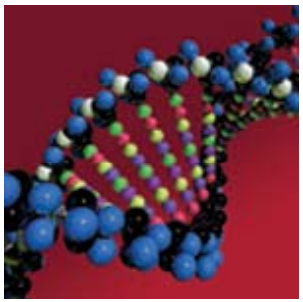
A Screening Method for Ozone Impacts of New Sources based on High-Order Sensitivity Analysis of CAMx Simulations for Sydney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  - http://www.environment.nsw.gov.au/

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Outline

- Motivation
- 3-D Modeling of new source ozone impacts
- Screening Tool
- Framework for evaluating ozone impacts
- Summary

Motivation

- The Sydney Greater Metropolitan Region exceeds applicable ozone standards
  - 1-hr average of 100 ppb
  - 4-hr average of 80 ppb
- Need methods to quantify ozone impacts of proposed new sources
  - Photochemical grid modeling is scientifically rigorous but resource intensive
  - Need a technically sound screening tool to efficiently evaluate which new sources require photochemical grid modeling
- Need a framework to evaluate when ozone impacts are significant

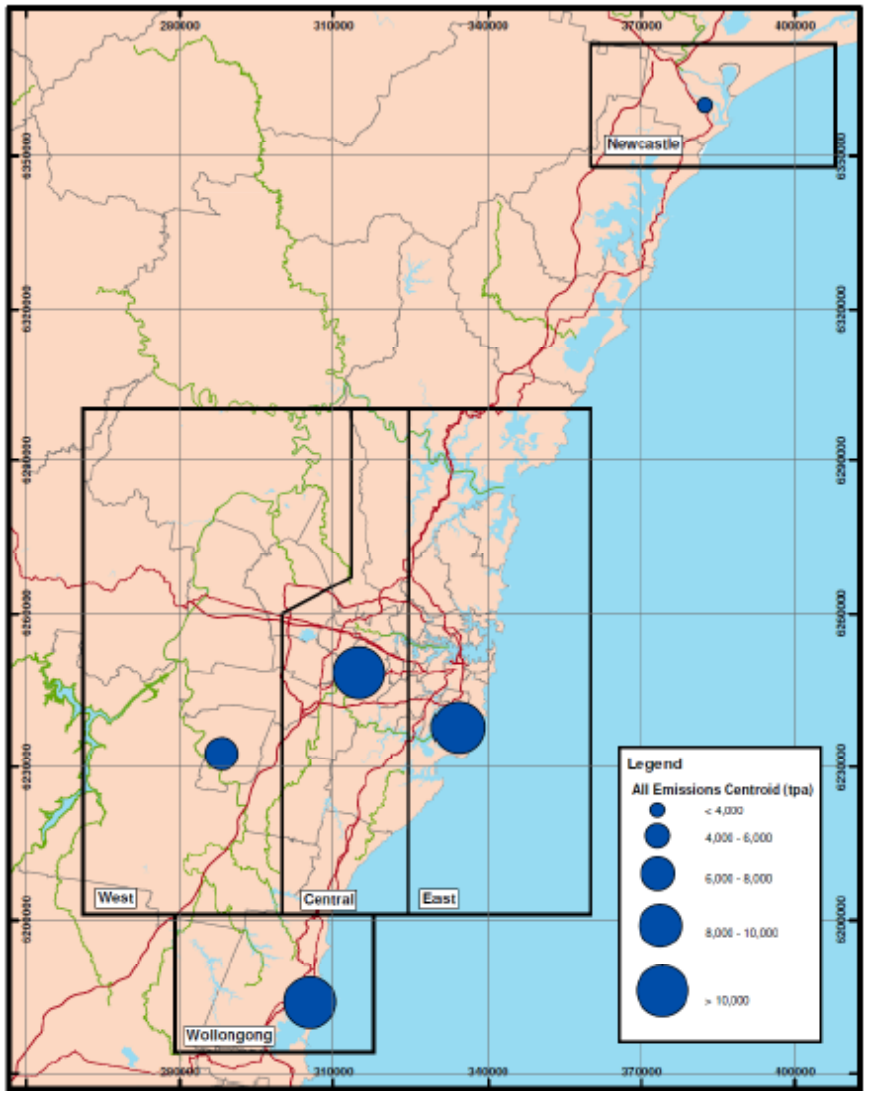
Overview of Methodology

- Reviewed literature to identify defensible methods
  - Photochemical grid modeling
- Model several prototypical new sources using a photochemical grid model (CAMx) for Sydney
- Use a sensitivity method (HDDM) in CAMx to develop a parametric model of the prototypical source impacts
  - O_3 impact = f(NO_X emissions, VOC emissions, source location)
- Implement the parametric model in a screening tool (spreadsheet) that can extend results for prototypical sources to any new source
  - Screening Tool
- Develop criteria to evaluate impacts using a tiered approach
  - Level 1 – screening tool sufficient for sources with "small" impact
  - Level 2 – photochemical modeling required for sources with "large" impact

CAMx Model Application for Sydney GMR

- Domain
  - 3 km grid (70 by 90)
  - 25 levels to 8,000m
- Episodes
  - Two summer periods
    - Dec 2003 / Jan 2004
    - Dec 2003 / Jan 2004
- CAMx version 5.3
  - CB05 chemistry
- Meteorology
  - TAPM prognostic model
- Emissions
  - OEH anthropogenic
  - MEGAN biogenic
- Boundary conditions
  - MOZART4

Prototypical “new sources”



- Locations and magnitude based on analysis of existing sources
- 5 locations selected
  - Newcastle
  - Sydney East, Central, West
  - Wollongong
- Each 500 tonnes/annum
  - VOC + NO_X combined
  - VOC/ NO_X ratio of 1.24
- Stack parameters that produce minimal plume rise for maximum impact

Parametric model using HDDM sensitivity

- The high-order decoupled direct method (HDDM) computes O_3 sensitivity to selected emissions within CAMx
  - Computes first and second order derivatives

- Taylor series describes source impact (ΔO_3)

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

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

Evaluating the HDDM parametric model

- Compare source impacts by the DDM parametric model to brute force differences

  – DDM parametric model impact

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

  – Brute force impact

    O_3 with new source – base case O_3 without source

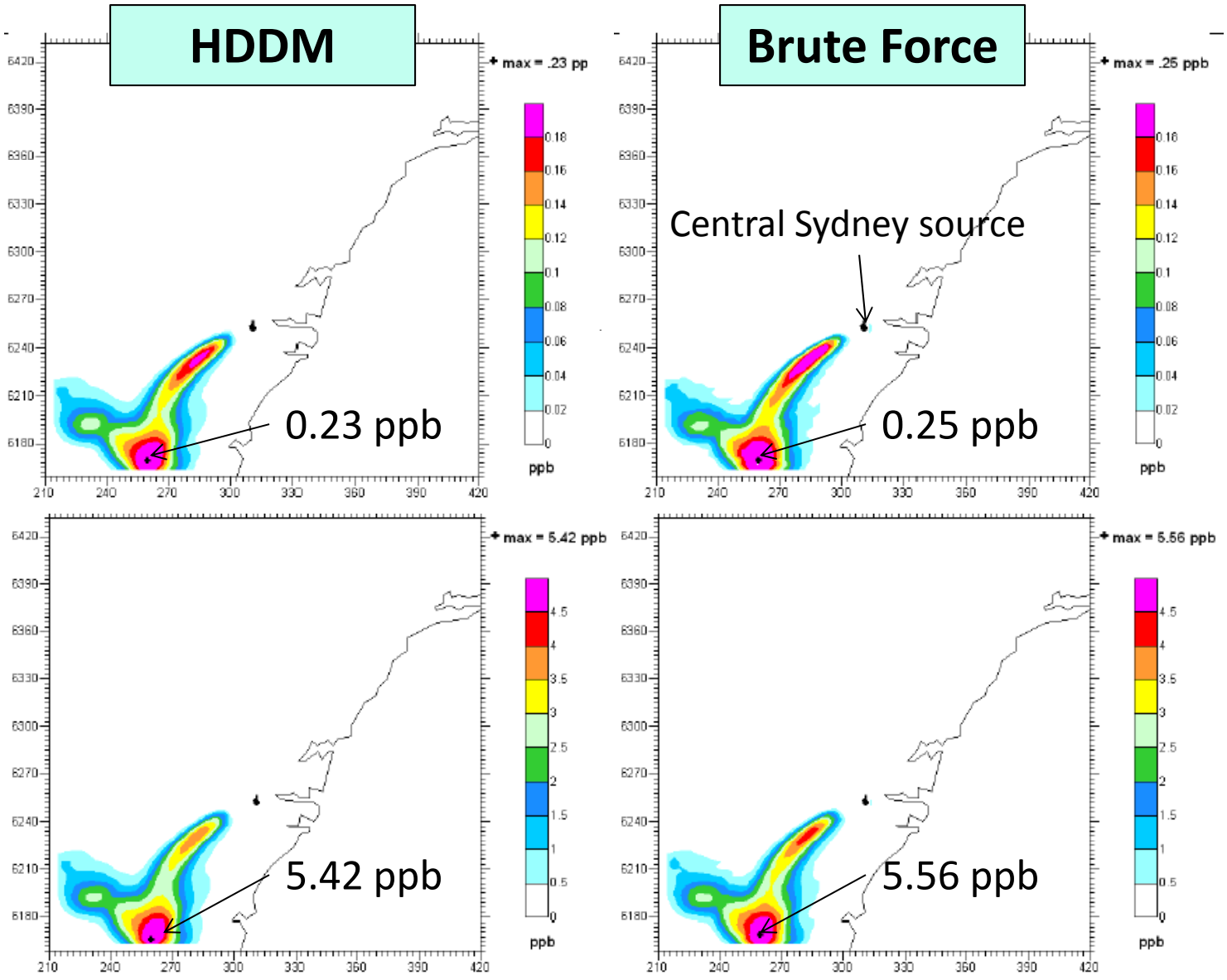
Evaluation: Location of source impacts

500 Tonnes/yr

Source used to develop method

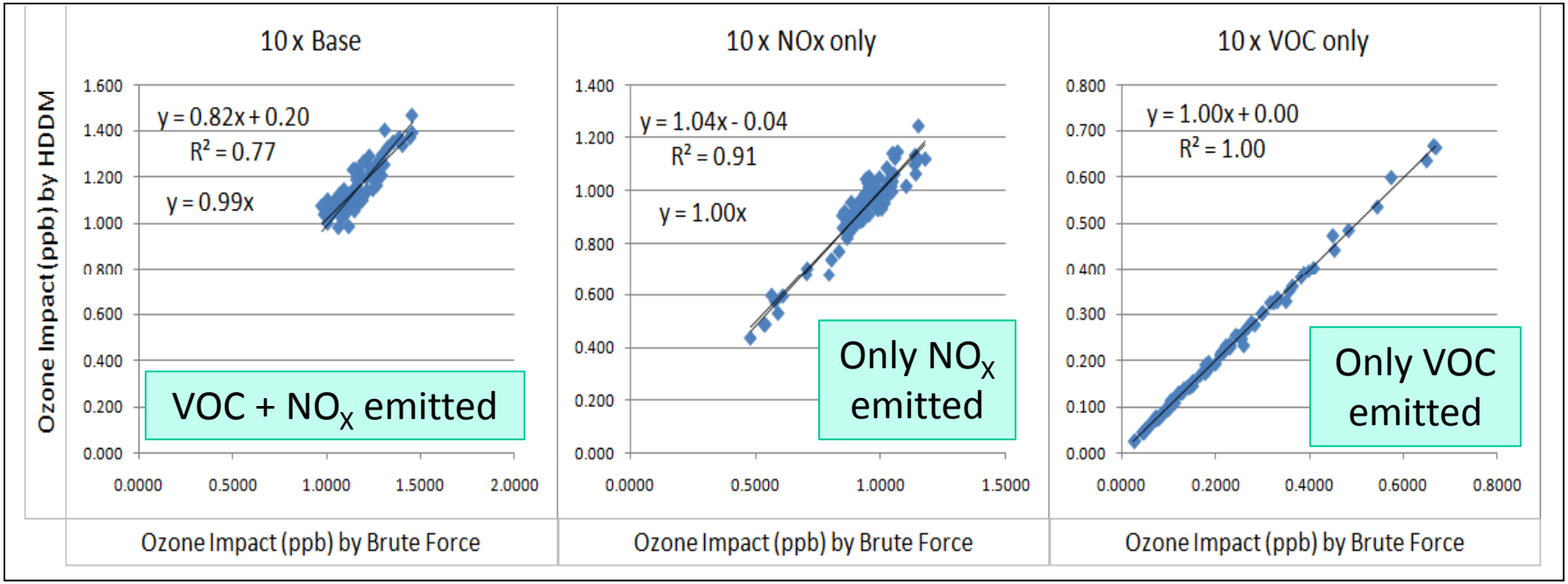
12,500 Tonnes/yr

25 x larger source



Evaluation: Different source VOC/NO_X ratios

- Scatter plot the brute force vs. HDDM result for 300 grid cells with the greatest O_3 impact
  - 5000 tonne/yr source in Central Sydney emitting VOC + NO_X, VOC only and NO_X only
- Very good agreement even when VOC/ NO_X ratio is changed
  - Screening tool accurately describes non-linearity in O_3 formation
  - Good accuracy for sources 25 x larger used to develop the method
  - Used to set upper bound on range of applicability



Criteria for Evaluating Ozone Impacts

- Factors to consider
  - Magnitude of source impact
  - Source located in O_3 attainment or nonattainment area
  - In all cases, sources must satisfy other regulator requirements

- Criteria established (not yet final)
  - Significant Impact Level (**SIL**)

    Source impact below 0.5 ppb not measureable ➔ level 1 analysis is sufficient

  - Maximum Allowable Impact (**MAI**)

    MAI = 1 ppb for nonattainment areas

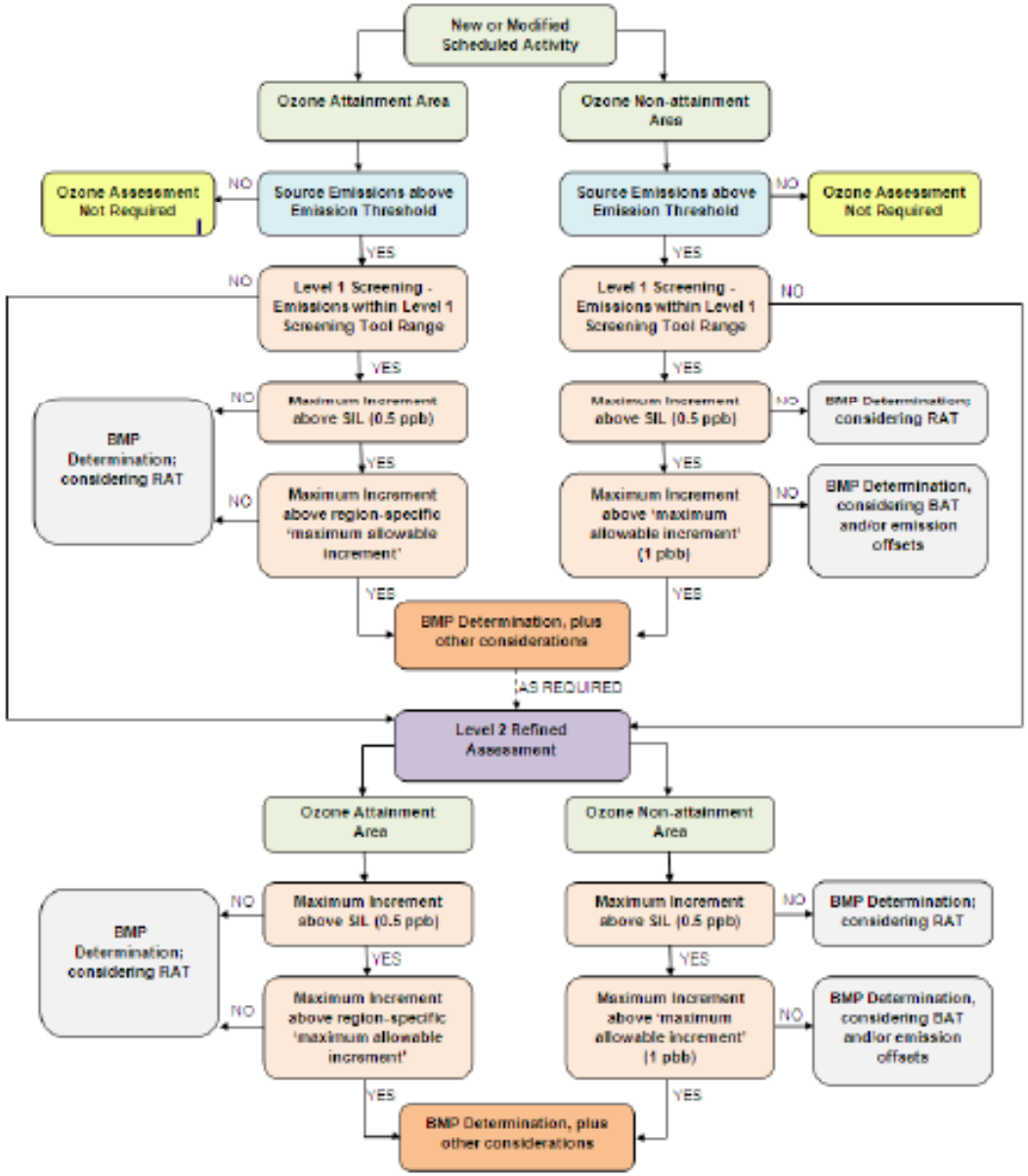
    For attainment areas, MAI = 25% of the difference between measured maximum O_3 and the level of the standard

    e.g. standard = 80 ppb; measured max O_3 = 60 ppb; MAI = 5 ppb

    Source impact below MAI ➔ level 1 analysis is sufficient

Criteria for Evaluating Ozone Impacts

Flow chart to guide source proponents through the evaluation



Level 1: Use Screening Tool

Level 2: Use a model like CAMx

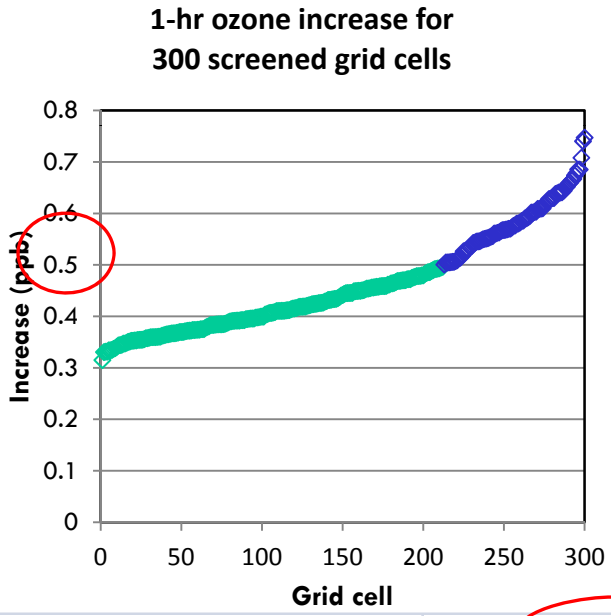
Screening Tool: Spreadsheet Macro

Source data input

Source Region	Newcastle
VOC Input Option	Default VOC Reactivities
CH4 (tonnes/day)	0.000000
CO (tonnes/day)	0.000000
NOx (tonnes/day)	1.000000
VOC (tonnes/day)	1.000000

Calculate O3 Impacts

Ozone impacts compared to SIL



Maximum 1-hr Incremental	0.74735	ppb

Maximum Allowable Impact (MAI) for source location

Location		
Source Location	Newcastle	
Baseline Ozone (1-hr)	68.8	ppb
Baseline Ozone (4-hr)	62.4	ppb
Region Classification	Attainment	
Maximum Allowable Increment (1-hr)	7.8	ppb
Maximum Allowable Increment (4-hr)	4.4	ppb
Ozone Standard (1-hr)	100	ppb
Ozone Standard (4-hr)	80	ppb

Compare maximum impact to the MAI

Screening Tool: VOC Speciation

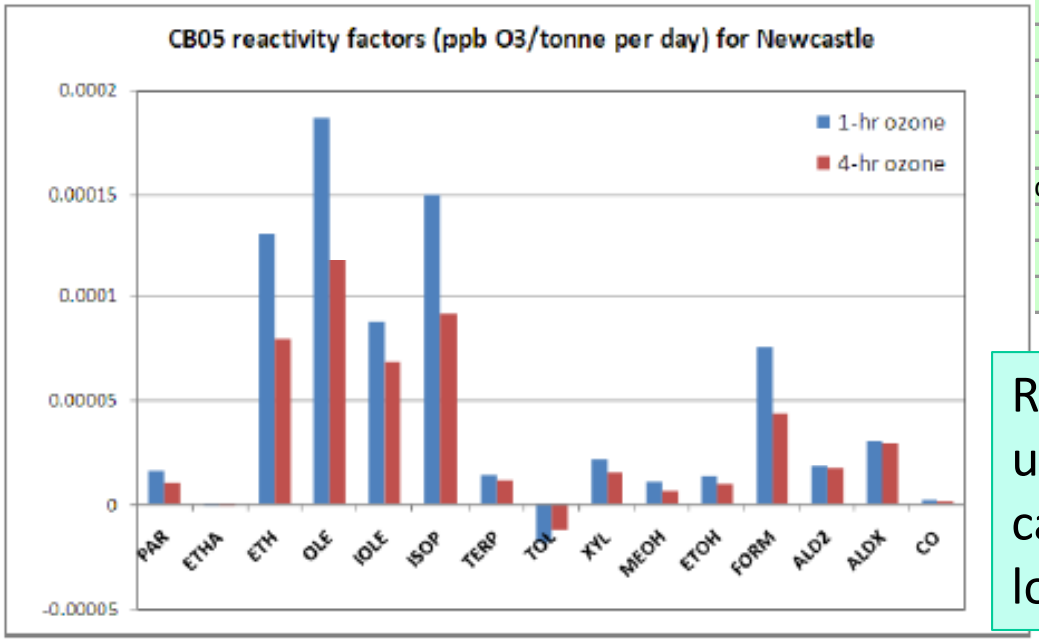
Option to input source-specific VOC

Source Region	Newcastle
VOC Input Option	User Specified Emissions
CH4 (tonnes/day)	0.000000
CO (tonnes/day)	1.000000
NOx (tonnes/day)	1.000000
VOC (tonnes/day)	1.000000

Calculate O3 Impacts

User Specified Emissions: Input VOC list

Description	Mwt	C	H	O	CAS	tonnes/day
formaldehyde	30.03	1	2	1	50-00-0	
formic acid	46.03	1	2	2	64-18-6	
methyl alcohol	32.04	1	4	1	67-56-1	
acetylene	26.04	2	2		74-86-2	
glyoxal	58.04	2	2	2	107-22-2	
Glyoxylic Acid	74.04	2	2	3	298-12-4	
oxalic acid	90.03	2	2	4	144-62-7	
ethylene	28.05	2	4		74-85-1	
	44.05	2	4	1	75-07-0	
	44.05	2	4	1	75-21-8	
	60.05	2	4	2	64-19-7	
	60.05	2	4	2	107-31-3	
	76.05	2	4	3	79-21-0	
d}	76.05	2	4	3	79-14-1	
	30.07	2	6		74-84-0	
	46.07	2	6	1	64-17-5	
	46.07	2	6	1	115-10-6	



Reactivity adjustment applied using VOC reactivity factors calculated for each source location using HDDM

Summary

- An efficient screening method developed
  - Scientifically defensible and robust
  - Defined range of applicability
  - Suitable for “smaller” sources
  - Use to focus resources on sources that require more detailed evaluation
- This method could be applied in other regions
  - Parameters in the screening tool are location specific and would need to be re-derived
  - Develop parameters for new location using a photochemical grid model
- Evaluation framework developed
  - In tune with local ozone standards and regulatory practices
    - Not yet finalized
  - Concepts could be adapted for new locations and jurisdictions