
DIETHYLENE GLYCOL BUTYL ETHER ACETATE {2-2-(BUTOXYETHOXY)ETHYLACETATE}	204.26	10	20	4	124-17-4
DIHYDROXYACETONE	90.08	3	6	3	96-26-4
DI-ISOBUTYL ETHER	130.23	8	18	1	628-55-7
DIISOPROPYL CARBONATE	146.18	7	14	3	6482-34-4
DIISOPROPYL ETHER	102.17	6	14	1	108-20-3
DI-ISOPROPYL KETONE	114.19	7	14	1	565-80-0
DIISOPROPYLENE GLYCOL; 1,1'-OXYDIPROPAN-2-OL	134.17	6	14	3	110-98-5
DIMETHOXYMETHANE (METHYLAL)	76.09	3	8	2	109-87-5
DIMETHOXYPROPANE	104.15	5	12	2	77-76-9
DIMETHYL ADIPATE (DIMETHYLHEXANEDIOATE)	174.19	8	14	4	627-93-0

Description	Mwt	C	H	O	CAS
DIMETHYL CARBONATE	90.08	3	6	3	616-38-6
DIMETHYL ETHER	46.07	2	6	1	115-10-6
DIMETHYL INDAN	146.23	11	14		53563-67-0
DIMETHYL PHTHALATE	194.18	10	10	4	131-11-3
DIMETHYL SUCCINATE (DIMETHYL BUTANEOATE)	146.14	6	10	4	106-65-0
DIMETHYL, ISOPROPYL BENZENE	148.24	11	16		25321-29-3
DIMETHYLHEPTANOL (2,6-DIMETHYL-2-HEPTANOL)	144.25	9	20	1	13254-34-7
DIMETHYLPENTANOL (2,3-DIMETHYL-1-PENTANOL)	116.20	7	16	1	10143-23-4
DIMETHYLTEREPHTHALATE	194.18	10	10	4	120-61-6
DI-N-PENTYL ETHER	158.28	10	22	1	693-65-2
DIPROPYLENE GLYCOL ETHYL ETHER	162.23	8	18	3	15764-24-6
DIPROPYLENE GLYCOL METHYL ETHER ACETATE ISOMER #1	190.24	9	18	4	
DIPROPYLENE GLYCOL METHYL ETHER ACETATE ISOMER #2	190.24	9	18	4	
DIPROPYLENE GLYCOL METHYL ETHER ISOMER (1-METHOXY-2-[2-HYDROXYPROPOXY]-PROPANE)	148.20	7	16	3	
DIPROPYLENE GLYCOL N-PROPYL ETHER ISOMER #1	176.25	9	20	3	
DIVINYL BENZENE {VINYL STYRENE}	130.19	10	10		1321-74-0
D-LIMONENE	136.23	10	16		5989-27-5
ETHANE	30.07	2	6		74-84-0
ETHANONE, 1-(4-HYDROXY-3,5-DIMETHOXYPHENYL)-	196.20	10	12	4	2478-38-8
ETHYL ACETATE	88.11	4	8	2	141-78-6
ETHYL ACRYLATE	100.12	5	8	2	140-88-5
ETHYL ALCOHOL	46.07	2	6	1	64-17-5
ETHYL BUTYRATE	116.16	6	12	2	105-54-4
ETHYL ETHER	74.12	4	10	1	60-29-7
ETHYL FORMATE	74.08	3	6	2	109-94-4
ETHYL ISOPROPYL BENZENE	148.24	11	16		26573-16-0
ETHYL ISOPROPYL ETHER	88.15	5	12	1	625-54-7
ETHYL LACTATE	118.13	5	10	3	97-64-3
ETHYL METHACRYLATE	114.14	6	10	2	97-63-2
ETHYL N-BUTYL ETHER	102.17	6	14	1	628-81-9
ETHYL PROPIONATE	102.13	5	10	2	105-37-3
ETHYL T-BUTYL ETHER	102.17	6	14	1	637-92-3
ETHYL-3-ETHOXYPROPIONATE	146.18	7	14	3	763-69-9
ETHYLBENZENE	106.17	8	10		100-41-4
ETHYLCYCLOHEXANE	112.21	8	16		1678-91-7
ETHYLCYCLOPENTANE	98.19	7	14		1640-89-7
ETHYLDIMETHYLPHENOL	150.22	10	14	1	85528-07-0
ETHYLENE	28.05	2	4		74-85-1
ETHYLENE GLYCOL	62.07	2	6	2	107-21-1
ETHYLENE GLYCOL DIACETATE	146.14	6	10	4	111-55-7
ETHYLENE GLYCOL DIETHYL ETHER; 1,2-DIETHOXYETHANE	118.17	6	14	2	629-14-1

Description	**Mwt**	**C**	**H**	**O**	**CAS**
ETHYLENE GLYCOL PROPYL ETHER {2-PROPOXYETHANOL}	104.15	5	12	2	2807-30-9
ETHYLENE OXIDE	44.05	2	4	1	75-21-8
ETHYLHEXANOATE (ETHYL N-HEXANOATE)	144.21	8	16	2	123-66-0
FORMALDEHYDE	30.03	1	2	1	50-00-0
FORMIC ACID	46.03	1	2	2	64-18-6
FURAN	68.07	4	4	1	110-00-9
FURANCARBOXYLIC ACID	112.08	5	4	3	26447-28-9
FURFURYL ALCOHOL	98.10	5	6	2	98-00-0
GAMMA- BUTYROLACTONE	86.09	4	6	2	96-48-0
GERANIOL	154.25	10	18	1	106-24-1
GLUTARALDEHYDE (A DIALDEHYDE)	100.12	5	8	2	111-30-8
GLYCEROL	92.09	3	8	3	56-81-5
GLYCERYL TRIACETATE	218.20	9	14	6	102-76-1
GLYCOL ETHER DPNB {1-(2-BUTOXY-1-METHYLETHOXY)-2-PROPANOL}	190.28	10	22	3	29911-28-2
GLYCOLIC ACID {HYDROXYACETIC ACID}	76.05	2	4	3	79-14-1
GLYOXAL	58.04	2	2	2	107-22-2
GLYOXYLIC ACID	74.04	2	2	3	298-12-4
GUAIACOL-TMS	124.14	7	8	2	90-05-1
HEPTANAL	114.19	7	14	1	111-71-7
HEXADIENE	82.14	6	10		42296-74-2
HEXANAL (HEXANALADEHYDE)	100.16	6	12	1	66-25-1
HEXYLCYCLOPENTANE	154.29	11	22		4457-00-5
HEXYLENE GLYCOL (2-METHYLPENTANE-2,4-DIOL)	118.17	6	14	2	107-41-5
HOMOVANILLIC ACID	182.17	9	10	4	306-08-1
HYDROQUINONE	110.11	6	6	2	123-31-9
HYDROXY ACETONE (ACETOL)	74.08	3	6	2	116-09-6
HYDROXY METHACROLEIN (2-(HYDROXYMETHYL)-2-PROPENAL)	86.09	4	6	2	40364-84-9
HYDROXYCITRONELLAL	154.25	10	18	1	107-75-5
HYDROXYPROPYL ACRYLATE	130.14	6	10	3	2918-23-2
INDAN	118.18	9	10		496-11-7
INDENE	116.16	9	8		95-13-6
ISOAMYL ACETATE (3-METHYLBUTYL ACETATE)	130.18	7	14	2	123-92-2
ISOAMYL ALCOHOL (3-METHYL-1-BUTANOL)	88.15	5	12	1	123-51-3
ISOAMYL ISOBUTYRATE	158.24	9	18	2	2050-01-3
ISOBUTYL ACETATE	116.16	6	12	2	110-19-0
ISOBUTYL ACRYLATE {2-PROPENOIC ACID}	128.17	7	12	2	106-63-8
ISOBUTYL ALCOHOL	74.12	4	10	1	78-83-1
ISOBUTYL ISOBUTYRATE	144.21	8	16	2	97-85-8
ISOBUTYL METHACRYLATE	142.20	8	14	2	97-86-9
ISOBUTYLCYCLOHEXANE (2-METHYLPROPYL CYCLOHEXANE)	140.27	10	20		1678-98-4
ISOBUTYLCYCLOPENTANE (2-METHYLPROPYL CYCLOPENTANE)	126.24	9	18		3788-32-7
ISOBUTYRALDEHYDE	72.11	4	8	1	78-84-2
ISOBUTYRIC ACID	88.11	4	8	2	79-31-2

Description	**Mwt**	**C**	**H**	**O**	**CAS**
ISOEUGENOL-TMS , ALSO NOTED AS "ISOEUG"	164.20	10	12	2	97-54-1
ISOPHORONE {3,5,5-TRIMETHYL-2-CYCLOHEXENONE}	138.21	9	14	1	78-59-1
ISOPRENE	68.12	5	8		78-79-5
ISOPROPYL ACETATE	102.13	5	10	2	108-21-4
ISOPROPYL ALCOHOL	60.10	3	8	1	67-63-0
ISOPROPYL CYCLOPROPANE	84.16	6	12		3638-35-5
ISOPROPYL FORMATE	88.11	4	8	2	625-55-8
ISOPROPYLCYCLOHEXANE (2-METHYLETHYL CYCLOHEXANE)	126.24	9	18		696-29-7
ISOPROPYLCYCLOPENTANE	112.21	8	16		3875-51-2
ISOPULEGONE (5-METHYL-2-(1-METHYLETHENYL)-CYCLOHEXANONE)	152.23	10	16	1	29606-79-9
ISOVALERALDEHYDE (3-METHYLBUTANAL)	86.13	5	10	1	590-86-3
LINALOOL	154.25	10	18	1	78-70-6
MALEIC ANHYDRIDE	98.06	4	2	3	108-31-6
MALIC ACID	134.09	4	6	5	6915-15-7
M-CRESOL (3-METHYL-BENZENOL)	108.14	7	8	1	108-39-4
MENTHOL	156.27	10	20	1	89-78-1
MENTHOL (RACEMIC)	156.27	10	20	1	15356-70-4
MESITYL OXIDE (2-METHYL-2-PENTEN-4-ONE)	98.14	6	10	1	141-79-7
METHOXY ACETONE	88.11	4	8	2	5878-19-3
METHOXYBENZENE; ANISOLE	108.14	7	8	1	100-66-3
METHOXYPROPANOL ACETATE	132.16	6	12	3	84540-57-8
METHYACRYLIC ACID	86.09	4	6	2	79-41-4
METHYL ACETATE	74.08	3	6	2	79-20-9
METHYL ACRYLATE	86.09	4	6	2	96-33-3
METHYL ALCOHOL	32.04	1	4	1	67-56-1
METHYL AMYL ACETATE (4-METHYL-2-PENTANOL ACETATE)	144.21	8	16	2	108-84-9
METHYL AMYL KETONE	114.19	7	14	1	110-43-0
METHYL BENZOATE	136.15	8	8	2	93-58-3
METHYL BUTYRATE	102.13	5	10	2	623-42-7
METHYL CARBITOL {2-(2-METHOXYETHOXY)ETHANOL} {DEGME}	120.15	5	12	3	111-77-3
METHYL CELLOSOLVE ACETATE	118.13	5	10	3	110-49-6
METHYL ETHYL KETONE (MEK) (2-BUTANONE)	72.11	4	8	1	78-93-3
METHYL FORMATE	60.05	2	4	2	107-31-3
METHYL GLYOXAL	72.06	3	4	2	78-98-8
METHYL ISOAMYL KETONE	114.19	7	14	1	110-12-3
METHYL ISOBUTYL KETONE	100.16	6	12	1	108-10-1
METHYL ISOBUTYRATE	102.13	5	10	2	547-63-7
METHYL ISOPROPYL CARBONATE	118.13	5	10	3	51729-83-0
METHYL ISOPROPYL KETONE	86.13	5	10	1	563-80-4
METHYL LACTATE	104.10	4	8	3	547-64-8
METHYL METHACRYLATE	100.12	5	8	2	80-62-6
METHYL N-BUTYL ETHER	88.15	5	12	1	628-28-4

Description	**Mwt**	**C**	**H**	**O**	**CAS**
METHYL N-BUTYL KETONE	100.16	6	12	1	591-78-6
METHYL PIVALATE	116.16	6	12	2	598-98-1
METHYL PROPIONATE	88.11	4	8	2	554-12-1
METHYL PROPYL KETONE (2-PENTANONE)	86.13	5	10	1	107-87-9
METHYL SALICYLATE (AN ESTER)	152.15	8	8	3	119-36-8
M-ETHYL STYRENE	132.20	10	12		7525-62-4
METHYL T-BUTYL ETHER (MTBE)	88.15	5	12	1	1634-04-4
METHYL T-BUTYL KETONE (PINACOLIN)	100.16	6	12	1	75-97-8
METHYLACETOPHENONE	134.18	9	10	1	26444-19-9
METHYLCYCLOHEXADIENE	94.15	7	10		30640-46-1
METHYLCYCLOHEXANE	98.19	7	14		108-87-2
METHYLCYCLOOCTANE	126.24	9	18		1502-38-1
METHYLCYCLOPENTADIENE	80.13	6	8		26519-91-5
METHYLCYCLOPENTANE	84.16	6	12		96-37-7
METHYLDIHYDRONAPHTHALENE	144.21	11	12		39292-53-0
METHYLETHYLPENTANOATE	144.21	8	16	2	
METHYLHEPTYNE (6-METHYL-2-HEPTYNE)	110.20	8	14		51065-64-6
METHYLINDENE	130.19	10	10		29036-25-7
METHYLPARABEN (4-HYDROXYBENZOIC ACID, METHYL ESTER)	152.15	8	8	3	99-76-3
M-ETHYLTOLUENE	120.19	9	12		620-14-4
METHYLVINYL KETONE	70.09	4	6	1	78-94-4
M-TOLUALDEHYDE	120.15	8	8	1	620-23-5
M-XYLENE	106.17	8	10		108-38-3
MYRCENE	136.23	10	16		123-35-3
NAPHTHOL	144.17	10	8	1	1321-67-1
NAPTHALENE	128.17	10	8		91-20-3
N-BUTANE	58.12	4	10		106-97-8
N-BUTYL ACETATE	116.16	6	12	2	123-86-4
N-BUTYL ACRYLATE	128.17	7	12	2	141-32-2
N-BUTYL ALCOHOL	74.12	4	10	1	71-36-3
N-BUTYL BENZOATE	178.23	11	14	2	136-60-7
N-BUTYL BUTYRATE	144.21	8	16	2	109-21-7
N-BUTYL FORMATE	102.13	5	10	2	592-84-7
N-BUTYLBENZENE	134.22	10	14		104-51-8
N-BUTYLCYCHOHEPTANE	154.29	11	22		
N-BUTYLCYCLOPENTANE	126.24	9	18		2040-95-1
N-DECANE	142.28	10	22		124-18-5
N-DECANOIC ACID	172.26	10	20	2	334-48-5
N-HEPTANE	100.20	7	16		142-82-5
N-HEPTANOIC ACID	130.18	7	14	2	111-14-8
N-HEPTYL ACETATE	158.24	9	18	2	112-06-1
N-HEXANE	86.18	6	14		110-54-3
N-HEXANOIC ACID	116.16	6	12	2	142-62-1
N-HEXYL ACETATE	144.21	8	16	2	142-92-7
N-NONANE	128.26	9	20		111-84-2
N-NONANOIC ACID	158.24	9	18	2	112-05-0

Description	**Mwt**	**C**	**H**	**O**	**CAS**
N-NONYL ACETATE	186.29	11	22	2	143-13-5
N-OCTANE	114.23	8	18		111-65-9
N-OCTANOIC ACID	144.21	8	16	2	124-07-2
N-OCTYL ACETATE	172.26	10	20	2	112-14-1
NONANAL	142.24	9	18	1	124-19-6
N-PENTANAL (N-VALERALDEHYDE)	86.13	5	10	1	110-62-3
N-PENTANE	72.15	5	12		109-66-0
N-PENTANOL	88.15	5	12	1	71-41-0
N-PENTYL PROPIONATE	144.21	8	16	2	624-54-4
N-PENTYLBENZENE	148.24	11	16		538-68-1
N-PENTYLCYCLOHEXANE	154.29	11	22		29949-27-7
N-PROPOXYPROPANOL	118.17	6	14	2	30136-13-1
N-PROPYL ALCOHOL	60.10	3	8	1	71-23-8
N-PROPYL BUTYRATE	130.18	7	14	2	105-66-8
N-PROPYL FORMATE	88.11	4	8	2	110-74-7
N-PROPYL PROPIONATE	116.16	6	12	2	106-36-5
N-PROPYLBENZENE	120.19	9	12		103-65-1
N-UNDECANE	156.31	11	24		1120-21-4
N-UNDECANOIC ACID	186.29	11	22	2	112-37-8
O-CRESOL (2-METHYL-BENZENOL)	108.14	7	8	1	95-48-7
OCTANAL	128.21	8	16	1	124-13-0
OCTANEDIOIC ACID	174.19	8	14	4	505-48-6
OCTYNE (1-OCTYNE)	110.20	8	14		32073-03-3
O-ETHYLTOLUENE	120.19	9	12		611-14-3
O-HYDROXYBENZALDEHYDE (SALICYLYLALDEHYDE)	122.12	7	6	2	
O-TOLUALDEHYDE	120.15	8	8	1	529-20-4
OXALIC ACID	90.03	2	2	4	144-62-7
O-XYLENE	106.17	8	10		95-47-6
P-CRESOL (4-METHYL-BENZENOL)	108.14	7	8	1	106-44-5
PENTAERYTHRITOL	136.15	5	12	4	115-77-5
PENTAMETHYLBENZENE	148.24	11	16		700-12-9
PENTANEDIOIC ACID, DIMETHYL ESTER (DIMETHYL GLUTARATE)	160.17	7	12	4	1119-40-0
PENTYL CYCLOHEXANE	154.29	11	22		4292-92-6
PENTYLCYCLOPENTANE	140.27	10	20		3741-00-2
PENTYLIDENECYCLOHEXANE	152.28	11	20		39546-79-7
PEROXYACETIC ACID	76.05	2	4	3	79-21-0
P-ETHYLTOLUENE	120.19	9	12		622-96-8
PHENOL (CARBOLIC ACID)	94.11	6	6	1	108-95-2
PHENOL, 2,6-DIMETHYL-	122.16	8	10	1	576-26-1
PHENOL, 2-METHOXY-4-(1-PROPENYL)-, (E)-; TRANS-ISOEUGENOL	174.28	10	22	2	
PHENOL, 2-METHOXY-4-PROPYL-	166.22	10	14	2	2785-87-7
PHENOL, 4-ETHYL-2-METHOXY-	152.19	9	12	2	2785-89-9
PHENYLACETIC ACID	136.15	8	8	2	103-82-2
PHTHALIC ANHYDRIDE	148.12	8	4	3	85-44-9
PIPERYLENE {1,3-PENTADIENE} (MIXED ISOMERS)	68.12	5	8		504-60-9

Description	**Mwt**	**C**	**H**	**O**	**CAS**
P-ISOBUTYL TOLUENE; 1-METHYL-4(2-METHYLPROPYL) BENZENE	148.24	11	16		5161-04-6
POLYPROPYLENE GLYCOL	76.09	3	8	2	25322-69-4
PROPANE	44.10	3	8		74-98-6
PROPENYLCYCLOHEXANE	124.22	9	16		5364-83-0
PROPIONALDEHYDE	58.08	3	6	1	123-38-6
PROPIONIC ACID	74.08	3	6	2	79-09-4
PROPYL ACETATE	102.13	5	10	2	109-60-4
PROPYLCYCLOHEXANE	126.24	9	18		1678-92-8
PROPYLCYCLOPENTANE	112.21	8	16		2040-96-2
PROPYLENE	42.08	3	6		115-07-1
PROPYLENE CARBONATE	102.09	4	6	3	108-32-7
PROPYLENE GLYCOL	76.09	3	8	2	57-55-6
PROPYLENE GLYCOL BUTYL ETHER {1-BUTOXY-2-PROPANOL}	132.20	7	16	2	5131-66-8
PROPYLENE GLYCOL METHYL ETHER {1-METHOXY-2-PROPANOL}	90.12	4	10	2	107-98-2
PROPYLENE GLYCOL MONOMETHYL ETHER ACETATE {2-(1-METHOXY)PROPYL ACETATE}	132.16	6	12	3	108-65-6
PROPYLENE GLYCOL N-PROPYL ETHER	118.17	6	14	2	1569-01-3
PROPYLENE GLYCOL PHENYL ETHER (2-PHENOXY-1-PROPANOL)	152.19	9	12	2	4169-04-4
PROPYLENE OXIDE	58.08	3	6	1	75-56-9
PROPYLENEGLYCOL-T-BUTYLETHER{1-(1,1,-DIMETHYLETHOXY)-2-PROPANOL}	132.20	7	16	2	57018-52-7
PROPYLPARABEN	180.20	10	12	3	94-13-3
P-TOLUALDEHYDE {4-METHYLBENZALDEHYDE}	120.15	8	8	1	104-87-0
P-XYLENE	106.17	8	10		106-42-3
PYRUVIC ACID	88.06	3	4	3	127-17-3
RESORCINOL	110.11	6	6	2	108-46-3
SABINENE	136.23	10	16		3387-41-5
SAFROLE	162.19	10	10	2	94-59-7
S-BUTYL ACETATE	116.16	6	12	2	105-46-4
SEC-BUTYL ALCOHOL	74.12	4	10	1	78-92-2
SEC-BUTYLCYCLOHEXANE	140.27	10	20		7058-01-7
S-PENTYLBENZENE	148.24	11	16		29316-05-0
STYRENE	104.15	8	8		100-42-5
SUCCINIC ACID-TMS	118.09	4	6	4	110-15-6
SYRINGALDEHYDE-TMS	182.17	9	10	4	134-96-3
SYRINGOL-TMS , ALSO NOTED AS "SYRGOL"	154.16	8	10	3	91-10-1
T-AMYLMETHYLETHER (TAME)	102.17	6	14	1	994-05-8
T-BUTYL ACETATE	116.16	6	12	2	540-88-5
T-BUTYLBENZENE	134.22	10	14		98-06-6
T-DECAHYDRONAPHTHALENE (TRANS-DECALIN)	138.25	10	18		493-02-7
TEREPHTHALIC ACID (P-BENZENEDICARBOXYLIC ACID)	166.13	8	6	4	100-21-0
TERPINENE	136.23	10	16		99-85-4
TERPINOLENE	136.23	10	16		586-62-9

Description	Mwt	C	H	O	CAS
TERT-BUTYL ALCOHOL	74.12	4	10	1	75-65-0
TETRAETHYLENE GLYCOL	194.23	8	18	5	112-60-7
TETRAHYDRO-2-FURANMETHANOL	102.13	5	10	2	97-99-4
TETRAHYDROFURAN	72.11	4	8	1	109-99-9
TETRAHYDROPYRAN	86.13	5	10	1	142-68-7
TETRALIN	132.20	10	12		119-64-2
TETRAMETHYLHEXANE	142.28	10	22		79004-85-6
TOLUENE	92.14	7	8		108-88-3
TRANS 1,2-DIETHYL CYCLOHEXANE	140.27	10	20		13990-95-9
TRANS 1,3-DIETHYL CYCLOHEXANE	140.27	10	20		13990-94-8
TRANS 1,3-HEXADIENE	82.14	6	10		
TRANS 1,3-NONADIENE	124.22	9	16		56700-77-7
TRANS 1,4-DIETHYL CYCLOHEXANE	140.27	10	20		13990-93-7
TRANS 1,4-HEXADIENE	82.14	6	10		
TRANS 1-METHYL-2-PROPYL CYCLOHEXANE	140.27	10	20		42806-77-9
TRANS 1-METHYL-3-PROPYL CYCLOHEXANE	140.27	10	20		34522-19-5
TRANS 1-METHYL-4-ETHYLCYCLOHEXANE	126.24	9	18		6236-88-0
TRANS 1-METHYL-4-PROPYL CYCLOHEXANE	140.27	10	20		28352-42-3
TRANS 2,2-DIMETHYL 3-HEXENE	112.21	8	16		690-93-7
TRANS 2,5-DIMETHYL 3-HEXENE	112.21	8	16		692-70-6
TRANS 4,4-DIMETHYL-2-PENTENE	98.19	7	14		690-08-4
TRANS 4-METHYL-2-NONENE	140.27	10	20		121941-01-3
TRANS OCTAHYDRO INDENE	124.22	9	16		3296-50-2
TRANS, TRANS-2,4-HEPTADIENAL	110.15	7	10	1	4313-03-5
TRANS,CIS-1,2,4-TRIMETHYLCYCLOHEXANE	126.24	9	18		7667-60-9
TRANS,TRANS-1,2,4-TRIMETHYLCYCLOHEXANE	126.24	9	18		1678-80-4
TRANS,TRANS-1,3,5-TRIMETHYLCYCLOHEXANE	126.24	9	18		1795-26-2
TRANS,TRANS-2,4-HEXADIENE	82.14	6	10		5194-51-4
TRANS-1,2,3,4-TETRAMETHYL-1-CYCLOBUTENE	110.20	8	14		3200-65-5
TRANS-1,2-CIS-4-TRIMETHYLCYCLOPENTANE	112.21	8	16		4850-28-6
TRANS-1,2-DIMETHYLCYCLOHEXANE	112.21	8	16		6876-23-9
TRANS-1,3-DIMETHYLCYCLOHEXANE	112.21	8	16		2207-03-6
TRANS-1,3-DIMETHYLCYCLOPENTANE	98.19	7	14		1759-58-6
TRANS-1,3-PENTADIENE	68.12	5	8		2004-70-8
TRANS-1,4-DIMETHYLCYCLOHEXANE	112.21	8	16		2207-04-7
TRANS-1,CIS-2,3-TRIMETHYLCYCLOPENTANE	112.21	8	16		
TRANS-1,METHYL-2N-PROPYLCYCLOHEXANE	140.27	10	20		4291-79-6
TRANS-1-2-DIMETHYLCYCLOPENTANE	98.19	7	14		822-50-4
TRANS-1-ETHYL-2-METHYLCYCLOHEXANE	126.24	9	18		4923-78-8
TRANS-1-ETHYL-3-METHYLCYCLOHEXANE	126.24	9	18		4926-76-5
TRANS-1-METHYL-3-ETHYLCYCLOPENTANE	112.21	8	16		2613-65-2
TRANS-1-PHENYL-1-PENTENE	146.23	11	14		16002-93-0

Description	Mwt	C	H	O	CAS
TRANS-1-PHENYLBUTENE	132.20	10	12		133753-32-9
TRANS-2,2,5,5-TETRAMETHYL-3-HEXENE	140.27	10	20		692-48-8
TRANS-2,2-DIMETHYL-3-HEPTENE	126.24	9	18		
TRANS-2-BUTENE	56.11	4	8		624-64-6
TRANS-2-DECENAL	154.25	10	18	1	3913-71-1
TRANS-2-ETHYLMETHYLCYCLOPENTANE	112.21	8	16		930-90-5
TRANS-2-HEPTENE	98.19	7	14		14686-13-6
TRANS-2-HEXENAL	98.14	6	10	1	6728-26-3
TRANS-2-HEXENE	84.16	6	12		4050-45-7
TRANS-2-METHYL-3-OCTENE	126.24	9	18		52937-36-7
TRANS-2-NONENE	126.24	9	18		6434-78-2
TRANS-2-OCTENE	112.21	8	16		13389-42-9
TRANS-2-PENTENE	70.13	5	10		646-04-8
TRANS-3-HEPTENE	98.19	7	14		14686-14-7
TRANS-3-HEXENE	84.16	6	12		13269-52-8
TRANS-3-NONENE	126.24	9	18		20063-92-7
TRANS-3-OCTENE	112.21	8	16		14919-01-8
TRANS-4-DECENE	140.27	10	20		19398-89-1
TRANS-4-ETHYL-2-OCTENE	140.27	10	20		74630-09-4
TRANS-4-METHYL-2-DECENE	154.29	11	22		101823-01-2
TRANS-4-NONENE	126.24	9	18		10405-85-3
TRANS-4-OCTENE	112.21	8	16		14850-23-8
TRANS-5-UNDECENE	154.29	11	22		764-97-6
TRIETHYLENE GLYCOL	150.17	6	14	4	112-27-6
TRIETHYLENE GLYCOL MONOBUTYL ETHER	206.28	10	22	4	143-22-6
TRIMETHYLCYCLOHEXANOL	142.24	9	18	1	1321-60-4
TRIMETHYLENE OXIDE (1,3-EPOXYPROPANE)	58.08	3	6	1	503-30-0
TRIPROPYLENE GLYCOL	192.25	9	20	4	24800-44-0
TRIPROPYLENE GLYCOL MONOMETHYL ETHER ([2-(2-METHOXYMETHYLETHOXY)METHYLETHOXY]-PROPANOL)	206.28	10	22	4	25498-49-1
UNDECANAL	170.29	11	22	1	112-44-7
UNSPECIFIED C5 UNSATURATED CARBONYL ISOPRENE PRODUCT	100.12	5	8	2	
VANILLIN	152.15	8	8	3	121-33-5
VINYL ACETATE	86.09	4	6	2	108-05-4
VINYLACETYLENE	52.07	4	4		689-97-4