

Location-Specific Sustainability Metrics for Hydrogen Energy Systems

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Statement of Originality

Declaration

I declare that the work presented in this thesis is, to the best of my knowledge and belief, original and my own work, except as acknowledged in the text, and that the material has not been submitted, in whole or in part, for a degree at this or any other university.

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List of Publications and Presentations

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Publications by the Candidate Relevant to the Thesis but not Forming Part of it

1. Hydrogen Economy Options for Australia, McLellan, B.C., Diniz da Costa, J.C., Dicks, A.L., Rudolph, V., Pagan, R.J., Wall, T.F., 2003 National Environment Conference, Environmental Engineering Society, Brisbane, 18-20 July 2003 pp105-110
2. Hydrogen Economy Options for Australia, McLellan, B.C., Diniz da Costa, J.C., Dicks, A.L., Rudolph, V., Pagan, R.J., Wall, T.F., Developments in Chemical Engineering and Minerals Processing Journal, 12 (5-6), pp447-460, 2004.
3. Hydrogen from Coal: A Pathway for the Future, McLellan, B.C., Dicks, A.L., Diniz da Costa, J.C., CCSD Report, June 2003.
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Abstract

The aim of the current work is twofold – it seeks to complete the knowledge gaps in relation to sustainability assessment of hydrogen energy systems in Australia, but in doing so, a new methodology of sustainability metrics assessment incorporating location-specific environmental factors by way of an emissions transport model is developed.

The major contributions of this research are:

1. Validation of the hypothesis of environment-dependent sustainability with a process model for environment-industrial interaction and the unique use of long-term historical data from an isolated Australian power station.
2. A novel sustainability metrics model which assesses the deviation due to the plant against the environment's carrying capacity, based on site-specific environmental signatures and process emissions.
3. Determining the sustainability metrics in terms of soil acidification for coal gasification, natural gas steam reforming and conventional coal electricity powered electrolysis, in the context of providing hydrogen to Brisbane, Australia.

These contributions are achieved by:

1. Determining the Fuel Cycle Inventory of emissions and inputs of the selected hydrogen production technologies;
2. Development of a methodology of sustainability assessment that incorporates local environmental limitations;
3. Development of a process model for environmental transmission of contaminants to provide the basis for the sustainability metrics;
4. Validation and proof of the model with historical data (intermittent years from 1983 to 1987 and 2006) from Tarong power station;
5. Incorporation of this model in the sustainability metrics and application of these metrics to the selected hydrogen production processes.

It is found that the emissions transport model (ETM), incorporating atmospheric and hydraulic transport is able to be validated with historical data, providing an accurate model of the soil sulphur concentrations at sites around the Tarong power station. The availability of historical data of the kind used in this validation for such an isolated pollutant source, which can be claimed to be the only contributor to local emissions, is very limited, thus offering a unique opportunity in terms of developing an accurate ETM. It is shown that the assumption made in current methodologies, that the load of emissions can be used as the only indicator of sustainability is false. This work shows that for soil acidification impacts, environmental dispersion and sensitivity is a non-linear process, and that the specific environment in which a plant is located is particularly important to the overall sustainability.

The validated ETM is then used as the basis for the development of a set of sustainability metrics (SM) that incorporate local environmental transport, sensitivity and limitations. The new SM model is applied to the selected hydrogen production technologies, and the model is shown to vary significantly in its output from the current methodologies. In particular, the incorporation of “critical loads” to give the environmental susceptibility to acidification gives the SM model the ability to measure sustainability in an absolute, rather than relative, sense. The spatial and temporal variability of sustainability is shown, and contours of sustainability, highlighting “hot spots” of low sustainability are produced.

Further work is recommended to expand the scope of hydrogen systems examined and the number of sustainability impacts assessed.

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List of Abbreviations

B	– “Baseline” – the ambient concentration of a compound in the environment
CC	– “Carrying Capacity”, “Buffering Capacity” – the allowable level of a compound in the environment, beyond which excessive damage will occur
CCSD	– Cooperative Research Centre for Coal in Sustainable Development
DEH	– Department of the Environment and Heritage
EB	– Environmental Burden
EIA	– Environmental Impact Assessment
EPA	– Environmental Protection Agency
ETM	– Emissions Transport Model
ExternE	– Externalities of Energy program in the EU
FCI	– Fuel Cycle Inventory
GHG	– Greenhouse Gases
ICHEME	– the Institution of Chemical Engineers
LCIA	– Life Cycle Impact Assessment
NO _x	– Generic term for Oxides of Nitrogen
NPI	– National Pollutant Inventory
PM ₁₀	– Particulate matter less than 10 microns in diameter
RAINS-ASIA	– Regional Air Pollution Information and Simulation (Asia)
SM	– Sustainability Metrics
SO _x	– Generic term for Oxides of Sulphur
TRACI	– Tool for the Reduction and Assessment of Chemical and other environmental Impacts
TVOCs	– Total Volatile Organic Compounds

Chapter 1

Introduction

1.1 Background

Increasingly in recent decades, society has come to realise clearly, the existence of causal relationships between pollutant emissions from human activity, and the health of both humans and the natural environment. In particular, recognition of global warming, acid rain and smog in connection with the emissions from fossil fuels use in stationary electricity and transport has lead to regulation and research into how to ameliorate the situation. Modern society is energy-intensive, and demand for energy is predicted to rise rather than decline in the coming decades (EIA, 2006; Azar, 2003; IEA, 2004). The energy sector is an essential area of human endeavour, and is also the largest emitter of Greenhouse Gases (GHG's) and acidifying compounds (NO_x and SO_x) in most areas (NPI, 2005), thus it is vitally important to reduce the environmental impacts of this industry.

From the extensive research into the options for reducing human GHG and local pollutant emissions from stationary energy and transportation applications, the “Hydrogen Economy” is emerging as one of the current frontrunners. The hydrogen economy, with its fuel-cell-driven vehicles emitting only water, offers the potential to eliminate local pollutants in cities, and drastically reduce, if not eliminate, the emissions of GHG's from electricity production if coupled with carbon capture and storage. To achieve this Eutopia, billions of research dollars are being spent in the US (USDOE, 2006), Europe (HFP, 2005) and Japan (Takahara, 2005) in particular, developing fuel cell and hydrogen production technology.

However, amid the hype and hope of Hydrogen, it is also seen to be increasingly important to assess the potential impacts of any such development in regards to the human, natural and economic environment. From past bitter experience of human short-sightedness when introducing new scientific developments to deal with

problems (perceived or real), it is obvious that, although we have twenty-twenty hindsight, our foresight has been rather limited through lack of knowledge, patience or breadth of vision. Then, how can these emerging technologies be assessed? How can their long-term impacts be determined, and how can we ascertain the level of impact that is acceptable? What does “acceptable” in fact mean? These questions lead us to the science of sustainability.

Sustainable development has been defined famously by Brundtland (1987) as development that "meets the needs of the present without compromising the ability of future generations to meet their own needs". This is a very broad statement, which leaves much room for interpretation, but also allows maximum applicability. In terms of the current question of the hydrogen economy, this statement may be translated as: *“How do we produce enough energy to fuel society’s needs now and on into the future without diminishing the ability to produce all further energy requirements or destroying the quality of life and environment currently experienced?”*. However, even with this more specific translation, we still come to the question of how we know if the chosen technology or process is actually leading us down a sustainable path? Also, in the case of the hydrogen economy, where there are various methods of producing and utilising hydrogen, which is the most sustainable? This is where measurement of sustainability becomes vital, which is the focus and importance of the current work.

In modern sustainability science, it is common to utilise a “triple bottom line” approach – incorporating environmental, economic and social factors into the aforementioned statement of Brundtland. In the ultimate analysis, the economy is heavily reliant on the environmental and social factors – costs rise and fall in direct response to consumer attitudes and physical realities of the environment. The economy is an element of modern civilisation that has no actual physical or tangible existence, and relies purely on theoretical definitions for measurements of its quality. In contrast, the environment, whilst complex, consists of physical realities that may be assessed, and which cannot be returned to their original state by simple redefinition of parameters. Likewise, although difficult to quantify, social factors such as quality of life which depend on health parameters, are quantifiable, and rely strictly on physical realities. In particular, when attempting to predict long-term sustainability, the

influences of political policy changes in response to public perception or actual environmental degradation are impossible to account for, so that all estimates must essentially be based on supposition. In an attempt to remain as close to the predictable realities, it is thus most effective to reduce the scope of sustainability to those measurable, physical aspects of environmental and social health.

Figure 1 depicts the concept of sustainability, as it is commonly conceived. Many species emitted by industrial sources also exist naturally in the environment (though typically at lower concentrations). Thus there can be said to be an environmental “baseline” level, from which the process causes a deviation (either decreasing or increasing from the background level). Diurnal, seasonal, locational and annual variation of environmental characteristics can make the baseline very difficult to quantify. Environmental resilience, or carrying capacity, is the ability of the environment to accept variations from the baseline without causing degradation of environmental quality. Until this carrying capacity is breached, the environmental impact will be minimal. Thus the sustainability of a new industrial process is dependent upon whether or not the ensuing impact or emission disturbs the environment beyond its carrying capacity.

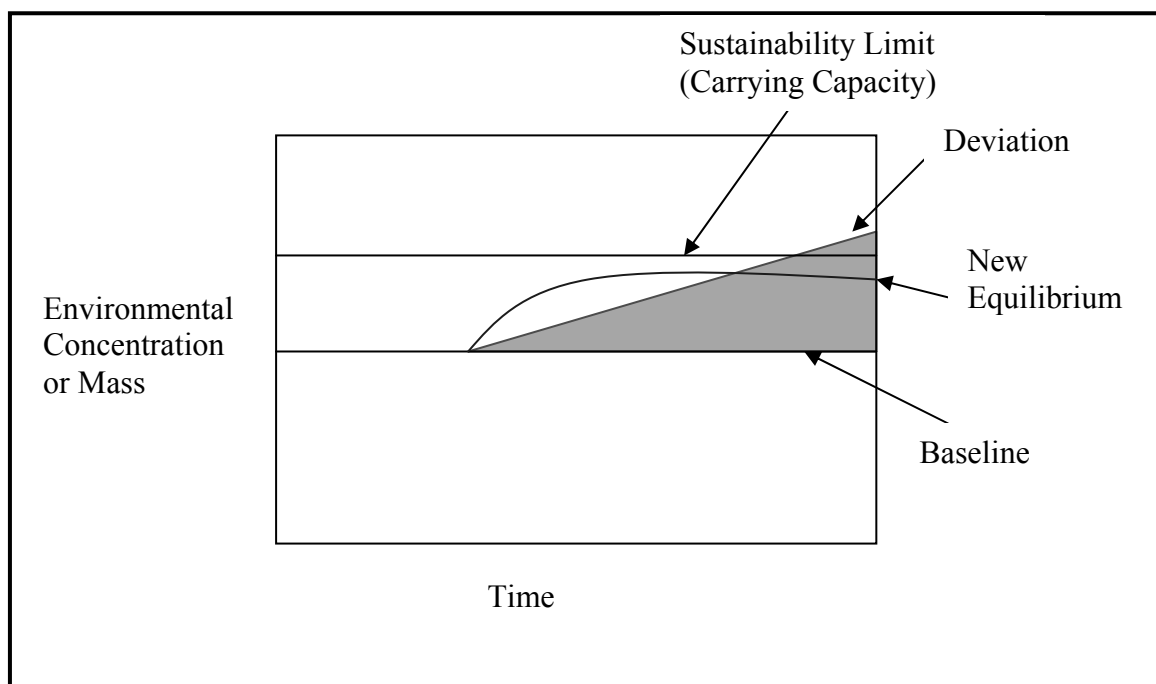


Figure 1: Conceptual Description of Sustainability

1.2 Scope

It is a complex exercise to ascertain the point at which the carrying capacity is breached for a particular environment. This is the major focus of the current work, coupled with the issue of how best to measure ecological sustainability (hereafter *sustainability*) of hydrogen energy systems.

After a preliminary review of the available options for hydrogen energy systems (McLellan, 2003; McLellan, 2004) it was concluded that the most likely near-term opportunities for an Australian hydrogen economy would be in the production of hydrogen from coal or natural gas. These options also offer the most scope in terms of the operational cycle impacts for sustainability assessment, and hence were ideal for the current work.

In any environment, there are natural processes occurring at any time, in tandem with direct and synergistic impacts deriving from human activities. The intention of sustainability assessment or any general environmental impact assessment, is to separate the natural from the anthropogenic emissions and subsequent effects. In many industrialised nations, the complexity of this exercise is enormous, as in any environment of concern there is a large matrix of emissions from a multitude of industries. However, in many regions of Australia, power generation is the major industry, if not the only industry in a single catchment area or airshed. This offers a significant opportunity to use the energy generation industry in Australia as a base line for gauging the sustainability of a developing hydrogen economy – particularly if the fossil fuel routes are followed.

1.3 Contribution to Knowledge

The most important novel features of this work are the development of a set of sustainability metrics that incorporates location-specific environmental parameters, and the subsequent validation and application of these metrics. The metrics are developed based on 3 fundamental stages:

6. Development of a process model for environmental transmission of contaminants;

7. Validation and proof of the model with historical data (intermittent years from 1983 to 1987 and 2006) from Tarong power station;
8. Incorporation of this model in a system of sustainability metrics and application of these metrics to selected hydrogen production processes.

The resulting contributions to knowledge are:

4. Validation of the hypothesis of environment-dependent sustainability with a process model for environment-industrial interaction and the unique use of long-term historical data from an isolated Australian power station.
5. A novel sustainability metrics model which assesses the deviation due to the plant against the environment's carrying capacity, based on site-specific environmental signatures and process emissions.
6. Determining the sustainability metrics in terms of soil acidification for a number of hydrogen production technologies in the context of providing hydrogen to Brisbane, Australia.

1.4 Structure of the Thesis

The structure of this document was aimed to allow the reader to follow logically through the thought processes behind the development and implementation of the current sustainability methodology. The proceeding chapters are as follows:

Chapter 2 - Literature Review

This chapter contains a description and appraisal of the current state-of-play of sustainability assessment and hydrogen energy systems, from which an appropriate basis and direction for the sustainability assessment was obtained. This examination shows significant gaps in knowledge in both areas of interest – in particular in the relation of sustainability metrics to the environment, and the sustainability of Hydrogen energy systems.

Chapter 3 - Methodology

The methodological development is described, based on the direction and understanding of knowledge gaps provided in Chapter 2. Features of the assessment

methodology that are incorporated to overcome the shortcomings of previous methodologies are highlighted.

Chapter 4 - Fuel Cycle Inventory

The fuel cycle inventory (FCI) forms the basis for the sustainability assessment of hydrogen energy systems. This chapter describes the techniques used to develop the FCI for the selected hydrogen production technologies. The results of the FCI are assessed internally and against existing processes and studies.

Chapter 5 - Model Description

Based on the methodology described in Chapter 3, a model is developed that overcomes the shortfalls of previous models for sustainability. This sustainability model is described, with a detailed explanation of the model development, equations and assumptions. Further, this chapter highlights the way in which the current model fills gaps in knowledge.

Chapter 6 - Model Validation

Without validation, the model would remain a theoretical methodology which could only be debated in terms of its inherent philosophy and mathematical fundamentals. This chapter presents an assessment and validation of the model as a reflection of real-world processes by comparison with historical data from an Australian power plant, which presents a globally unique opportunity.

Chapter 7 – Sustainability Metrics Scenario Analysis

The sustainability metrics model developed over the preceding chapters is applied to a number of selected hydrogen production technologies. Through this assessment and sensitivity analysis, the model is proven as a measure of sustainability, covering the inadequacies of previous methodologies. The model is also compared with existing methodologies of assessment.

Chapter 8 - Conclusions and Recommendations

The outcomes and contributions to knowledge of the project are summarised in this chapter. Suggestions for future developments in assessment of hydrogen technologies and sustainability models are raised.

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Chapter 2

Literature Review

2.1 Introduction

This chapter provides the essential footing for the current work, premised on the requirement to assess the sustainability of hydrogen energy systems as an example of potential solutions to global emissions from increasingly energy-intensive societies (Chapter 1). Thus the aim of this chapter is first to examine what work has been done in the field of sustainability assessment – identifying existing methodologies and especially any work that has been done on hydrogen energy systems. From these methodologies one must be chosen that most closely fits the needs of the assessment, or which may be developed to cover the inadequacies of previous work. This is followed by a brief review of the prevalent pathways for production and utilisation of hydrogen to identify the most applicable methods for the purpose of this assessment.

2.2 Approaches to Sustainability Assessment

As mentioned in Chapter 1, “sustainability” here has been taken to imply “ecological sustainability”, as the underlying foundation of both human social and economic systems is the natural environment. The literature in the field of sustainability and environmental impact is extensive, so this concise review has covered the relevant state of the field as it stands.

The science of sustainability, though broad in its applicability and philosophy, has consistently returned to the concept of indicators or metrics in an attempt to provide a yardstick to determine how closely the reality of a human impact fits with the ideal of sustainability. All of the various models of sustainability assessment that have been discussed in the literature fit into this category, although the approaches and specific metrics chosen have been slightly different – some indicators are qualitative, some

quantitative, some formed of a single number and some including vast sets of mathematical equations. However, they ultimately strive for the same goal – measuring sustainability, or as some might say – measuring the immeasurable (Bell and Morse, 1999).

Bossel (1999) appropriately sums up the matters of importance in the search for an appropriate set of indicators as “knowledge of what is important for the viability of the systems involved, and how that contributes to sustainable development”. It is also worth noting that the set of indicators should be the smallest allowable indicative set (neither too few to measure important factors, nor too vast a set to be practical). With these points in mind, the following sets of indicators are examined.

2.2.1 Parameters and Equations

Scientists and engineers prefer to quantify and model mathematically, where possible, the measures of any important parameter in the operation of a process plant or industrial operation. Likewise, when it comes to the concept of sustainability, many equations and system parameters have been derived in an attempt to provide general, quantifying measures of system performance.

In their work, Badin and Tagore (1997) described a method for energy pathway analysis with specific emphasis on hydrogen fuel cycles. This included the factors of:

1. capital and tax costs;
2. energy efficiency over the cycle; and,
3. environmental emissions as an overall output.

All of these factors are appropriate indicators, in themselves, of the performance of the plant, but they are directed at economic and technological as well as environmental impacts. When examining sustainability from the perspective of environmental sustainability, the first 3 indicators are unnecessary, whilst the final indicator, as an aggregate of all emissions, does not provide the necessary detail – especially when it is considered that there are a variety of environmental effects arising from the different emissions of a process.

Several researchers have used the concepts of “Net Energy Ratio” (Akai, Nomura et al., 1997) or “Integrated Energy Balance” (Matsuhashi and Ishitani, 1997) – the ratio of energy produced to energy expended – as shown in (Equation 1) - and Specific CO₂ emissions (Equation 2) (Akai, Nomura et al., 1997) to compare different fossil fuel power plant and sequestration options.

$$R = \frac{E_{out}}{E_{in}} = \frac{\varepsilon_o L}{\varepsilon_i + \varepsilon_{op} L} \quad [1]$$

$$C = \frac{[C_i + (C_{op} + C_g)L]}{\varepsilon_o L} \quad [2]$$

This limited set of equations is again, an under-specified set, but the specific emissions equation approach could be extended to include other pollutants. This approach is also appropriate for assessing technologies’ inherent qualities and allowing comparison, and could be easily adapted to hydrogen production. However, there are some queries as to whether a specific emissions figure is valid in terms of localised impacts, as the impact of the total mass load is often more important, and is hidden by using the specific emissions approach.

Matsuhashi and Ishitani (1997) also expanded their approach and derived an equation for determining sustainability limitations, which they applied to CO₂ removal options (Equation 3):

$$a + r + s - b + \frac{C_o c}{(1 - C_o)} \geq \frac{D_o}{\mu_o R_o} (1 - C_o) = \frac{P_o}{R_o} \quad [3]$$

To generalise, Equation 3 is a mass balance of existing (a), replacement (r), substituted (s) and recycled (C₀) resources, and demand for those resources (D₀), rate of increase of recycling (c) and demand (b). The final outcome is that when production is greater than resource availability, the system is unsustainable. A measurement of the sustainability of resource use based purely on mass flow is useful, but the incorporation of a variety of estimated factors such as “rate of resource substitution” and “rate of change of energy efficiency” which are highly unpredictable as they pre-empt future technological developments, is dubious in terms of accuracy.

A well-known expression or indicator of the environmental impact of a process or activity is the concept of the ecological footprint (Rees and Wackernagel, 1996) which calculates the equivalent area of land required to provide inputs and sinks for the process. This approach offers an interesting method of combining and comparing the impacts of an activity, and could be applied to the concept of sustainability in much the same way as other technology indicators. However, it also has the deficiency of being a single indicator (thus providing little indication of individual impacts), and does not include the important variables of time and distance. Variation or effect of impact over time is of crucial importance, as this is the determining factor of sustainability – if the indicator gives only a once-off impact, it is impossible to determine whether that impact will cause the process to be sustainable over a year, ten years or more into the future. The ecological footprint is also deficient in its lack of a measure of distance from the site in which the impact is occurring (i.e. – inputs can come from any part of the globe) whereas in reality it is vital to know where and when the impact is occurring, so that the true continuing effect can be determined.

2.2.2 Externalities

The method of measuring sustainability or ongoing environmental impact of a process or industry as a cost to be included in product pricing is the concept of Externalities. The cost of impacts is estimated from the cost to society of the various health and environmental impacts from emissions. This has been widely applied, with the most obvious ongoing application, the ExternE (Externalities of Energy) project of the European Union (EU, 1991). This approach suits modern policy makers, who tend to understand monetary equivalents more readily than other units.

Ogden, Williams et al. (2002) have also utilised economic equivalents to estimate the societal lifecycle costs of cars with alternative energy systems including hydrogen. They utilised values from the ExternE program and adapted these values to United States population densities. There is some concern as to whether or not this approach gives valid results, as many other factors are involved in health and environmental impacts – such as local climate, socio-economic and associated health factors (e.g. quality of diet). Ogden, Williams et al. (2002) calculate this Societal Life Cycle Cost

(LCC) in terms of the per vehicle costs for a variety of different energy systems (including hydrogen fuel cell vehicles) via Equation 4:

$$LCC = VFC + PVLC \quad [4]$$

Where LCC is the Life Cycle Cost of a vehicle (\$/vehicle), VFC is the initial expenditure on car purchase (\$/vehicle), and PVLC is the present value of the lifetime costs for fuel and maintenance, pollutant damages, greenhouse effects and oil supply insecurity costs. One difficulty with this method is the availability of data on the human health and pollution costs of the different emissions or even an entire industry sector – studies into this have been completed in the USA (Norris, 2003) and Europe (EU, 1991), but Australian data is unavailable (although attempts at modifying overseas data on human and ecotoxicity have been made (Lundie, Huijbregts et al., 2006)). In the complex industrial-environmental-social web, it is also very difficult to separate the impacts from a certain emitted species or emitter, hence the level of accuracy is called into question. As aforementioned, with all of the impacts rolled up into a single indicator, the weighting of different impacts is not obvious, such that important impacts may be hidden and thus policy development be affected.

The use of monetary equivalents is also potentially flawed in the increasingly global society, as the equivalent cost of locating an uncontrolled power plant in a developing country would most certainly be lower than locating the same plant within the bounds of a developed country although, especially in Eurasia, the two locations may not be particularly distant from each other. Utilising monetary equivalents would also require constant updating of costs, which is highly data-intensive.

2.2.3 Fundamental Principles Approaches

Much work has been done on developing methodologies for assessing sustainability from fundamental physical and chemical principles. In principle, these approaches would appear to be valid, but much of the meaning is lost in the “denaturalisation” of the objects and processes involved, leaving outcomes that are objective, perhaps, but not strictly relevant to the end-user.

A number of thermodynamic approaches have been applied to the concept of sustainability, including Exergy (Balocco, Papeschi et al., 2004) and Emergy (Brown, Odum et al., 2004) analyses. The concepts of emergy and exergy have also been applied to the concept of the “ecological footprint” (Zhao, Li et al., 2005). These approaches may have some validity in the expression of the theoretical energy flows within the environment, but they do not address environmental problems in explicit form (i.e. what happens when a certain emission enters the environment). Thus, a process may, in terms of energy flows, be declared sustainable, but may produce an emission that has highly detrimental effects on the surrounding human and environmental populations. In addition, the language and concepts of these analyses are not utilised among the common populace, thus the outcomes of such analyses convey little sensible information to those who must make decisions in matters of policy.

Another methodology is the HANPP “Human Appropriation of Net Products of Photosynthesis” model (Vitousek, Ehrlich et al., 1986). This model tries to quantify the amount of total “biologically fixed solar energy” that is utilised by humans. This method is limited in the inputs it utilises, but nonetheless offers some indication of sustainability of human activity. A further advancement of this theory is the “Material and Energy Flow Accounting” (MEFA) method, which provides an analysis of energy and mass flows in society and its interaction with nature (Haberl, Fischer-Kowalski et al., 2004; Haberl, Wackernagel et al., 2004). The MEFA method is more explicit in the direction of internal flows, rather than limited to the external inputs of the HANPP method. Both of these methodologies tend to be applied at the “whole of society” level, although they could be applied at the plant-level, but with more difficulty in detaching a sub-set of society from the whole. An advantage of these methodologies is that they take into account the differences in the society or industry and the local environment, thus making them applicable to the comparison of societies located in entirely different regions.

A generalised resource-based approach to measuring sustainability providing 3 indicators shown in Figure 2 uses ratios of changed to “normal” factors in order to quantify the change caused by a process as a fraction. The input data is a simple mass

balance. This approach is useful if the difference in the changed and normal values are within an appropriate range (i.e. if the values are too close together, the ratio will be close to 1, whereas if the values are too far apart, the value will tend towards 0, and the significance of any differences may be questionable), but this does not provide any long-term predictive capabilities, only being able to compare technologies, locations and improvement from past measurements. If the baseline value of an environmental emission can be calculated or measured however, and the potential for change estimated, these indices may provide a useful method of comparison.

<p>(1) Depletion index = $-(\text{present time rate of change of a resource stock}) / (\text{stock})$ $-(\text{accrual})$ or 0 (stasis) is better; $+(\text{depletion})$ is worse.</p> <p>(2) Dependence index = $(\text{gross import}) / (\text{internal use})$ Zero is better; $+$ is worse.</p> <p>(3) Disturbance index = $(\text{present flux}) / (\text{natural flux}) - 1$ Zero (undisturbed) is best, and $-$ (reduced flux) or $+$ (increased flux) are worse.</p>
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Figure 2: Resource-based Sustainability Indicators (Herendeen and Wildermuth, 2002)

Again, this methodology does not give any indication of where and what specific impacts are occurring. Divorcing the environment (and thus the environmental impacts) from the indicator appears to be the option that most analysts take in the search for an objective indication of sustainability. However, the assumption that such an “objective” indicator is more appropriate is flawed – it is like the case of a person who selects to serve apples over oranges by weight only, not including the fact that their guest does not enjoy apples. Likewise, if an emission is not connected to the location and time, its true, subjective, ongoing impact cannot be determined.

2.2.4 Environmental Burden Approach

The Environmental Burden Methodology uses a set of multipliers (potency factors) to determine the contribution of an emitted substance to a given environmental impact (e.g. - Global Warming, Photochemical Smog, Atmospheric Acidification). These potency factors are based on the theoretical contribution of the substance relative to a standard substance (e.g. Methane’s contribution to Global Warming is calculated as 21 times that of Carbon Dioxide (Tallis, Azapagic et al., 2003)). The total weighted

contribution to the particular environmental impact is designated as the “Environmental Burden” (EB) as per Equation 5.

$$EB_i = \sum_{N=1}^n (W_N)(PF_{i,N}) \quad [5]$$

The Institution of Chemical Engineers (IChemE) has released a recommended procedure for measuring sustainable development progress in the process industries utilising the typical Environmental Burden approach (Tallis, Azapagic et al., 2003). They then normalise the Environmental Burden over the amount of product or profit to give a sustainability indicator. This approach has been applied to general industrial applications, and for specific industries (Azapagic and Perdan, 2000; Azapagic, 2004).

The IChemE approach is general in nature, and offers a system of metrics which act mostly as “technology indicators”, in that they assess inherent sustainability of the plant or system only in terms of quantity of emissions, without connecting it to its environment, except by implication in the selection of metrics and indirectly through the potency factor. This approach can be used to compare different processes, or the performance of a given plant over time (without long-term predictive capacity), with lower emissions being considered more sustainable. This approach is satisfactory in terms of comparisons of similar processes for a given product and given location, but it does not provide much assistance in terms of comparing different processes in different locations, as it does not include factors that indicate the sensitivity of the environment to a given impact.

Advances made on this technique by Diniz da Costa, et al. (2004) and Diniz da Costa and Pagan (2006) go some way towards addressing this problem, but still retain some limitations. As they point out, the EB approach offers a potential for impact only, rather than indicating the actual impact of the process in terms of its local environment.

They thus extend the metrics to include factors from the local environment that affect whether the potential impact is realised in full or not in the area of impact. This incorporates the potential for the environment to buffer the emissions or impacts of

the process. The Specific Environmental Burden (SEB) (Equation 6) is thus derived by multiplication of a factor K, which is an empirical multiplier derived from assumed relationships between environmental parameters and emissions rates leading to variation of impacts.

$$SEB_i = (EB_i)(K_i) \quad [6]$$

This approach allows the simple integration of local environmental factors, and the comparison of plants in different locations. The development of the metrics to include local environmental conditions is intuitively an improvement in terms of predicting and comparing the relative sustainability of different plants or processes that are located in different environments. However, the method of obtaining the specific environmental dose value (K) is under-developed and largely empirical. It would be preferable to have a K value, or even a function K, that was based strictly on accepted laws of environmental interaction of the species in question, rather than empirical factors that may not apply to all localities. The authors also attempt to incorporate spatial and temporal factors by normalising the SEB over an area of impact and the time period of impact – by incorporating a model or function for distribution of the emission, the actual location of impact can be pin-pointed, and spatial and temporal factors automatically incorporated.

2.2.5 Impact Assessment

During the 1980's and 90's, and continuing to the present day, advances in identification and measurement of environmental causal relationships have lead to the creation of a field of study that looks at the impact of human activity on the environment. Impact Assessment has two common sub-streams – Life Cycle Impact Assessment and Environmental Impact Assessment – with the major differences being in the scope and specificity of the assessment of environmental impacts.

2.2.5.1 Life Cycle Impact Assessment

Life Cycle Impact Assessment (LCIA) studies (particularly) the environmental aspects and assesses the impacts of a product or process through the life cycle of the product from “cradle to grave” – through all stages from raw materials acquisition to final disposal (ISO 14040:1998). LCIA’s tend to be once-off analyses of product impacts which, although they assess the whole-of-life-cycle emissions, do not delve into the ongoing or cumulative effects and their spatial distribution. The LCIA approach to sustainability in its most relevant form has been applied to the Australian electricity generation industry by May and Brennan (2006).

Although the general methodology of LCIA has been standardised, there is still a wide variety of software packages and corresponding approaches available (over 36 cited in Wibberley (2004)).

Typically an LCIA does not incorporate spatial or temporal parameters (Wibberley, 2004) although the concept has been debated over the years (Huijbregts, 1999; Bellekom, Potting et al., 2006). LCIA’s are most commonly applied to products, which makes spatial parameters difficult to incorporate (Bellekom, Potting et al., 2006) except as “characterisation factors” (Norris, 2003; Lundie, Huijbregts et al., 2006). One example, TRACI (Tool for the Reduction and Assessment of Chemical and other Impacts) (Bare, Norris et al., 2003) is an LCIA tool that tries to incorporate the spatial distribution of impacts through the use of factors based on fate analysis by the United States Environmental Protection Agency (US-EPA). It is typical of many LCIA’s which incorporate spatial and temporal factors only implicitly through the use of data derived in the course of the study, or even from unrelated studies. Thus, although spatial distribution and temporal rates of change prior to final human or environmental consumption are necessary parts of the initial fate analysis, they do not appear explicitly in the final LCIA, and neither does the final LCIA relate to its specific environment (the lowest level of characterisation is a state-wide average). In addition, as for many other techniques, sustainability is not examined as an ongoing process, but more as a once-off impact.

2.2.5.2 Environmental Impact Assessment

Environmental Impact Assessment (EIA) is a methodology that has come to be a legal requirement for large developments within Australia. It is very similar to the LCIA process, but tends to regard only the construction and operational phases of a project. An EIA is often more targeted and specific than an LCIA, as it takes into account the specific surrounding environment and the impacts from the proposed plant on that local environment (Wibberley, 2004). EIA's typically incorporate spatial or temporal factors in the form of pre-modelling of transport of emissions to air, water and land. The EIA methodology is thus useful in the assessment of sustainability if the modelling results (and assumptions) are explicitly stated, but EIA's still tend to be once-off, ad hoc reports which can add complexity to the comparison of alternatives.

2.2.6 Summary

It is apparent that the issue of sustainability, and in particular its measurement, has been approached in various ways by numerous authors. To determine where these methodologies fall down, it is important to refer back to what is necessary for the measurement of ecological sustainability, namely:

- a) analysis of long term temporal variation,
- b) understanding and incorporation of the relationship between the process and its environment (chemico-physico-biological impacts)
- c) understanding of the location of impacts (spatial variation)
- d) incorporation of and response to limitations on resources and environmental capacity
- e) ability to easily and reliably compare options across locations

Table 1 shows how the different methodologies examined hold up in comparison to the criteria listed.

Table 1: Comparison of Methodologies with Sustainability Requirements

Methodology	Temporal Variation	Process / Environmental Relationships	Spatial Variation	Recognising Limits	Comparability of Locations
Parameters & Equations		implicit			
Fundamental Principles		implicit		X	
Externalities	implicit	implicit	implicit		Data intensive
Environmental Burden	Monitoring method	implicit			
Modified EB ^a	implicit as time of impact	implicit	implicit as area of impact		X
LCIA	implicit	implicit	?	implicit	Data intensive
EIA		implicit	implicit	implicit	Data intensive

^a Modified EB refers to the methodology of Diniz da Costa and Pagan (2006)

It is apparent that none of the methodologies examined fits all of the criteria for accurately measuring sustainability of a process, although the Externalities, modified EB and EIA approaches can fulfil the majority of the requirements. It is therefore necessary to adapt current methodologies to explicitly cover all the categories listed. In addition, it would be preferable to reduce the data intensity, such that comparison of different localities is made simpler (i.e. – techniques such as EIA and LCIA are still typically once-off assessments of single technologies and locations that need to be entirely repeated to compare with other options).

From this assessment, it is observed that there is a knowledge-gap in as far as sustainability studies do not cover spatial and temporal processes, and much of the information on environmental impacts is implicit rather than explicit. Thus one of the major improvements that must be attempted in this work is to include spatial and temporal processes the assessment methodology for sustainability. In particular, for the assessment of hydrogen energy systems, the directly impacted environment is of

most concern. Furthermore, it is important that environmental relationships and limitations be explicitly included wherever possible in the metrics, and that flexibility to allow comparison of alternative sites and processes be incorporated.

2.3 Hydrogen Energy Systems

Much of the material in this section comes from a review paper submitted to the International Journal of Hydrogen Energy (McLellan, Diniz da Costa et al., 2004), which is appended to the current document (Appendix 1). In addition, the work that has been done on sustainability-related assessment of hydrogen energy systems is reviewed.

2.3.1 Hydrogen Sources and Production Methods

Hydrogen can be produced from a wide range of source materials, including fossil fuels, biomass, some industrial chemical by-products and water via electrolysis. Australia is in the fortunate position of having the full range of options within the borders of a single country. The choice of source for hydrogen production in Australia, as elsewhere, would depend on various local factors including location of resources, available reserves, cost of extraction, cost of utilisation and transportation. Table 2 shows some of the factors affecting the choice of hydrogen source in Australia.

Table 2: Australian Resources for Hydrogen Production (McLellan, Diniz da Costa et al., 2004)

Resource	Reserves (yrs)	Price (US\$)	Source to End- User Average Distance (km)	Notes
Coal	261 – 500	28.04 / t (~ 0.7 / GJ) <i>Black</i>	<500 (~200 East Coast)	Extensive Infrastructure
References	(Williams, 2001; BP, 2002)		(SKM, 2001)	(ISR, 2001)
NG	78 – 130	~ 3 / GJ	560 (810 outside Victoria)	Extensive Infrastructure, Cleanest fossil fuel option
References	(BP, 2002; AGA, 2003)		(Encom, 2000)	
Oil	10 – 14	38.30 / bbl (~ 6.50 / GJ)	530	Some Infrastructure
References	(ABARE, 2002; BP, 2002; Petrie, 2002)		(PPA, 2003)	
Biomass	Limited to available land	Source Dependent	100 - 200	Some Infrastructure, Potentially inexpensive, Renewable Resource
References			Estimate from Geographical Data	
Water	Limited by other industry / residential requirements	Source Dependent	<100	Extensive Infrastructure, Limited by availability in rural locations, Potential for use on seaboard,
References			Estimate from Geographical Data	
Chemical	Limited by industrial production	Source Dependent	Source Dependent	Uncertain amount of Infrastructure, Potential for using pollutant / waste-products, Reliability and lifetime an issue
References			Estimate	

It is apparent from Table 2 that of all the possible sources of hydrogen, NG and coal present the most likely options in terms of current infrastructure, widespread and long-term availability, although distances from reserves to end-usage point are typically further than other sources. In particular, water usage is becoming an issue of great importance in Australia, which may preclude electrolysis from becoming a widespread option for hydrogen production.

The technique utilised to produce hydrogen from the source will depend on technology development, required infrastructure investment, efficiency, location and

suitability of local supplies. In a country as vast as Australia, with such a wide variety of environments, it is likely that a variety of production routes will be used. Table 3 lists the various production methods available and corresponding parameters used in the selection of a potential technique.

Table 3: Summary of Hydrogen Production Methods (McLellan, Diniz da Costa et al., 2004)

Method	Fuels	Overall Efficiency (%)	H2 Cost (US\$/GJ)	TCI (US\$/GJ H ₂ Capacity)	Notes
Steam Reforming	NG, Oil	65-75 (LHV)	5-8	9-15	Well-established, Extensive infrastructure,
References	(Dicks, 1996; Dicks, 2003)				
Partial Oxidation	NG, Oil	50 (LHV)	7-10	9-22	Minimal infrastructure, Well-established, Variety of fuels
References	(Dicks, 1996; Dicks, 2003; Walsh, 2003)				
Auto-thermal Reforming	NG	N/A	N/A	N/A	No infrastructure,
Thermal Decomposition	NG	N/A	N/A	N/A	No infrastructure, Low emissions / easy waste handling, Potential for use with solar energy
Gasification	Biomass, Oil, Coal	42.5-46.5 (LHV)	10-12 9-13	33-34 20-42	Minimal infrastructure, Concentrated CO ₂ stream ideal for sequestration, Uses cheap fuels, Potential for use with solar energy
References	(Williams, 2001; Iwasaki, 2003)				
Pyrolysis	Biomass, Coal	47.9 (HHV)	9-13	15-19	No infrastructure, Uses cheap fuels, Concentrated CO ₂ stream ideal for sequestration
References	(Iwasaki, 2003)				
Electrolysis	Water, H ₂ S	35-42 (HHV) (Electricity source included) 70 (NG assisted)	20-25 (Large) 11-42 (Small)	3-30 (Large) 32-486 (Small)	Potential zero emissions with renewable electricity, Environmental / economic benefits depend on electricity supply, Water supply possibly unreliable
References	(Martinez-Frias, Pham et al., 2003)				
Biological Processes	Biomass	N/A	N/A	N/A	Undeveloped, Control and scale-up issues
Plasma Reforming	NG, Oil, Biomass	N/A	~10	N/A	Unproven commercially, Electricity source can affect environmental benefits
References	(Bromberg, Cohn et al., 1997; Bromberg, Cohn et al., 1999)				

Notes: a) TCI = Specific Total Capital Investment (Padro and Putsche, 1999)
b) Some costs could not be converted to AU\$, so all values were left in US\$ for reasons of comparison

In terms of cost, efficiency and currently available infrastructure, Table 3 shows that NG steam reforming would be the obvious choice. However, combining the conclusions of both Table 2 and Table 3, indicates that the location and estimated quantity of existing reserves of coal, as well as the current high dependency on it (in the order of 42% of primary energy usage and 84% of stationary power production according to BP (2002)), make coal gasification another option to be closely assessed. Biomass could also prove to be a successful candidate for hydrogen production, being in close proximity to the end user, and with the benefits of being a renewable source. However, the costs associated with it are uncertain at the present time.

2.3.2 Sustainability Assessment of Hydrogen Energy Systems

Little, if any, work has been done on the subject of sustainability of hydrogen energy systems. What work exists, focuses more specifically on comparing emissions as a technology indicator rather than examining what the actual meaning of those emissions is in terms of environmental impacts in the long term (Williams, 2001; Ogden, Williams et al., 2002; Bargigli, Raugei et al., 2004). Thus much of this work can only be used to find the relative theoretical environmental merit of a technology in comparison to other existing or proposed technologies, and improvement in terms of sustainability is only measured as improvement from the status quo. Assessment in Australia is particularly lacking, with no work completed on assessing the environmental implications of different hydrogen energy systems in the particular circumstances of this country. A number of reviews of economic viability have been examined for single or multiple technologies (Walker, Blinderman et al., 2001; Blinderman and Jones, 2002; ACIL, 2003), and some technology reviews have been completed (Innes, 2003; McLellan, Dicks et al., 2003; Walsh, 2003; McLellan, Diniz da Costa et al., 2004), but on the whole, the subject of sustainability in terms of hydrogen energy systems has not yet been addressed.

Although the utilisation of hydrogen in and of itself offers little in the way of environmental impact (hydrogen utilisation in devices such as fuel cells produces only water as an output), when viewed on the scale of the full fuel cycle – from raw materials extraction, transport and hydrogen production and utilisation – the impacts

can be much more significant. Hence it is necessary to examine the full energy system from a holistic perspective. In terms of sustainability assessment, this brings in the added complexity of a potentially very wide spatial range over which the process impacts, which must be accounted for in the methodology utilised for assessment.

In terms of global environmental impacts, the benefit or detriment of hydrogen generated from fossil fuels is highly dependent on the use of CO₂ sequestration. Capture and sequestration technologies are energy intensive and an energy balance is required to verify the feasibility of each system. In the case of Australia, where the majority of the population is distributed through a number of centres separated by long distances, the effects of product and feed transportation also become very important.

In terms of environmental benefit, it is essential to carry out sustainability assessment on each process to determine which actually contributes the least damage over time. At this stage, no analysis is available in terms of Australian production, although some LCIA and extensive technology assessment work has been done on individual technologies in other parts of the world (Wihersaari, 1996; Boman and Turnbull, 1997; Gupta, Turk et al., 2000; Haupt and Zimmermann, 2001; Spath, 2001; Lettens, Muys et al., 2003). Other authors have looked more broadly at comparing multiple hydrogen energy pathways, but tend to focus mostly on the economic and greenhouse emissions only (Nicoletti, 1995; Ogden, Williams et al., 2002; Koroneos, Dompros et al., 2004; Granovskii, Dincer et al., 2006).

Thus there appears to be a significant gap in research in terms of the ecological sustainability of hydrogen energy systems – particularly across a wide range of technologies and a complete range of emissions. In addition, the lack of work in the Australian context provides a further avenue for investigation.

2.3.3 Summary

It is clear that sustainability assessment of hydrogen energy systems has not been considered specifically by any of the previous work. In addition, the related work – LCIA's and technology assessment – is either incomplete in its scope (does not address all environmental issues or technologies) and is not focused on determining the long term impacts of producing and utilising hydrogen. Even hydrogen related work is limited in the Australian context.

Hydrogen energy systems themselves add a number of complexities to the sustainability assessment:

- a) Full fuel cycle analysis necessary to determine true ecological sustainability
- b) Wide spatial range necessary to incorporate the full fuel cycle
- c) Comparison of different processes for production, transportation and utilisation must be possible.

Table 4 describes how the previously discussed methodologies for sustainability assessment hold up under the requirements for assessing hydrogen energy systems.

Table 4: Comparison of Methodologies for Hydrogen Energy System Assessment

Methodology	Full Fuel Cycle	Comparison of Process Options	Wide Spatial Variation
Parameters & Equations	X	X	
Fundamental Principles	X	X	
Externalities	X	X	implicit
Environmental Burden	X	X	
Modified EB	X	X	implicit as area of impact but difficult to justify
LCIA	X	Data intensive	
EIA	X	Data intensive	Possible with some difficulty

Thus, it is apparent from Table 4 that any of the Externalities, Modified EB or EIA approaches would be able to satisfy the requirements of assessing the sustainability of hydrogen energy systems, but with some reservations as to the difficulty of application, the openness of the method and the ability to justify comparisons if the area of impact is too large.

2.4 Conclusions

It is apparent from the literature review that hydrogen energy systems have never been adequately assessed in terms of sustainability. Moreover, any work on sustainability assessment has been limited within Australia. Thus the proposed application of sustainability assessment in the context of hydrogen energy systems in Australia is particularly novel.

From the work reviewed in this chapter, it is apparent that the Environmental Impact Assessment, Modified Environmental Burden and Externalities approaches are the only methodologies that fulfil most of the criteria necessary to assess ecological sustainability in its truest sense, and particularly in the case of hydrogen energy systems (Table 5).

However, even these methodologies are flawed in that they do not fulfil all of the criteria necessary for sustainability assessment, and many of the criteria are only fulfilled implicitly. In terms of the outputs from the different methodologies, EIA's often offer subjective comparisons of the impacts, while the reduction of all environmental impacts to a cost may not adequately weight the importance of conflicting impacts. The modified EB method offers perhaps the most useful outputs, in that it provides potential for impacts based on a mass-weighted figure, with potency factors being the dubious aspect, as they may not be globally equal and applicable.

In preference over the monetary equivalent given by the Externalities method, the EB method is considered to be a more adequate starting point to extend to a methodology that can fulfil all the requirements. Chapter 3 describes the methodology advanced to

overcome the current flaws in sustainability assessment as observed in the present chapter.

Table 5: Overall Assessment Table of Existing Sustainability Assessment Methodologies

Criteria	Methodology	Externalities	Modified EB	EIA
Sustainability Assessment Requirements	Temporal Variation	implicit	Implicit as time of impact	
	Process / Environmental Relationships	implicit	implicit	Implicit
	Spatial Variation	implicit	implicit as area of impact	Implicit
	Recognising Limits			Implicit
	Comparability of Locations	Data intensive	Implicit	Data intensive
Hydrogen Energy System Assessment Requirements	Full Fuel Cycle	X	X	X
	Comparability of Processes	X	X	Data intensive
	Wide Spatial Variation	implicit	Implicit as area of impact but difficult to justify	Possible with some difficulty

Nomenclature

a = rate of increase of μ_o (%)

b = rate of increase of D_o (%)

C_o = rate of recycle of resources or cascading (for energy resources) (%)

c = rate of increase of C_o (%)

C = specific CO₂ emissions (t CO₂ / GJ)

C_i = Construction emissions (t)

C_{op} = annual operating emissions (t/yr)

C_g = annual emissions from fuel usage (t/yr)

D_o = demand of the resources at initial time period (GJ)

EB_i = i th Environmental Burden

E_{out} = Life Cycle energy output (GJ)

E_{in} = Life Cycle energy input (GJ)

ϵ_o = annual energy output (GJ/yr)

ϵ_i = initial energy input for construction (GJ)

ϵ_{op} = annual operating energy input (GJ/yr)

L = Lifetime of the plant (yr)

μ_o = life cycle integrated energy balance of the resources at initial time period

P_o = production of the resources at initial time period (GJ)

$PF_{i,N}$ = Potency Factor for substance N , for Environmental Burden i

R = Net energy ratio

R_o = reserves of the resources at initial time period (GJ)

r = rate of increase of R_o (%)

s = rate of substitution by other resources (%)

W_N = mass of substance N emitted, including accidental and unintentional emissions (kg/yr)

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Chapter 3

Methodology

3.1 Introduction

On examination of the literature in regards to sustainability assessment, it was found that none of the existing methods covers all the needs of a sustainability assessment for hydrogen energy systems. In this chapter therefore, a methodology is proposed to overcome the shortcomings of the existing methodologies of sustainability assessment. The proposed approach seeks to define the link between the process and its environment more solidly, and to provide a more holistic approach to sustainability assessment, by adding environmental processes in a temporal and spatial matrix. Therefore, this chapter aims at providing the framework needed for sustainability metrics model development, analysis and validation in subsequent chapters.

3.2 Fundamental Issues in Sustainability Metrics

A fundamental question that this work is endeavouring to address is whether the environment can process, buffer or recycle emissions. If the environment can sustain such processes without breaching its carrying capacity, then in principle anthropogenic emissions can be perceived as sustainable processes. Many models dealing with environmental emissions are “loading” models, which is also the general approach in sustainability metrics (Tallis, Azapagic et al., 2003). There are many merits in these models as they provide a yard stick to compare different processes and impacts. However, fundamentally these sustainability metric models do not take into consideration environmental processes resulting in temporal and spatial variations.

Another point of importance when we are dealing with issues of environmental impact is the concept of midpoint as compared to endpoint impact. An appropriate limit must be placed on the assessment, such that the interminable chain of causality is not followed to an excessive extent (Bare, Norris et al., 2003; Jin and High, 2004).

For example, acidification of soils could cause the loss of biodiversity among the microbial population, which may in turn lead to effects on higher species, and eventually effect the human population. Were we to take the end-point of the human effect, the assessment would become far too complex, and the level of accuracy would drop away with every step. Hence it is argued for the assessment of sustainability, that the assignation of an appropriate mid-point is essential.

In order to address the shortcomings of the existing methodology, it is proposed to incorporate environmental processes into the sustainability metrics, based on the following considerations:

1. explicit use of a simple emissions transport model (ETM) to determine (to some extent of accuracy) the spatial fate of emissions and correlation with receptors
2. inclusion of rates of on-going dynamic environmental processes to determine the temporal fate of species
3. quantification of the carrying capacity (environmental resilience and limitations) of the local environment from intrinsic properties of the environment that might easily be obtained by the user
4. Spatial discretisation of impacts to allow pinpointing of areas of critical importance
5. Ensuring that the model is not excessively data-intensive, but capable of comparison of different locations and processes.

The following sub-sections provide an insight into the approach taken in this work aiming at addressing these fundamental issues in sustainability metrics.

3.3 Methodology

3.3.1 Introduction

To assess the sustainability of a proposed hydrogen energy system, fulfilling the requirements of the previously mentioned criteria, a mathematical model of the process and its environment was created. This consisted of 3 main sections – the

model of the process in terms of a full fuel cycle inventory; the model of the environmental transport of the emissions from the process; and, the incorporation of locational environmental resilience through the carrying capacity in the sustainability metrics. The proceeding sections elaborate on these steps.

3.3.2 Fuel Cycle Inventory

An inventory of inputs and outputs over the process is a fundamental initial requirement for assessing the sustainability of the process. As argued in Chapter 4, the most appropriate level of inventory is one which covers the full fuel cycle – from the extraction of the hydrogen or electricity feedstock, to the operation of the plant, and incorporating the transportation steps in between (see Figure 3). This does not include the construction and decommissioning of infrastructure that would be found in a full Life Cycle Assessment, but previous studies (Nunn, Cottrell et al., 2001; Spath, 2001) have shown that the operational impacts are most significant for fossil fuel based systems, and in terms of sustainability they present the most important long-term factors. For renewable energy systems, the other life cycle phases may impact more highly on the overall sustainability, and should thus be included.

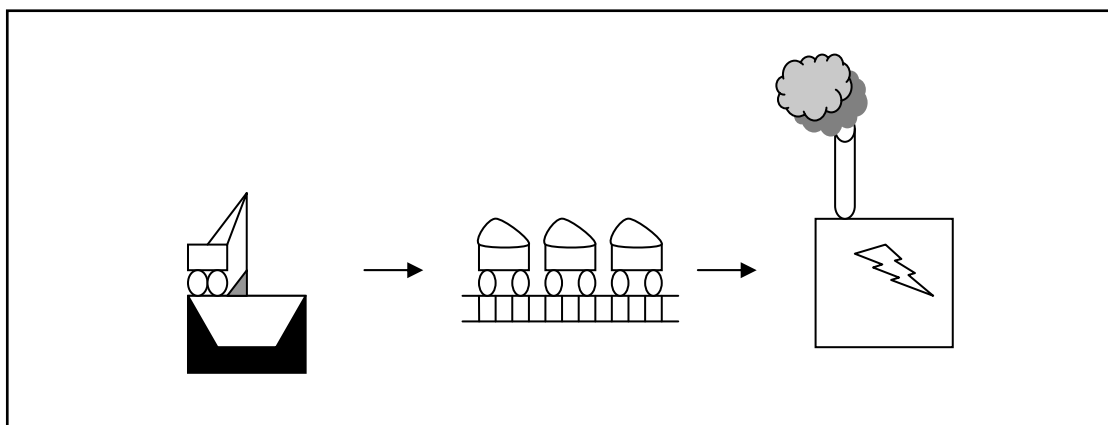


Figure 3: Operational Units Considered in the Fuel Cycle Inventory

Data on a wide range of emissions was obtained from the fuel cycle analysis (Chapter 4) however, for the validation of the current work, only the acidifying compounds were considered.

3.3.3 Process Approach to Emissions Transport

To incorporate dynamic spatial and temporal factors into the sustainability metrics, the emissions from the process were initially assumed to be inflows to the airshed, which was modelled as a “tank” or reservoir of set radius and height, with the assumption of perfect mixing (Figure 4). The bottom of the tank was the earth within the radius of the airshed and the only fluxes out of the tank were via wind and deposition to soil. The tank could also incorporate reactions (aqueous and other atmospheric reactions).

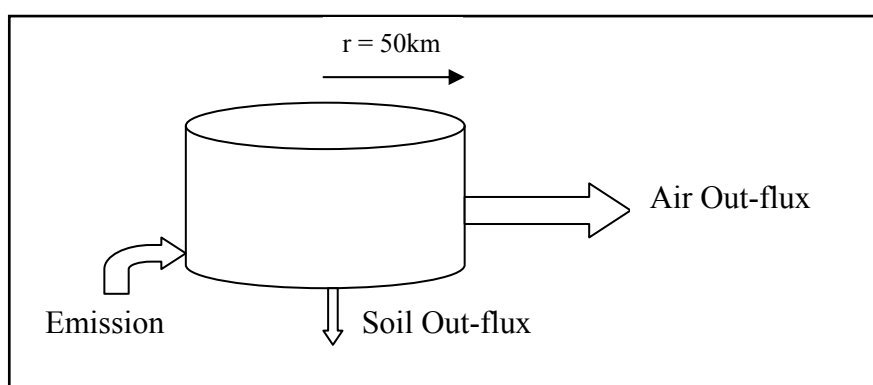


Figure 4: Single Airshed Tank Model

Treating the airshed as a single tank or reservoir obviously introduced high levels of error, as the radius of the airshed may be in the range of 50-100km or more, for which the assumption of perfect mixing is not valid, and the environmental resilience parameters may vary widely. To better fit reality, the sustainability model was expanded, continuing the process engineering approach, by breaking down the receiving environment into a series of smaller reservoirs, with flows between them modelled as “pipes” (Figure 5).

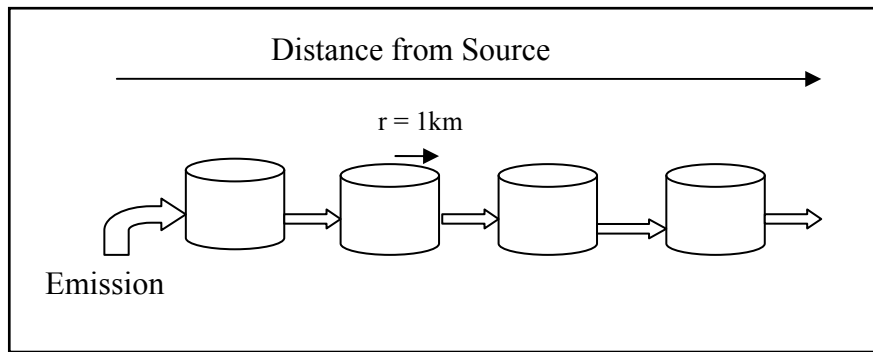


Figure 5: Process "Reservoir" and "Pipe" model of Environmental Transmission

The result of the creation of these “sub-airshed” tanks, was that the model conformed more closely with the reality of the environment, and that the environment (and subsequently all impacts) was already discretised.

The utilisation of such a simple methodology may seem inherently flawed in the face of the complexities of the environmental interactions that the work is attempting to model. This argument is valid, however, the underlying aim of this work is not so much to have the most accurate of models, but to demonstrate that the sustainability assessment can and should have local environmental factors integrated into it. A simple model also minimizes data requirements, but can still provide a reasonably accurate assessment. In fact, to make the model over-complex would perhaps be to assume that too high a degree of accuracy is possible – an assumption that has often been proved foolish when dealing with a subject as complex as the environment.

In addition, by incorporating such a simple model, it is possible to make all the assumptions and outcomes explicit in the sustainability assessment. This overcomes the downfalls of previous methodologies, where the incorporation of spatial and temporal factors via ETMs was either implicit only, or the ETMs themselves were too complex to apply to any given situation without high levels of data and time.

3.3.4 Space

The Emissions Transport Model (ETM) incorporates the physical dimensions of the surrounding environment via modelling the progress of emissions through a series of “reservoirs”. Each reservoir’s radius is used in calculating the environmental flows, and the distance of receptors from the emission point.

3.3.4.1 Spatial Discretisation

The combined effect of this approach is to give a polar grid of receptors, with the environmental flows discretised by sub-airshed. This allows the incorporation of local environmental data specific to each grid section in order to model the actual environment surrounding the process to a greater level of detail.

3.3.5 Time

The model is a dynamic model, where time is incorporated into the model via the reaction and deposition or uptake rate of emitted species, and by the accumulation and associated fluxes within the reservoirs. Thus the progressive environmental depletion or accumulation, which relates directly to the long term viability of the system, can be estimated.

3.3.6 Carrying Capacity

Intrinsic environmental physico-chemico-biological parameters of soil, vegetation, water bodies, climate, animal and human populations are utilised in an attempt to quantify the environmental resilience within a given reservoir. This is the factor that truly determines the sustainability of the process over time, and hence the comparison of performance against these levels forms the sustainability indicator. Carrying capacity may be estimated from local environmental factors, and is closely aligned with the chosen mid-point. If the mid-point is chosen appropriately, the estimation of carrying capacity will be enhanced in its relevance and ease of acquisition (Jin and High, 2004). The derivation of carrying capacity is a matter that is given closer analysis in Chapter 5.

3.3.7 Validation

In order to validate the process approach to the ETM, and the requirement for location-specificity, the model is tested using historical data from an isolated Australian power station. With the elimination of many of the typical causes of interference in more highly industrialised areas, this was deemed to be a great advantage in proving the validity of the current work.

3.4 Application of the Metrics to Hydrogen Energy Systems

As mentioned previously, review of the methods of hydrogen production indicated that the most likely short-term options for Australia would come from coal gasification or natural gas steam reforming. Thus these options are utilised as the basis for application of the sustainability metrics. A number of scenarios are examined for the environmental and internal process parameters.

3.5 Conclusion

The development and application of the current sustainability metrics methodology for the assessment of hydrogen energy systems in Australia was followed in this way to fulfil the necessary criteria. The following chapters 4-7 describe in more detail each step of the development process and the application of the metrics.

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Chapter 4

Fuel Cycle Inventory

4.1 Introduction

The first step in deriving both a comprehensive set of Sustainability Metrics (SM) and the emissions from the plant that would form the input to the Emissions Transport Model (ETM), is the Fuel Cycle Inventory (FCI).¹ The Fuel Cycle Inventory for this work is based on a typical Life Cycle Assessment approach, but the emphasis on the operational cycle was deemed to be valid for fossil fuel based systems, as the majority of sustainability issues, and indeed the issue of sustainability itself, has most relevance to this phase of the project. In addition, it has been shown in previous work that the major emissions-based impacts result from the operational phase (Nunn, Cottrell et al., 2001; Spath, 2001).

4.2 Basis, Scope and System Boundaries

By performing a straight-forward mass and energy balance over the plant to be assessed, the potential important emissions could be quantified, and thus the input to the ETM determined. 3 important potential hydrogen production technologies were chosen for examination – coal gasification (gasification), Natural Gas steam reforming (NG-SR) and conventional coal-based electrolysis (electrolysis). Gasification and NG-SR were chosen based on earlier work (McLellan, Dicks et al., 2003; McLellan, Diniz da Costa et al., 2004) which indicated their high potential for hydrogen production in Australia, whilst electrolysis is chosen for comparison as a technology that is easily modelled as a direct translation from conventional coal power stations.

¹ Initially a full Life Cycle Inventory was considered however, it was determined that the main variation of impacts between plant localities would depend on the Fuel Cycle, rather than the Construction and Decommissioning phases of the life cycle.

The scope of the fuel cycle impact assessment was limited to the operations directly involved in the extraction, transport and production steps of the hydrogen energy system. As such, the upstream emissions and impacts of industrially important materials and fuel have not been included. Thus, the operational aspects of the process only, are assessed, and the supply of fuel and chemical components is assumed to be outside the scope of the assessment. A full life cycle analysis would typically involve many of these upstream impacts, but for the sake of this project, only primary impacts were examined, with secondary and higher order impacts ignored.

The FCI is completed in spreadsheeting software over proprietary LCIA tools due to the complete freedom in adjusting parameters within the process, as well as the clarity, simplicity and openness that a spreadsheet allows. It also allows the handling of solids and the use of advanced technologies such as fuel cells to be more easily modelled. In potential commercial applications, it is most likely that the process design will be complete to the point where the mass and energy data are already available.

For the sake of brevity, only the major emissions are given here. More complete FCI's are described in Appendix 2. Furthermore, the descriptions here are based on the gasification option, which is examined most thoroughly.

The functional unit or basis for the comparison of results will be the provision of 1000MW (178kt/yr) of hydrogen at the site of the current Tarong power station, for transport to Brisbane, Australia.

The system consists of resource extraction, transport and hydrogen production (Figure 6). Coal is assumed to be sourced from the current Meandu mine, and NG sourced from existing gas fields in Roma. Coal transport is assumed to be via rail, and NG transport by pipeline, as this allows for simple comparison of long and short distance transport. Operation of rolling stock or piping is the only process considered.

Hydrogen plant operation under normal operating conditions is considered, with allowance for scheduled down-time. The system boundaries for inventory purposes

are drawn spatially around the three main units, so that any emissions from or inputs to the unit operations from the environment are included.

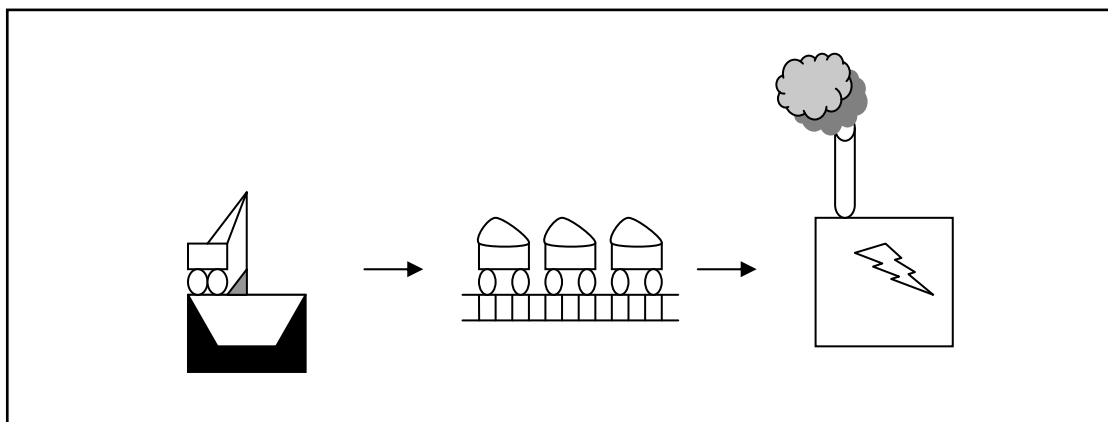


Figure 6: Fuel Cycle Operational Units

4.2.1 Extraction Operations Inventory

The extraction operation includes mining and washing of the coal or extraction of NG. The major inputs to an existing coal mine are diesel fuel and water, with outputs of pollutant emissions to land, water and air and the main product – coal (Figure 7). NG wells are taken mainly as a source of fugitive NG emissions. The resource requirements calculated in the hydrogen production section determine the required coal or NG output (with a factor to count for loss). For the coal options, the current work derives multipliers from a simple ratio of the annual substance emissions for coal mining in Queensland given by the National Pollutant Inventory (NPI) (NPI, 2005) and the total Queensland annual coal output (NRM, 2004). For NG, the emissions are taken mainly from Spath (2001). Various mines also report annually on their specific emissions, such that where the source is specified, more specific data may be used. NPI workbooks can also be used to determine pollutant emissions corresponding to the coal requirements from the given set of factors (NPI, 2005).

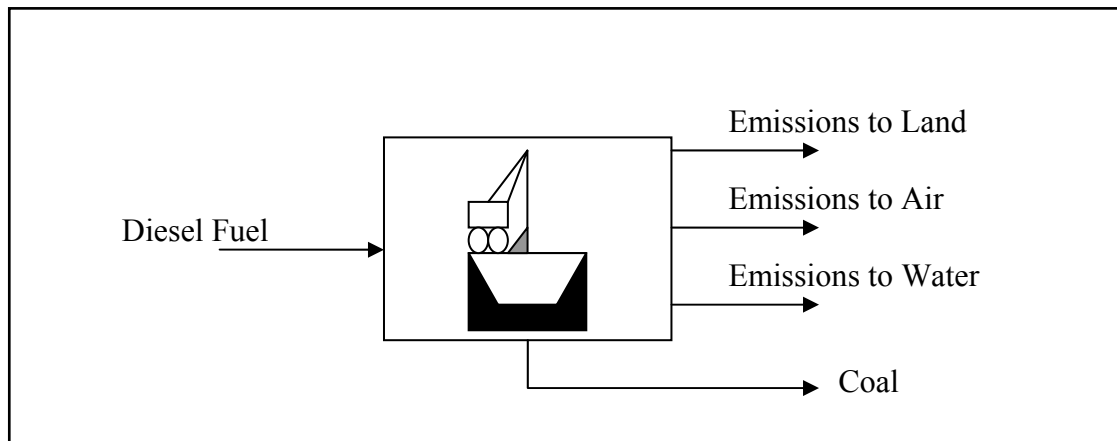


Figure 7: Mining Inventory Flows

The emissions monitored by the NPI, and the corresponding emissions factors as calculated in the current work, are given in Appendix 2. Organic compound emissions are typically the fugitive emissions released from coal during and after excavation, as well as a contribution from diesel fuel use. Metals and particulates are emitted in dust from the mine, as well as in the emissions from diesel fuel usage.

4.2.2 Resource Transportation Inventory

The inputs to the coal transportation unit were predominately coal and diesel fuel, with outputs of pollutant emissions to land, air and water, and the load of coal being delivered to the hydrogen generation plant (Figure 8). NG emissions are assumed to be due to leakage, and account for an estimated 1% over the 450km from Roma to Tarong (Ogden, 1999; AGA, 2003; NPI, 2006). Coal is assumed to be lost at a rate of 0.5% between the mine and the plant due to loading, unloading and operational losses.

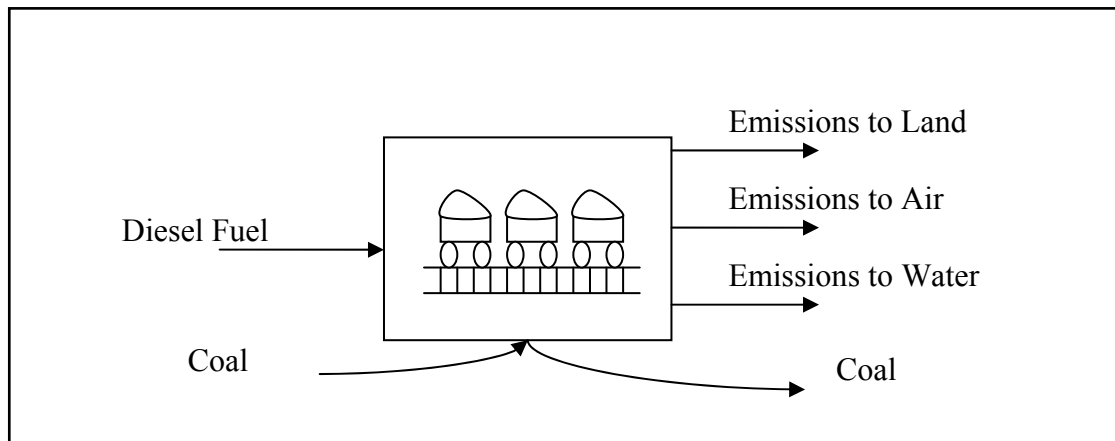


Figure 8: Coal Transportation Inventory Flows

The emissions from coal transportation were derived from the NPI workbook on rail emissions (NPI, 1999), with the fuel efficiency and CO₂ emissions derived from the Queensland Rail report on emissions from rail transport (QR, 2002). The distance from the mine to the plant was taken to be 5km.

Metals emissions are limited by the content of the diesel fuel utilised. Products of combustion may vary based on the efficiency of reaction in the engine, and catalytic conversion.

4.2.3 Electricity and Hydrogen Production

The gasification plant is modelled as an oxygen-blown, entrained gasifier technology, with desulphurisation and particulate capture technology. The report by (Innes, 2003) for the Cooperative Research Centre for Coal in Sustainable Development (CCSD), indicates that the Entrained Flow Gasifier is the most flexible in terms of feed coal properties and along with fluidised bed gasifiers, provides the highest power output for an Integrated Coal Gasification Combined Cycle (IGCC) plant. This report further concluded that this gasifier-type is the most appropriate for most Australian coals. The flexibility of an IGCC plant to produce electricity or hydrogen is an advantage for this technology.

The electrolysis plant is modelled on the current Tarong power station, with rates of required energy consumption for the electrolyser per unit of hydrogen taken as 4.3-4.9 (kWh / m³ H₂) (Ullmann, 1986). The emissions from the plant were scaled from the

existing Tarong power station to the energy output requirements for the electrolyser. The NG-SR plant emissions are determined by input-output factors derived from Spath, et al. (2001).

The major inputs to either hydrogen or electricity production would be water, coal (or NG) and chemicals (e.g. – amines for desulphurisation) (Figure 9). Major outputs are the emissions of pollutants to air, water and land, and the major product – hydrogen or electricity – to the end user.

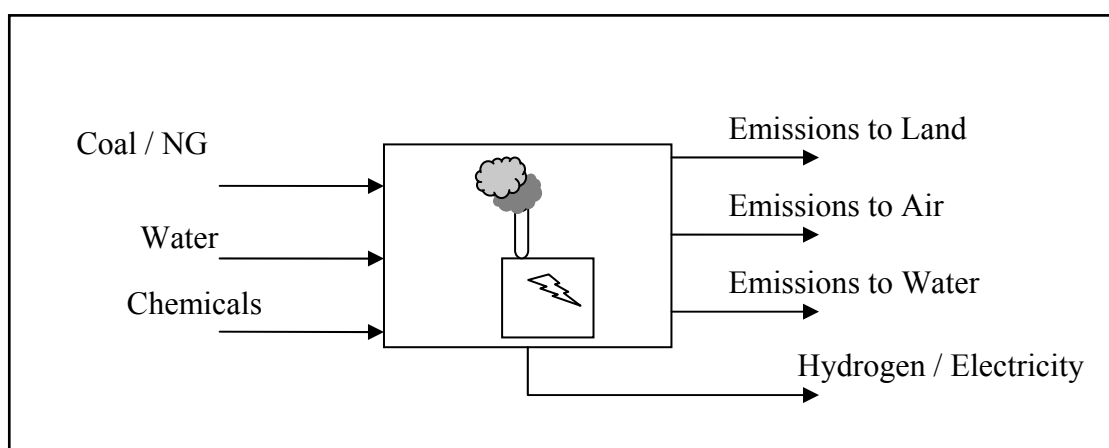


Figure 9: Hydrogen and Electricity Production Inventory Flows

Figure 10 shows, in simplified form, the flow sheet for the production of hydrogen or electricity via coal gasification. (Note: - GT = Gas turbine; ST = Steam turbine; ASU = Air separation unit; WGS = Water gas shift reactor;)

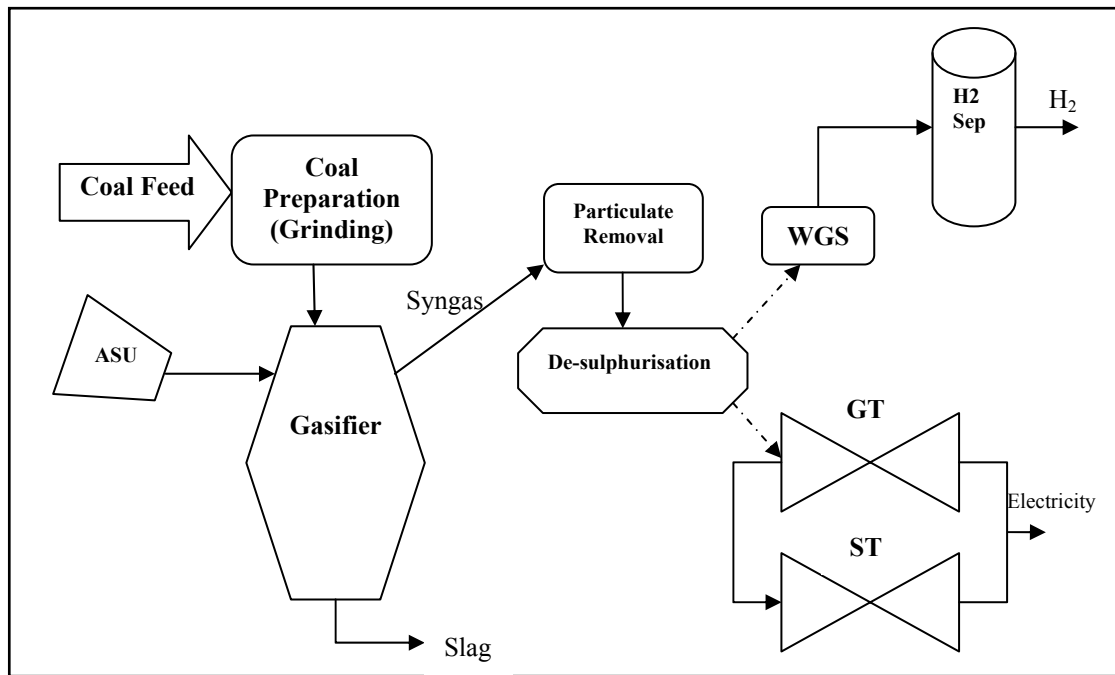


Figure 10: Simplified IGCC Flowchart for Hydrogen or Electricity

For the gasification plant, shortcut design equations were used to calculate the mass and energy flows, with major parameters sourced from the literature. The shortcut equations and the overall mass and energy balance emissions in tabular form are summarised in Appendix 2.

Particulate matter (PM_{10}) and metals emissions for all options are limited by the total amount present in the feed, and reduced by clean-up processes. The electrolysis plant assumes only particulate removal, whilst the gasification plant has higher requirements on gas clean-up. Organic compounds are products of gasification and are removed in clean-up to some extent. Combustion products (CO , CO_2 , SO_x) are limited by the presence of oxygen and the amount of non-oxygen element in the feed coal. SO_x is mostly removed by clean-up due to technical requirements of the gasification plant (Innes, 2003). NO_x is mainly produced when electricity is being produced, from nitrogen present in the coal, and in the provided oxygen (1-5% nitrogen remaining). Combustion conditions in the electrolysis scenario lead to higher NO_x emissions. A summary of the main operating parameters of the plants is given in Table 6.

Table 6: Main Operating Parameters for Plants Producing 1000MW (2.26×10^7 GJ of H₂)

Process	Electrolysis	NG SR	Coal Gasification
Overall Efficiency	27.6 % HHV	89.3 % HHV	60 % HHV
Unit Efficiencies	Coal PF – 35%, Electrolyser – 4.9kWh / m ³ H ₂	-	-
Fuel Energy Input	4.46 Mtpa = 9.143×10^7 GJ/yr	0.744bcm/yr = 2.83×10^7 GJ/yr	1.76 Mtpa= 4.21×10^7 GJ/yr
C Conversion Rates	-	99%	99%
WGS Conversion Rates	-	98%	98%
Syngas Flowrate (kmol/s)	-	7.22	8.64
Operating Conditions – Main Units			
T (°C)	80	800	1600
P (bar)	1	26	31

Notes:

1m³ H₂ = 12.8 MJ (HHV)

1 kg = 141.9 MJ

1 kWh = 3600 kJ

Total = 178,000 tpa H₂ = 2.526×10^7 GJ/yr

Coal = 20.5 MJ/kg

NG = 38 MJ / m³

CH₄ = 33.8 MJ / m³

4.2.4 Data Sources

4.2.4.1 Coal Composition

The Ultimate Analysis – composition of Nitrogen, Sulfur, Carbon, Oxygen, Hydrogen – moisture and ash content of coal is relatively easy to acquire (Spero, 1997; Tarong, 2006), which supplies the main source of input data for process reactions and flows in the FCI. Trace component compositions are more difficult to determine, so where specific data is unavailable, generic emissions data is utilised from the National Pollutant Inventory (NPI, 2005).

Ash composition, slagging temperature and flux requirements at various temperatures are acquired from reports by the CCSD (Do and Patterson, 2004).

4.2.4.2 Plant Equipment Shortcut Equations and Process Assumptions

The gasification plant for this work is modelled off the Buggenum IGCC plant (Netherlands), which utilises the Shell / Demkolec entrained flow gasifier. Details of the emissions, efficiencies and input requirements are available in Williams (2001) and Innes (2003). This gives a basis for comparison of SO₂, NO_x and PM₁₀, as well as different plant conditions such as gasifier temperature and pressure. Plant utilisation rate and efficiency are taken from Nunn, Cottrell et al. (2001) and Ogden (2003).

Shortcut design calculations for ancillary units are considered sufficient for the purposes of the project, as specific design is not necessary for a sufficiently-accurate FCI. The majority of shortcut calculations are taken from Branan (1994).

4.2.5 Air Emissions

Table 7 - Table 9 show a summary of some of the more important air emissions from the entire fuel cycle. The full emissions summary is provided in Appendix 2.

Table 7: FCI Major Substance Results for Hydrogen Production Operation

Substance Emissions (t/yr)	Gasification^a	Electrolysis	NG-SR
CO	34,971.59		1,233
NO _x	561.58	33,944	
PM ₁₀	30.73	4,193	
SO ₂	88.43	22,631	
CH ₄	232.61		91,844
CO ₂	5,074,424	5,924,936	1,809,016
Usage Rates			
Coal (Mt / yr)	1.76	4.46	-
NG (bcm / yr)	-	-	0.744
Water (ML / yr)	4,176	470,384	1,514

^a NO_x emissions are from the combustion of syngas in the IGCC electricity production option

Table 8: Emissions from Resource Transport

Substance emissions (t/yr)	Gasification	Electrolysis	NG-SR
CO	0.363	0.736	
NO _x	2.860	5.798	0.55
PM ₁₀	0.067	0.136	0.013
SO ₂	0.125	0.254	0.061
Total Volatile Organic Compounds (assume mainly CH ₄)	0.123	0.249	617.2
Fuel Usage and Emissions			
Diesel Fuel Usage (kL / yr)	48.4	98.1	
CO ₂ Emissions (t/yr)	130.68	264.88	33.72

Table 9: Emissions from Resource Extraction

Substance Emissions (t/yr)	Gasification	Electrolysis	NG-SR
CO	121.6	246.4	
NO _x	243.1	492.8	9.5
PM ₁₀	950.4	1,926.4	0.4
SO ₂	12.2	24.6	5.5
Total Volatile Organic Compounds (TVOCs) (assume mainly CH ₄)	33.2	67.2	14.1
Fuel Usage			
Diesel Use (kL / yr)	7,151	14,496	-
CO ₂ Emissions from Diesel Use (t/yr)	19.0	39.1	-

The contribution of each stage of the process to the overall emissions is graphically demonstrated in Figure 11 - Figure 13. In each scenario, only the extraction and hydrogen production operations show an important contribution to the overall emissions. This is the expected outcome in particular with the coal transportation, which is over the very short distance of 5km.

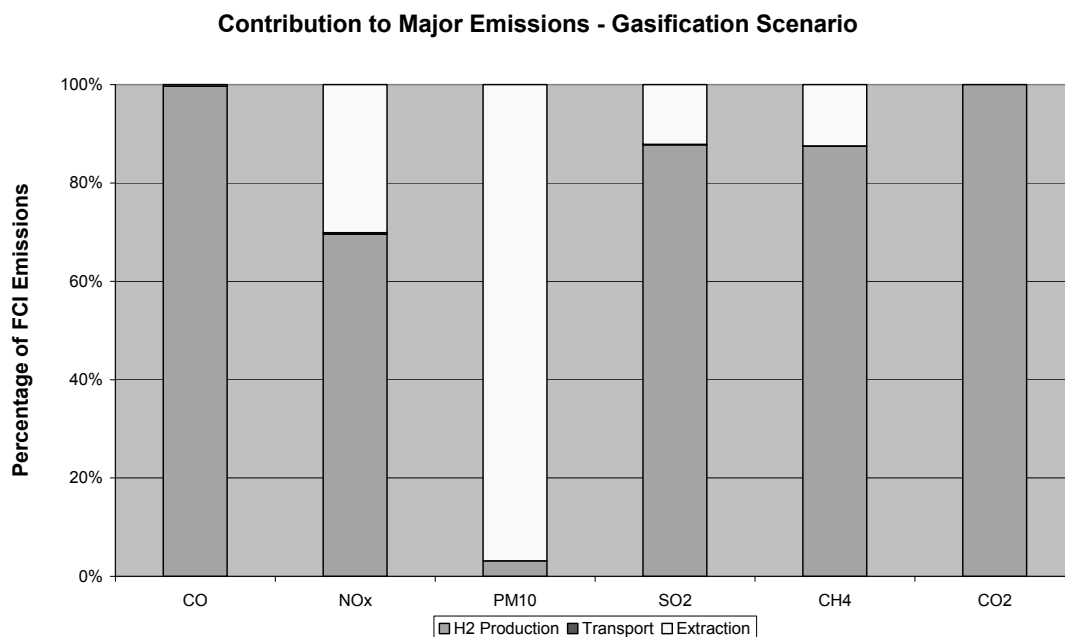


Figure 11: Contribution of Fuel Cycle Stages to Overall Emissions - Gasification

The high rate of particulate emissions from mining relative to the hydrogen production plant in the gasification situation Figure 11 is due to the high removal efficiency of particulates required by the process. Particulate emissions from mining include coal dust, dust from excavation and emissions from diesel fuel use primarily.

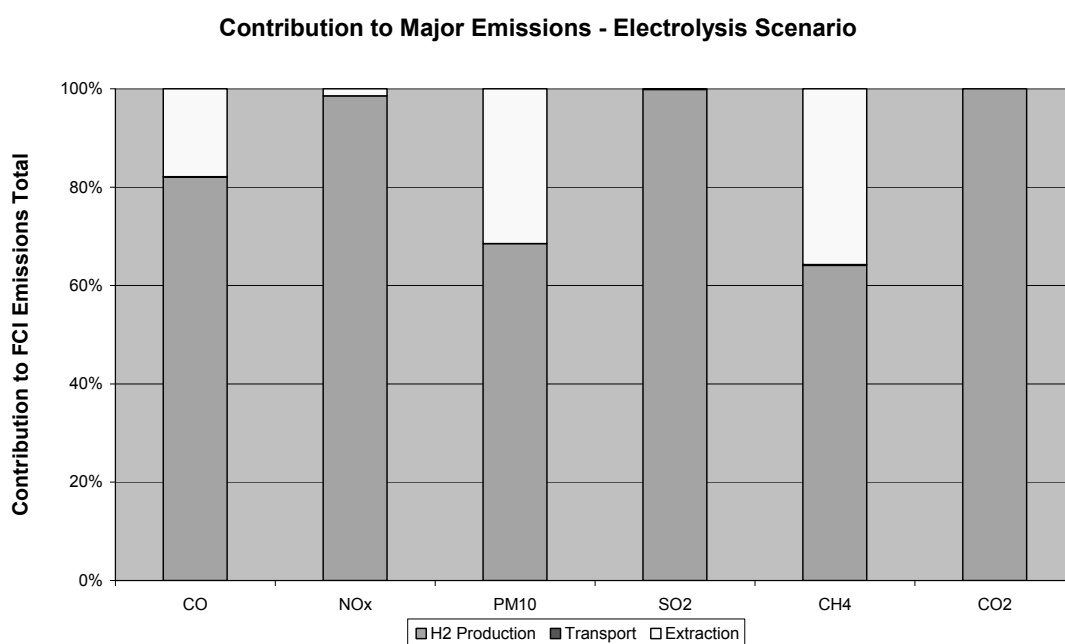


Figure 12: Contribution of Fuel Cycle Stages to Overall Emissions - Electrolysis

Again, in Figure 12 it is observed that the emissions of particulates are high from the extraction operation however, the electrolysis plant has a lower efficiency of particulate removal and thus in this case, the production stage has higher emissions than extraction. SO_x contribution from coal extraction is also lower, as the electrolysis plant has no desulphurisation, which leads to higher emissions, whereas the gasification plant necessarily has low sulphur rates to avoid damage to the plant (Innes, 2003).

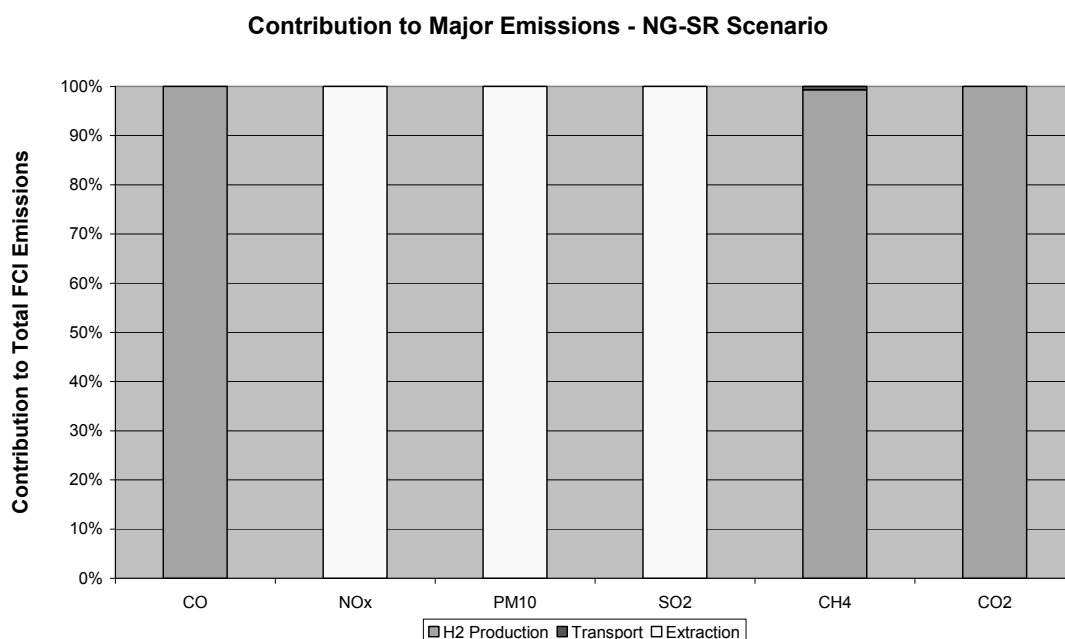


Figure 13: Contribution of Fuel Cycle Stages to Overall Emissions - NG-SR

Fugitive emissions and flaring of gas lead to comparatively high NO_x, PM₁₀ and SO_x emissions from extraction in the NG-SR scenario (Figure 13). The levels of emissions from this scenario are low in overall terms as well, which provides an excellent contrast with the coal scenarios.

4.3 Comparison with Existing Work

A comparison of the FCI results with existing work gives an indication of the accuracy of the modelling and estimation methods utilised. The emissions from the

electrolysis scenario will not be compared, as they are modelled directly off the Tarong power station, so that the comparison would be an exact match.

4.3.1 Gasification

The comparison of the gasification scenario can be made on the basis of the IGCC configuration of the plant for electricity production (at the coal feed rate as for hydrogen production). The major work in the field with data allowing comparison is that of Nunn, Cottrell et al. (2001). This study used a basis of 1MWh of electricity to compare a number of technologies for the production of electricity on a Life Cycle Basis. The scope included construction, extraction and provision of fuels and consumables, transportation emissions and waste disposal. Table 10 shows the emissions given for the different stages compared with the current work. The comparison was made as close as possible by utilising the same distance of transport and the same coal composition.

Table 10: Comparison of Emissions for IGCC Fuel Cycle for the Current work and ACARP (Basis: 1MWh of electricity, 44% overall plant efficiency (HHV))

	ACARP				Current Work			
Emission	Total	Electricity	Mining	Transport²	Total	Electricity	Mining	Transport
GHG³ (kg CO₂-eq)	766	739	19	4	726	722	4	0.05
NO_x (kg)	0.59	0.54			0.15	0.09	0.05	0.001
SO_x (kg)	0.15				0.02	0.02	0.002	~0
PM₁₀⁴ (g)	20.7	19.9			190	6	181	0.03
Power Station Parameters								
Coal Usage (kg)			345			334		
Fly Ash (kg)	17.8					31		

² Both assessments assume 20km transport of coal

³ Power station construction contributes <0.25% to Greenhouse Gas Emissions (GHG) so was not removed from this figure

⁴ Fugitive emissions of dust from coal stockpiles not included in ACARP

The GHG emissions for the Electricity production stage match closely due to the assumption of identical coal composition, with some minor differences due to plant efficiency (45% in the current work versus 44% in the compared work). GHG emissions from Mining are 5 times lower for the current work, while transport emissions are roughly 1% of the ACARP values. The mining value difference is most likely owing to the inclusion by ACARP of the fugitive methane emissions, which are not included in the current work, as the NPI workbooks do not cover these emissions. The difference in transport emissions is unusual, for although the current work has been based on rail transport, which may typically emit 3 or 4 times less than road transport, 80-100 times less is more than the typical variation. The assumptions of Nunn, Cottrell et al. (2001) are not explicit in the rates of transport emissions used, so further analysis cannot be undertaken, but fuel consumption rates and assumed fuel conversion rates could be behind the difference. Nunn, Cottrell et al. (2001) compared their own overall GHG results with other existing LCA's and found that all of them were within a range of 12-15% of each other. The current work fits well within this range (only 5% lower than Nunn, Cottrell et al. (2001)).

NO_x emissions in the current assessment are 6 times lower, and SO_x an order of magnitude lower than the ACARP assessment. This may be due to the different data sources – the current work is based on extrapolation from data from the Buggenum plant (Williams, 2001), whereas the ACARP assessment uses a different source.

The current work calculates particulate emissions from mining using data from NPI workbooks and other government monitoring and policy bodies (NRM, 2004; NPI, 2005). The ACARP assessment has a much lower total emissions rate (an order of magnitude). This may reflect the general nature of the data used in the current work, and in particular the inadequacies of the NPI workbooks, or the significance of omitting the loss from coal stockpiles that was assumed in the ACARP assessment.

4.4 Conclusion

The Fuel Cycle Inventory was performed, and analysed in terms of internal and external comparability. It is apparent that the GHG emissions match closely with

existing work for Australia, but assumptions in regard to transport and particulate and acid emissions may have contributed to some major differences in non-GHG emissions. Taken as a whole, these results validate the FCI to be further used as the basis for assessing the sustainability of hydrogen generation systems in Chapter 7.

One of the most important outcomes of the FCI, is identification of the fact that the highest emitting stage of the fuel cycle is the hydrogen production facility for almost all emissions, by significant amounts.

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Chapter 5

Sustainability Metrics Model

5.1 Introduction

This chapter is concerned with the development of the sustainability metrics model to simulate the environmental effects of emissions to the environment. It is the aim of this chapter to provide a detailed description of the model developed for the current work, both from a conceptual and a mathematical perspective. To address the limitations of current sustainability metrics assessment, the approach taken in this work is to build a model based on emissions to the environment as air sheds and catchment areas, atmospheric reactions, soil take up, percolation and run off. To describe the complexities associated with environmental conditions, the model is integrated as a series of tanks, reactors, pipes and control systems. This approach leads to an engineering systems assessment, which allows the spatial discretisation of sites, thus giving a more realistic description of locations based on their specific environmental conditions.

5.2 Sustainability Metrics

As previously mentioned, the model was developed from the Environmental Burden (EB) approach described in the literature (Tallis, Azapagic et al., 2003), incorporating the following advances that should improve the accuracy of sustainability assessment:

1. an emissions transport model (ETM)
2. reaction rates and other on-going dynamic environmental processes
3. quantification of the carrying capacity (environmental resilience and limitations) of the local environment
4. Spatial discretisation of impacts
5. Ensuring that the model is non-data-intensive, but capable of comparison of different locations and processes.

These factors will be explained explicitly hereafter.

5.2.1 General Form of the Metrics

There are two major impact categories in terms of ecological sustainability that can be readily measured and incorporated as metrics: contaminant increase and resource depletion. These categories can be examined in terms of the airshed, watershed and land impacts as the fundamental, underlying support bases for both the economic and social systems.

5.2.1.1 Contaminant Increase

Emissions from a process enter the surrounding environment and cause a deviation from the natural or ambient baseline concentrations. Often, especially in the case of non-reactive atmospheric emissions, it is possible to estimate the pattern of increase as a function of distance and time. In this work, the atmospheric transport model described in the proceeding sections is used for this purpose.

The effects of such deviations from natural conditions are difficult to predict in many cases, due to the complex nature of ecosystems – in particular the biological components. However, based on an understanding of the various processes and components within the environment, it is possible to estimate the carrying capacity of an environment, against which the process may be weighed to determine the ecological sustainability.

Figure 14 shows the theoretical baseline, carrying capacity and process influence on contaminant concentrations in a theoretical volume around a process for a time period of 1 year. For the sake of simplicity, it is shown here as a two dimensional graph, neglecting the third axis, which is time, and the forth dimension, which would be a second measure of distance or direction in order to give 2 spatial dimensions. Figure 14 shows that not only the process contribution, but also the carrying capacity may vary over distance (as indeed the baseline may – especially in the case of soil

contamination). This is due to the influence of environmental factors. For example, if the contaminant in question affects humans more readily than the rest of the environment, then an area with more people would have a lower carrying capacity than a deserted area. Typical sustainability metrics do not take the spatial location of impacts into account, however, it is obvious from even this simple example that spatial location is very important.

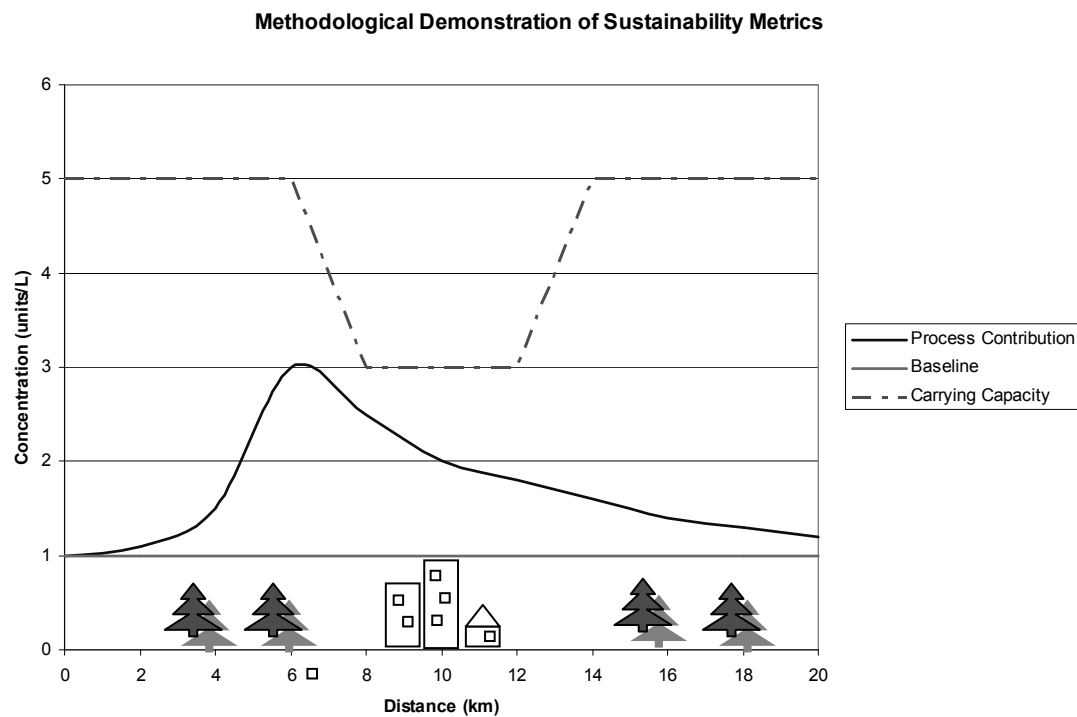


Figure 14: Sustainability Metrics Concept for Contaminant Increase Spatially

Temporally, the typical sustainability metrics consider the concept of contaminant increase as per Figure 15 - the plant emits contaminant at a steady rate, which causes constant increase in the environment. Thus the emissions from the process can be taken as the ultimate sustainability metric.

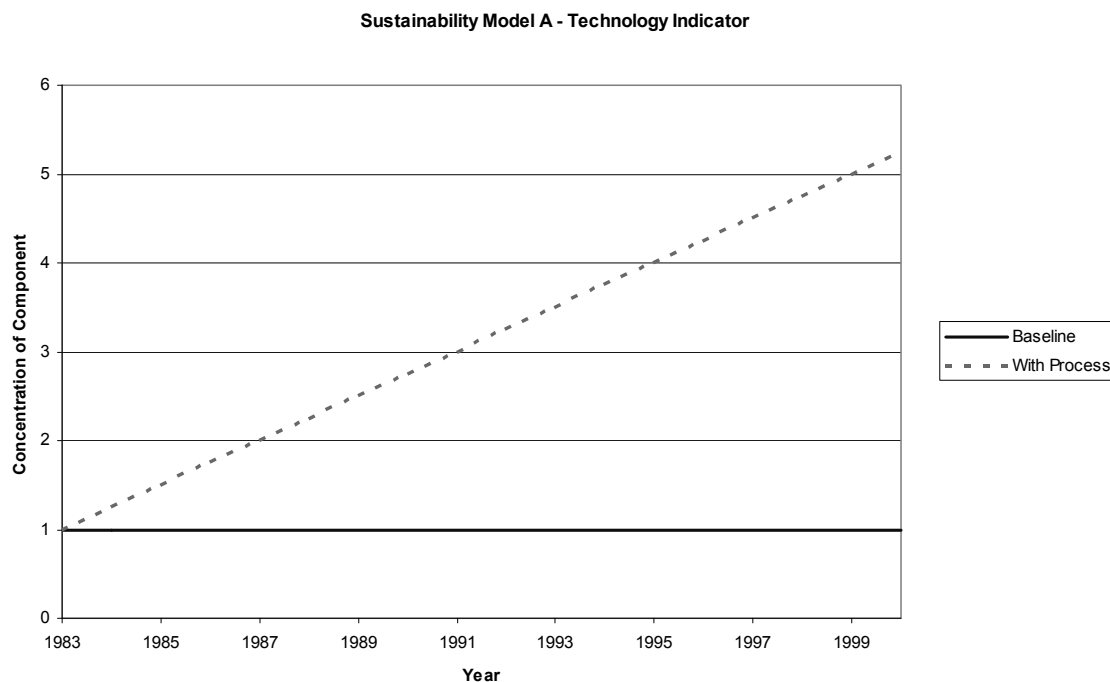


Figure 15: Typical Sustainability Model

However, it is apparent from past experience that there is always a limit to contaminant increase before detrimental environmental or human health effects begin to occur. This threshold or limit of environmental resilience is termed the “carrying capacity” in this work. Utilising the existing model of sustainability metrics, with the addition of the carrying capacity, we observe that, over the lifetime of the process, emissions may breach the environmental limitations as in Figure 16.

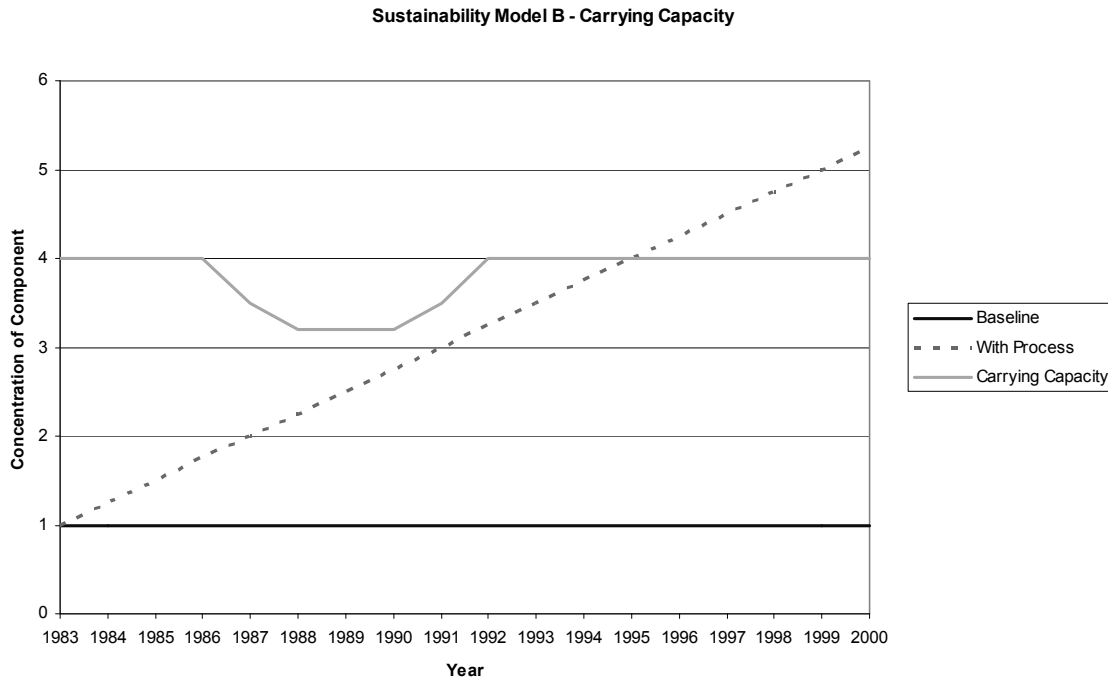


Figure 16: Typical Sustainability Concept with Threshold

When we consider the actual processes that occur in the environment, it is apparent that there are many fluxes, sources and sinks of contaminant components that imply that the released contaminants do not remain solely in the immediate vicinity of the process, and that somehow many components are broken-down or processed in the environment for useful purposes. Thus the concentration of a compound emitted to the environment in many cases does not increase in a linear fashion, but its impact is “buffered” by the environment. Depending upon the rates of emission, dilution, removal by physical, chemical and biological processes, the concentration of contaminant may reach a new equilibrium level before breaching the carrying capacity of the environment (Figure 17). The baseline and carrying capacity vary with the receiving environment, which will be a significant factor in terms of comparison of sustainability across localities.

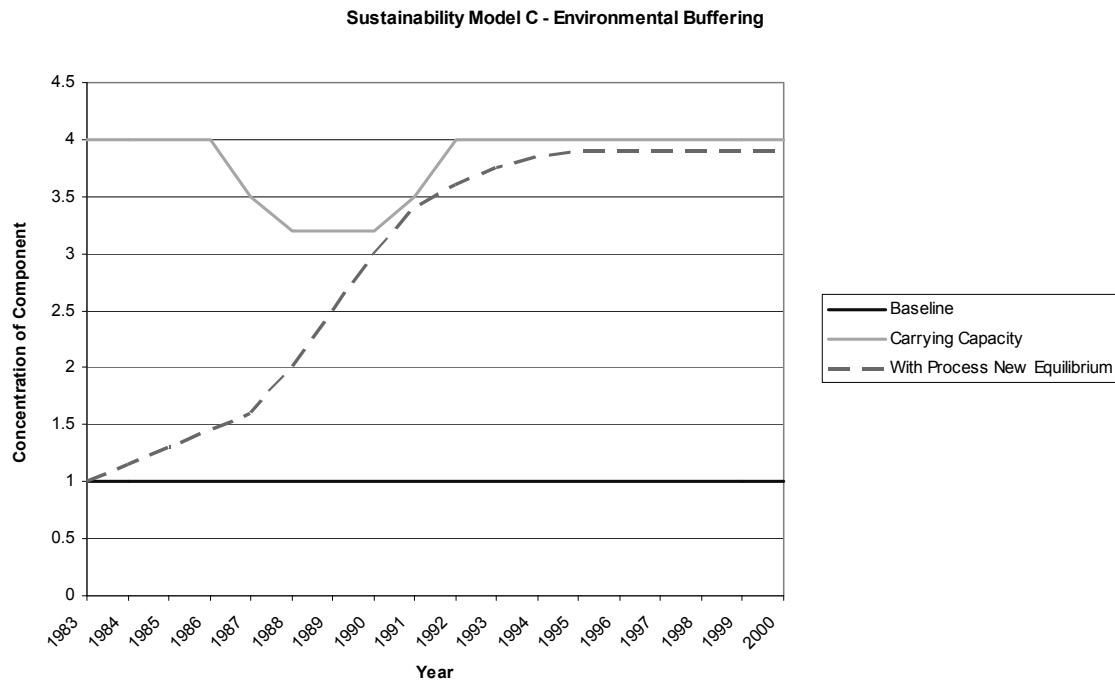


Figure 17: Sustainability with Environmental Buffering

The situation in Figure 17 is however, still a very idealised one, in which the baseline of the contaminant as naturally found in the receiving environment is constant, and the flows in and out of the system are nicely controlled, such that the increase in the concentration follows a beautiful, smooth equilibrium curve. Reality is rather different unfortunately, as the baseline varies with diurnal, seasonal, physical and climatic variation. Thus the real state of contaminant increase in the environment may be something more similar to Figure 18.

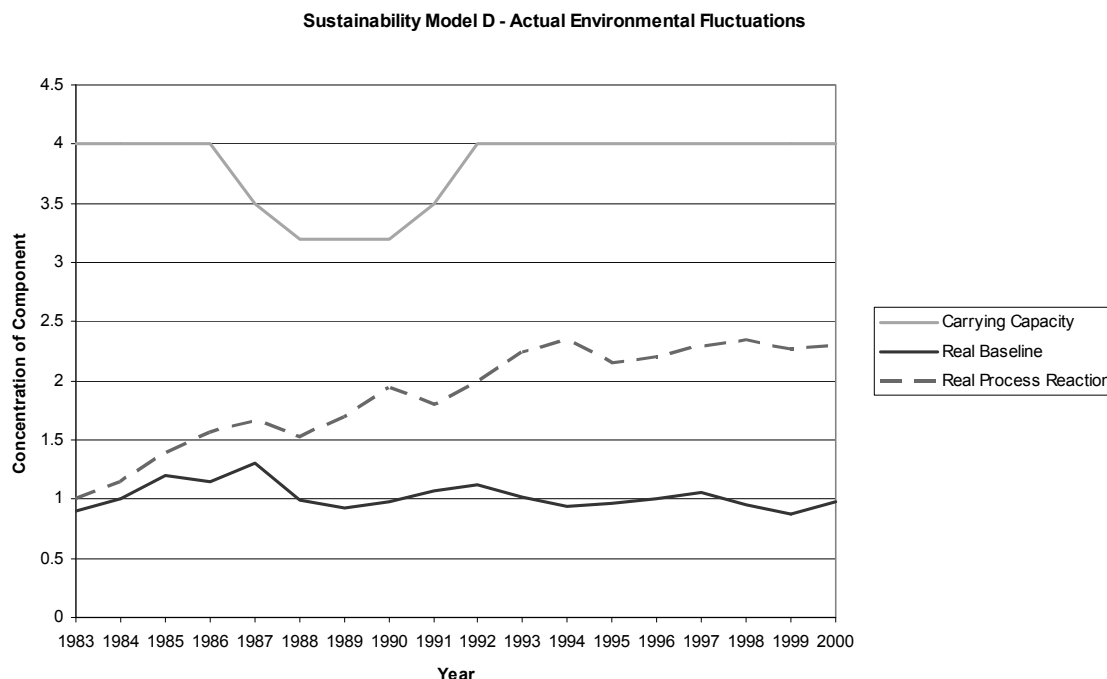


Figure 18: Sustainability with Actual Environmental Behaviour

The purpose of the current work then, and the challenge of a new methodology of sustainability assessment, is the development of metrics which incorporate a model that predicts environmental variation of emissions, compares the situation with the “no process” situation, and comes out with a measurable indicator that can compare differences in receiving environment.

5.2.1.1.1 Variability of the Carrying Capacity

Before continuing, a note on the variability of the carrying capacity is warranted. Figure 19 indicates a number of ways in which the carrying capacity may vary – reversibly, non-reversibly or partially reversibly. The situations indicated are for a negative variation in carrying capacity, but the positive variations are also possible.

As an example of non-reversible change in carrying capacity, we may take the building of a city in the vicinity of the process. If the contaminant affects human health, then the introduction of people into the receiving environment will reduce the capacity of the environment to carry an emission. A city is a relatively permanent addition to the environment which would therefore cause a permanent, irreversible reduction in carrying capacity. Along the same lines, a temporary pipeline

construction camp would be a reversible reduction in carrying capacity, as it would be gone after completion of the project at hand. A partially reversible change might be the construction of an adjacent process plant, which would have a large number of people on site for construction, followed by an operational phase with a much lower on-site population.

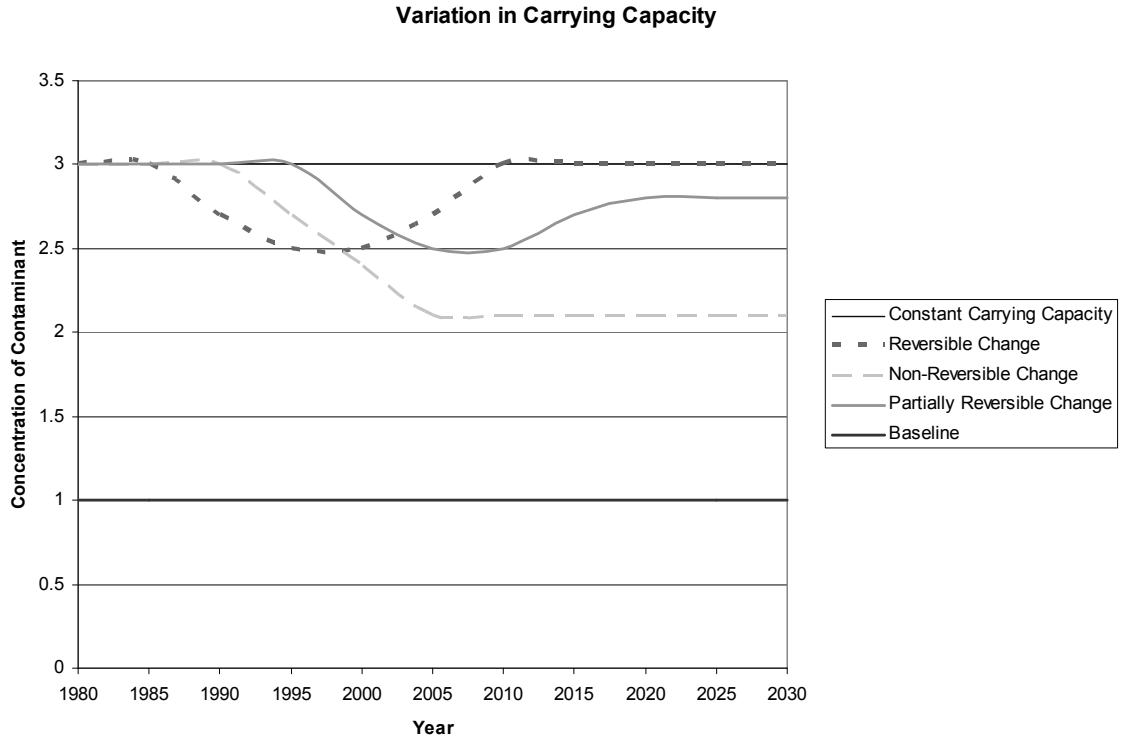


Figure 19: Variability of Carrying Capacity

5.2.1.1.2 Sustainability Metrics

Thus the sustainability metric can be derived from knowledge of the baseline, carrying capacity and the equation or form of the contaminant contribution curve by determining the percentage overall breaching of the carrying capacity over the 2 spatial dimensions. Hence, Equation 7:

$$SM_i = \left\{ 1 - \frac{\iint_{d_1, d_2} f(d_1, d_2)}{\iint_{d_1, d_2} [CC(d_1, d_2) - B(d_1, d_2)]} \right\} \times 100\% \quad [7]$$

Where, f , CC and B are the emissions function, carrying capacity and baseline, respectively in terms of the two spatial dimensions, and SM_i is the sustainability metric for component i.

For a single time period, this is sufficient, however, looking at sustainability in the true sense as a time dependent function, we can create a time-series of the sustainability metric outputs for a given component, thus giving a further graph for comparison, or where possible, can incorporate time and integrate prior to the spatial integrations. Hence, Equation 8:

$$SM(t)_i = \left\{ 1 - \frac{\iiint_{d_1, d_2, t} f(d_1, d_2, t)}{\iint_{d_1, d_2} [CC(d_1, d_2, t) - B(d_1, d_2, t)]} \right\} \times 100\% \quad [8]$$

Special cases of contaminant increase are the globally important substances such as greenhouse gases and ozone depleting substances. In such cases, the spatial dimensions become unimportant, as the effect is assumed to be equivalent no matter what the location. Thus the equations may be simplified down to Equation 9:

$$SM(t)_i = \left\{ 1 - \frac{\int_t f(t)}{\int_t [CC(t) - B(t)]} \right\} \times 100\% \quad [9]$$

however, the magnitude of the total carrying capacity in comparison to a single process is vastly larger, thus the metric would diminish in comparison to the overall global capacity. Therefore, in the case of impacts of a global scale, it is deemed most useful to utilise the actual emission of substance from the process, as used in most standard metrics (e.g.-(Azapagic and Perdan, 2000)).

The overall conclusion of the SM approach taken here, is that the higher the SM percentage value, the closer the plant is to 100% sustainable. The carrying capacity indicates the value of the contaminant level beyond which the environment can no longer buffer the effects of the plant impact, and hence when the SM value is 0% or below (i.e. – where $f / (CC-B) \geq 1$) the sustainability can be considered 0. Negative sustainability values only help to indicate the magnitude of carrying capacity

excedence, hence for the current work, negative sustainability values are considered to be 0.

5.2.1.2 Resource Depletion

The category of Resource Depletion is applied to the usage of non-renewable resources, land-use and water consumption. In a slightly different manner to contaminant increase, resource depletion categories can be measured in terms of the baseline resource availability. The difference with resource depletion is that it is more likely to be viewed as a regional or global scale problem, rather than as a spatially-specific variable. In this case, it is possible to discard spatial variation, and look solely at the time-variability of the resource.

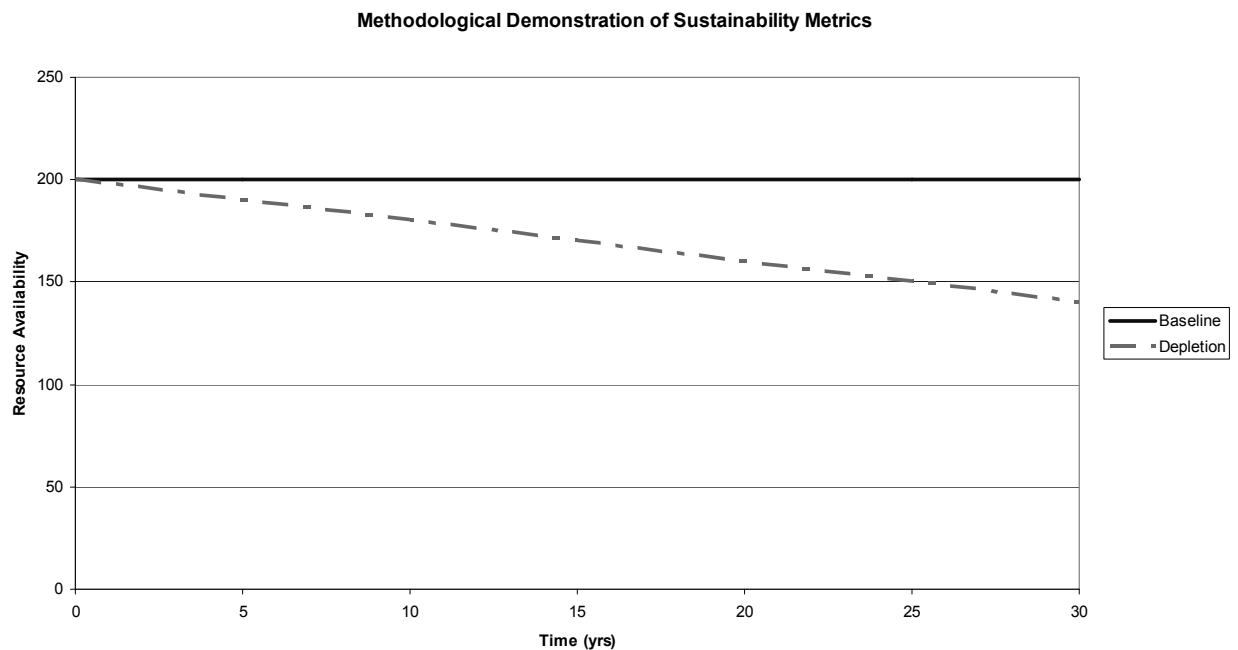


Figure 20: Sustainability Metrics Concept for Resource Depletion

The sustainability metrics could then be derived as a percentage usage of total available resource over the time period of interest, Equation 10:

$$SM_i = \left\{ 1 - \frac{\int_t f(t)}{\int_t [CC(t) - B(t)]} \right\} \times 100\% \quad [10]$$

One difficulty with this is that the baseline of available resources may vastly outweigh the resource depletion, in which case, the sustainability metric will approach one, and differentiation between alternatives will be difficult. In such cases, the regional availability may be used to reduce the baseline.

5.2.1.3 Determining the Baseline and Carrying Capacity

Determination of the baseline concentrations of contaminants or the current availability of a given resource may be difficult to achieve accurately due to lack of monitoring or inherent uncertainties in estimation methods. Added to the difficulty in terms of the contaminant concentrations is the fact that much of their presence in nature depends heavily on seasonal factors and ongoing climatic trends that make for a variable baseline. In order to eliminate the influence of these latter factors, it is proposed to use the long term annual average where available. In terms of the resource availability, data sources must be chosen wisely, so as to hopefully achieve a reasonably accurate result – however, if the same figure is used for comparison of alternatives, it can at least be assured that any errors will be uniform.

The carrying capacity is even more difficult to accurately predict, as in most cases it is only realised when catastrophic ecological collapse occurs within an ecosystem. Some fields are more advanced than others in the determination of carrying capacities. Much work has been done on the effects of acid compounds on soils and plants, and some work has examined the eutrophication of waterbodies. Where there is no certain estimation technique, the EPA's environmental emissions limits can be utilised as a surrogate carrying capacity.

5.3 Emissions Transport Modelling

5.3.1 Model Design

The modelling of the emissions transport and environmental system, and the integration of sustainability metrics is accomplished using the Microsoft Excel spreadsheeting program, as with the FCI. Environmental transport, reaction and impact assessment of pollutant emissions are all integrated into a single model, with a process approach allowing simple model development. Airsheds and soil are modelled using a set of simple “fixed-box” model type “tanks” connected in series radially outward from a central emissions point (as described in De Nevers (2000)), with reactions assumed to occur in reactors within the tanks (see Figure 21). A number of sub-airsheds are linked together to model the overall transport of emissions throughout an airshed (as per Figure 22).

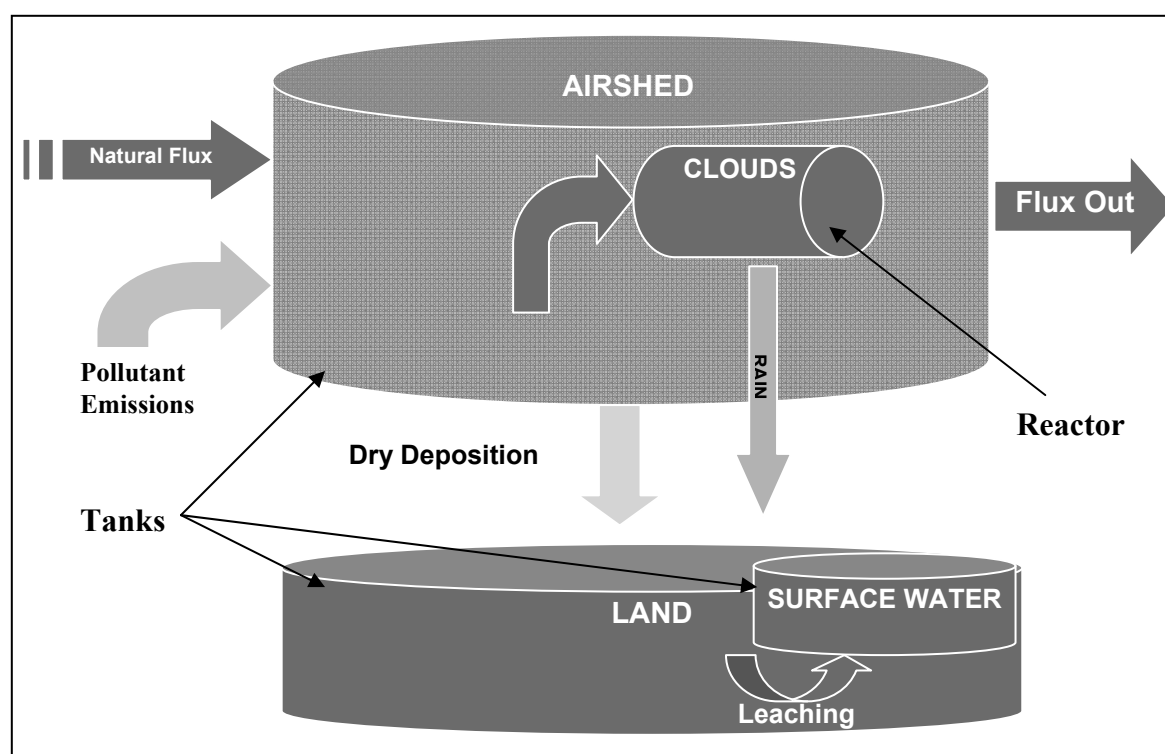


Figure 21: Process Modelling of Environmental Transport and Reaction

As shown in Figure 21, the pollutant is emitted to the first sub-airshed, where it is assumed to be instantaneously diluted to give a uniform concentration across the sub-airshed. Based on a percentage of cloud cover, some of the pollutant enters clouds within the airshed, where most atmospheric aqueous-phase reactions occur. Pollutant is deposited to soil and water via both dry and wet deposition, while some of the remaining airborne pollutant is passed on to the next sub-airshed in a wind-related flux. Some of the deposited pollutant is leached from the soil to the water-bodies within the sub-airshed. Ground water and Surface water reservoirs have not been modelled here due to the lack of historical data on the relevant contaminant concentrations, but they are the ultimate environmental sink for contaminants. It is recommended that further work, beyond the scope of the current study, examine the integration of ground and surface water quality into the model, with monitoring data collected for validation purposes. This would provide a more accurate indication of overall sustainability.

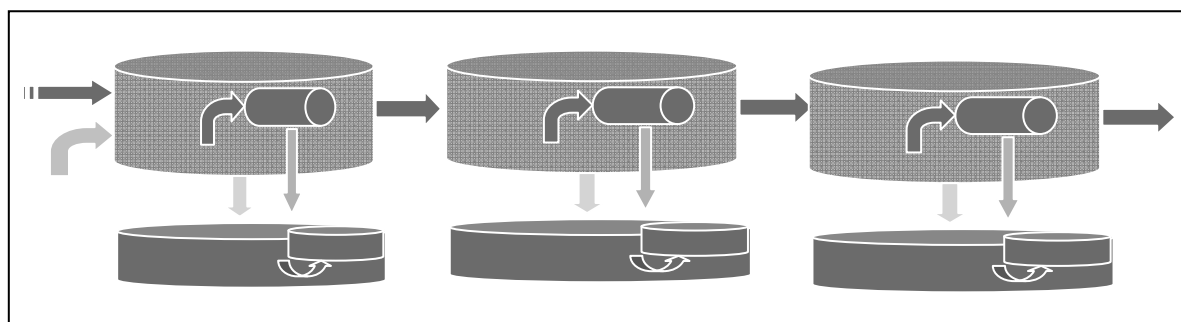


Figure 22: Linked Sub-airsheds for Overall Airshed Modelling

Expanding the process engineering approach further, we can develop a Process Flow Diagram for the environment-process system (Figure 23). The distribution of contaminant between clouds and the remaining “clear air” is modelled as a flow splitter, whilst the environmental relationship between rainfall and leaching is modelled as a flow control loop.

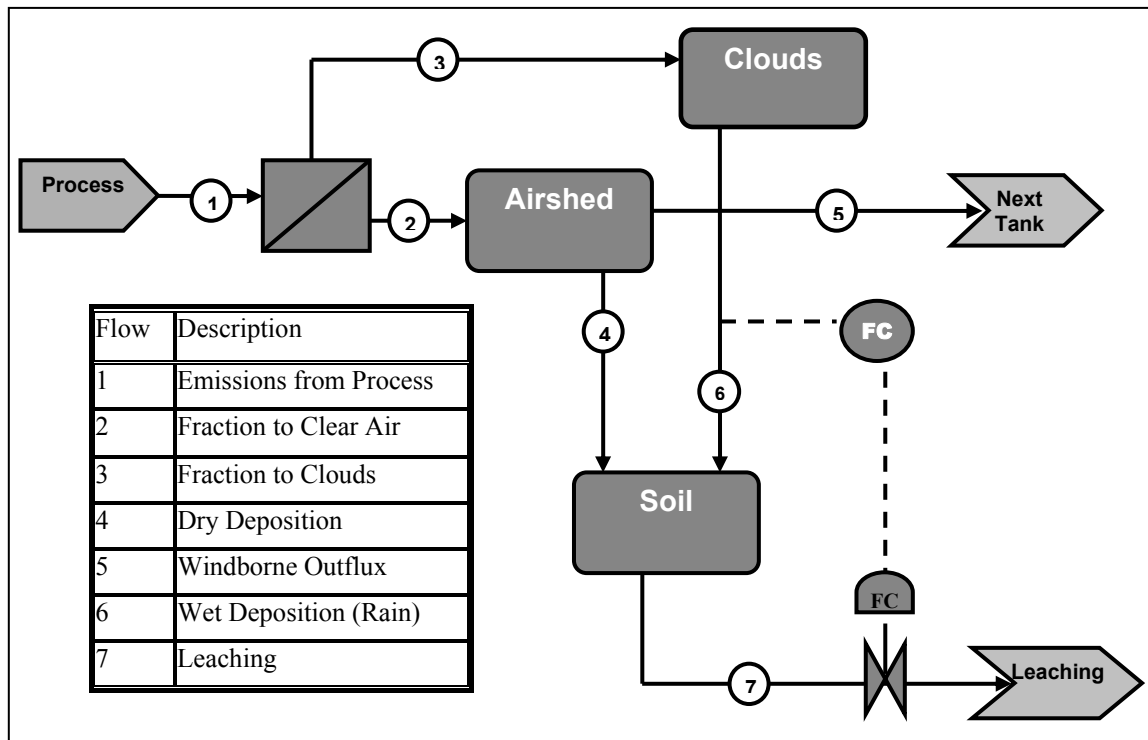


Figure 23: "Single Tank" Process Flow Diagram for the Emissions Transport Model Tank

Existing models typically utilise Gaussian plume models for the transport of air-borne emissions, but few of them apply this any further than determining the concentrations and deposition rates at various distances from the source. The current methodology allows variations in local conditions to be modelled by adjustment of environmental parameters within the airshed or indeed any individual sub-airshed.

5.3.2 Sub-Airshed Volumes

As theoretical mixing volumes, rather than actual tanks, the sub-airsheds can be modelled as volumes of any geometrical shape. Here, the model has been considered in terms of cylindrical tanks, which lend themselves to ease of calculation as separate sub-airsheds, but not necessarily when they are placed as part of the complete model. Emissions are assumed to travel only in a radial direction from the plant, carried by the wind. Intuitively, dilution of emissions with increasing distance suggests that the sub-airsheds in the model should increase in volume with increasing distance from the plant (as shown in Figure 24).

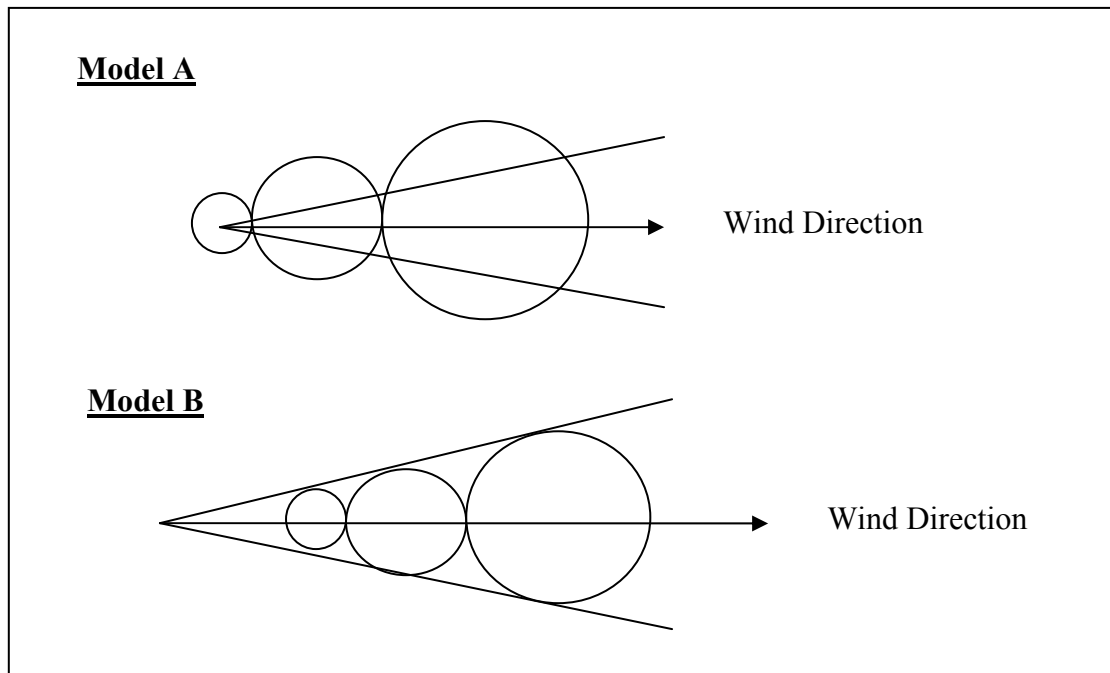


Figure 24: Cylindrical Sub-airsheds of Increasing Radius for ETM

As shown in Figure 24, the cylindrical sub-airsheds either extend outside, or do not completely fill the sector of interest. This is not a critical flaw, due to the prior assumption of inherent error however, it is possible to remedy this by assuming that the overall airshed is shaped as a large cylinder, with sub-airsheds being sectors of the cylinder as depicted in Figure 25.

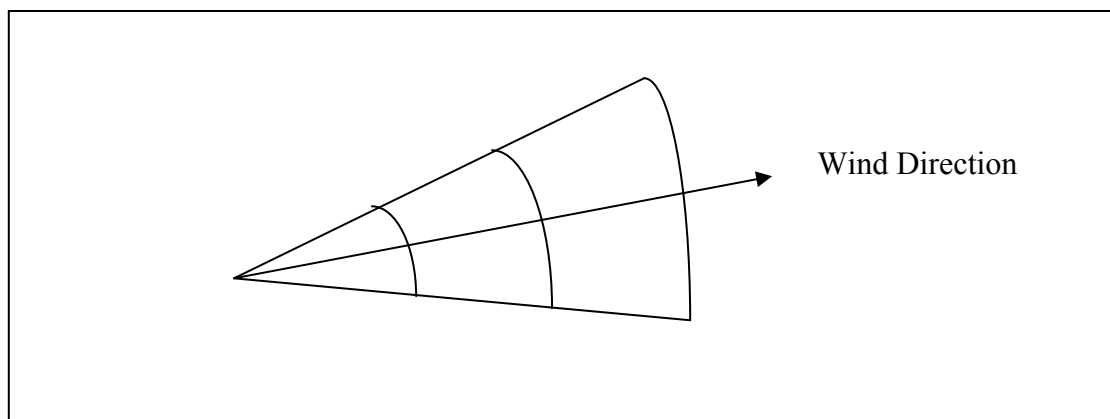


Figure 25: Radial, Sectoral Model of Airsheds for ETM

Figure 26 shows the overall picture in terms of the overall airshed. The suggested model uses flux over the fraction of the surface of the inner sub-airshed within a given

arc at a set wind velocity to determine the flowrate of pollutant from sub-airshed to sub-airshed.

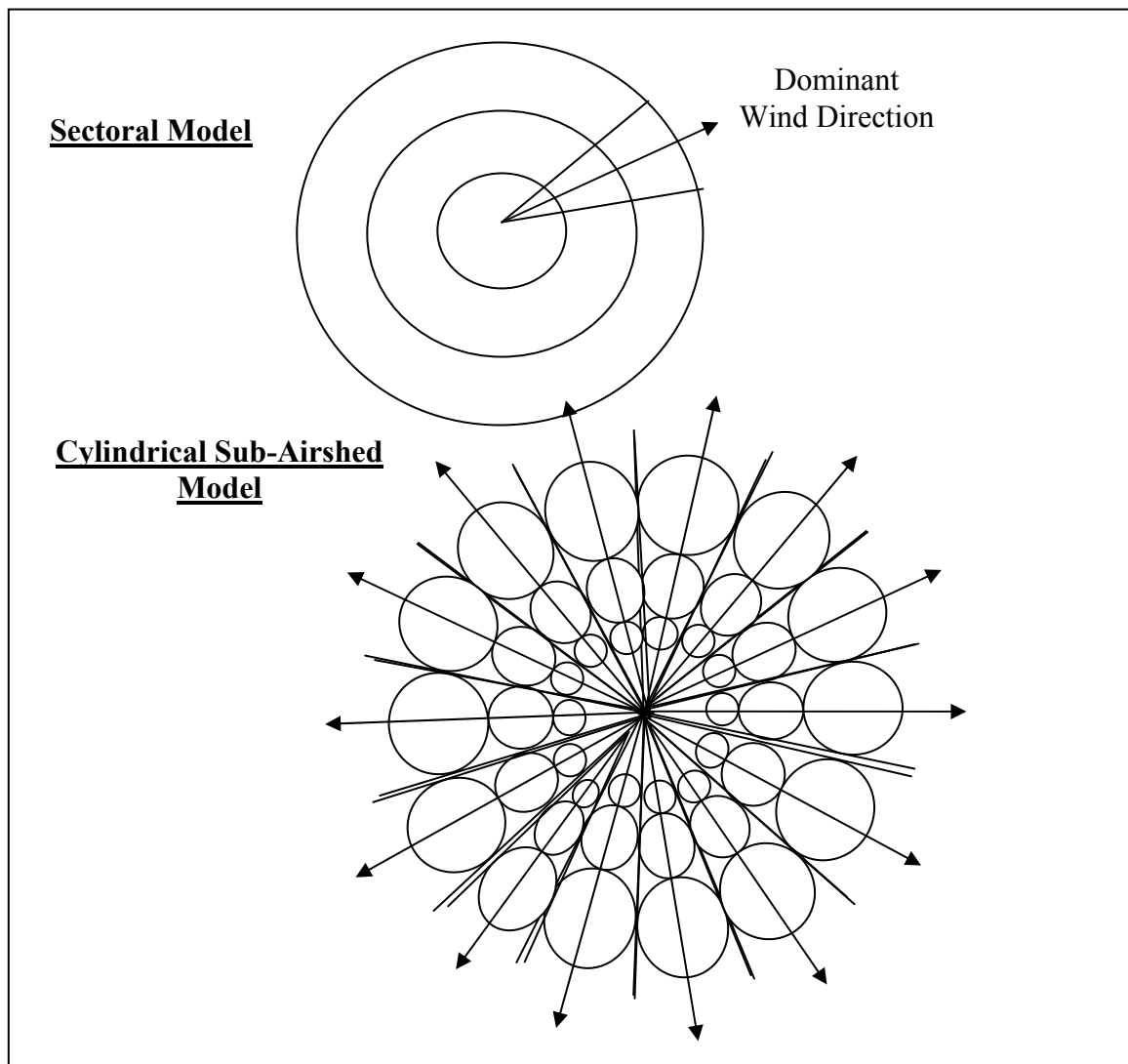


Figure 26: Sub-Airshed Volume Shape Models

The “Cylindrical Sub-airshed Model” was chosen in the end, due to the reduction in mathematical complexity resulting, although the “Sectoral Model” model may conform more closely to reality. The chosen model allows simple *discretisation of impacts* in the context of an *Emissions Transport Model* incorporating *reactions and ongoing environmental processes*, thus fulfilling criteria 1-4 of the methodology.

5.3.3 Equations Resulting from the Process Approach

The mathematical derivations of equations utilised in the ETM for the contaminant increase metrics is given in the proceeding sections. Following the process approach, a mass balance over the relevant tanks, and application of first principles was utilised to determine change in concentration over time.

5.3.3.1 Temporal Variation of Contaminant Concentration in Sub-Airsheds

Using the innermost sub-airshed as an example, a simple mass balance of the form:

$$\text{accumulation} = \text{in} - \text{out} + \text{generation}$$

we derive the following equation:

$$\frac{dM}{dt} = NF_i + E_i - NF_o - D \quad [11]$$

where:

$$NF_i = \text{Natural Flux In} = b.v.SA_1 \text{ (}\mu\text{g / s)}$$

$$E_i = \text{Emissions Rate (}\mu\text{g / s)}$$

$$NF_o = \text{Natural Flux Out} = c.v.SA_2 \text{ (}\mu\text{g / s)}$$

$$D = \text{Deposition} = u.c.FSA \text{ (}\mu\text{g / s)}$$

$$M = \text{Total Mass of Compound (s)}$$

$$b = \text{background concentration (}\mu\text{g / m}^3\text{)}$$

$$c = \text{concentration (}\mu\text{g / m}^3\text{)}$$

$$v = \text{wind velocity (m / s)}$$

$$u = \text{deposition velocity (m / s)}$$

$$FSA = \text{bottom surface area (m}^2\text{)}$$

$$SA = \text{vertical surface area (m}^2\text{)}$$

Under the assumption of steady state, this can be shown to lead to the concentration equation:

$$c = \frac{b.v.SA_1 + E_i}{v.SA_2 + u.FSA} \quad [12]$$

If however, we assume a dynamic system, with accumulation, then the subsequent derivation of the 1st order differential equation follows:

$$\begin{aligned}
\frac{dM}{dt} &= b.v.SA_1 + E_i - c.v.SA_2 - c.u.FSA \\
\frac{V.dc}{dt} &= [b.v.SA_1 + E_i] - [v.SA_2 + u.FSA]c \\
\frac{dc}{dt} &= \frac{[b.v.SA_1 + E_i]}{V} - \frac{[v.SA_2 + u.FSA]}{V}.c \\
\therefore \frac{dc}{dt} &= Q - P.c \\
\therefore c &= \frac{Q}{P} + \alpha.e^{-Pt}
\end{aligned}$$

for the known conditions ($t = 0$, $c = b$):

$$c = \frac{Q}{P} + \left[b - \frac{Q}{P} \right] e^{-Pt} \quad [13]$$

Likewise, if we follow the substitution and solution of the differential equations for each sub-airshed, we will be able to determine an equation giving the concentration assumed to be at the centre of each sub-airshed over time. The factor of distance can be left separate for the time being, in order to simplify the process, and is the simpler variable to incorporate, as it will depend on either a basic trigonometric or linear function in the radial direction. The subsequent derivations are given in Appendix 3, with the resulting concentration equations in terms of time given below for the next 3 sub-airsheds:

$$\begin{aligned}
c_2 &= \frac{vSA_2}{V_2} \left[\frac{Q}{PP_2} + \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) e^{-Pt} \right] + Ke^{-P_2t} \\
c_3 &= \frac{v^2SA_2SA_3}{V_2V_3} \left\{ \left[\frac{Q}{PP_2P_3} + \left(\frac{b - \frac{Q}{P}}{(P_2 - P)(P_3 - P)} \right) e^{-Pt} \right] + \left[\frac{bV_2}{vSA_2} - \frac{Q}{PP_2} - \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) \frac{e^{-P_2t}}{(P_3 - P_2)} \right] \right\} + K_2e^{-P_3t} \\
c_4 &= \frac{vSA_4}{V_4} \left\{ \frac{vSA_3}{V_3} \left[\frac{vSA_2}{V_2} \left[\frac{Q}{PP_2P_3P_4} + \left(\frac{b - \frac{Q}{P}}{(P_2 - P)(P_3 - P)(P_4 - P)} \right) e^{-Pt} \right] + \frac{Ke^{-P_2t}}{(P_3 - P_2)(P_4 - P_2)} \right] + \frac{K_2}{(P_4 - P_3)} e^{-P_3t} \right\} + K_3e^{-P_4t}
\end{aligned}$$

However, on examining the limits of the dynamic equations in comparison with the steady state system, it can be seen that the dynamic system rapidly approaches the steady state ($-P.t$ approaches $-\infty$ rapidly when t is in seconds). For example, if the airshed radius and height are both 1km:

$$\begin{aligned}
P &= \frac{[v.SA_2 + u.FSA]}{V} \\
&= \frac{(3 \times \pi \times 1000 \times 1000 + 0.008 \times \pi \times 1000^2)}{\pi \times 1000^2 \times 1000} \\
&= 0.003
\end{aligned}$$

If $P = 0.003$, then $P.t = -1$ after 333s or 5.55min, and after an hour the dynamic system is already close to steady state. Hence in the case of atmospheric pollutants, it is acceptable to utilise the steady state approximation, which leads to the following equations for the subsequent airsheds:

$$\begin{aligned}
c_2 &= \frac{c_1.v.SA_1 + b.v.(SA_2 - SA_1)}{v.SA_2 + u.FSA_2} \\
c_3 &= \frac{c_2.v.SA_2 + b.v.(SA_3 - SA_2)}{v.SA_3 + u.FSA_3} \\
&\dots
\end{aligned}$$

5.3.3.1.1 Clouds

Clouds can be incorporated in the model, either as reactors, or merely as a vessel to allow a different route for deposition – i.e. wet deposition. Cloud contaminant concentrations may be assumed to be in equilibrium with the surrounding atmosphere, with concentrations determined by Henry’s law. For the moment, we assume the form of the contaminant is unimportant, so that we can disregard aqueous reactions. Thus, the cloud mass balance becomes Equation 14:

$$0 = q_r.k.P - q_r.c_r \quad [14]$$

As the air “tank” concentration is assumed to be steady state, the concentration of contaminant in the air, and hence the concentration of contaminant in rain water, is constant within each “tank”.

5.3.3.2 Temporal Variation of Contaminant Concentration in Soil

The soil tank is of much interest due to the potential for deposition resulting in impacts such as soil acidification and land contamination that could cause health impacts on flora and fauna. Most existing models neglect the transport of contaminants out of the soil, with the impact assumed to be due to the entire load deposited. The inputs and outputs to the soil are indicated in Figure 27.

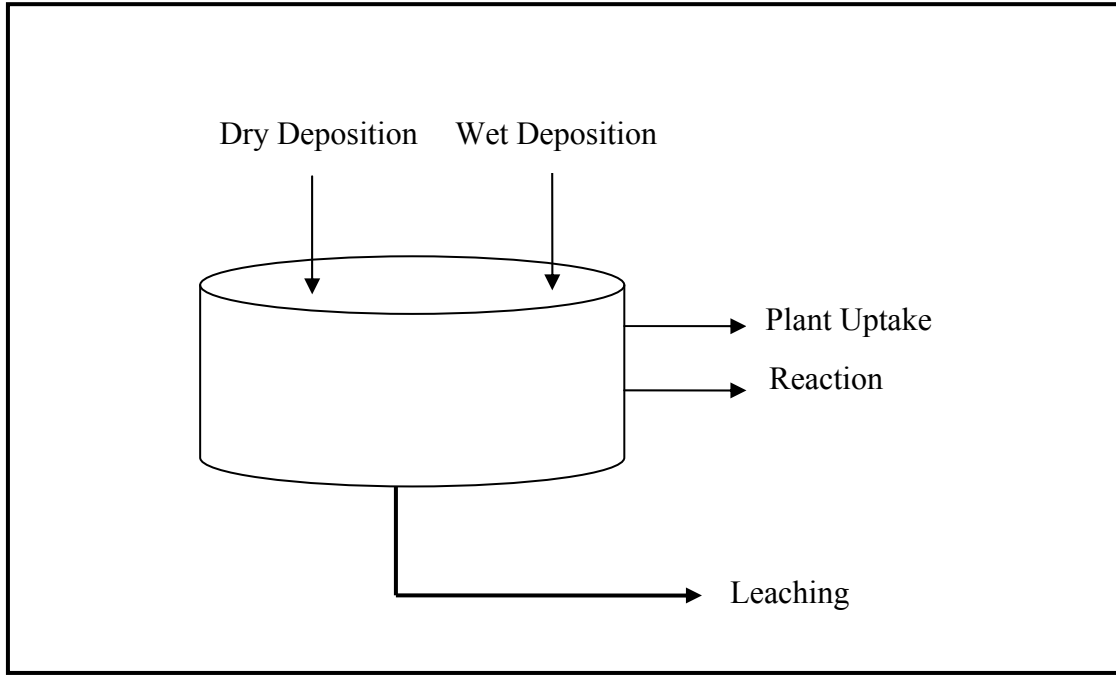


Figure 27: Inputs and Outputs to the Soil "Tank"

Thus the mass balance over the soil may be written as:

$$\frac{dM}{dt} = u.c_1.FSA.(1 - \mu) + q_r.c_r.FSA.(1 - \mu) - r_p.FSA.(1 - \mu) - K_L q_r.c_s - r_s \quad [15]$$

K_L here, is a factor incorporating the fraction of rainfall that is removed by run-off (F). K_L is also the control function of the flow controller in Figure 23. The value of F is related to the rate of run-off (slow, medium, high).

$$K_L = F \left(\frac{q_{r(t)}}{q_{r(N)}} \right) \quad [16]$$

After determining the general solution of the differential equation, a second factor (G), based on the permeability of the soil, which determines the relative effect of permeating rainwater on the bulk neutral soil component concentration, is incorporated in the constant of integration.

$$K_P = G \left(\frac{q_{r(N)}}{q_{r(t)}} \right) c_{s0} \quad [17]$$

These location-specific factors are used to adjust the fraction of rain over a neutral, average value that contributes to wash-out of contaminants. Each site has its own permeability and run-off rates, which show a close connection to the contaminant concentrations (see Chapter 6).

Assuming no soil reactions (this will be included in the carrying capacity estimation) and removal by vegetation, the mass balance may be written in simplified form as:

$$\begin{aligned}\frac{dc_s}{dt} &= Q - P \cdot c_s \\ \therefore c_s &= \frac{Q}{P} - \alpha \cdot e^{-Pt} \\ c_s &= \frac{(u \cdot c_1 + q_r \cdot c_r)}{K_L \cdot q_r} - \alpha \cdot e^{-\frac{K_L \cdot q_r \cdot FSA \cdot (1-\mu)}{V_s} t} + K_p\end{aligned}\quad [18]$$

Where the factor α can be determined from the initial conditions: $t = 0$, $c_s = c_{s0}$;

This dynamic process can be modelled in a spreadsheet by discretisation into yearly values, which allows the incorporation of annual rainfall data (obtained from the Bureau of Meteorology).

5.3.3.3 Incorporation of Spatial Dimensions

Some spatial dimensions of individual sub-airsheds (Surface area, Volume) are already incorporated within the temporal modelling equations given above. However, to track the dispersion, and the sustainability indicator, over at least the simplified 2 dimensions of the Earth's surface in the location of interest, equations or methods of integration are necessary. A polar co-ordinate set was chosen, as most processes can be seen as having some centre, which is the major emitter of pollutants and the major economic focus. This also lends itself to ease of incorporating some of the climatic data and conversion to compass bearings from the plant. Based on these assumptions, we will first examine the radial dimension.

As described previously, the sub-airshed tanks are considered to expand in size within the tangential limits of a sector of the compass – with an inner angle of nominally 45° to fit the typical wind rose data format. Most large modern emission sources are designed with dispersion to required limits in mind, thus incorporating high stacks. This usually means that little of the pollutant actually enters the air within close

proximity of the plant. According to initial work and other models (Katestone, 2005), the typical initial point of impact seems to be in the range of 2-4km. If we assume a first sub-airshed, r_1 , as having a radius of 1.5km, then geometrically, we can determine the radii of subsequent sub-airsheds and the central airshed.

The central radius, r_c , is calculated from the angle of increasing radius by:

$$r_c = \frac{\left(1 - \tan\left(\frac{45^\circ}{2}\right)\right) \times r_1}{\tan\left(\frac{45^\circ}{2}\right)} \quad [19]$$

The location of the centre of the first sub-airshed can then be calculated:

$$d_1 = r_c + r_1 \quad [20]$$

and subsequent airshed radii can be calculated by:

$$r_2 = \frac{\tan\left(\frac{45^\circ}{2}\right) \times (d_1 + r_1)}{\left(1 - \tan\left(\frac{45^\circ}{2}\right)\right)}$$

$$r_{n+1} = \frac{\tan\left(\frac{45^\circ}{2}\right) \times (d_n + r_n)}{\left(1 - \tan\left(\frac{45^\circ}{2}\right)\right)}$$

It is possible to expand the model to an unlimited number of airsheds however, for the current work, it was believed that as soon as 100km was reached, that would be sufficient. Mt Isa mines work (Gilmour, Mayhew et al., 2001) has indicated that this assumption is reasonable, and with an angle of increase set at 45° , this means that the radii of the tanks do not increase beyond reasonable limits. The total number of sub-airsheds would, including 5 concentric rings of 8 sub-airsheds and the inner airshed, thus amount to 41.

In order to locate the impacts in terms of radial distance then, the impact over a given sub-airshed is assumed to be the average impact occurring at the centre of the sub-airshed.

The airsheds expand in radius as we move radially outwards from the central airshed. This means that the surface area increases, whilst the concentration of sulphur decreases. As the concentration decreases, relative error due to inaccuracies in data or

tuning of model parameters, is likely to increase. These characteristics may also lead to differences in sensitivity in the outer airsheds, as compared with the inner airsheds. This effect was not examined, as the results of the model matched closely with existing Gaussian plume models, which was considered acceptable as validation.

5.4 Application of the Metrics

The equations thus derived, give temporally and spatially discretised output data covering the surroundings of the process for the entirety of its operational lifetime.

With the environment of the process being thus discretised, it is possible to determine the specific local effects within each sub-airshed. To determine the overall sustainability of the process for a given impact category, the respective sustainability as compared to the carrying capacity should be the average over the land area of each sub-airshed, and this overall average utilised as the overall indicator.

This method should provide a good estimate of the sustainability in most cases, however the case may arise (due to unusual environmental conditions) where the carrying capacity is breached in one of the sub-airsheds, but all other airsheds are well within the limitations. Using an average in this case would not reveal the local sustainability for that particular section of the environment. It may be possible to provide an indicator for each airshed, but the practicality of this – where 41 indicators were involved for each category of impact - would seem limited. Instead, it may be more practical to utilise not only an overall average per unit of area, but also to include an average for each “band” of sub-airsheds. Thus the 8 innermost airsheds would be averaged together, the 2nd set of 8 out from the centre, and so on, with the central airshed counted separately. Thus, with the overall average, there would be merely 7 indicators. However, with this method as well, it is possible for important results to be concealed, in the case of 7 low and only one high score. So it is advisable that all high scores be flagged in addition to the use of averages.

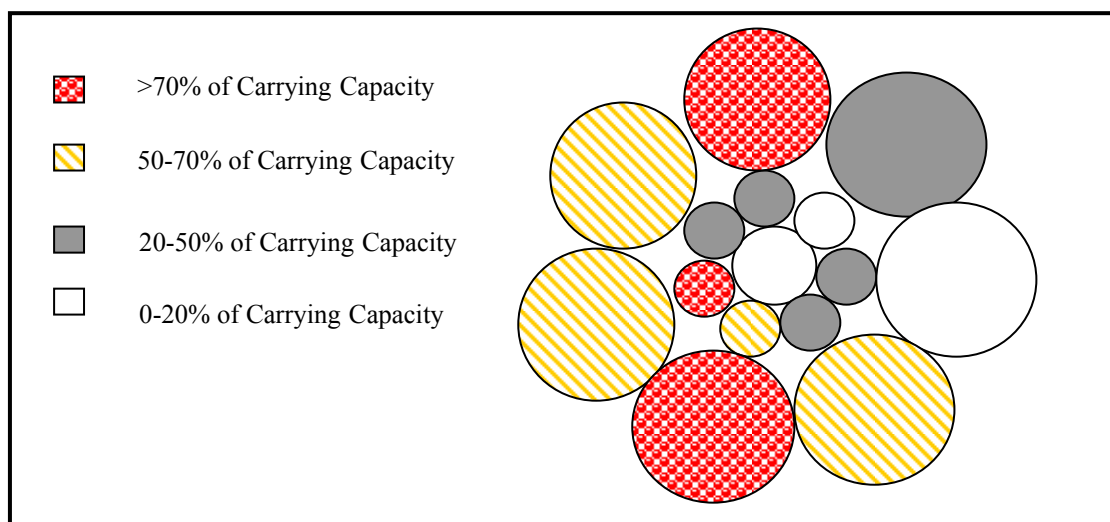


Figure 28: Pictorial view of the Sustainability Metrics Model as the Effect on Surrounding Environment

5.5 Conclusion

The model developed in the current work, and described in this chapter, overcomes the inadequacies of previous sets of sustainability metrics through the incorporation of an *Emissions Transport Model* and the inclusion of a method of comparison with the *environmental baseline* and *carrying capacity* of the receiving environment. Specific locational factors such as permeability and run-off rate are included in the ETM to trace the fate of contaminant emissions. Likewise, the carrying capacity and baseline of each site or airshed will depend on the specific soil conditions at that site. Some challenges are involved in the application of the metrics, as to the selection of an appropriate averaging method or flagging measurements that are in the critical level, such that their importance is not lost in an overall average.

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Chapter 6

Validation of the Model

6.1 Introduction

The fundamental hypothesis of the sustainability metrics (SM) model used in this work, as described in Chapters 3 and 5, is that local environmental parameters should be incorporated in metrics to overcome the flaws in existing models, which ignore local conditions. The Emissions Transport Model (ETM) forms the connection between the process emissions and the environment that allows local conditions to be incorporated in the metrics. This chapter describes the validation of the ETM based on historical data from Tarong power station. In addition to model validation, this chapter also addresses a sensitivity analysis to model parameters to verify the effectiveness of the model developed in Chapter 5. Environmental data always poses some dilemmas due to variations, and this is discussed in terms of the scope of the developed model.

6.2 Essential Data

As mentioned in Chapters 1-3, it may be argued that Australian coal-fired power plants offer the most suitable point of comparison for gauging the impacts of new energy technologies from the point of view of their relative seclusion, monitoring requirements and similarity of emissions to fossil-fuel based hydrogen production facilities (Murray, 1984; Diniz da Costa and Pagan, 2006). This avoids the difficulty of separating the contribution of the source to a given environmental impact from a complex matrix of emissions sources which poses challenges in other regions (Migon and Caccia, 1990; Thunis and Cuvelier, 2000; Tao, Larson et al., 2005; Wang, Carmichael et al., 2005). With this in mind, data was obtained from Tarong power station (Plenderleith, 1989) and augmented to provide 23 years of intermittent historical data. A similar study on deposition rates at a forest site in the USA over 23 years is the closest comparison available, but does not incorporate a single emissions

source (Likens, Bormann et al., 1990), which is the uniqueness of the current work. Apart from the operational and environmental monitoring data required, the climatic data was obtained from the Bureau of Meteorology (BOM), soil and land use data was obtained from Tarong Energy (Plenderleith, 1989), and from the Queensland Government Department of Natural Resources and Mines (NRM). Data requirements are listed in Table 11. Acquired ETM and SM data is provided in Appendix 4. Tarong emissions data and analysed data that is not under commercial-in-confidence is provided in Appendix 5.

Table 11: Data Requirements for Model Validation

Parameter	Source	Appendix
Fuel Cycle Inventory		
Coal Usage	(Buckley, 1989; Tarong, 2006)	5
Coal Analysis	(Buckley, 1989)	5
Emissions Rates	(NPI, 2006; Tarong, 2006)	5
Power Output	(Tarong, 2006)	5
Emissions Transport Model		
Daily Rainfall	(BOM, 2006)	4
Wind Patterns	(BOM, 2006)	4
Topology	(Woodward-Clyde, 1998)	4
Surface Water %	(Woodward-Clyde, 1998)	4
Sustainability Metrics		
Soil Characteristics	(Plenderleith, 1989), (AFFA, 2006; DPI, 2006)	4
Land Use	(Plenderleith, 1989; DPI, 2006)	4
Total Australian Coal Production	(BP, 2002)	4

The Tarong Crop and Forestry Study (Plenderleith, 1989) provides soil characterisation for the sites monitored over the period 1983 – 1987. Soil sampling and testing methodologies are described in Appendix 6. In order to validate the model, it was necessary to obtain data for the current situation. Therefore, using

identical testing methods to the original study, 3 of the sites deemed as the most appropriate (described in Appendix 6) were re-examined. Of the emissions from the plant, SO_x was selected for the purpose of model validation as one of the few contaminants which was monitored in Plenderleith (1989), one which has some comparative models for other countries (IIASA, 2001), and one of the most significant in terms of potential impacts (Larssen, Knudsen et al., 2006; NPI, 2006).

6.3 Model Results

Sites 15, 17 and 32 from the original study by Plenderleith (1989) were tested in 2006, and the data obtained was used to validate the model. The model was matched as closely as possible to the historical data by variation of location-specific factors. The relevant information on the selected sites is given in Table 12.

Table 12: Examined Site Details Relevant to the Model

Site Characteristics	Site 15	Site 17	Site 32
Landform	Hillslope (3degrees)	Hillslope (6degrees)	Footslope (3degrees)
Drainage	imperfect	well drained	poor
Permeability	moderate	high	slow
Runoff Rate	moderately rapid	very slow	moderately rapid
Distance from Stack (km)	19.3	7	4.3
Elevation (m)	550	590	400
Bearing from Plant (degrees)	274	181	335
Wind Direction Probability (%)	20.0	9.3	23.9
Atmospheric SO_x Concentration (µg/m³)	3.09	2.94	13.21

The following graphs show the soil concentration variation over time given by the model, with a calculated baseline value (indicating the soil concentration as it would be without the plant), and historical data with error bars based on the variation of sample measurements for each year (as obtained from Plenderleith (1989)). Please note that, as each site had a different base concentration of sulphur, the scales on each graph are necessarily different. The calculated baselines are solely based on background sulphur values (i.e. with no power plant in the airshed). For comparison purposes, the model can provide information on how the sulphur concentration of the soil varies in the case of: (i) baseline for background concentration only, (ii) full loading as conventionally used showing continuous accumulation of sulphur on soils,

and (iii) the model based on plant emissions incorporating environmental interaction. Calculated baselines are indicated in the legends as “Base”, model results as “Model” and historical data is indicated by the site number.

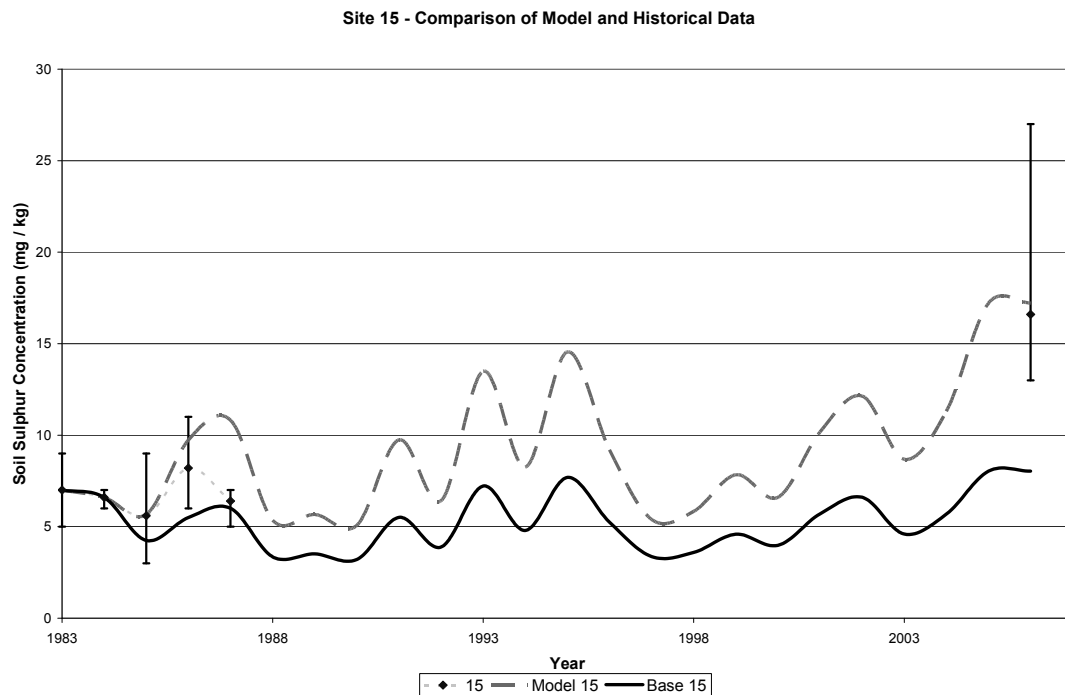


Figure 29: Site 15 - Soil Concentration Performance - Model, Baseline and Historical Data

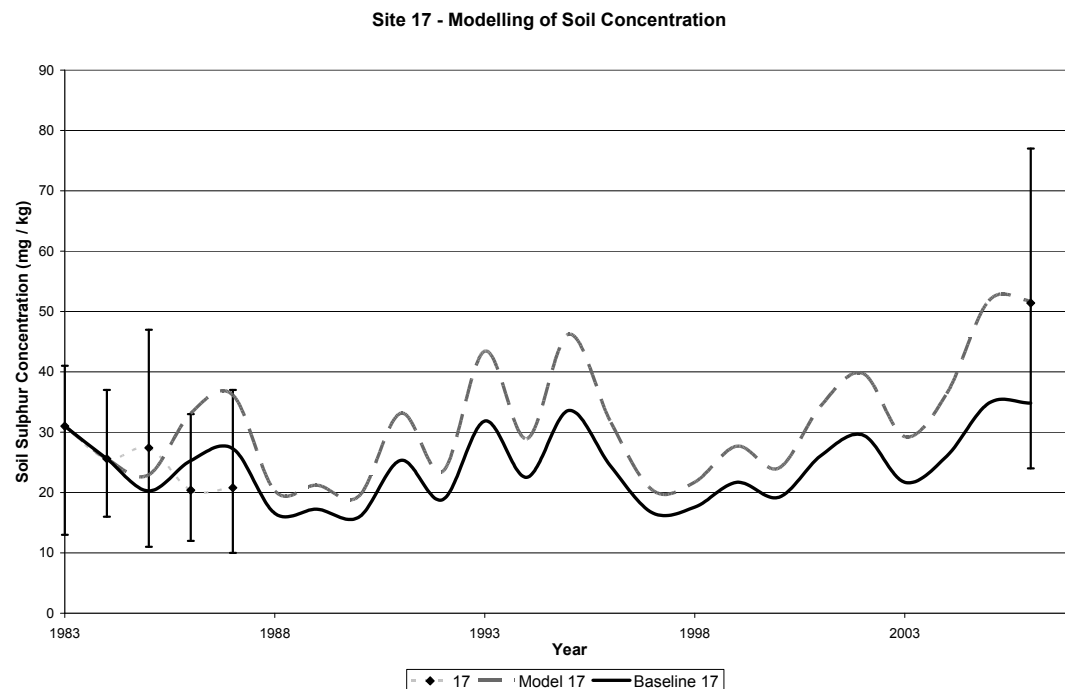


Figure 30: Site 17 - Soil Concentration Performance - Model, Baseline and Historical Data

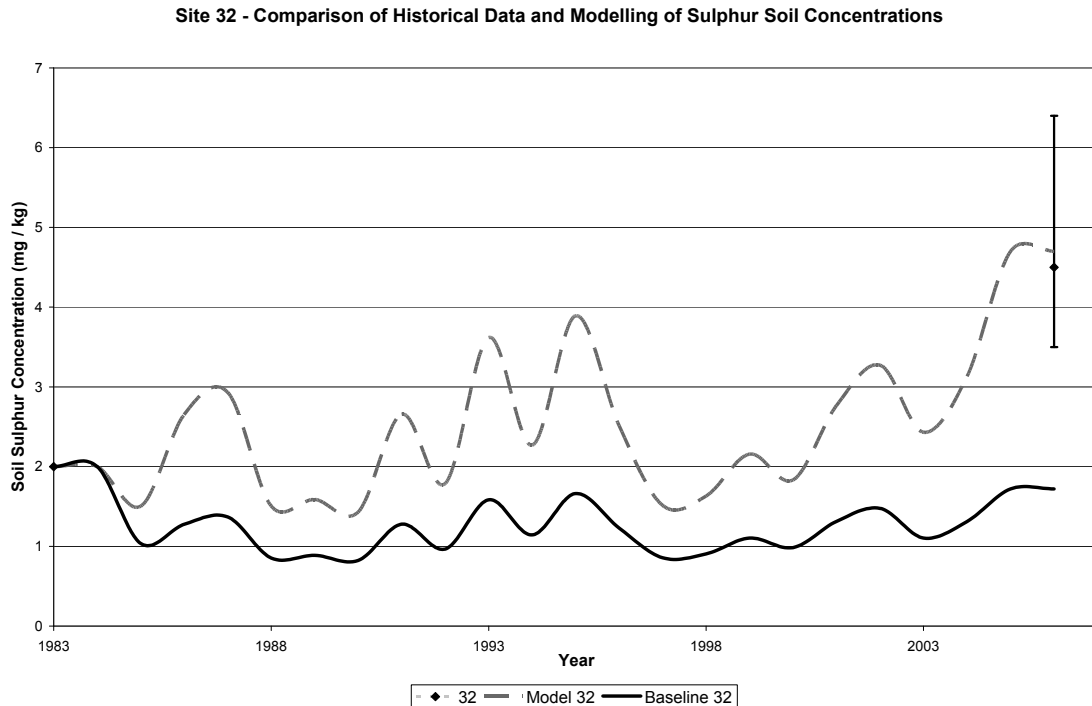


Figure 31: Site 32 - Soil Concentration Performance - Model, Baseline and Historical Data

Observing Figure 29 - Figure 31, a number of points may be noted:

1. The soil Sulphur concentration does not remain constant although the emissions are considered to be constant over most of the lifetime of the plant (with variations due to plant commissioning and extension).
2. The soil concentration varies in the same way across each of the sites.
3. The model results stay mostly within the range of the variation of measurements.
4. The baseline varies similarly to the model.
5. The difference between the model and the baseline is larger towards the end of the period.
6. The difference between the model and the baseline is larger during dry periods.
7. For site 17, and some parts of site 15, the baseline is within the range of error as well as the model.

To explain these observations, we must refer back to the process model utilised in this work, as illustrated in Figure 32.

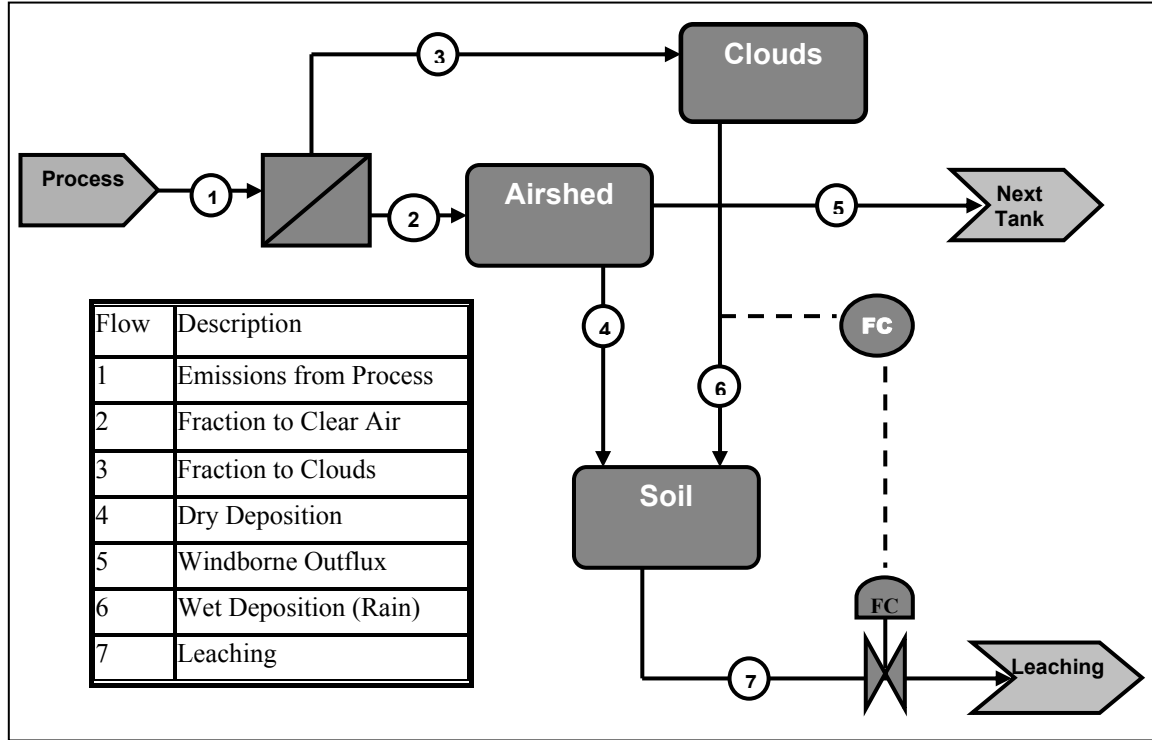


Figure 32: Process Flow Diagram for the ETM

Equation 19 gives the concentration of Sulphur in the soil or ground water, based on the mass balance.

$$c_s = \frac{(u.c_1 + q_r.c_r)}{K_L.q_r} - \frac{(u.c_1 + q_r.c_r)}{K_L.q_r} . e^{-\frac{K_L.q_r.t}{V_s}} + K_p \quad [21]$$

Where the control valve on the leaching output from the soil tank, has the flow control functions:

$$K_p = G \left(\frac{q_{r(N)}}{q_{r(t)}} \right) c_{s0} \quad [22]$$

and

$$K_L = F \left(\frac{q_{r(t)}}{q_{r(N)}} \right) \quad [23]$$

The physical reality of this theoretical depiction of the soil tank, is that contaminant is deposited at a constant rate onto the surface of the soil, but is removed to ground or surface water at a rate that is related to the rate of rainfall, and whether or not it exceeds the average rainfall which is the major control system for contaminant concentration in soils. To explain further, the model assumes that, prior to the construction of the process, the environment had reached an equilibrium level of

contaminant, whereby the natural processes of deposition and leaching were balanced at the average historical rainfall level. In years where an excess of rain fell, the concentration would be depleted by excess run-off and leaching, but in periods of drier weather, the deposition would outweigh removal rates (Shaw and Thorburn, 1985). In summary, the historical average rainfall could be considered the equilibrium point, and the leaching and run-off rates would be higher when rainfall exceeded that point, thus driving concentrations down, whilst less rainfall would lead to an increased concentration. Figure 33 shows the annual rainfall, and the historical average annual rainfall. By comparison with Figure 29 - Figure 31, it is apparent that, on the whole, the model follows the rainfall trend in the inverse, as would be expected (Hagedorn, Schleppi et al., 2001; Bolland, Yeates et al., 2003). In contrast to the rainfall however, the addition of atmospheric emissions from the process increases the atmospheric concentrations, which in turn increases the deposition rates. This causes the equilibrium soil concentration to shift to a higher level over time – augmented towards the end of the period of observation by a number of consecutive dry years.

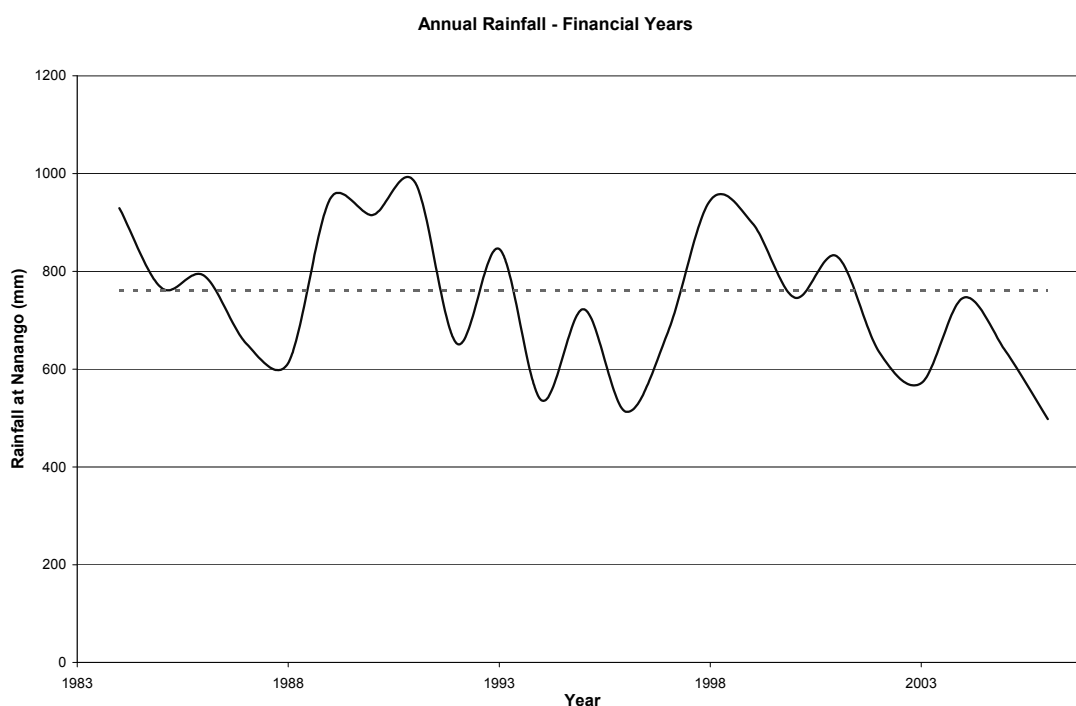


Figure 33: Annual Rainfall at Nanango Showing Historical Average

The baselines plotted in Figure 29 - Figure 31 are based on the atmospheric concentration of sulphur continuing at the pre-plant ambient level over the lifetime of

the process. The environmental variation due to rainfall occurs constantly, such that the baseline itself varies annually as is observed in the graphs. However, it is also to be noted that the baseline does not vary as widely, or reach a new, higher equilibrium, due to this constant, lower atmospheric concentration.

The only factor that changes between the process and no-process (baseline) situations is the atmospheric concentration. The fact that the model is differentiated more widely from the baseline in times of low rainfall, must therefore be due to the effect of the run-off and permeability terms on the removal rate, accentuating the difference in deposition due to atmospheric concentration difference. When the rainfall is high, the run-off factor has a higher impact on decreasing the concentration, whilst when the rainfall is low, the permeability plays the major role in causing an increase in concentration. This is true mathematically, and also when we consider the physical reality – in periods of high rain, the soil saturation is high, so the ground water flow is facilitated and wash-out occurs from the upper soil layers, whilst in periods of low rain, soil is unsaturated, hence sulphur removal is restricted. This agrees with the theoretical underpinnings of Fetter (1993) and Iwata, Tabuchi et al. (1995) and the findings of Bolland, Yeates et al. (2003) and Renck and Lehmann (2004).

The variability of measurements over each site – as demonstrated in particular by the variation in site 17 – make it difficult to clearly maintain that a variation between the baseline and the process-added situation occurs. However, for the other sites, most of the measured points are distinctly different from the baseline values, indicating some change due to the process operation. The reason that site 17, and some points from site 15 show this behaviour is that the atmospheric sulphur concentration at those sites is low, hence the differentiation is less than for site 32, at which the sulphur concentration difference is much higher.

Given that the sulphur concentration is much higher at site 32 due to its proximity to the plant, it would be considered that the soil concentration would increase more rapidly. In fact, the situation given no environmental processes other than deposition would lead to the situation shown in Figure 34. However, the measured sulphur content is not as high as would be predicted in the “full-loading” situation, which indicates that the model, which fits the observed data well, is more realistic – that in

fact much of the deposited sulphur is removed by environmental processes. This has direct consequences for the sustainability metrics methodology, as it proves that a loading-only model is not applicable to all situations, as actual environmental processes can reduce the overall impact of an emission.

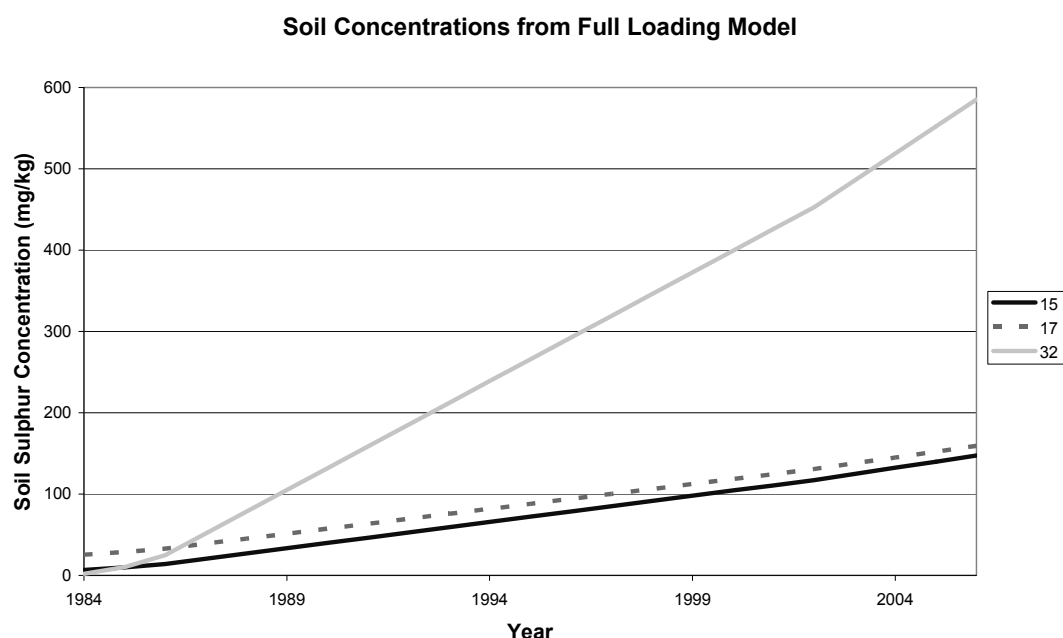


Figure 34: Full-Loading Model Behaviour on Soil Sulphur Concentration

A number of authors have examined this issue of loading versus incorporation of environmental parameters (Jin and High, 2004; Diniz da Costa and Pagan, 2006), and it is from this fundamental background that the idea of critical loads and carrying capacities (Cresser, 2000; Yossapoll, Caudill et al., 2002) has emerged. The obvious divergence of sulphur content in soils from the total loading idea expressed in Figure 34 gives an argument for moving towards a sustainability metrics system that includes environmental parameters, as being the ideal methodology for both comparison and absolute assessment of sustainability.

To examine the particular behaviour of each site, the slow permeability and moderately high run-off rate of site 32, mean that the sulphur is rapidly removed from the topsoil layers, keeping the concentration low. By contrast, site 17, having a slow run-off rate and high permeability, retains much of the deposited sulphur within the soil, thus the sulphur concentration increases to a high level over the period. Site 15

has characteristics similar to site 32, but has a lower removal rate, thus the concentration at that site increases to a moderate level over time.

Some of the measurements show trends that are counter-intuitive and thus the model does not fit such points well. These differences may be due to unincorporated environmental processes such as plant interactions, or high variation in site-specific local rainfall. These short-term dynamic processes are difficult to incorporate in the model without an intricate knowledge of the particular sites, and monitoring that is beyond the resources or practical limitations of any organisation, as identified in Cresser (2000). The limitation of the quantity of historical data available (3-6 points of data) also makes it difficult to determine whether or not the model is statistically valid however, the validation was completed to the extent possible within these limitations. As the model kept within the limits of the measurements on the most part, it was considered acceptable to omit further complexity, whilst admitting the limitations that environmental complexity imposes.

Although these major complexities are acknowledged, we argue that the natural system is in a steady state for the period of time tested in this work. Steady state is a typical assumption in acid deposition and critical load work – e.g. (Iivonen, Kamari et al., 1993; Hettelingh, Posch et al., 1995; Duan, Xie et al., 2001). In the current instance, the natural system being examined is a forest with minimal anthropogenic interaction. The only emission to the forest originates from the coal power plant. In fact, this is a unique situation in terms of the global experience, where the environmental effect can be directly allocated to one emissions source only. In most countries, the emissions from multiple sources need to be separated and impacts allocated accordingly. As the forest in question is mature, the rate of sulphur uptake by plants is compensated for by the sulphur release rate by decomposition of foliage deposited on the soil. As this work investigates the environmental effects over a 30 year period, any short term dynamic effects are considered to be insignificant. So for the purpose of this work, these biological parameters are not limiting factors on the concentration of sulphur in the soil. This agrees with the findings of Quilchano, Haneklaus et al. (2002).

Thus the behaviour of the model is observed to fit with the logical and mathematical predictions. Likewise, it is observed that fitting with the historical data indicates a high level of correspondence between the model and the actual environmental behaviour. The following sections analyse the model further in terms of sensitivity.

6.4 Model and Data Analysis

The errors inherent in the system are analysed in the proceeding sections to give some notion of both the precision of the model results, and the necessity for precision. The model applied in the current work takes a process systems approach with limitations in view of availability of historical data (in number of parameters and number of data points). In contrast, the reality of soil chemistry is exceptionally complex, involving a variety of factors that can change soil concentrations – in particular vegetation species, weathering rate, deposition of acid-neutralising compounds, decomposition rate of litter and soil matter (Berden, Nilsson et al., 1987; Likens, Bormann et al., 1990; Cresser, 2000). This can cause highly complex patterns of variation in sulphur concentration which cannot be accounted for with the current model. Hence, error is to be expected in the comparison of the model with the historical data - although it is seen from Figure 29 - Figure 31 that the general trend is closely matched. It is important to quantify the level of error in the model, and determine whether this is acceptable. Likewise, analytical methods have inherent error which contributes to the total error, but which is more easily quantified.

6.4.1 Errors in Analytical Methods

The soil analysis completed in the case of the most recent tests at the University of Queensland, indicates the error in the values obtained (Table 13) which is in agreement with other sources – e.g. (Budden and Collins, 1998; SPAC, 2000).

Table 13: Errors in Analytical Methods

Analysed Characteristic	Error (+/-)
pH	0.15
S	2.2 (mg/kg)

Thus, with the particular focus on Sulphur compounds, it is apparent that lower Sulphur content samples (Site 32), may be highly susceptible to error, as the error is of a similar value to the actual measurement. Errors in this case are summative, such that the error due to sample variation and the error in analytical variation should be summed to give the true potential variation of each point.

6.4.2 Variability over the Site

Table 14 and Table 15 show the variability for the most recent measurements over the sample site for Sulphur concentration and pH respectively. The 5 samples taken from each site indicate high variability over the small area of 400m² tested.

Table 14: Site Sample Sulphur Measurement Variability 2006

Site	2006 Sulphur Concentration Measurement (mg/kg)					
	Variability (mg/kg) / (% of Mean)	1	2	3	4	5
15	2.3 / 14	11.0	13.3	12.1	12.9	12.4
17	53.2 / 103	32.8	50.3	77.3	72.4	24.1
32	2.9 / 64	3.9	5.0	3.5	3.5	6.4

The results in Table 15 show that some sites appeared to have greater variability than others, whilst the variability itself is shown to be very wide. The implications of this are examined later. This data shows variability within the range shown in soils in Sweden (Berden, Nilssen et al., 1987), in northern Queensland soils (Noble, Middleton et al., 2002) and in northern New South Wales soils (Singh, Odeh et al., 2003).

Table 15: Variability and Error in pH Measurements 2006

Site	2006 pH Measurement					
	Variability (pH units) / (% of Mean)	1	2	3	4	5
15	0.35 / 5.5	6.45	6.50	6.23	6.58	6.26
17	1.8 / 32	6.06	4.59	5.0	6.39	6.0
32	0.47 / 8.4	5.50	5.87	5.40	5.62	5.8

From this sample data alone, it is apparent that the variability in terms of sulphur content in particular is very high over each sample site. This variability could cause deviations from the true mean value over the sample site. Given that only 0.02% of the surface area of the site is sampled, the statistical accuracy of the sampling methodology may be questioned (although to take more samples would be both time consuming and destructive to the site). Having said this, we had to maintain the same sampling methodology on the same sites as carried out in the initial sampling program from 1983 to 1987. This is the only way to show consistency and validity in data acquisition.

When compared with the analytical error, the variation over the site is much higher, thus the range into which the model must fit can be assumed to be within the variability of the site measurements, rather than limited to the error of the analytical methods.

6.4.3 Temporal Variability at Each Site

Temporal variability of the soil measurements is shown in Table 16. The variability of the soil analysis at each site over the first 5 years in particular, can be compared with natural variability. It is apparent that this variability of the mean for the sites of interest is within the variability of measurements from even a single site in all cases. Studies confirming the temporal variability over such a long term are scarce, however the work of Berden, Nilsson et al. (1987) indicates a range of 0.4 – 0.7 pH units variation over 20 years in Sweden, which is comparable with the variation seen here.

Table 16: Temporal Variation of pH Measurements

Site	Mean pH Measurements						
	Variability (pH units) ^a / (% of Mean)	1983	1984	1985	1986	1987	2006
15	0.24 / 3.7	6.36	6.38	6.52	6.6	6.42	6.4
17	0.48 / 8.0	6.3	5.82	5.96	6.2	5.9	5.6
32	0.14 / 2.2				6.3	6.16	5.6

^a Variability does not include 2006 measurements

Sulphur variation shown in Table 17 over the first 5 years of the trials indicates variability in the range of 40%. If this were taken to be the natural variability, then it is certain that there has been a significant change in Sulphur concentration in soil at all sites in 2006.

Table 17: Temporal Variation of Sulphur Measurements

Site	Mean Sulphur Measurements						
	Variability (mg / kg) ^a / (% of Mean)	1983	1984	1985	1986	1987	2006
15	2.6 / 38.5	7	6.6	5.6	8.2	6.4	16.6
17	10.6 / 42.3	31	25.6	27.4	20.4	20.8	51.4
32	2 / 0	2			2	0 ^b	4.5

^a Variability does not include 2006 measurements

^b This value is believed to be an error in measurement – as previously mentioned, analytical error is high in comparison to the actual measurement at this site.

It may be concluded from the variation in the samples and the error in the measurements that the range of acceptable variability of results is quite wide. This may bring into question the perceived trend in the soil sulphur concentration. It would be recommended that future studies take more samples per site, in order to reduce the effect of outlying values on the mean, such that the confidence limits can be drawn more tightly around the average. However, for the current study, the mean values must be taken as the accepted average value for the site, with error bars given to indicate the possible range of variation.

6.5 Sensitivity Analysis

Model parameters were varied by 20% in either direction singly and in combination in order to gauge the effect of model parameter input on the output results. The parameters of particular interest which were varied to judge sensitivity are listed in Table 18.

Table 18: Parameters of Interest in Sensitivity Analysis

Parameter	Standard Value	Minimum	Maximum
Dry Deposition Velocity	0.005 (m/s)	0.004 (m/s)	0.006 (m/s)
Run-off Factor (F)	Location Specific	F x 0.8	F x 1.2
Permeability Factor (G)	Location Specific	G x 0.8	G x 1.2
Average Rainfall	760 mm	608 (mm)	912 (mm)
Annual Rainfall	Year Specific (mm)	$q_r \times 0.8$	$q_r \times 1.2$
Total Process Emissions	27,000 (t/yr)	21,600 (t/yr)	32,400 (t/yr)
Radius of 1 st Airshed	1.5 km	1.2 km	1.8 km
Height of Airshed	1.1 km	0.88 km	1.32 km

6.5.1 Effect of Variation of Parameters

Site 15 is used in the following graphs (Figure 35 - Figure 42) to illustrate the sensitivity of a single site to changes in the different parameters. The graphs for the remaining sites are given in Appendix 9.

It is apparent from Figure 35 that an increase in Dry Deposition Velocity creates a corresponding increase in soil sulphur concentration. This is the expected environmental and mathematical behaviour, as the deposition rate (q_{dd}) is dependent solely on the deposition velocity (u) and the atmospheric concentration (c_1), such that a change in either will produce a linear change in deposition, ($q_{dd} = u.c_1$) and hence a change in soil concentration. The dry deposition flow in the model increases linearly in response to increasing partial pressure of sulphur in the air “tank” above the soil tank, in line with fundamental principles (Seinfeld and Pandis, 1998; Potter and Colman, 2003). In this way, it is much like the response of drainage flowrates to increased head in the tank above.

Site 15 - Sensitivity to Dry Deposition Velocity

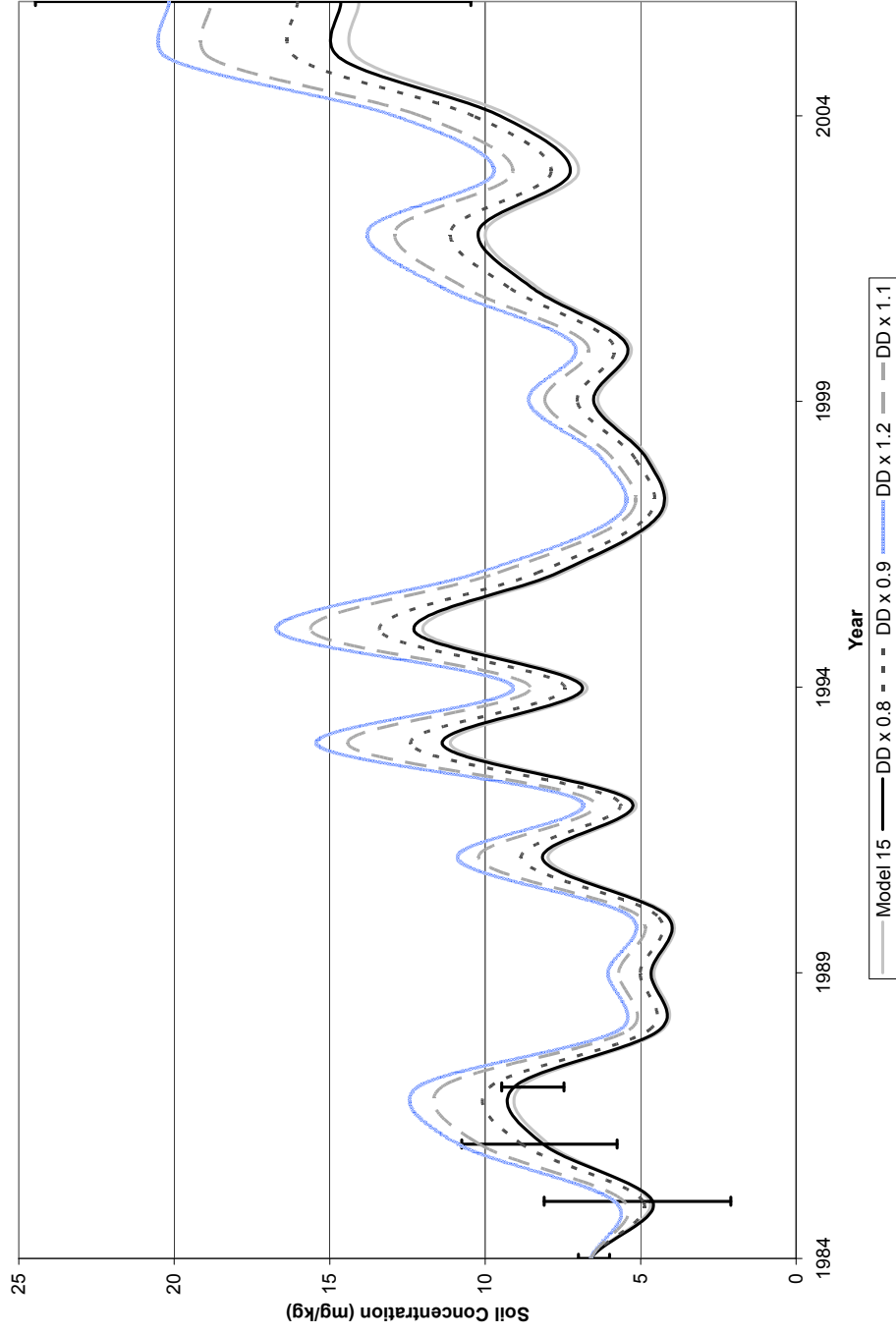


Figure 35: Site 15 Soil Sulphur Concentration – Sensitivity of ETM to Dry Deposition Velocity

Table 19 shows that the decrease in dry deposition rate creates a larger variation than an increase in dry deposition, indicating that the relationship between dry deposition and final soil concentration is partly non-linear in the model. The equation for concentration contains the deposition velocity in both the steady state and dynamic (exponential) terms. The steady state term is dominant, thus the response is almost linear, but the dynamic term has some contribution, which creates this non-linear behaviour.

Table 19: Percentage Variation from the Base Model in Response to 20% Parameter Variation

Parameter	Percentage Response to Variation (%)			
	Site 15 (-10%)	Site 15 (-20%)	Site 15 (+10%)	Site 15 (+20%)
Average Rainfall	-10	-20	+10	+20
Process Emissions	-4.09	-8.17	+4.09	+8.17
Dry Deposition Rate	-6.18	-12.37	+12.31	+6.16
Annual Rainfall	+18.81	+44.50	-14.25	-25.33
Run-off Factor (F)	+6.93	+15.60	-5.67	-10.40
Permeability Factor (G)	+4.18	+9.40	-3.42	-6.27
1 st Airshed Radius	+4.57	+10.27	-3.74	-6.86
Airshed Height	+4.67	+10.49	-3.83	-7.03

The variation between the lines in the first few years is much narrower than towards the end of the graph – this is due to the change in the process plant emissions over its lifetime. The emissions from the plant slowly increase during commissioning from 1984 until 1986 when the full capacity is achieved, then from 2003, an extension to the plant increases the emissions. Across the whole period, the variation of 20% for dry deposition rate still results in the model fitting well with historical data, which makes the case for a fairly robust model in terms of this parameter.

Site 15 - Sensitivity to Process Emissions Rate

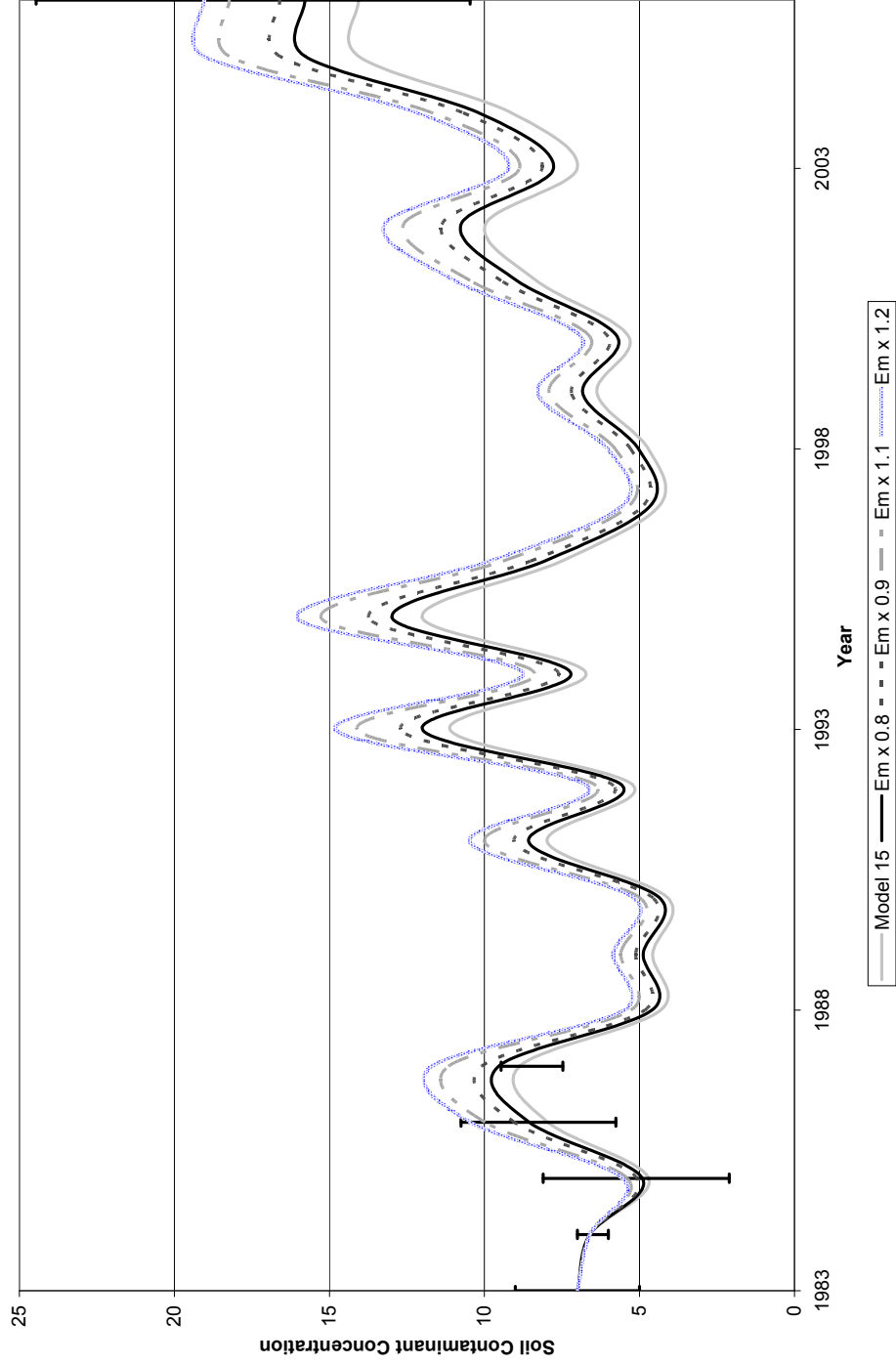


Figure 36: Site 15 Soil Sulphur Concentration – Sensitivity of ETM to Process Emissions Rate

Figure 36 shows that an increase in process emissions increases soil concentration, and likewise a decrease in process emissions decreases soil concentration. The environment is thus mirrored accurately in the behaviour of the model in response to this parameter. Again, the variation of the emissions remains within the error limits. From the experience with the deposition velocity, it would be expected that the concentration response to the variation of emissions would be slightly non-linear, however, from Table 19 it is apparent that the response is in fact linear. The reason for this discrepancy may be that the concentration of atmospheric sulphur (which is affected by the change in emissions) is a very small number in comparison to the deposition velocity. Thus any non-linearity is minimised in its impact, and does not show prominently in the results.

Figure 37 shows that the concentration of sulphur in soil follows the average annual rainfall in an inversely proportional manner. This is the expected behaviour when considering that decreasing the long term average rainfall implies an increase in the number of years in which rainfall exceeds the equilibrium level, and hence the years in which a higher washout of contaminant occurs. This response comes back to the idea of a flow control mechanism in the process model, whereby the equilibrium level of rainfall (corresponding to an equilibrium level of sulphur in the soil) is used as the set-point. When excess rainfall occurs, the water in the soil tank (and hence the sulphur) is discharged at a higher rate. When the set-point is moved to a lower value, excess rainfall occurs at a higher frequency, and the flowrate out of the tank is increased on average. This response was previously discussed in the Model Results section.

Site 15 - Sensitivity to Average Rainfall

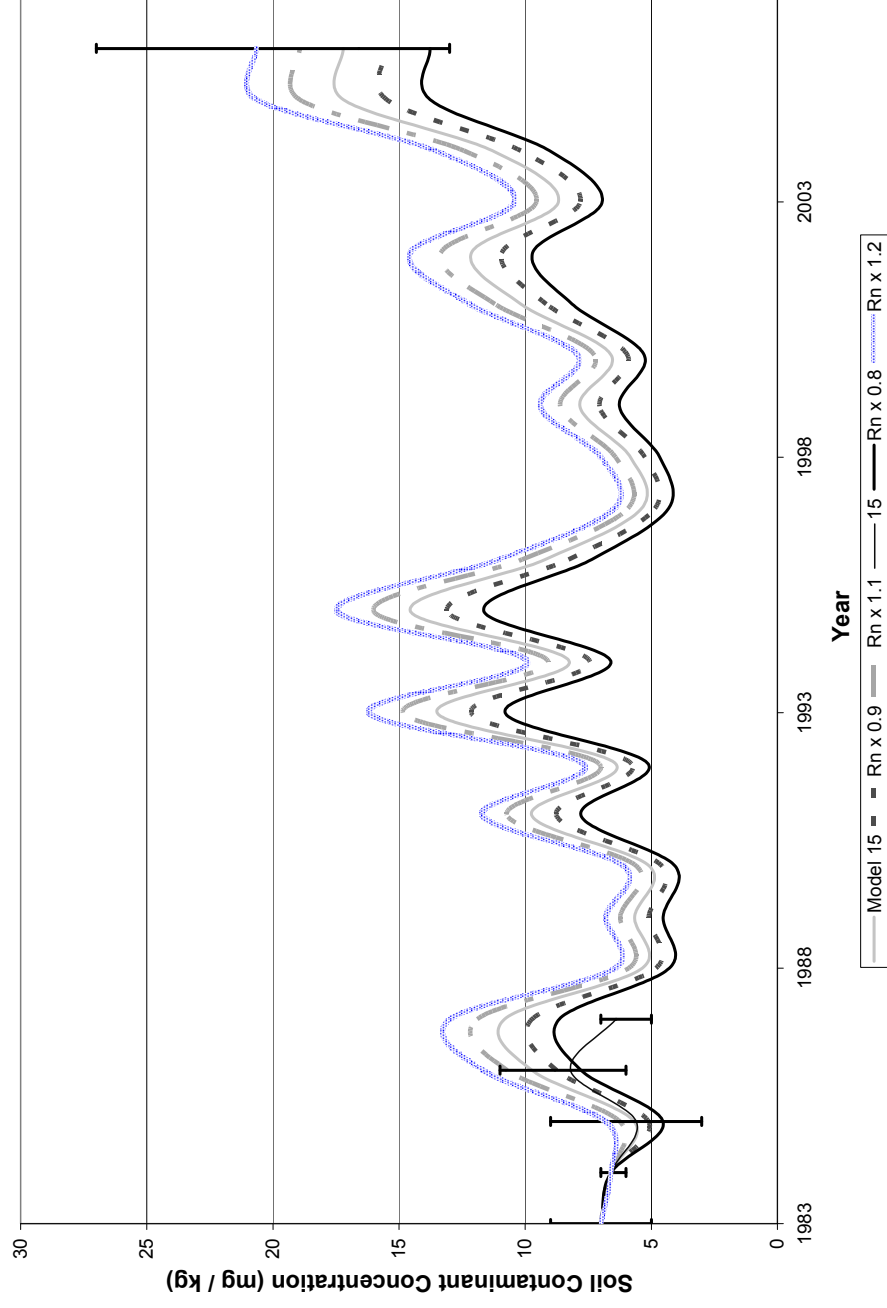


Figure 37: Site 15 Soil Sulphur Concentration – Sensitivity of ETM to Average Annual Rainfall

Table 19 indicates that there is a linear response to change in this parameter. This fits with the mathematical model, in that the r_N term appears in the steady state and permeability terms as a multiplier, and its importance may diminish in the dynamic term.

The sensitivity to annual rainfall shown in Figure 38 and Table 19 indicates that a large variation of Sulphur concentration is caused in response to rainfall variation. In general, the reduction in rainfall increases the sulphur concentration in soils. This is the expected behaviour from an environmental perspective, as the sulphur that is deposited at a constant rate by dry deposition will be removed via leaching and run-off proportional to rainfall rate, such that an increase rainfall will increase the removal of sulphur from the soil. The behaviour of the model over the +/- 20% range is close to linear, but examination of wider variation (factor of 2 variation) shows that the behaviour is in fact non-linear. When we refer back to the mathematical model, this is also the expected behaviour, as the rainfall factor is involved in all terms of the model, and in particular in an inversely proportional relationship to concentration in the steady-state and permeability terms. This is reflected in Figure 38, as a decrease in rainfall leads to an increase in Sulphur concentration.

The behaviour in response to rainfall is of particular interest in Australia at present, and looking towards the future with uncertainties in climatic variations under a global warming regime.

Sensitivity to Annual Rainfall - Site 15

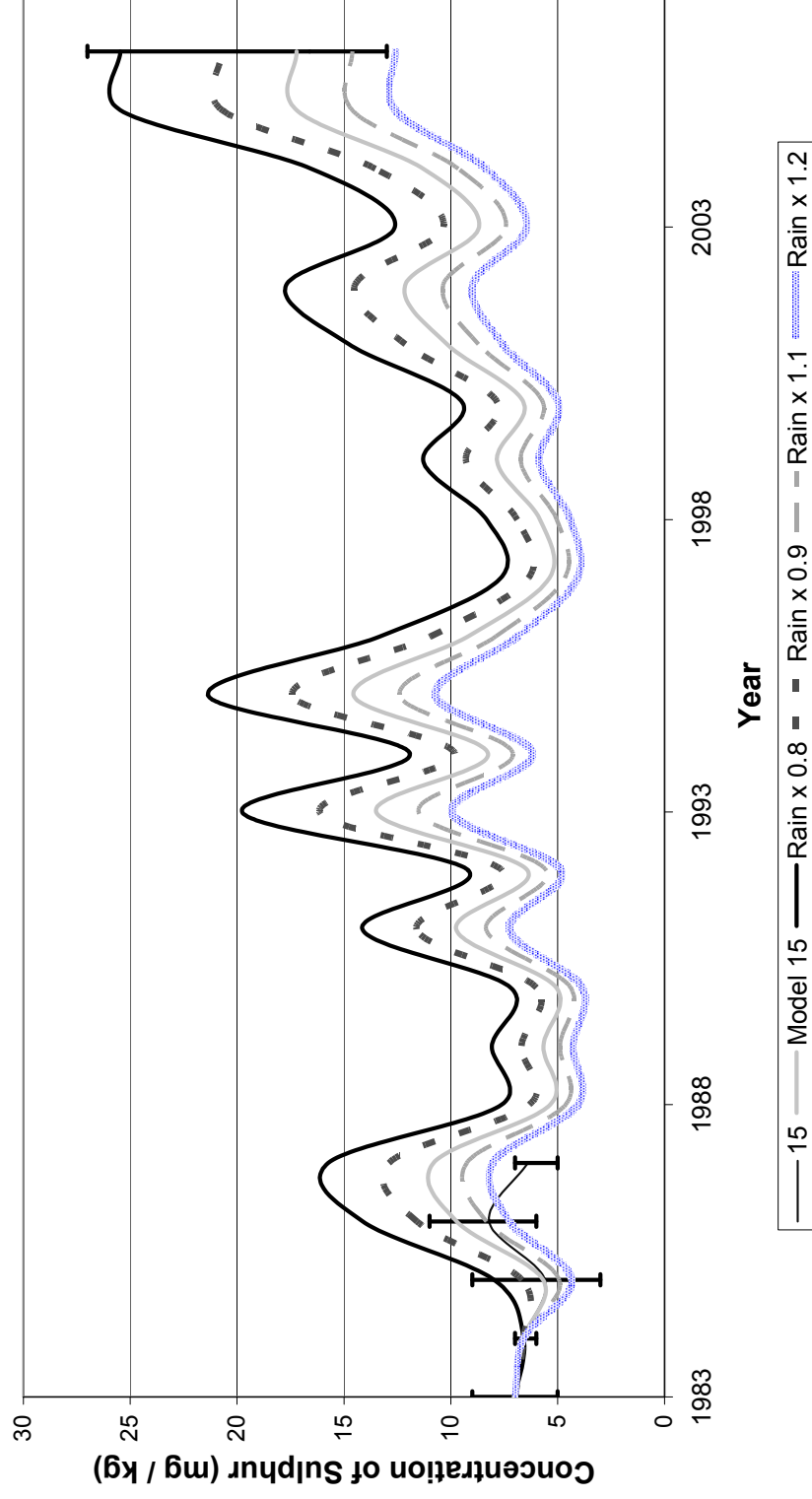


Figure 38: Soil Sulphur Concentration – Sensitivity of ETM to Annual Rainfall - Site 15

Site 15 - Sensitivity to Permeability Factor (G)

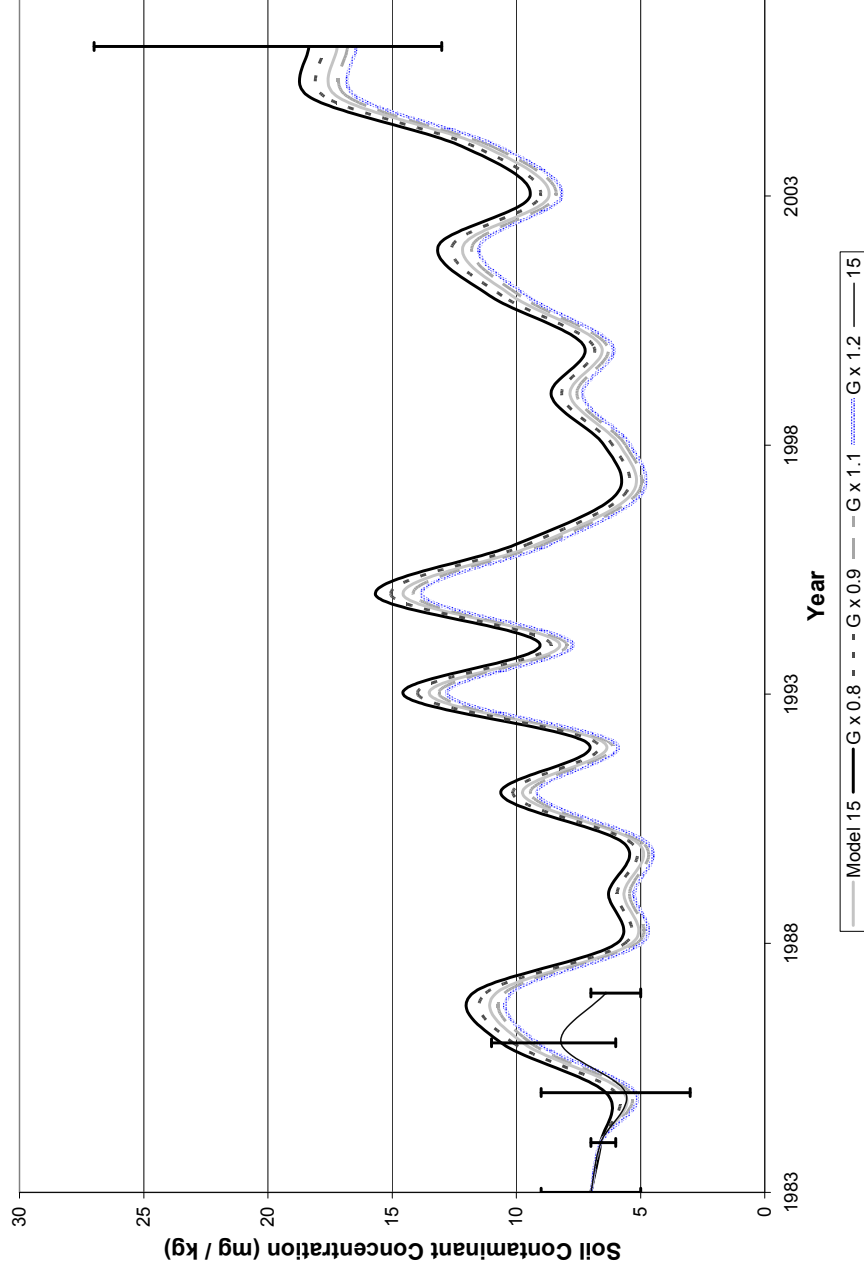


Figure 39: Site 15 Soil Sulphur Concentration – Sensitivity of ETM to Permeability Factor (G)

Reducing the permeability factor G , increases soil sulphur concentration, as shown in Figure 39. Considering the realities of the environment, soil that does not allow the passage of water easily, will tend to maintain a high surface level of sulphur, unless a swift run-off rate washes-out the surface sulphur. In the mathematical model, the permeability factor directly relates to the amount of residual sulphur that is washed-out, such that an increase in G will increase the effect of rainfall above the average, and therefore the wash-out of sulphur. The response to this parameter is linear, but the y-intercept consisting of the steady state and dynamic terms, makes this less obvious than previous factors. This is the mathematically predicted response.

The increase in run-off factor, F , decreases the soil sulphur concentration as per Figure 40. Increasing the run-off factor, increases wash-out from the top 1-2cm where most dry deposited contaminant is found, thus decreasing soil sulphur concentration. In the model, F is one of the two control parameters adjusting sulphur output in response to rainfall. Mathematically the factor F is found in both the steady state term, and in the coefficient and exponent of the dynamic term. Thus the behaviour in response to variations in this factor would be expected to be non-linear. This prediction is confirmed by examination of the sensitivity assessment, but the degree of linearity is high. Again, as per previous factors, it is projected that the non-linearity is muted due to the minor effect of the dynamic section of the concentration equation (due to the small magnitude of the exponential component).

Site 15 - Sensitivity to Run-off Rate Factor

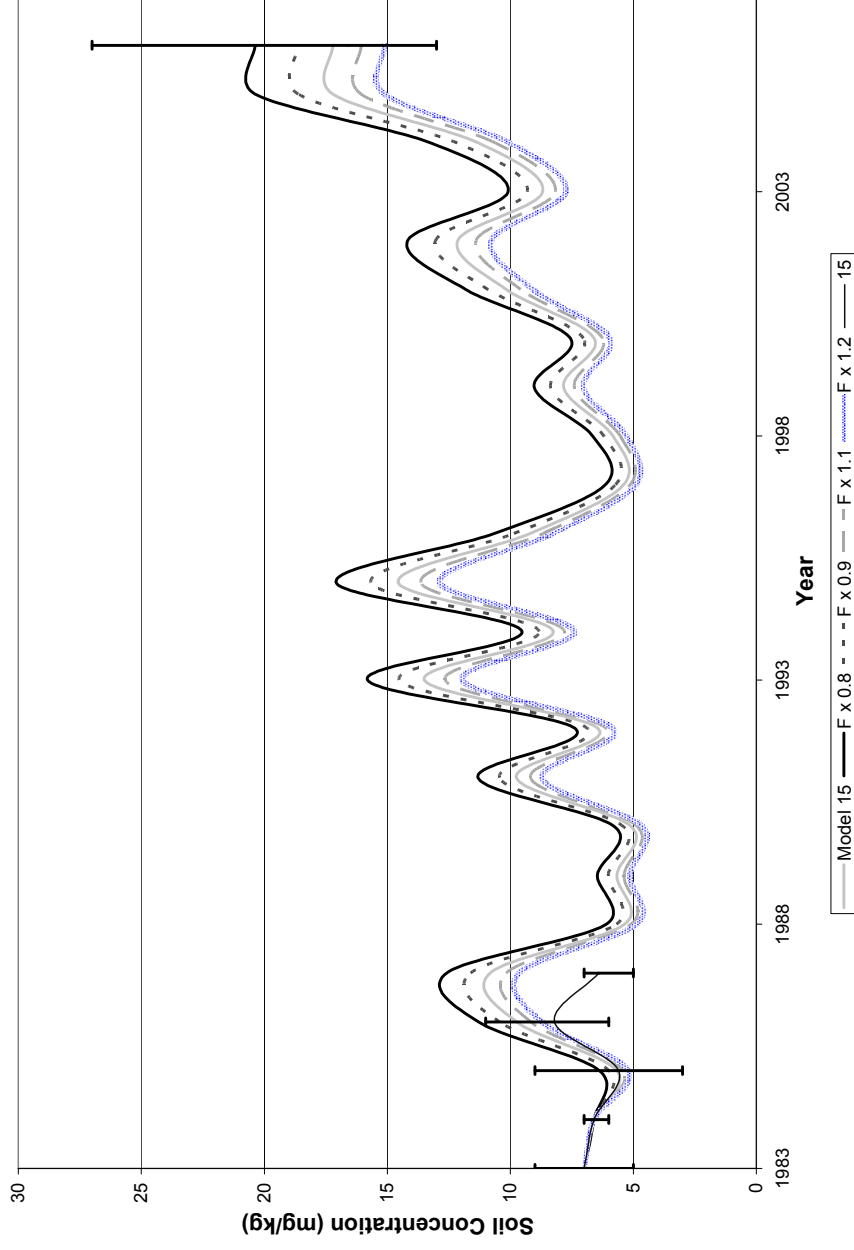


Figure 40: Site 15 Soil Sulphur Concentration – Sensitivity of ETM to Run-off Factor (F)

Sensitivity to 1st Airshed Radius - Site 15

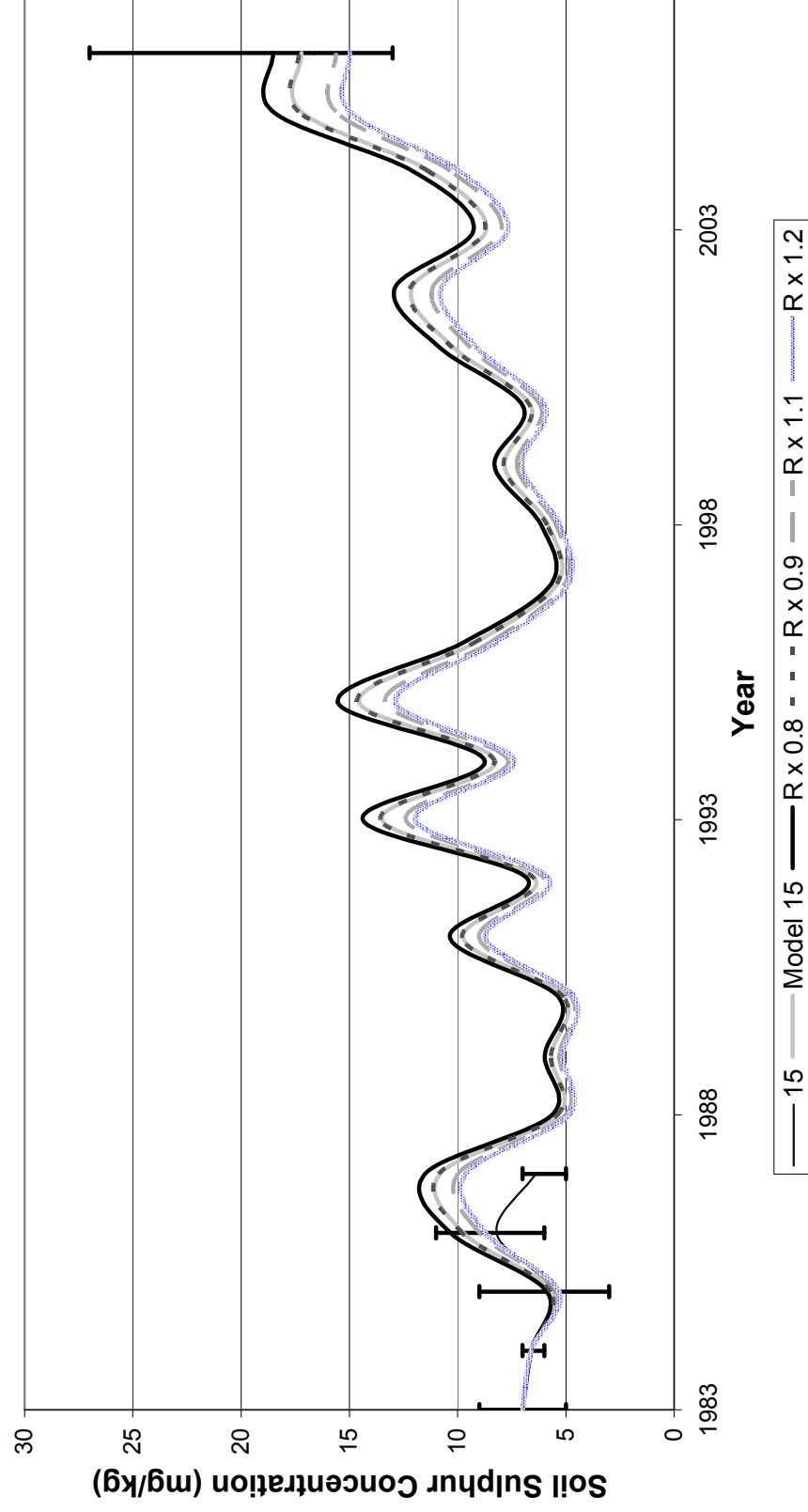


Figure 41: Site 15 Soil Sulphur Concentration – Sensitivity of ETM to Airshed Radius

Figure 41 shows that a decrease in the radius of the first sub-airshed (which is used to calculate the radii of all subsequent sub-airshed tanks) results in an increase in soil sulphur concentration. Decreasing the sub-airshed radius increases atmospheric concentration of contaminant in the model, as the emission is assumed to all flow into the tank, no matter the radius, hence the deposition will increase and the soil concentration will also increase as observed. It is also observed that, despite a large variation of the radius, the model remains within the limits of error of the historical data. Physically, this can be seen as changing the dilution rate – the emission is assumed to be diluted at a rate that is proportional to the volume of the tank, hence the larger the tank, the lower the concentration if the same amount of substance is contained within it. A higher or lower dilution rate could be attributed to unstable wind conditions and to variations in the wind direction, increasing or decreasing the probability of sulphur deposition.

The response behaviour is highly non-linear. Mathematically, this is expected, as the atmospheric concentration is related to the square of the radius, whilst the transfer from one airshed tank to another is related linearly to the radius, and the atmospheric concentration is a parameter in both the steady state and dynamic sections of the model.

Site 15 Sensitivity Analysis - Airshed Height

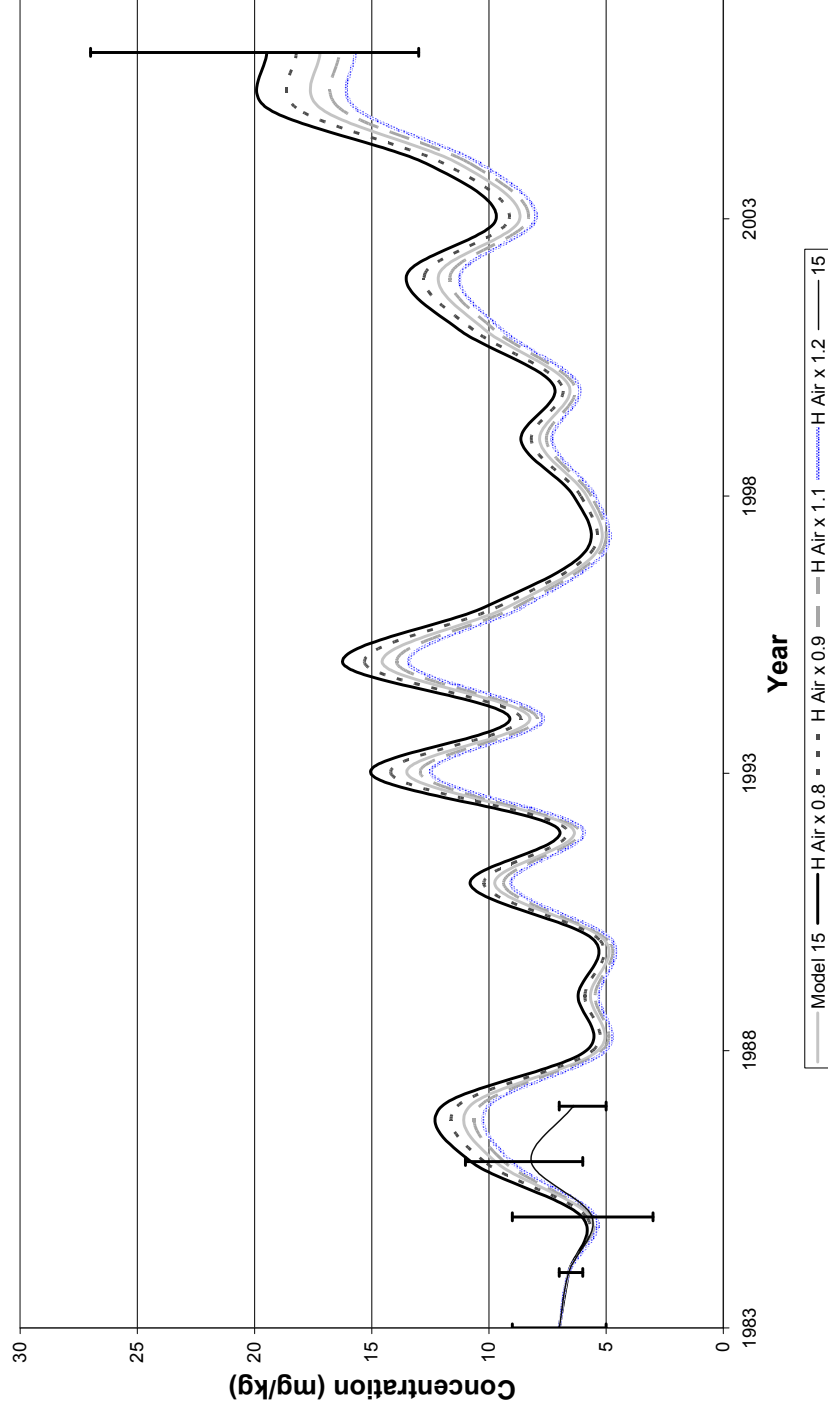


Figure 42: Soil Sulphur Concentration – Sensitivity of ETM to Airshed Height – Site 15

Figure 42 and Table 19 indicate that the variation of soil sulphur concentration in response to a change in airshed height (air “tank” height) is very similar to the variation in response to airshed radius. In the mathematical model, both these factors affect the atmospheric concentration of contaminant by changing the volume of the air tank, and the flux of contaminant between sub-airsheds by changing the surface area over which flux occurs. By affecting the atmospheric concentration, they affect the deposition rate, which in turn affects the soil sulphur concentration. Decreasing tank height increases the atmospheric and soil concentrations. It is apparent that the variation due to a 20% variation in height is still within the limits of error of the model, and also proves to be non-linear. The model would predict a non-linear response due to the inclusion of the atmospheric concentration in both the steady state and dynamic terms. The small variability due to error implies that the current airshed height can be used with confidence.

6.5.2 Summary of Sensitivity Analysis

Based on site 15, the parameters of the ETM were varied and the subsequent response of the model was graphed and analysed. As shown in Table 19, the parameters that impacted most on the model performance were the yearly rainfall, average rainfall, run-off factor and dry deposition velocity.

The yearly rainfall produced the largest deviation from the standard model, with a variation of 20% causing a variation of 26 – 47%. This has many implications – both for the model, and for the local impact of Australian emissions sources in general. In terms of the model, error may enter into the assessment of each individual site if the annual rainfall is not relatively constant across all “tanks”. This may be one source of error causing the model to deviate from the historical data at times. In terms of the local impact of Australian emissions sources, with the current national drought, and potential under a climate change paradigm to have reduced annual rainfall, the soil sulphur concentration (and hence the potential for soil acidification) may increase rapidly. This could be cause for concern, and is something that Australian decision makers should keep in mind.

Likewise, the average annual rainfall has shown a decrease over the past 30 years (BOM, 2006). If this trend continues, then the sulphur levels in the soil could be raised to a new equilibrium level. If the average rainfall and sulphur levels do not return to its previous levels, then the model would need to be reset around the new averages.

The effects of run-off factor and dry deposition rate are of lesser concern given that the model remains within the bounds of error under the variation of these factors. The run-off factor is site-specific, which can lead to difficulty in prediction of environmental response if the factor deviates too far from the best-fit however, given a simple classification of any site, such as that used in Plenderleith (1989), the model can be fitted with reasonable confidence.

The change in emissions rates by 20% results in less than 10% change in soil concentration. This is a point of particular interest in terms of the sustainability metrics, as it indicates that a loading-only, technology-indicator style metric could over estimate the impact of such a difference in emissions on the environment. This provides a significant argument for the incorporation of an ETM in the sustainability metrics.

From the sensitivity analysis, the model may be considered to be appropriately responsive to variations in parameters, but robust in regards to the behaviour compared with historical data.

6.6 Comparison of the ETM with Existing Models

To confirm the validity of the ETM, it was compared with the AUSPLUME Gaussian Plume Software and the RAINS-ASIA Acid Deposition Software. From these comparisons, it was hoped to ascertain the level to which the simplified model could be trusted in comparison with more complex models. The parameters of interest were the deposition and atmospheric concentration of SO_x .

6.6.1 Comparison with AUSPLUME

AUSPLUME is an Australian-based Gaussian Plume model, developed by Monash University and the Victorian Environmental Protection Agency. A terrain file and Meteorological file were developed using Geographic and Meteorological Data, and used in AUSPLUME for comparison with the current model.

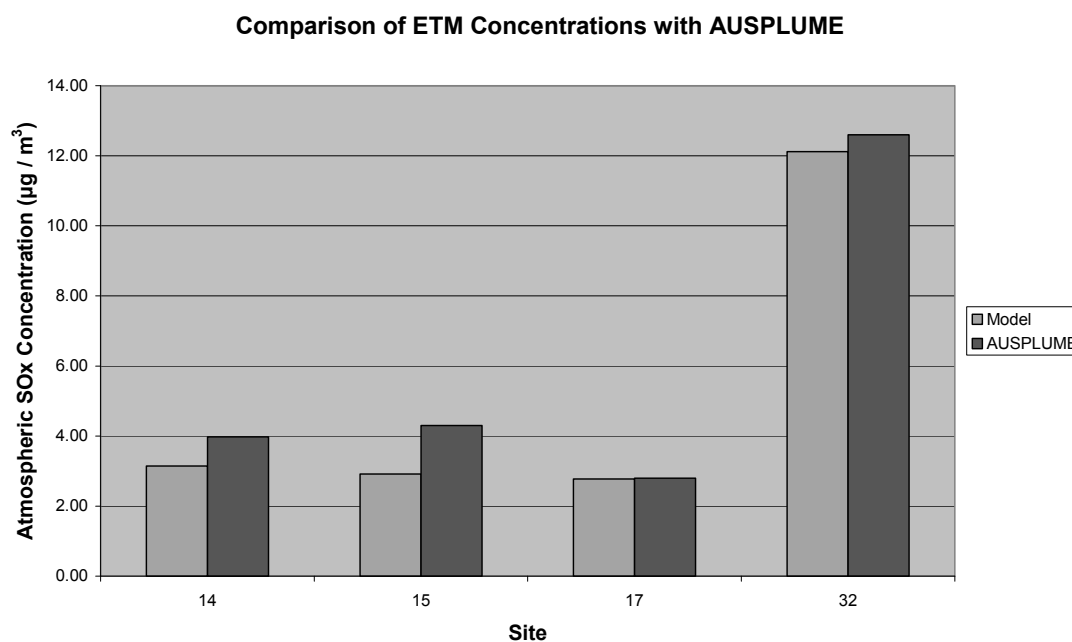


Figure 43: Comparison of Atmospheric SO_x Concentrations from ETM with AUSPLUME

From Figure 43, it is apparent that the current model provides concentrations that are close to those provided by the AUSPLUME software. Although it has been surpassed for specific air pollutant transport and reaction by TAPM (Hurley, 2002), the AUSPLUME model is widely used in the Australian context to model atmospheric emissions transport (Gilmour, Mayhew et al., 2001; Katestone, 2005), and is typical of a Gaussian plume model. With the close correlation shown with AUSPLUME results, the model can be used with reasonable confidence to predict the atmospheric concentration.

6.6.2 Comparison with RAINS-ASIA

RAINS-ASIA (Regional Air Pollution Information and Simulation)(IIASA, 2001) is a model allowing the examination of effects of control options on deposition of sulphur and acidification of the soil. It was developed for use in South Eastern Asia, hence is not directly applicable to Australia, but by selecting regions of Asia with similar climatic conditions to South-East Queensland, a comparison giving the magnitude of expected results can be obtained. Furthermore, RAINS-ASIA is a model specifically looking at the deposition of Sulphur and its contribution to acidification over long distances. The factors extractable from this model for comparison are the deposition rates per unit of area.

Examining the stationary point-sources, and the climatic data for the different regions of South Eastern and Central Asia that the model addresses, the Guang Zhou province of China proved to be the most comparable, with a single stationary source emitting 24,800 tonnes of SO_x, (similar to the emissions rate of 27,000 tonnes for the source examined in this validation) and climatic conditions similar to South East Queensland. The deposition contribution from this source is given in Table 20.

Table 20: Deposition Contribution from Point Source 1 in Guang Zhou, China (RAINS-ASIA)

Latitude	Longitude	mg/m ² /yr
23	113	170
23	112	83

From Figure 44, it is observed that the current model has a slight bias towards high values as compared with the RAINS-ASIA model for deposition. The differences between the current model and the RAINS value at the individual sites is due to RAINS only incorporating an average deposition over a large area (approximately 90km x 90km), whilst the current model examines deposition on a more local scale, with average values over the tank surface area (circles of radius 3 – 15 km for the sites of interest). The monitored sites are all in close proximity to the plant, which accounts for the higher deposition rate in comparison with the average. Comparing the overall average values however, shows that across the whole area of interest, RAINS and the current model give very similar deposition rates (see also Table 21).

Table 21: Comparison of Model with RAINS-ASIA Deposition

	Deposition (mg / m²)	Total Deposition (t)	Percentage of Emissions (%)
Model	151-1,695 (186 Average)	6,812	27.6
RAINS	170	6,013	24.2

Deposition Comparison of RAINS-ASIA and Current Model

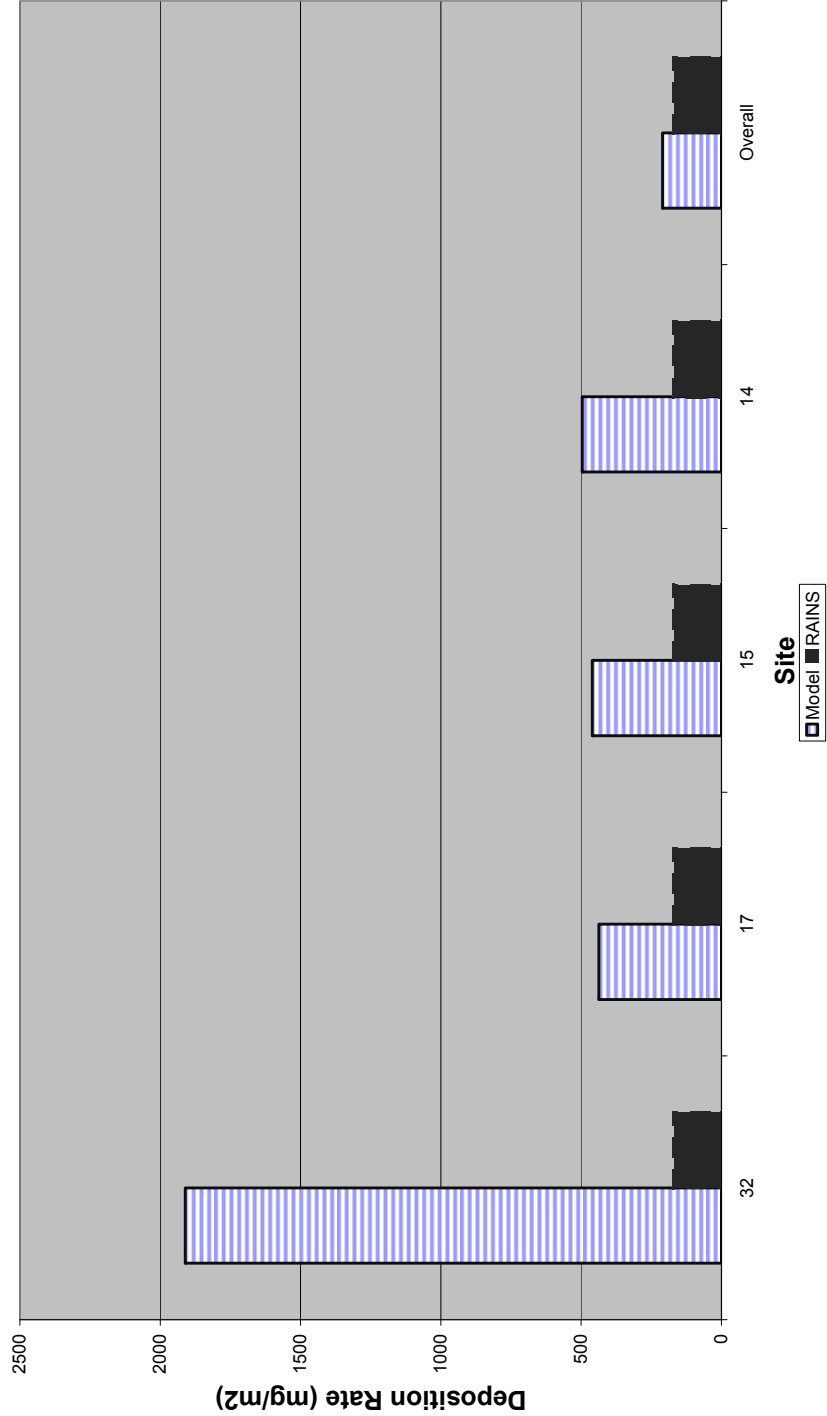


Figure 44: Comparison of Deposition Rates from RAINS-ASIA and Current Model

The comparison of the current model deposition rate with RAINS-ASIA shows that the results are quite close in terms of deposition. This result allows greater confidence in application of the model.

6.7 Conclusions

In this chapter, the first fundamental contribution to knowledge is showed by the validation of the Emissions Transport underlying the Sustainability Model. A major distinction of the proposed model is the introduction of environmental interactions for specific sites. This is a departure from conventional loading models which assume that all sites have the same environmental properties, and thus that the sustainability metrics are equally applicable to all sites. The concurrence of the model with the data, shows irrefutably that the location-specific environmental conditions cannot be ignored if a true picture of the environmental impact, and therefore the sustainability, is to be obtained. In addition, validation of the ETM for a period of 23 years was achieved using the data from the Tarong power station. This is a significant achievement, as the availability of such long term data monitoring a site from its pristine state to the present, with only a single major emissions source is almost impossible to duplicate anywhere else in the world.

However, environmental data is very complex, so this work takes the approach of using the midpoint of soil deposition and subsequent soil concentration variation based on purely physical processes. Omitting the biological and biochemical influences of the receiving environment naturally causes some error and unpredictability, however, inclusion of these exceedingly complex processes would belie the inherent error in prediction, thus giving a false appearance of precision. In truth, the inclusion and perfect modelling of even a single site would require resources and analysis beyond the scope of any corporation or study due to the vast number of parameters in constant flux. Given that the available data does not support a more complex model, and that the inclusion of only physical processes still allows validation within the limits of error, it is concluded that the omission of these processes is both warranted and valid.

The model was fitted to the empirical data using variation of multiple parameters derived from the process modelling approach described in Chapter 5. The validation of the model based on data from Tarong power station, and the comparison of results for deposition and atmospheric concentration with accepted existing models, indicates that it is able to mimic environmental behaviour within reasonable limits of accuracy. The sensitivity assessment shows that the model is robust in response to variation of parameters, and highlights that the parameters of highest impact are those factors which affect the removal of sulphur from the soil. The particularly strong influence of the annual rainfall rate has significant implications for the future acidification of the soil in the current drought conditions, and with the potential for decreasing annual rainfall in a future climate influenced by global warming. This factor could also be a strong influence when siting of a potential plant is considered, as the influence on soil may be mitigated under conditions of higher rainfall. The ultimate sink for any leached contaminants would be groundwater and surface water which are not examined here due to the lack of historical data for validation, but this is an area needing much further research.

The non-linearity of the response to emissions increase, and the difference in the percentage change of soil sulphur concentration in response to a change of 20% in emissions or other parameters, supports the utilisation of an ETM in the sustainability metrics. If a directly-proportional, linear response had been recorded for all parameters, it might be assumed that a loading-model metric system would be sufficient. However, a non-linear response to emissions variation in particular denies the validity of loading models of sustainability except for use in comparison of potential technologies. This finding contributes significantly to the debate on environmental sustainability, and throws the validity of technology-based sustainability metrics into question.

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Chapter 7

Sustainability Metrics Scenario Analysis

7.1 Introduction

This chapter integrates the Fuel Cycle Inventory (FCI) work for hydrogen production technologies from Chapter 4 into the proposed sustainability metrics (SM) model derived in Chapter 5 and the deposition model validated in Chapter 6. It is the aim of this chapter to provide an SM assessment, compare the current model with existing models and perform an internal analysis. The metrics are focused on soil acidification for Tarong and applied to hydrogen production systems providing hydrogen to Brisbane under a number of selected scenarios to elucidate the potential applicability of the proposed SM model.

The basis for assessment is the production and provision of 1000MW of electricity or equivalent hydrogen (178 kt/yr) to Brisbane, with production occurring at the current Tarong power station site. The time basis for operation of the process is considered to be 30 years, which is the typical expected lifetime of most power stations. With the selection of the site for delivery, currently exploited coal and gas fields are utilised as the feed fuel source to a coal gasification plant, a conventional coal electricity based electrolysis plant and a natural gas steam reforming plant. Although the FCI provides data for the transportation, extraction and hydrogen production operations, from this point onwards, the SM assessment will be applied only to the production stage, as this is the stage of highest emissions (see Chapter 4).

7.2 Metrics Model Analysis

Following the validation and sensitivity assessment of the emissions transport model (ETM) in Chapter 6, it was found that the model was robust, such that it could be applied to the situation of sustainability metrics for hydrogen energy systems with confidence. It was also observed that each site within the receiving environment has a

particular environmental signature, which the factors of run-off rate and soil permeability contribute to. The ETM was fit to these characteristics, thus giving a close match with historical data on the level of the individual site. Furthermore, the model showed similar average results for large areas (90 x 90km) when compared to the RAINS-ASIA acid deposition model (IIASA, 2001). Hence, a high resolution for each site can be achieved by the ETM whilst average values can also be delivered for large areas when specific environmental data is not available. The availability of data for the Tarong area thus made this the ideal site for testing the metrics.

7.2.1 Technology Scenarios

One scenario each for coal gasification, conventional coal power-based electrolysis, and natural gas steam reforming (NG-SR) hydrogen production were considered in examination of the sustainability metrics (Table 22). These scenarios were chosen to compare process options that were appropriate for delivering the basis amount of electricity or hydrogen to Brisbane.

Table 22: Scenarios for Testing the Sustainability Metrics

Scenario	H ₂ Source	Process	Location	Transport	FCI Data SO _x (t/yr)
1	NG	Steam Reforming	Tarong	Pipeline (NG - 250km) (H ₂ - 200km)	0.001
2	Coal	Gasification	Tarong	Train / Pipeline (Coal – 5km) (H ₂ – 200km)	40.5
3	Water (Coal PF)	Electrolysis	Tarong	Train / Pipeline (Coal – 5km) (H ₂ – 200km)	22,630

The factors for each scenario were used as input to the Fuel Cycle Inventory (FCI) (see Chapter 4), and the resulting emissions utilised as input to the SM model. Emissions rates are shown to correspond closely to the rates given by Nunn, Cottrell et al. (2001), Williams (2001) and Ogden (2003).

The sulphur contribution to soil acidification metrics at the Tarong site was used to demonstrate the applicability of the SM methodology. The sustainability of soils under the influence of a local emitter of acidifying compounds is one of the most important examples of the need to include local environmental parameters and transport mechanisms within a sustainability regime. Many other substance emissions are available from the FCI, but the full assessment is beyond the scope of the current work. Other metrics are included in Appendix 10 as further examples of the application of the general metrics model.

7.2.2 Carrying Capacity and Baseline

The buffering capacity of the soil is taken as the carrying capacity in terms of acidification. Another possible carrying capacity threshold could be the level at which severe effects on plants or animals occur, however, the data is not readily available on this option. Much research has been completed into the issue of acidification – especially in Europe – and hence many methodologies for measuring the carrying capacity of soil in relation to acidification are available. For this work, the critical load assessment work of Kuylensstierna, Cambridge et al. (1995), Cinderby, Cambridge et al. (1998) and IIASA (2001) and the buffering capacity work of the CSIRO (Noble, Middleton et al., 2002; Singh, Odeh et al., 2003) are utilised to estimate the carrying capacity.

The critical load concept assumes that there is some annual loading of acidifying substances, beyond which soil acidification will occur. The concept was developed in particular, in response to the acid rain problem in Europe, but there has been debate as to whether the concept is valid, in that it assumes a simple environmental response to emissions, neglecting known complexities (Cresser, 2000). Despite the significant omissions in the critical load models, the concept is being widely used and developed as an estimation technique (de Vries, 1993; Cinderby, Cambridge et al., 1998; Huijbregts, 1999; Cresser, 2000; Dupont, Clair et al., 2005). The most extensive work has been carried out by the International Institute for Applied Systems Analysis (IIASA) and the Stockholm Environmental Institute (SEI), who indicate that land in the vicinity of Tarong is largely in the least sensitive class, with no critical loads – i.e.

critical loads greater than 200 (mmol H⁺-eq/m²/yr) (Cinderby, Cambridge et al., 1998).

The work of Noble, Middleton et al. (2002) validated an equation relating soil characteristics (clay, silt and organic carbon content) to the potential resistance to pH change due to acid deposition (i.e. buffering capacity) Equation 24.

$$pH_{BC} = 6.28 - 0.11 \times \text{clay}\% + 3.71 \times \text{OC}\% - 0.16 \times \text{silt}\% + 0.03 \times \text{silt}\% \times \text{clay}\% \quad [24]$$

Applying Equation 24, based on the data from Plenderleith (1989) to the Tarong sites gives pH_{BC} of between 10 and 60 (mmol H⁺ / kg / pH Unit). This can be used to determine the resilience of the environment to change in pH, or applied to a given pH limit to determine a carrying capacity for the environment. In this case, we have applied a limit of reduction by 1 pH unit to determine the carrying capacity.

These methodologies are only truly comparable when a time period is specified, as the methodology of Cinderby, Cambridge et al. (1998) represents a yearly limit to acid deposition, whilst the methodology used by Noble, Middleton et al. (2002) is a total buffering capacity per unit pH.

Table 23: Comparison of Buffering Capacity and Critical Load Methodologies

Methodology	mmol H ⁺ / kg	mmol H ⁺ / kg / pH Unit	mmol H ⁺ / m ² / yr
Critical Load (Cinderby, Cambridge et al., 1998)	0.36 - >1.43 (1 year) 10.8 - >43 (30 years)		50 - >200
pH Buffering Capacity (Noble, Middleton et al., 2002)	10 – 60 (1 pH Unit)	10 – 60	

The carrying capacity in terms of SO_x may then be calculated as twice the molar H⁺ carrying capacity, as most deposition occurs in the form of SO₄²⁻ (Norris, 2003). Thus a carrying capacity in terms of SO_x concentration in soil can be calculated as shown in Table 24.

Table 24: Carrying Capacity and Average Sustainability Metrics at Tarong Sites for Electrolysis Option

Site	Carrying Capacity A (mg SO _x / kg) ^a	SM 1 (%)	Carrying Capacity B (mg SO _x / kg) ^b	SM 2 (%)
15	700	99.66	470	99.49
17	700	99.35	460	98.99
32	700	99.88	240	99.66

^a From Cinderby, Cambridge et al. (1998)

^b Derived from Noble, Middleton et al. (2002)

The lower carrying capacity calculated from Noble, et al. (2002) gives a higher variability in SM, is more site-specific, and is from work completed in Australia, hence this carrying capacity will be utilised in the subsequent sections.

7.3 Sustainability Metrics Applied to Technology Options

To refresh, the sustainability metrics equation (Equation 25) is the proposed SM model utilised in this work. In the case of the current application, the soil sulphur concentration is determined through the use of the ETM. This is then compared with the carrying capacity and baseline for each year and each sub-airshed tank over the lifetime and distance parameters of the model.

$$SM_i = \left\{ 1 - \frac{\int_t \int_{d_1, d_2} f(d_1, d_2, t)}{\int_t \int_{d_1, d_2} [CC(d_1, d_2, t) - B(d_1, d_2, t)]} \right\} \times 100\% \quad [25]$$

Using the model, graphs of the concentration of sulphur in the soil can be derived (example Figure 45), and the sustainability metrics equation applied to the concentration at each point for each year in simplified form shown in Equation 26.

$$SM_i = \left\{ 1 - \frac{C_{(s)}}{[CC_{(s)} - B_{(s)}]} \right\} \times 100\% \quad [26]$$

The discrete metrics can then be normalised over the area of the sub-airshed tank and the lifetime of the plant to determine the overall average sustainability.

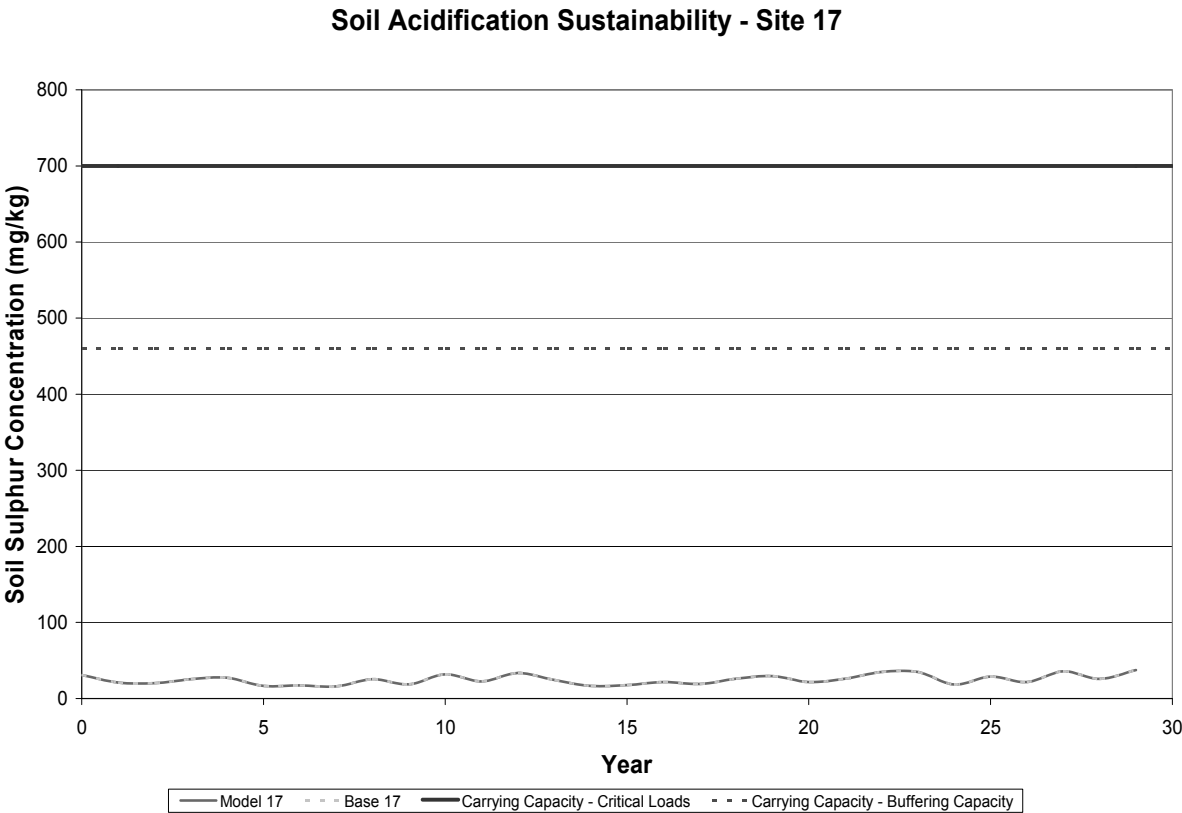


Figure 45: Base Case Sustainability - Site 15 - Electrolysis

Figure 45 demonstrates that the soil sulphur concentration is very low in comparison to the carrying capacity concentration. This is reflective of the fact that the local soils around Tarong are not exposed to a very high deposition rate of sulphur. The low rate of sulphur deposition is due in part to the low initial sulphur content of the local coals, and the effectiveness of sulphur removal by the environment. Applying the sustainability equations gives the metric for comparison. The sustainability metrics at site 17 from each technology for hydrogen production listed in Table 22 are shown in Figure 46.

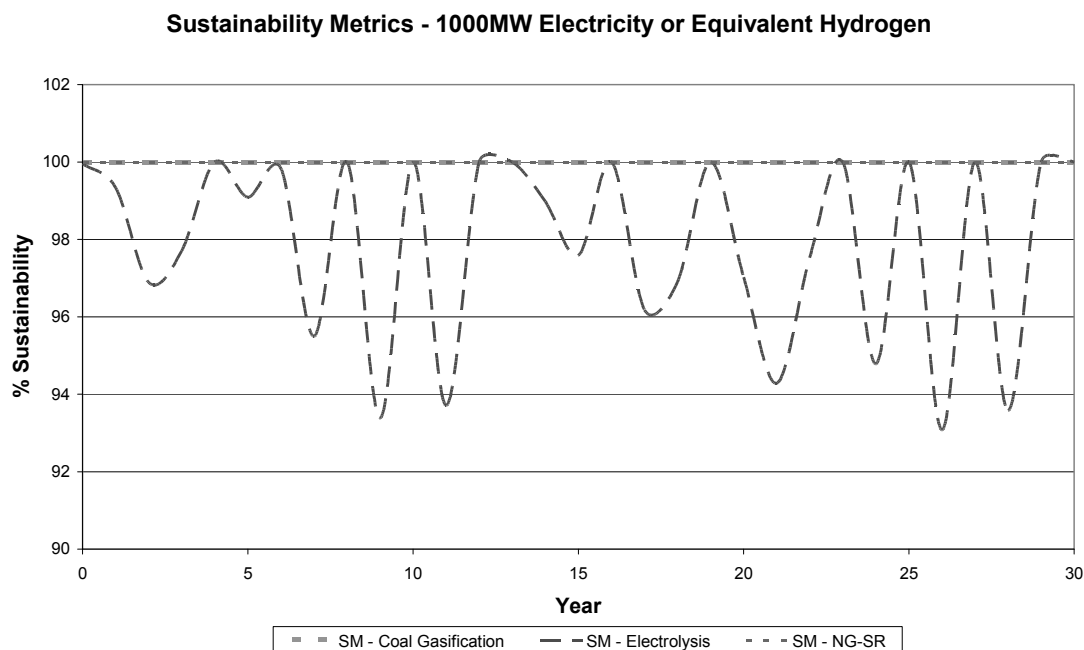


Figure 46: Comparison of Sustainability Metrics for the 3 Base Scenarios – Site 17

Figure 46 demonstrates that the sustainability is very high for all scenarios. The electrolysis option, which is based on the current Tarong power plant (scaled down to meet the basis requirements) is the highest emitter of sulphur, and hence the least sustainable. However, given that the sustainability metric for electrolysis is typically greater than 94% even for this option, all 3 scenarios can be said to be sustainable.

The high sustainability derives from 3 aspects:

1. very low sulphur content of the coal and NG
2. high levels of removal – especially in the gasification, where removal is more effective from both a technical and economic perspective than conventional coal based power generation due to the smaller volume of high pressure gas needing to be treated, and the inclusion of sorbents in the feed (Innes, 2003)
3. carrying capacity for the Tarong sites under assessment in this work is very high, as is shown in Table 24.

7.4 Comparison with Other Models for Sustainability

The current model for sustainability assessment can be compared against the IChemE's sustainability metrics, the TRACI model, which has been well received

within the Life Cycle Assessment community, and against the modified environmental burden approach of Diniz da Costa and Pagan (2006).

7.4.1 IChemE Metrics

The IChemE's metrics, or environmental burden (EB), in regards to acidification are given by the product of the mass of emissions (W) and their potency factor (PF), as in Equation 27 (Tallis, Azapagic et al., 2003).

$$EB_i = \sum W_N \times PF_{i,N} \quad [27]$$

This metrics equation constitutes a loading-type model of sustainability, where the comparison can only be drawn between the performance of a single plant or a number of plants in the same location. No environmental fate analysis is included, hence this metric can only be considered as a technology indicator (Diniz da Costa and Pagan, 2006). The potency factor for SO_x in relation to acidification is 1, so the environmental burden simplifies down to the sum of SO_x emissions from the plant.

Thus the relative sustainability of the 3 scenarios as described in Table 22, is that natural gas steam reforming (scenario 1) is 40,500 times more sustainable than coal gasification (scenario 2), which is in turn 560 times more sustainable than coal power electrolysis (scenario 3). This methodology can only be said to be effective when, as in the current situation, an assessment of yet-to-be-constructed, potential processes is being examined for a given site. This metric tells very little about the actual impact that the process has on the environment, which has been proven to be a limited methodology as shown in Chapter 6.

7.4.2 TRACI

TRACI is a life cycle impact assessment tool developed by the US-Environmental Protection Agency (Bare, Norris et al., 2003). The TRACI model is specific to the United States, so some question might be placed on the comparability, but the fate analysis / characterisation factors underlying it have recently been incorporated in some of the widely used LCA software, lending some credence to its use for

comparison. It has also been discussed in relation to the concept of sustainability metrics (Bare, 2005; Bare, Gloria et al., 2006).

TRACI uses midpoints to assess and compare the impacts of processes, hence we can draw a comparison between the level of acid deposition determined by TRACI for US conditions, and the model used here, which assumes that all Sulphur deposited contributes to acidification as SO_4 . The results of using TRACI are shown in Table 25.

Table 25: TRACI Results for SO_x Acidification Potential

Scenario	Acidification Contribution (mol H^+-eq)
Natural Gas Steam Reforming	0.00125
Coal Gasification	1.03×10^6
Coal Power Electrolysis	5.75×10^8

TRACI obtains these results by multiplication of the emission with an average characterisation factor for the US or a selected state of the US ($50.79 \text{ mol H}^+\text{-eq} / \text{kg SO}_x \text{ as S}$). This characterisation factor is the result of extensive regional fate analysis and makes the application to general situations more effective than the IChemE approach. However, the omission of a fate analysis on the specific plant-level location mean that the location of effects is not identified, and thus the local environmental sustainability cannot be truly assessed. We cannot tell from TRACI's output whether the acidification contribution is 100m, 1km or 1000km from the plant, or in what direction. Hence, in the final analysis, the sustainability can only be judged by comparison within and between process options, and relative sustainability will be the same as for the IChemE approach.

By comparison, the current methodology does not separate the deposition due to excess emissions, but shows that, due to atmospheric dispersion, the contribution of the excess emissions for natural gas steam reforming or coal gasification is insignificant. In the case of electrolysis, the current model indicates a contribution to acidification of $4.7 \times 10^4 \text{ (mol H}^+\text{-eq)}$ above ambient deposition within the range of

modelling in the ETM. The difference comes down to a matter of scale. While the current model examines a transport distance of up to 100km, the TRACI model is regional in its approach (the lowest level of spatial discretisation is the state), thus the TRACI acid deposition contribution accounts for a much larger percentage of the total emissions (approximately 80% of total potential contribution from the raw FCI output). Furthermore, TRACI does not indicate the level above ambient deposition – this is a key issue, in that by the time the sulphur contribution of the plant reaches 100-150km, the concentration has been diluted to the ambient level, hence there can be said to be no excess environmental deposition beyond that range.

The approach in TRACI is to simplify for the sake of general applicability in Life Cycle Assessment. By the same token, there are advantages in this approach, in particular in large industrial areas where it may be difficult to break down emissions from a large number of industries and the transportation sector. Hence, by working with average values and mid-points, TRACI provides a much faster first-cut result.

In the current work the desire is to quantify and locate the impacts of emissions, thereby providing an indicator of sustainability in a location-specific sense. This is the key advance in utilising the current metrics methodology. Most metrics, in ignoring the immediate environment and environmental transport, assume a direct linear relationship between the emissions and the level of sustainability, which is shown in this work to be inconsistent with the reality of environmental resilience. Hence, this is the second major contribution of this work and several scenarios are addressed in following sections to showcase the environmental fate and impact due to hydrogen energy systems over the lifetime of the plant.

7.4.3 Modified Environmental Burden Approach

As described in Chapter 2, Diniz da Costa and Pagan (2006) have suggested a modified approach to the “environmental burden” (EB) sustainability metrics recommended by the IChemE. Their approach in terms of acidification may be summarised by Equations 28 and 29, where they derive a specific environmental impact (S_{EI}) from the environmental burden (EB_i) modified by a dose value (K_i) which

incorporates environmental parameters – soil pH and days of rain (rf_{rain}) – with the impact normalised over an area of impact (A_{imp}) and time of impact (t).

$$S_{EI} = \frac{(EB_i)(K_i)}{A_{imp} \cdot t} \quad [28]$$

where:

$$K_i = \frac{\left[\left(1 - \frac{pH_{soil}}{pH_7} \right) + \left(\frac{rf_{rain}}{365} \right) \right]_i}{\left[\left(1 - \frac{pH_{soil}}{pH_7} \right) + \left(\frac{rf_{rain}}{365} \right) \right]_{high}} \quad [29]$$

In the current example, we are not comparing plants sited in different locations, but we can use this approach to compare different sites around Tarong and compare with the current sustainability metrics.

Table 26: Specific Environmental Impact Comparison of Sites

Site	pH	EB (t)	K	A _{imp} (ha)	S _{EI}	SM %
15	6.4	4515	0.73	17800	0.185	99.3
32	5.6	5418	1	686	7.9	99.56

Although the application is not exactly as the authors intended it (the approach is typically utilised for an entire site, comparing different plants and locations), the principle is the same for comparing sites in different directions around a single plant. Like the IChemE metrics the S_{EI} can only be used for comparison between options – it does not offer an absolute measure of sustainability. From the IChemE approach, the impact at site 32 would be considered to be 1.2 times worse than at site 15, whilst the modified EB approach indicates that the impact would be 42.7 times worse, and the current model indicates that site 32 is in fact 0.26% closer to fully sustainable than site 15.

It is notable from comparison of these 3 models alone, that the different models can indicate very different results. The current model stands out from these other models,

in that it incorporates the local environmental limitations of pH buffering, thereby attempting to obtain an absolute measure of sustainability, rather than merely a comparative measure.

7.5 Response of Sustainability to Technology Parameters

Australia is very fortunate, in that its coal and NG reserves are often very low in sulphur. For the base scenarios, a coal content of 0.29% sulphur (typical of the coal fed to Tarong power station) is used (Tarong, 2006). Adjusting the sulphur content to 1% to emulate some common coals in the USA (EIA, 2004) - the response of the metrics is shown in Figure 47. Although many plants use desulphurization units in the USA, the approach of this scenario is to examine the effect of high sulphur emissions on the soil acidification impact. It must be borne in mind that the focus here is on soils only, as high sulphur emissions are likely to affect plants and the water pH of natural water bodies.

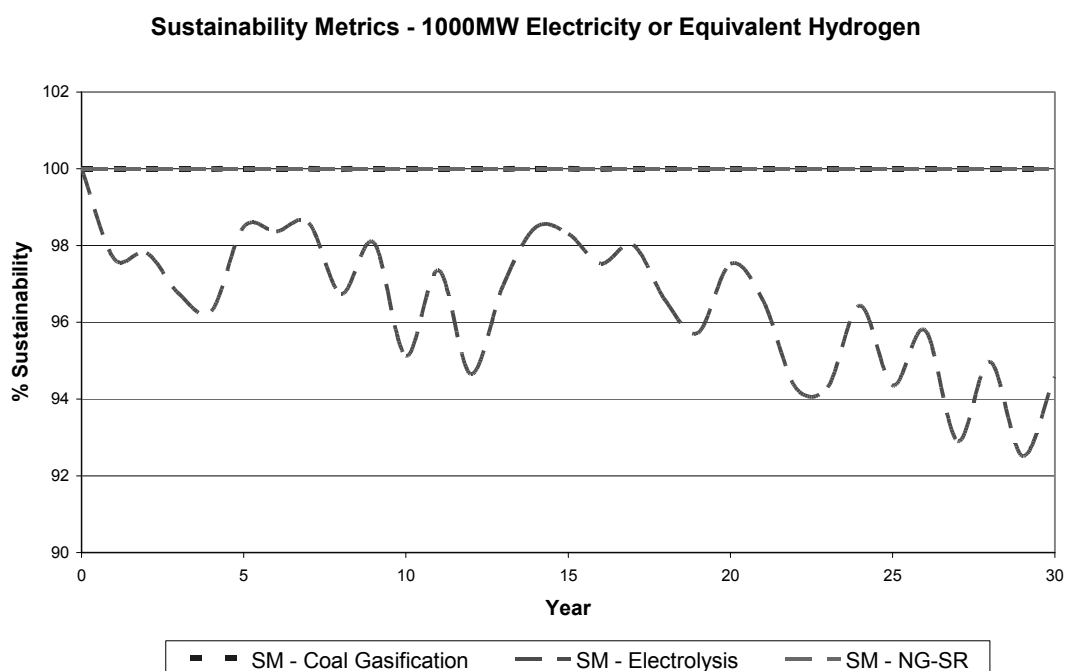


Figure 47: Response to Increase in Coal Sulphur from 0.3 to 1 wt% for each technology.

The response is most obvious in the case of electrolysis, considering that there is no sulphur capture in the Australian power station. For a 3-fold increase in sulphur content, the sustainability falls by only 3.5% from the base case, which shows that

significant flexibility in feed sulphur content is allowable within the realm of sustainability. IGCC requires high levels of sulphur removal to avoid catalyst poisoning and corrosion damage (Williams, 2001; Innes, 2003), hence the emissions still remain low and even with such high sulphur content the sustainability is still close to 100%. The increase in sulphur content will have flow on effects in the FCI, as increased rates of sorbent use will be necessary, hence higher energy and water usage will also be required, which may decrease the efficiency of the plant and decrease sustainability in other areas. The NG scenario has such low rates of sulphur emissions that the variation does not cause the sustainability to change.

7.6 Variation of Production Rate of Hydrogen

Production of 178kt of H₂ per year can fuel 1.4 million cars under the assumptions of Ogden (2003), which assumes an annual driving distance of 17,700km. For Queensland conditions (see Appendix 7), using the same fuel efficiency, the same amount of hydrogen would provide for 1.57 million cars. Examining rates of hydrogen production of 10%, 50%, 90%, 110%, 150% and 1000% of the current plant gives some idea of the relative impact and sensitivity of hydrogen production sustainability.

The coal gasification and steam reforming cases do not produce a high enough emission to cause any decrease in sustainability, even when the production rate is increased by an order of magnitude. Examining the change in relation to electrolysis gives the results shown in Figure 48.

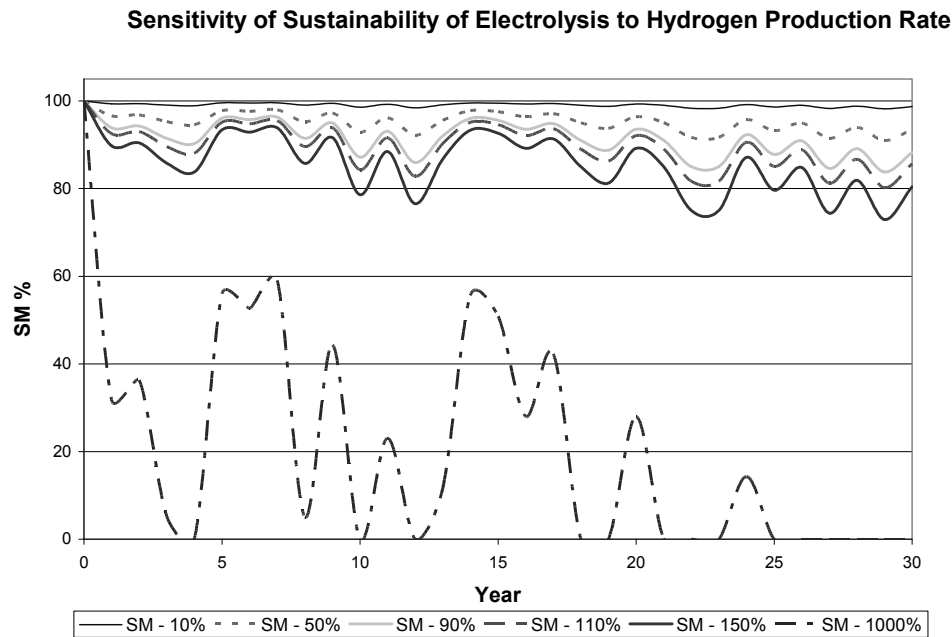


Figure 48: Sustainability Sensitivity to Hydrogen Production Rate - Electrolysis

It is apparent from Figure 48 that the sustainability of the plant does not decrease excessively for a variation of up to 50% in the hydrogen production rate, but that an order of magnitude increase – roughly equivalent in producing hydrogen to fuel all cars in Australia – would be unsustainable for a single plant at Tarong.

7.7 Response to Variation of Environmental Parameters

As indicated by the sensitivity assessment of the ETM in Chapter 6, some environmental parameters have significant impacts on the soil sulphur concentration. In particular, it was concluded that rainfall has a very large impact. Thus these parameters were examined in relation to the sensitivity of the sustainability metrics.

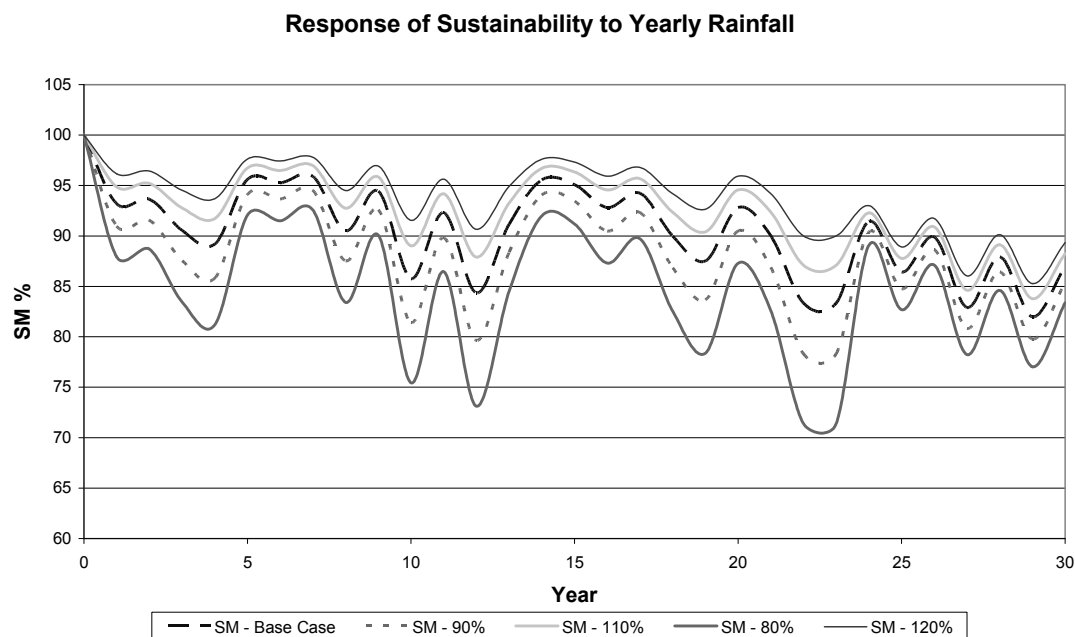


Figure 49: Sustainability Response to Yearly Rainfall Variation - Electrolysis Scenario

Using the electrolysis scenario as an example, Figure 49 shows the variation of sustainability in response to the change in yearly rainfall. It is apparent that, when there is a lower yearly rainfall, the sustainability decreases, due to the increase in sulphur retention in the soil. On average, a decrease in rainfall of 20% produces a decrease in sustainability of 3.3%, whilst an increase in rainfall of 20% produces an increase of 5.7% in sustainability.

The variation in response to rainfall has implications for the most appropriate siting of a plant, as well as the potential for reduction of sustainability under a global warming scenario. For example, Brisbane has an average rainfall approximately 10-20% above that of Tarong, such that, if soil sensitivity were considered equal, the siting of a plant in Brisbane would have higher sustainability. The current work does not include the groundwater or surface water sensitivity to acidification, due to lack of available data for validation of the model, but this is the major final sink for sulphur within the local environment. Thus, further research should be completed to determine whether the increased sulphur leaching due to excess rain would in fact be detrimental to fresh water sources. Work on water critical loads is being done in Europe (e.g. (Battarbee, Allott et al., 1995)).

7.8 Synergistic Effects of Technological Parameters

Environmental systems and industrial processes are similar, in that a change in one technological parameter typically leads to a change in a variety of other linked parameters. In truth, no single environmental parameter should be assessed in isolation, and nor should the effects of process parameters on the environment. For example, if we adjust the sulphur content of coal, yet require a constant sulphur removal effectiveness, then the rate of water usage would rise, the energy efficiency would fall, and hence the usage of coal and the plant emissions would rise. Examination of the associated effects of the variation of hydrogen production from the electrolysis and coal gasification scenarios follow (results in Table 27 and Table 28).

Resource depletion is an important inclusion in a set of sustainability metrics. It is commonly addressed in terms of the overall production (P) to reserve (R) ratios for resource analysis – e.g. (BP, 2002). With a small adaptation converting production rate (t/yr) to yearly production (t), this can be adapted to the concept of sustainability metrics as per Equation 30 (as discussed in Appendix 10). For the current example, we will apply a carrying capacity of the total Queensland coal reserves.

$$SM = \left[1 - \left(\frac{P \times t}{R} \right) \right] \times 100\% \quad [30]$$

Furthermore, water is a vital issue in Australia in particular (Diniz da Costa, 2003), with the current drought and global climate change raising concerns for future sustainability of water supply. Assuming a carrying capacity equal to 50% capture of rainfall on a 1km radius site (similar to the current Tarong power station), we can determine a water sustainability metric as well (Equation 31). The same equation can be utilised for global emissions such as greenhouse gases, if the emissions rate for a state or country is capped legally, and the Kyoto protocol targets (DEH, 2006; UNFCCC, 2006) for allowable emissions increase in Australia are used as the carrying capacity. (For further discussion, please see Appendix 10). In Equation 31, “E” represents plant water usage or greenhouse emissions.

$$SM = \left[1 - \frac{(E)}{CC} \right] \times 100\% \quad [31]$$

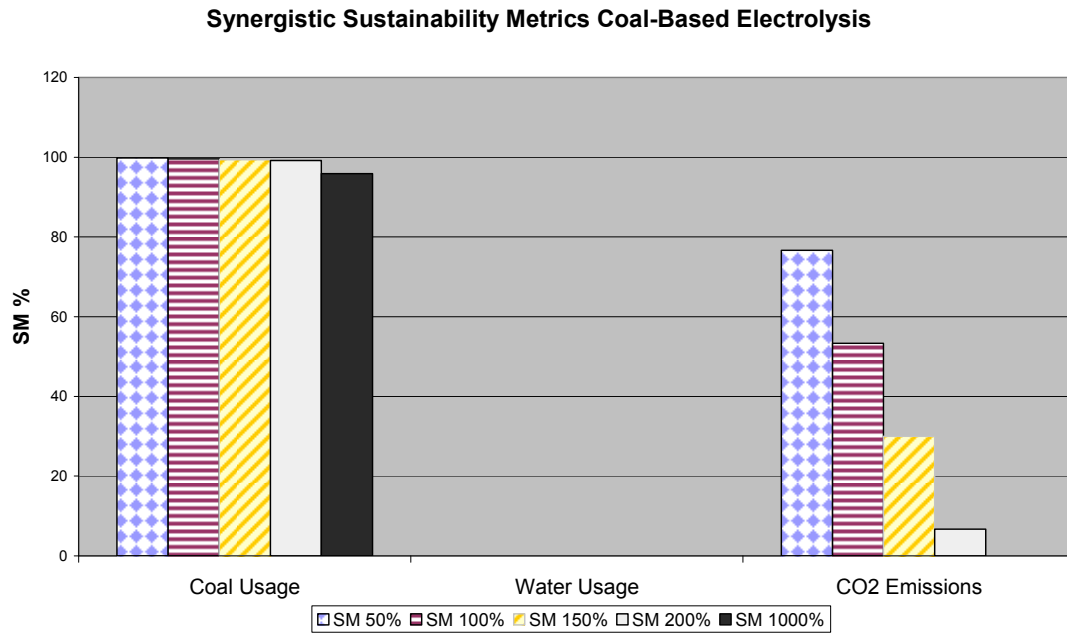


Figure 50: Electrolysis Synergistic Sustainability Impacts - Comparison of Variation of Hydrogen Production Rate

Table 27: Synergistic Impacts in Response to Variation in Hydrogen Production - Electrolysis

Parameter	SM for Hydrogen Production Rate of:				
	50%	100%	150%	200%	1000%
Coal Usage	99.8	99.59	99.39	99.18	95.91
Water Usage	0	0	0	0	0
CO ₂ Emissions	76.67	53.33	30.00	6.67	0

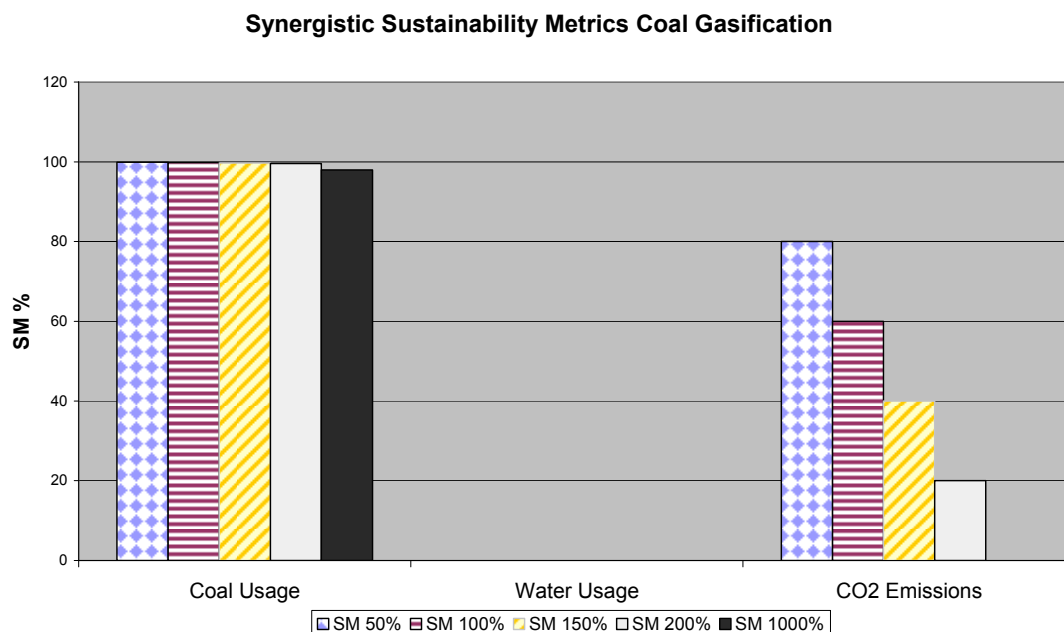


Figure 51: Coal Gasification - Synergistic Sustainability Impacts Response to Hydrogen Production Rate

Table 28: Synergistic Impacts in Response to Variation in Hydrogen Production – Coal Gasification

Parameter	SM for Hydrogen Production Rate of:				
	50%	100%	150%	200%	1000%
Coal Usage	99.90	99.80	99.70	99.59	97.97
Water Usage	0	0	0	0	0
CO ₂ Emissions	80.0	60.00	40.00	20.00	0

The results here, show the interconnectedness of the various technological and environmental parameters, where an increase of hydrogen production rate affects not only the sustainability in terms of acidification, but also the emissions of greenhouse gas emissions, and the usage of water and coal. It may be noted at this point, that the sustainability of the plant in terms of water usage is considered to be 0 for most options, as the plant cannot collect enough rainwater from the site to fulfil its requirements. Other definitions of the carrying capacity could potentially indicate a sustainable plant – for instance, basing on a larger plant area, or the flow of local creeks.

7.9 Worst (and Best) Case Scenarios

In order to obtain further information on the performance of the SM model, 2 extreme scenarios were examined. These scenarios tested the model performance assuming an error of 20% in each of the parameters of interest – thus examining the cumulative effect of moderate errors in parameters, or the potential for extreme variation in the environment. The direction of parameter variation is shown in Table 29.

Table 29: Direction of Change of Parameters for Worst Case Scenarios

Scenario	Best Case	Worst Case
Process Emissions (Coal Sulphur)	⬆	⬆
Yearly Rainfall	⬆	⬇
Run-off Factor	⬆	⬇
Permeability Factor	⬆	⬇
Carrying Capacity	⬆	⬇

The electrolysis example is used in the comparison for site 17. The worst case incorporates a doubling of the coal sulphur concentration, whilst the best case involves the incorporation of flue gas desulphurisation removing 90 % of SO_x . Results of the sustainability assessment based on the extreme cases, is shown in Figure 52.

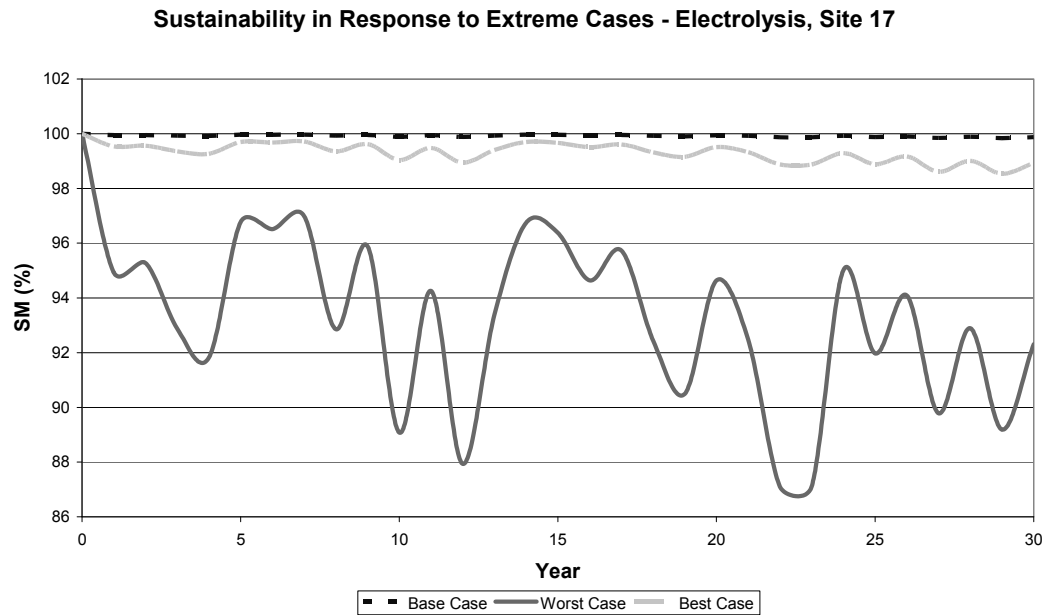


Figure 52: Sustainability Metrics in Response to Extreme Cases for Electrolysis, Site 17

The SM response to the worst case scenario shows that the sustainability under low rainfall conditions, with high sulphur coal, low run-off and low permeability, low carrying capacity soil drops significantly from the base case. Nonetheless, the sustainability remains above 86%. The best case scenario increases the SM to nearly 100%. It may be argued that, with the sustainability considered to be so high, even in the worst case, that there is no need for flue gas desulphurisation. This lends validity to the current situation at Tarong.

7.10 Sustainability Metrics Contour Lines

To this point, we have only shown the sustainability metrics for individual sites around Tarong, however, the model produces discretised data for each sub-airshed at 45 degree intervals around the emissions source (Figure 54, Figure 56 and Figure 58). The SM for each sub-airshed can be averaged over its areas to determine an overall sustainability metric. With interpolation using typical graphing software, we can produce contour maps of sustainability in the plant vicinity (Figure 53, Figure 55 and Figure 57). This gives an easy method of viewing the variation in sustainability over the local area. Calculating the area between each contour could be used as an

alternative method of combining the individual airshed metrics into a single figure for the entire plant.

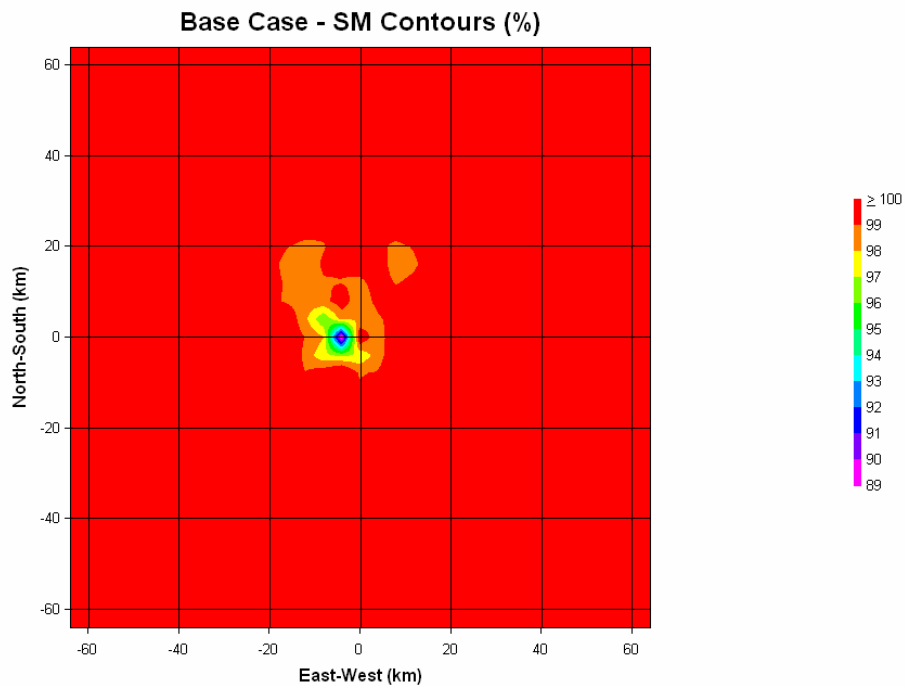


Figure 53: Sulphur Soil Acidification Sustainability Contours for Coal-based Electrolysis Base Case - Tarong

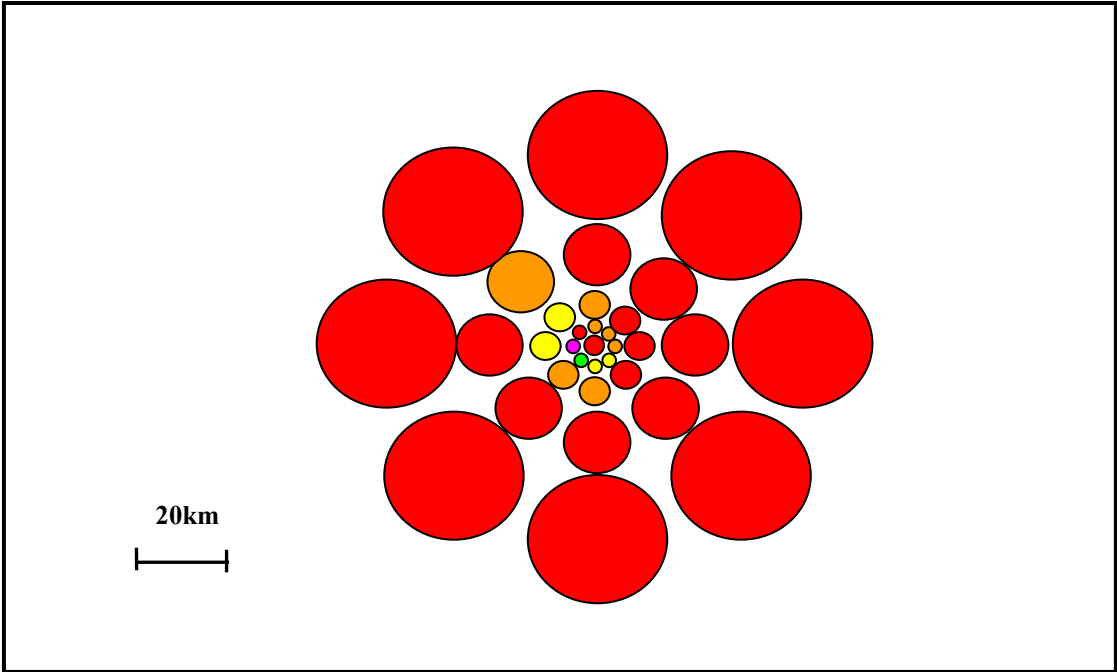


Figure 54: Sulphur Soil Acidification Sustainability Metrics Base Case Scenario – Coal-Based Electrolysis

99 – 100	98 – 99	97 – 98	95 – 96	89 – 90

Sustainability Metrics - Worst Case Scenario for Electrolysis at Tarong

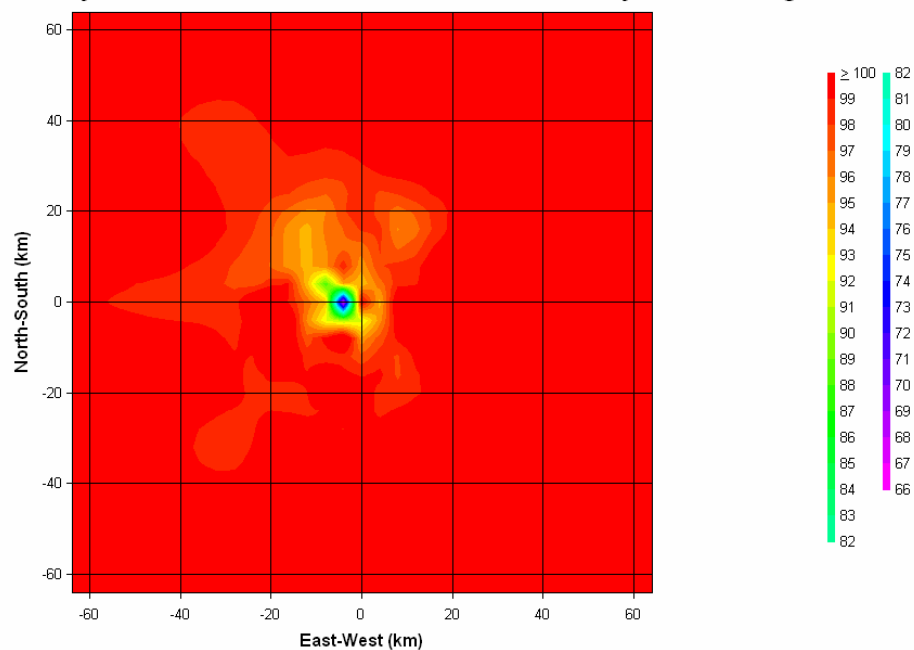


Figure 55: Sulphur Soil Acidification SM Contours for Tarong – Coal-based Electrolysis, Worst Case Scenario

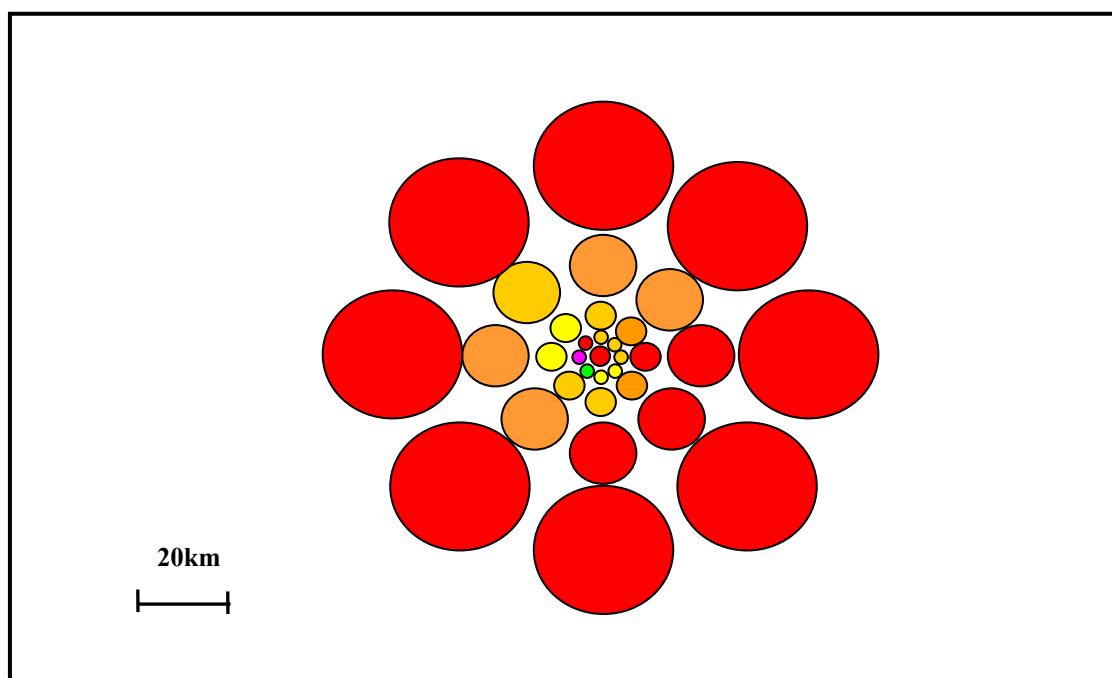


Figure 56: Sulphur Soil Acidification Sustainability Metrics Worst Case Scenario – Coal-based Electrolysis

98 - 100	96 - 98	94 - 96	91 - 94	86 - 88	66 - 67

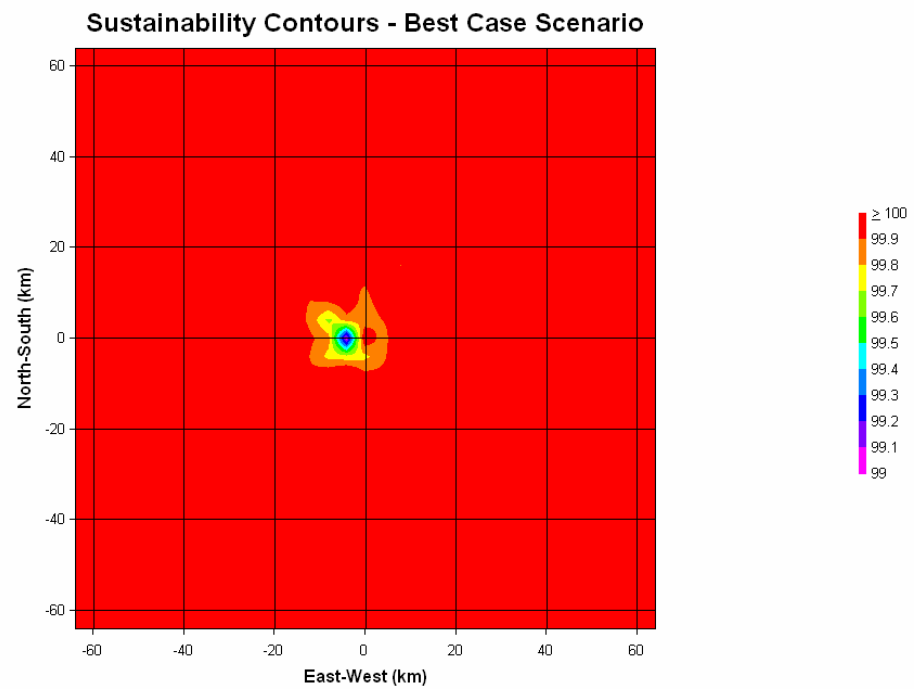


Figure 57: Sulphur Soil Acidification SM Contours for Tarong – Coal-based Electrolysis, Best Case Scenario

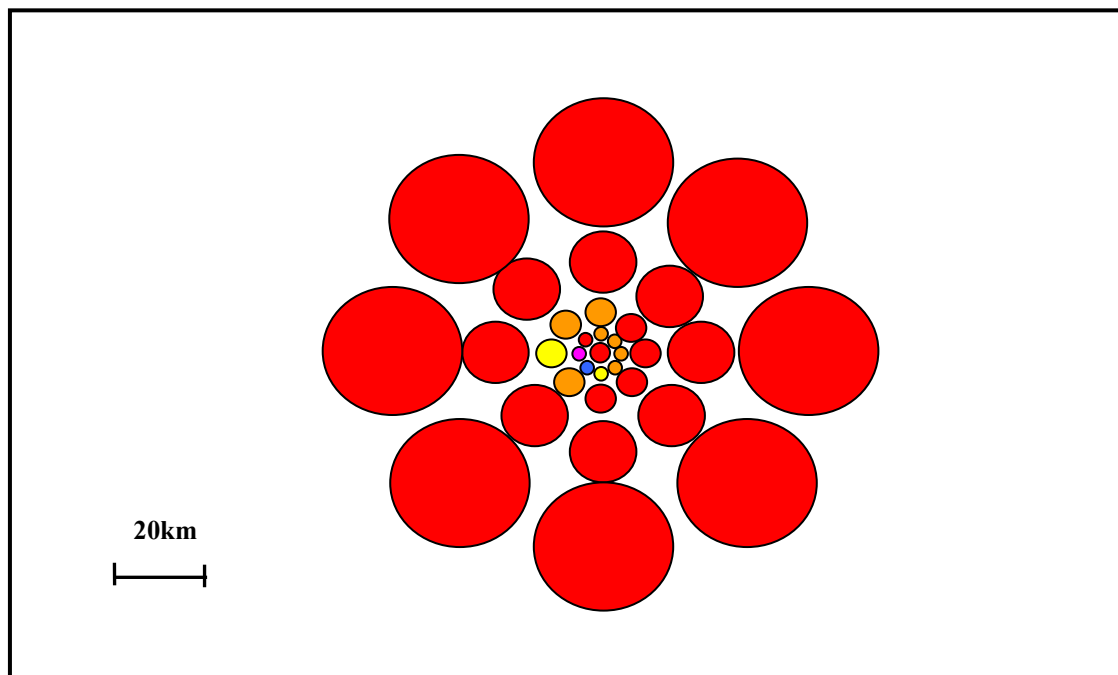


Figure 58: Sulphur Soil Acidification Sustainability Metrics Best Case Scenario – Coal-based Electrolysis

99.9-100	99.8 – 99.9	99.7 - 99.8	99.6 - 99.7	99.5 - 99.6	99 - 99.1

From the graphs, it is apparent that there are “islands” of higher or lower sustainability in some areas. These represent points of particularly high or low carrying capacity. It must be noted that the above SM contour lines are exclusively related to sulphur emissions from a potential plant sited at the current Tarong Power Station and derived mainly from average soil results for the area (other than the sites 15, 17 and 32 where full information is known). In addition, some of the land within the area assessed is used for agricultural or other purposes, where other sulphur emission activities may occur which are not related to Tarong power station. Nevertheless, the SM contour lines serve the purpose to illustrate the potential applicability of the SM model proposed in this work. The proposed ETM model and SM model in this work provides a site specific high resolution environmental impact and sustainability metrics. This can be used as a powerful tool in environmental management where the sustainability of “hot spot” areas or sinks needs to be properly ascertained and managed over time.

In comparison to the graphical method of representation, the combination of SM results from each sub-airshed by averaging over the area gives the results in Table 30.

Table 30: Overall Sustainability Metrics Averaged using Land Areas - Electrolysis

Scenario	SM %
Base Case	99.52
Best Case	99.73
Worst Case	99.07

It is apparent that the overall metrics vary much less widely than the results for individual sites. This indicates that, although the overall metric is an important number, and useful in its own right, the graphical representation gives a better picture of the location of impacts, and is able to highlight the areas of highest impact which is hidden in the single overall value. The larger area of the outer airsheds, which have higher SM values, weights them more heavily than the lower sustainability inner airsheds, which can be misleading in terms of site-specific impacts. Therefore it is recommended that the graphical approach be used preferentially, or that a weighting or banding method be used in averaging. An example of the banding averaging methods is shown in Table 31, where each concentric circle of sub-airsheds is

averaged together from the inside outwards. This method reduces the number of metrics from the total individual sites, but still hides the worst sites to some extent.

Table 31: Banding Method of Averaging - Electrolysis

Scenario	Airshed					
	Inner	1	2	3	4	5
Worst Case	100	90.39	95.67	97.67	99	99.57
Best Case	100	99.73	99.89	99.95	99.98	100
Base Case	100	96.77	98.59	99.28	99.67	99.87

7.11 Conclusions

In this chapter, the second major contribution of this work is presented in the application and analysis of the new sustainability metrics model to hydrogen production systems. By incorporating local environmental transport mechanisms and limitations on soil concentrations of acidifying compounds, the current SM model paints a more realistic picture of environmental sustainability than typical loading models.

The analysis of the model in terms of the site of Tarong power station, using acidification as the prime example of the new SM methodology, and the application of the metrics to specific hydrogen production technologies is a unique (if somewhat specific) application of sustainability assessment. The available data from the area surrounding Tarong power station, and the existing methodologies for acidification carrying capacity estimation made this the ideal location and metric for the current work. Likewise, comparison of 3 fossil fuel based hydrogen production technologies gives some insight into the relative performance of these technology options under various conditions. Due to the very low rates of sulphur and high rates of sulphur removal respectively, the NG-SR and coal gasification technologies were shown to be close to 100% sustainable under all variations considered. The electrolysis technology, based on conventional coal based electricity supply, proved to be the highest emitter of acidifying compounds by a significant margin, but still had a high level of sustainability under most conditions.

The response of the SM results to the sensitivity of the soil, the variation of hydrogen production rates and the rainfall around the site was examined. The assessment culminated in the examination of sustainability under best and worst case scenarios, showing that the sustainability of the electrolysis scenario could be improved to close to 100% by incorporating sulphur removal in an environment with high leaching removal, and that the worst case scenario would reduce the sustainability to close to 86%. This variability is typical of the current model - whereas the loading changes by almost 100% in either direction from the base case, the sustainability varies by considerably less. The resulting SM data was then presented in graphical form.

The current work has presented only the sustainability in regards to acid deposition as an example of the new SM methodology however, the true sustainability of the plant relies on the performance in regards to a combination of different environmental impact categories – including resource depletion, water usage and global impacts such as greenhouse gas emissions. Likewise, the variation of a single process parameter can lead to significant change in the SM in regards to other impacts. Some simple metrics were shown to illustrate the synergistic effects of the variation of sulphur emissions on other impacts. The further development of a full set of metrics is recommended to assess the overall sustainability over all relevant categories.

When the model was compared with some existing SM methodologies, it was shown that the current model is markedly different in its results. The existing methodologies involve the use of environmental loads directly as the metric (Tallis, Azapagic et al., 2003), or with minimal adjustment through multiplication with a characterisation factor (Bare, Norris et al., 2003). As long as the characterisation factor does not vary between distinct localities within a larger region, the sustainability remains a general concept, rather than relating directly to the location and extent of the process impacts. The modified EB methodology (Diniz da Costa and Pagan, 2006) offers a more location-specific characterisation factor, but the derived metrics still vary by many orders of magnitude. Furthermore, all the current methodologies examined offer only a comparative assessment option – i.e. a relative measure of sustainability. On the other hand, the new SM model allows selected plants in their specific environment to be assessed individually, and an absolute measure of sustainability to be obtained. It was shown that the variation of emissions rates within these loading models does not

reflect accurately the variation in final impacts, due to the lack of dispersion and soil sensitivity assumptions. Thus, although a variation in acid emissions caused an equal variation in sustainability indicated by the loading models, the current SM model showed that much of the increased load is buffered or dispersed, which causes the sustainability changes to be much lower than the loading change.

The spatial discretisation and tracking of sustainability impacts is another important aspect of the current SM model. Existing methodologies cannot locate the impact of the plant in its environment or determine the sustainability at a given point around the plant, whereas the current SM model can. This can be particularly useful in the graphic representation of sustainability variation shown in the final section of this chapter. With the identification of “hot spots” of high vulnerability, mitigation and monitoring procedures can be targeted appropriately, rather than in a more expensive broad-sweep approach. By comparison, an overall single value metric can potentially hide the sensitivity or extent of an impact at individual sites through the heavy weighting towards sub-airsheds of higher area, which tend to be in the lower impact regions towards the outer edges of the area of interest.

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Chapter 8

Conclusion

8.1 Introduction

The fundamental aims of this work have been to evaluate the sustainability of potential hydrogen energy systems for the Australian context and in the process, to develop a new methodology of sustainability assessment that covers the gaps in current methods. The literature review indicated that the assessment of the environmental sustainability of hydrogen had not been completed and that, on the whole, the current methodologies for sustainability assessment neglect the explicit incorporation of the local environment, spatial and temporal variation.

With these gaps in current knowledge in mind, five stages of work were undertaken to achieve these goals:

1. The current methodologies of sustainability assessment were reviewed, and the most appropriate methodology for development was chosen as the sustainability metrics (SM) model.
2. An Inventory of the Fuel Cycle Emissions and Resource Usage of selected hydrogen energy systems was undertaken to supply the underlying data to assess the sustainability of these systems.
3. The theoretical SM model was developed, incorporating an Emissions Transport Model (ETM) to connect the plant to its environment and allow the spatial and temporal analysis of sustainability at different locations, under different environmental conditions.
4. Historical data for the Tarong power station, an isolated Australian power plant, was used to validate the ETM, and show that the importance of environmental dispersion and transport processes cannot be ignored in the assessment of sustainability.
5. The validated SM model was applied to a number of hydrogen production scenarios for the impact of acidification, thus providing an assessment of the

performance of the current model under various conditions, a comparison with existing models of sustainability, and an indication of the sustainability of the hydrogen technologies examined.

8.2 Discussion of Contribution

This work has provided two major contributions to existing knowledge – the validation of the ETM underlying the SM model, and the application and analysis of the SM model to the unique application and location of hydrogen production systems in Australia.

Much research and development has been achieved in the field of atmospheric transport of process emissions however, it is rare for a model to progress beyond the atmospheric concentration or pollutant deposition rate. The current ETM has used a process approach to model the short to mid-range transport of emissions from fossil fuel based hydrogen plants, and moved beyond simple atmospheric concentration or deposition rates to examine the balance of sulphur in the soil. The results and approach have been validated using historical data from Tarong power station, which represents one of the most unique and valuable aspects of this work, due to the isolation of the plant and availability of environmental data for pre-plant and current conditions. Such opportunities for the assessment of environments under the influence of a single pollutant source are extremely rare.

The ETM developed here, was limited to physical processes due to the limitations of data, which can lead to deviations where other complex environmental interactions such as weathering, site-specific rainfall and vegetation change are at work. However, even given the limitations, the results of the validation showed a very close correlation with currently accepted transport models, and with the historical data.

With the validation of the ETM, the SM model was applied with confidence to the production of 1000MW of hydrogen from electrolysis with conventional coal electricity, coal gasification and NG steam reforming. The metrics were applied for the case of acidification specifically, due to the prior validation of the ETM in

response to sulphur emissions, and the availability of carrying capacity estimation methods.

The most important aspect of the new SM model, and the second major contribution to knowledge, was the demonstration that the response of sustainability in the local environment is not necessarily in the same magnitude as the change in loading, and that the environmental resilience or limitations have a major role in sustainability. Thus it was shown that, unlike current loading models, an increase in magnitude of emissions by 100% does not create a decrease in sustainability from 98% to 49% for instance. Furthermore, the new SM model, properly calibrated, allows an absolute assessment of sustainability, rather than the solely-comparative assessment that current methodologies allow. It was also shown that the concept of a single indicator number (as the only option from a loading model) can actually be very deceptive, as the average can often hide higher damage at specific sites. Thus the graphical and spatially discretised output of the new SM model is very useful in allowing the highlighting of “hot spots” of high impact. Finally, the application of the metrics to the production of hydrogen in Australia is a novel one, in that minimal work on sustainability of hydrogen has been completed, and the work on sustainability within Australia is also limited.

8.3 Recommendations for Further Research

Although this work has covered some of the gaps in current knowledge in relation to the sustainability of hydrogen, and the new SM model has been developed to more accurately determine the sustainability of a plant in its local environment, there are a number of aspects that could be extended.

Firstly, although the SM model has been validated for sulphur deposition and its contribution to soil acidification, there are numerous other impacts that have not been included. It was shown that the synergistic effects of the variation of a single technological or environmental parameter can vary widely in regards to associated impacts. Thus, to get a true indication of the sustainability of a process, further work

is needed to develop the metrics for other emissions, and the resource usage metrics could be developed further.

Secondly, the current ETM and sustainability assessment covers only the potential for acidification of soils as the endpoint of the model. The ultimate sink for the acidifying compounds will be ground and surface water, hence it is suggested that further work be done to estimate the flows and final destination of run-off. It is possible that this work may include the integration of more complex models of soil hydraulics and atmospheric transport and reaction. However, it would be suggested that, where possible, simplifications be used such that the SM model is readily applied in any environment.

Finally, the assessment in this case has only covered 3 potential hydrogen energy systems, and has focussed solely on the hydrogen production phase of the fuel cycle. Thus there is a much wider scope for assessment of the full fuel cycle and full range of hydrogen production and utilisation technologies in a “well-to-wheel” type study.

Appendices

Appendix 1

Review Paper

This paper appeared in the International Journal of Hydrogen Energy in 2005. The work on hydrogen production is solely my own work, whilst the other sections are mainly the work of the other authors.

Hydrogen Production and Utilisation Opportunities for Australia

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ABSTRACT

Worldwide, research and policy momentum is increasing in the move towards a hydrogen economy. Australia is one of the highest per capita users of energy, but relies heavily on fossil fuels to fulfil its energy requirements – thus making it one of the highest per capita polluters. It is also a country rich in natural resources, giving it the full range of options for a hydrogen economy. With the first Australian Hydrogen Study being completed by the end of 2003, there has as yet been little analysis of the options available to this country specifically. This paper reviews the resources, production and utilisation technology available for a hydrogen economy in Australia, and discusses some of the advantages and disadvantages of the different options. It points out that coal, natural gas, biomass and water are the most promising hydrogen sources at this stage, while solid oxide and molten carbonate fuel cells may hold the advantage in terms of current expertise for utilising hydrogen rich gases for stationary power in Australia.

Keywords: fuel cells; hydrogen; hydrogen production; Australia; fossil fuels;

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1. INTRODUCTION

Concerns over the effect of global carbon dioxide (CO₂) emissions and other local air pollutants such as nitrogen and sulphur oxides (NO_x and SO_x) and fine particulates on the environment and human health have led to significant research into the use of alternative energy carriers. Currently the forerunner in the race for the new energy industry appears to be hydrogen, with vast amounts of research funding, and hopes of a greenhouse friendly fuel vested in it.

Hydrogen can be produced from a variety of sources including fossil fuels, biomass, water and some industrial waste chemicals, and can be used in fuel cells or other engines or turbines to provide energy. Overall, emissions in a hydrogen energy cycle are expected to be lower than for today's carbon energy cycle, but the centralised production of hydrogen offers the extra advantage of enabling large scale capture and sequestration of CO₂ emissions. Sequestration, along with the efficiency improvement due to fuel cell technology, could make a major difference in emissions from a hydrogen economy.

Australia is a country of vast natural resources, especially coal, which is both beneficial and detrimental in terms of environmental improvements in energy delivery. In favour of a hydrogen economy is the availability of so much potential hydrogen fuel, while the current reliance on fossil fuels, the low price of "dirty" energy delivery and the established nature of the coal power industry may make it difficult to increase industrial momentum towards hydrogen.

Various types of fuel cells are being developed, with different applications appropriate for each type. Australia has a particular expertise in high temperature fuel cells, but how they will fit with hydrogen production technology – especially coal Integrated Gasification Combined Cycle (IGCC) systems – is yet to be examined thoroughly using Australian coals.

2. HYDROGEN SOURCES AND PRODUCTION METHODS

Hydrogen can be produced from a wide range of source materials, including fossil fuels, biomass, some industrial chemical by-products and water via electrolysis. Australia is in the fortunate position of having the full range of options within the borders of a single country. The choice of source for a future hydrogen economy in Australia, as elsewhere, would depend on various local factors including location of resources, available reserves, cost of

extraction, cost of utilisation and transportation. The technique utilised to produce hydrogen from the source will depend on technology development, required infrastructure investment, efficiency, location and suitability of local supplies. In a country as vast as Australia, with such a wide variety of environments, it is likely that a variety of production routes will be used.

2.1 Natural Gas

Natural gas (NG) is the cleanest of all fossil fuels and has the highest hydrogen to carbon ratio, as it consists almost entirely of methane. Especially in Australia, it has very low amounts of impurities such as sulphur compounds and heavy metals, which means that it requires the least pre-processing and produces less waste per unit of hydrogen produced.

Hydrogen from NG for the ammonia and petroleum industries represents the largest portion of the current global production market (Geiger, 2003). Hydrogen can be produced from NG directly via various processes, including steam reforming, partial oxidation, auto-thermal reforming and thermal decomposition (Dicks, 1996; Dicks, 2003), as well as indirectly via electrolysis using electricity and/or heat from gas combined cycle processes.

Estimates are that in Australia approximately 250,000 t/yr of hydrogen are produced from SR for ammonia production, whilst Brin's Oxygen Company (BOC) produces or purifies another 20,000 t/yr approximately for the chemical and petrochemical industries (Walsh, 2003). BOC also operates a POX hydrogen production system producing 25,000-30,000 t/yr for hydro-cracking in a petroleum refinery (Walsh, 2003).

The NG decomposition process offers the benefits of production of a solid carbon phase, which can be relatively easily separated, handled and disposed of, and a gaseous H₂ phase of very high purity, without CO and CO₂. It is also a single-step process, requiring none of the water gas shift (WGS) reactors needed by SR systems. The major drawback of the process is the energy lost by not utilising the solid carbon to produce still more hydrogen, along with (ultimately) CO₂ (Hirsch, Epstein et al., 2001). This process was commercialised in the past, although it has been supplanted by SR as the major producer of hydrogen (Poirier and Sapundzhiev, 1997).

The source of heat is also of crucial importance to both the efficiency and environmental impact of the processes. Extensive research is being carried out into the use of concentrated solar energy for this purpose, as it offers the potential of unlimited renewable, low-emissions

energy (Kogan, 1998) (Hirsch, Epstein et al., 2001) (Ohya, Yatabe et al., 2002). Australia has the highest average insolation rate of any continent, which could make the solar options particularly attractive. These processes still have a variety of challenges to overcome before a commercially feasible process becomes established however, they may become more viable in future (especially with NG) in the case of greenhouse gas (GHG) mitigation strategies and carbon taxes becoming more widespread.

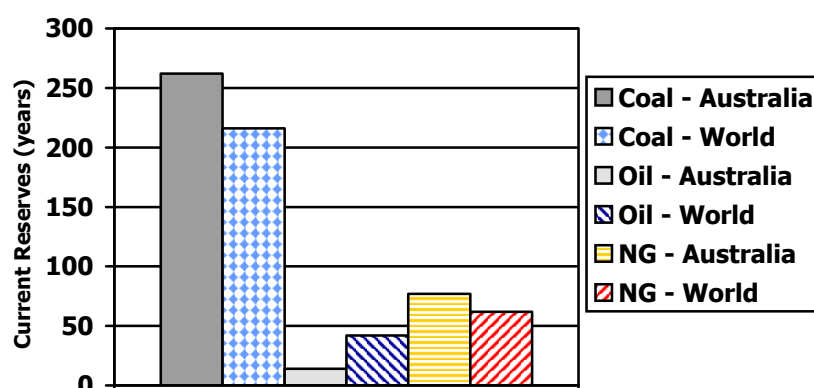
Estimates of NG reserves in Australia vary quite dramatically depending on the source. BP, 2002 estimates Australian reserves at $2.55 \times 10^{12} \text{ m}^3$ and production at a rate of $32.7 \times 10^9 \text{ m}^3/\text{yr}$ (compared to consumption of $22.5 \times 10^9 \text{ m}^3/\text{yr}$ or 874.8 PJ), which implies a lifetime of 77.9 years, compared with an expected 61.9 years globally. The Australian Gas Association (AGA, 2003) estimates reserves at 157 343 PJ ($4.09 \times 10^{12} \text{ m}^3$) with production at 1232.1 PJ and consumption at 996 PJ, implying a lifetime of 127.8 years. This variability in the different sources may be due to their definitions of reserves – commercially recoverable or theoretically recoverable – and the source of their data. In either case, the longevity of NG reserves in Australia is greater by 25 – 200% than global expectations, which puts Australia in an advantageous situation in terms of the global market. With a relatively short supply of NG available, and with constantly increasing demand, predictions are that resource costs are likely to increase along with oil, whilst coal costs are predicted to fall slowly (Ogden, Williams et al., 2001).

NG trade is globally established, and Australia exports approximately 20% of its total production, thus there is an extensive infrastructure already in place across the country. Pipelines connect all capital cities, and many other major industrial or residential centres as detailed in (Encom, 2000). The total pipeline infrastructure amounts to over 17,000 km across the country. In most cases, the length of pipeline from source to usage point is over 100 km, and indeed, the average length is in excess of 560 km overall or 810 km outside of the state of Victoria. These large distances may become important if carbon dioxide captured by centralised hydrogen production plants was to be utilised to enhance NG recovery or for sequestration in exhausted gas wells because the costs associated with the CO_2 and H_2 transportation could change optimal plant locations or even make the process economically unviable. Infrastructure exists in most of the major centres for the production and distribution of NG in the form of LNG, which is an advantage for distributed production of hydrogen at the residential or refuelling station levels. It may be possible to use existing NG transmission pipelines to transport hydrogen or hydrogen / NG blends however, this would depend strongly on the ability of current pipeline materials to withstand hydrogen embrittlement (Ogden, 1999) and diffusion losses.

2.2 Oil / Petroleum

Total recoverable oil reserves in Australia are estimated at between 1 and 3.5 billion barrels (0.4 billion tonnes), by Geoscience Australia (Petrie, 2002) and BP (2002) respectively. This equates to approximately 14 years supply at current production levels, or only 10 years at current consumption levels of 38.1 million tonnes/yr or between 1600 and 1800 PJ/ yr (ABARE, 2002). This is approximately one third of the 40 years estimated for the total global oil reserves to be used up (see **Figure 1**), which puts Australia in an undesirable situation in terms of its dependence on imported oil within 20 years, unless new reserves become available or major changes in fuel efficiency and use of light personal vehicles occur. These limits on supply provide a strong case for moving away from oil-based energy production and also show that if production from oil were to become the major hydrogen source, then it could only be for a relatively short start-up period, if it were found to be economically viable.

Figure 1: Current Fossil Fuel Reserves (BP, 2002)



Major oil pipelines already installed between current oil fields and major industry or residential centres are shown in Table 1. The distance between major oil reserves and usage points is greater than 200km in almost all cases, with an average pipeline length of 530 km between the well and usage ends (PPA, 2003). It is also apparent that most major centres in Australia do not currently have access to piped-in oil, which may be a disadvantage for those centres. This distance from the point of usage must be taken into account when comparing the possible sources of hydrogen, as it can have a major affect on the economic viability of the process.

Existing infrastructure in the form of pipelines (for potential centralised or distributed hydrogen production) and gasoline refuelling stations (for distributed production) is a definite advantage for any hydrogen source however, as has been noted, pipeline infrastructure is relatively minimal at the moment. The advantages and disadvantages of installing new pipelines for the centralised production of hydrogen at the extraction site and subsequent piping to end use, as another option, should be considered in an assessment of the viability of oil as a hydrogen source.

Table 1: Australia's Major Oil Pipelines (Pipeline Publications Australia Pty Ltd, 2003)

Well End	Usage End	Approximate Length (km)
Jackson	Moonie ^a	850
Moonie	Brisbane	250
Ballera	Moomba ^b	250
Moomba	Port Bonython	700
Mereenie	Alice Springs	250
Longford	Long Island Point (Melbourne)	200
Newcastle ^c	Sydney	150

^a Jackson oil continues to Brisbane in Moonie-Brisbane pipeline

^b Ballera oil continues to Port Bonython in Moomba-Port Bonython pipeline

As a liquid, petroleum would hold an advantage for applications such as on-board reforming for fuel cell vehicles, or where large quantities of fuel are required to be stored, as it is easily stored and transportable.

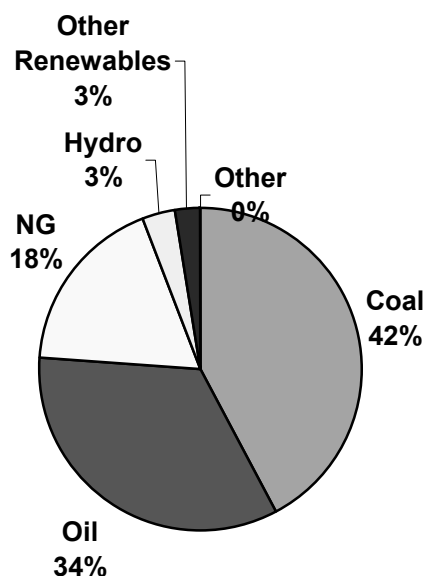
2.3 Coal

Coal is the most abundant fossil fuel on the planet, with current estimates of 216 years global recoverable reserves and 261 years Australian reserves (BP, 2002) at current usage rates. As with other fossil fuels, reserve accuracy is unreliable however, most estimates are greater than the values quoted, with some over 500 years (Williams, 2001). This indicates that the longevity of coal supplies is almost certain to surpass that of NG by over 100 years. Currently coal is the main source of primary energy in Australia, as can be seen in Figure 2. Furthermore, it is the predominant fuel for electricity production, with approximately 84% produced from coal (Riedy and Diesendorf, 2003). Coal power generation is also the largest

source of greenhouse gas emissions, producing approximately half of the total Australian emissions (Riedy and Diesendorf, 2003).

Figure 2: Australian Primary Energy Sources (BP, 2002)

2001 Primary Energy Sources



Hydrogen can be produced from coal by two main methods - gasification, and use of coal-generated electricity to electrolyse water. Of these, gasification may offer the greater potential for CO₂ sequestration, as well as the reduction of other pollutants such as NO_x and SO_x.

Of all fossil fuels, coal has the lowest hydrogen to carbon ratio, so more CO₂ is produced per mole of H₂. Much research has been done on Integrated Gasification Combined Cycle (IGCC) processes, with 5 prototype plants in operation worldwide – 3 in USA and 2 in Europe – with efficiencies close to 50% (Haupt and Zimmermann, 2001)), and the (Australian) Commonwealth Science and Industrial Research Organisation (CSIRO) is currently undertaking research and development into this area. With sequestration, coal gasification produced hydrogen has the potential to be a very low emissions fuel on a life cycle basis. More research into sequestration and gasification in the Australian context is necessary before widespread implementation can occur.

As of February 2003, worldwide, there were 417 active or planned gasification projects, with a total production capacity of 428 866 510 Nm³/d (IGO, 2003). Australia has 2 active gasification projects producing 805 000 Nm³/d of syngas for hydrogen production and 20 208 Nm³/d for electricity production respectively (SFA, 2000).

Variations on this technique, such as using concentrated solar thermal energy to provide the necessary heat for gasification, and underground coal gasification (UCG) (where the coal is not removed from the ground but gasified in situ) are also being developed. A pilot plant using UCG to produce syngas for electricity is being trialled at Chinchilla in Queensland, with a current capacity of 80 000 Nm³/h of low calorific value gas (Blinderman and Jones, 2002). This gas could also be used to produce hydrogen.

Australia's high dependence on coal in the energy market has both advantages and disadvantages for a future hydrogen economy. In terms of infrastructure, the coal extraction, transportation and power generation industry is well established, such that the required infrastructure would be the gasification plants and hydrogen distribution system. Coal reserves (export, domestic, proven and potential economic reserves) are located within 200km of the eastern Australian capitals (Brisbane, Sydney, Melbourne, Canberra, Hobart), with almost all reserves within 500km of major centres (SKM, 2001). An extensive rail transportation system exists, with over 3050km of rail in Queensland and New South Wales used for coal transportation (mainly for export) (ISR, 2001).

The established nature of current power generation, and the long lifetime of current plants may limit the willingness to adopt a new approach to energy production, which could be disadvantageous. Social reaction may also be adverse or sceptical unless a widespread educational campaign was undertaken. The low cost of coal as compared to other sources is also an advantage to its use, especially in Australia.

2.4 Biomass

There are two main types of biomass from which hydrogen fuel may be derived – (a) biomass from organic municipal waste, sewage, food production, agriculture and forestry industry organic waste and (b) dedicated energy crop plantations. As the biomass fuel sources are so varied and so widely distributed, it is difficult to quantify the potential resources available, and more research is required in this area.

In Australia especially, bagasse (the crushed outer stalk of sugar cane) is the focus of much research and development, as it is a large resource currently under-utilised by the sugar industry. Currently some bagasse is used to produce electricity (250 MW installed capacity Australia-wide) (AAS, 1999), while the rest is either burnt or used as mulch/fertiliser. Hydrogen could be produced from bagasse by gasification in the same way as coal, giving a new potential market for Australian sugar cane growers who are having difficulty competing in the global market.

Landfill gas from refuse dumps can be collected and reformed, as can sewage treatment gas. Currently landfill gas is collected at just over a dozen tips, and utilised to produce electricity (72 MW installed capacity), as is sewage gas (7.5 MW installed) (AAS, 1999). This represents another under-utilised source, which is expected to increase dramatically (sewage electricity to triple by 2010), and this fuel that is currently burnt could be reformed to produce hydrogen as with NG (AAS, 1999). Hydrogen can be produced from solid biomass via gasification, pyrolysis or biological processes.

The feedstock price is the largest component of operating costs for the biomass gasifier, accounting for approximately 40% of the cost of hydrogen (US\$9-17) from large facilities (producing 0.7-2.2 million Nm³/d) (Padro and Putsche, 1999). The feedstock prices vary depending on the source of the biomass – the higher costs are for dedicated biomass production and the lower costs are for waste biomass. Some industrial producers of waste biomass (such as bagasse in the sugar industry), would be able to obtain feedstock at minimal cost.

Energy conversion of 47.9% (HHV) for a system producing 5.9 t/d (2740 Nm³/h) of H₂ from 100t/d of biomass has been reported by Iwasaki (Iwasaki, 2003). Based on a comparison with this work, it was estimated that the potential hydrogen production capacity via pyrolysis/gasification from the bagasse currently used for electricity alone would be 231 t/d. This is more than the estimated amount of hydrogen to fuel 10% of Brisbane's current passenger vehicles (90,000) (Ogden, 1999; ABS, 2001; ABS, 2003). The process produces minimal CO and has the potential to produce electricity or hydrogen, as well as a number of by-products (Padro and Putsche, 1999; Iwasaki, 2003).

Under the right conditions, various bacteria can be made to produce H₂ from a variety of feedstocks (usually biomass), via a number of different processes including direct / indirect biophotolysis and photo/dark-fermentation. The reactions and bacteria involved are too

numerous to mention here – for further information the reader is directed to other sources – e.g. (Levin, 2002). These processes are yet to be proven on a large scale, and issues of control and health risks may make this method of production impractical. The feedstock requirements also cannot be too stringent if it is to be a useful process. Most of Australia experiences relatively mild winters, which could make temperature control less energy intensive than colder countries.

2.5 Water

Electrolysis of water can produce very high purity hydrogen with high efficiency. Australia is one of the driest countries in the world. As such, water is a particularly valuable resource, especially for rural areas that rely on agriculture as the main source of income. There is also a strong move to renew environmental flows in the over-utilised Murray River system that provides for agriculture in 3 states. Most of the major centres are situated on the seaboard, so seawater is a possible source that would not interrupt fresh water usage.

The electrical energy required, may be produced by a wide variety of methods, and it is this electricity source that is the strongest determining factor in the environmental benefit of using this process. Most Australian electricity is produced from the combustion of coal, which is one of the highest producers of GHGs in terms of energy production. If the electricity supplied to the electrolyser was produced in this manner, the environmental benefits of the produced hydrogen would be less than electricity produced from a renewable/carbon neutral resource (unless sequestration were implemented). In addition, when looking at the overall efficiency of the process, coal-fired power plants have efficiencies up to approximately 40% (Diniz da Costa, 2003), which would reduce the efficiency of the electrolysis process to on average 35%, and at most 42%. In addition significant amounts of CO₂ are emitted. NG assisted electrolysis (where NG is oxidised, providing heat and reducing chemical potential by removing oxygen) has been shown to offer overall efficiencies of up to 70% (based on the assumption of 40% electricity production efficiency) (Martinez-Frias, Pham et al., 2003). Other electricity production options, such as renewables, can reduce GHG output during generation, but have inhibitive high capital costs at present.

Extensive research has been carried out on the production of hydrogen for storage of electricity from renewable sources such as wave (Woodbridge and Woodbridge, 1996), wind (Dutton, Bleijs et al., 2000) and especially photovoltaic (PV) cells (e.g. the German-Saudi

Hysolar project). In Australia, solar energy would certainly be a viable option if the capital costs were reduced, due to the high average daily insolation.

Some of the major gas companies use electrolysis of water at the point of usage due to the high cost of transportation (BOC produces 135m³/h in two locations) (ACTED, 2000; Walsh, 2003). A recent proposal has been for the mass production of hydrogen from seawater using tidal power in the Kimberley region, and initially putting it into the existing natural gas pipeline at volumes of 10 – 20%, for either separation at the point of use, or burning with the NG to reduce CO₂ emissions (Zorbas, 2003).

2.6 Chemical

Various chemical sources – mainly by-products of industrial processes or impurities in other fuel sources - exist for the production of hydrogen. One source of particular interest is hydrogen sulphide (H₂S), which can be formed as a by-product during the H₂ reduction and acid bleaching of sulphides as well as from the hydro-desulphurisation of petroleum and other fossil fuels, and can be contained at a high percentage (up to 80% by volume) (Tambwekar and Subrahmanyam, 1997) in sour gas streams from geothermal sources. It is also an undesirable gas associated with sewage and decomposition processes. H₂S can be separated into its component hydrogen and sulphur by electrolytic or photocatalytic separation processes with more ease than water. This produces pure hydrogen and sulphur, with the environmental benefit of removing the foul smelling H₂S that also contributes to acid rain. As previously mentioned, Australia's sewage gas is currently under-utilised in terms of energy production, and it may be that future plant upgrades would include facilities for both methane and hydrogen sulphide collection.

Other industrial flue gases may potentially offer the opportunity for hydrogen production by WGS of CO, as has been examined in Iceland (Arnason and Sigfusson, 2000). The use of chemical by-products to produce hydrogen is still very much in the initial stages of research and development, although there has been interest in it since the late 1960's (Funk, 2001). This approach would also fit in with the ideals of cleaner production. The current capacity for hydrogen production via such processes is yet to be identified, but especially in areas of high industrial density such as Gladstone there is potential for flue gas from various industries to be utilised at a central point.

Table 2: Australian Resources for Hydrogen Production

Resource	Reserves (yrs)	Price (US\$)	Source to End-User Average Distance (km)	Notes
Coal	261 – 500	28.04 / t (~ 0.7 / GJ) <i>Black</i>	<500 (~200 East Coast)	Extensive Infrastructure
NG	78 – 130	~ 3 / GJ	560 (810 outside Victoria)	Extensive Infrastructure
Oil	10 - 14	38.30 /bbl (~ 6.50 / GJ)	530	Some Infrastructure
Biomass	Limited to available land	Source Dependent	100 - 200	Some Infrastructure, Potentially inexpensive, Renewable Resource
Water	Limited by other industry / residential requirements	Source Dependent	<100	Extensive Infrastructure, Limited by availability in rural locations, Potential for use on seaboard,
Chemical	Limited by industrial production	Source Dependent	Source Dependent	Uncertain amount of Infrastructure, Potential for using pollutant / waste- products, Reliability and lifetime an issue

3. FUEL CELL SYSTEMS

After decades of research and development, fuel cells of all types are taking their first steps out of the laboratory into the commercial market. Fuel cells offer much higher power generation efficiencies than conventional generation systems, based on engines and turbines, and the preferred fuel for these technologies is hydrogen. There are five main types of fuel cell, illustrated in Table 3.

The low temperature proton exchange membrane fuel cell (PEMFC) and alkaline fuel cell (AFC) requires very pure hydrogen (less than 10ppm CO), whereas the phosphoric acid fuel cell (PAFC) can tolerate up to 1% CO in the feed. The high temperature molten carbonate

(MCFC) and solid oxide (SOFC) fuel cells will run on fuels containing several percent of CO. The Alkaline Fuel Cell (AFC) requires an oxidant of either pure oxygen or CO₂-free air, and so has not been favoured by developers for any applications other than niche markets. The PEM fuel cell has been chosen by most of the automotive companies as the power source for future vehicles. The Phosphoric Acid Fuel Cell (PAFC) is the most developed in terms of hardware and demonstrations, but has been overtaken recently by the PEM fuel cell. The high temperature fuel cells (Molten Carbonate and Solid Oxide) offer the best potential for use with hydrocarbon-derived fuels such as would be obtained from coal gasification.

3.1 High temperature fuel cells (MCFC and SOFC)

There are several reasons to focus attention on solid oxide fuel cells (SOFCs) and molten carbonate fuel cells (MCFCs):

- If fuel cells are going to succeed commercially, they will need to penetrate the stationary power generation market before they gain widespread acceptance in vehicles. It will be much easier to compete with a small, stationary reciprocating engine or microturbines at installed costs of \$1,000 to 1,500 per kW than an internal combustion engine at \$50 per kW. The price tolerance and operating conditions in the stationary markets are also much less severe than in vehicles. Furthermore, high-temperature fuel cells are thermodynamically better suited to stationary applications than other kinds of fuel cells.
- Unlike low-temperature fuel cells, which need fairly pure hydrogen, both MCFCs and SOFCs can tolerate carbon oxides, as found in reformed hydrocarbon fuels, so common feedstocks can be used more efficiently and with lower processing costs.
- Both types are well suited to combined-cycle and cogeneration applications because of their high operating temperatures.
- High-temperature operation allows fuel processing to be integrated closely or directly into the fuel cell, also raising system efficiency and simplifying designs.

The leading companies developing MCFCs and SOFCs are ramping up production for commercial sales. One company, FuelCell Energy (FCE), is now selling commercial products and already has a backlog of orders for systems starting at 250kW installed capacity. FCE is currently the only manufacturer of molten carbonate fuel cells in the U.S. and is likely to dominate the large stationary fuel cell market as it develops in the immediate future. However other companies are also coming along, including Siemens Westinghouse who are focusing on utility scale SOFC based plants at over 1MW installed capacity. There are other SOFC manufacturers, like Sulzer Hexis in Switzerland and Acumentrics in the U.S., who have their sights set on building a larger number of smaller systems. These

manufacturers are developing smaller-scale fuel cells for the residential and telecommunications market. Though in principle SOFCs could provide power over a range of applications – everything from 1 kW for residential power to several MW for utility power generation, MCFCs are only really suitable for systems above a few hundred kW. This is because the design of an MCFC system is inherently more complex. A detailed description of how MCFC and SOFC systems work is given elsewhere - e.g. (Larminie and Dicks, 2003).

Table 3: Fuel cell characteristics

Fuel Cell Type	Operating Temperature [°C]	Electrolyte	Fuel	Oxidation Media	Typical Unit Sizes [kW _e]
Alkaline Fuel Cell (AFC)	70 – 100	Alkaline hydroxide	H ₂	Oxygen	< 100 (stack)
Proton Exchange Membrane Fuel Cell (PEM) also known as the solid polymer fuel cell	50 – 100	Perfluorated sulphonated polymer	H ₂ and reformed H ₂	Oxygen from air	0.1-500 (stack)
Phosphoric Acid Fuel Cell (PAFC)	160 – 210	Stabilised phosphoric acid	H ₂ reformed from natural gas	Oxygen from air	5-200 (stack) (plants up to 11,000)
Molten Carbonate Fuel Cell (MCFC)	650	Molten carbonate	H ₂ and CO from internal reforming of natural gas or coal gas	Oxygen from air	100-300 (plants up to 2,000)
Solid Oxide Fuel Cell (SOFC)	800 – 1000	Ceramic solid	H ₂ and CO from internal reforming of natural gas or coal gas	Oxygen from air	0.5-100 (plants up to 1,000)

Australia's real advantage currently lies in the area of SOFC development and commercialisation. Several companies are competing internationally to get their planar SOFC products to market first. While many are rushing to be the first to release a commercial fuel cell, the reality is that most companies are still researching, developing products, and testing them. Only a handful will be ready to sell a fuel cell in the coming 2 years. The most notable are Sulzer Hexis in Switzerland (aiming at 1 kW scale systems for residential applications), and Ceramic Fuel Cells Ltd. in Australia (initially focused on 40 kW natural gas fuelled stationary power systems).

3.2 Fuel Cell/Gas Turbine Hybrids and Integrated Coal Gasifier Systems

It is possible to combine either an SOFC stack or MCFC stack and a gas turbine, into a system in which the gas turbine acts as a bottoming cycle. The high temperature SOFC is particularly suitable for use in a hybrid system, as it can be run at elevated pressure and has a high exhaust gas temperature. Such a hybrid arrangement can yield efficiencies of 60% with simple gas turbines and over 70% with more complex turbines depending on the design and size. A pressurised SOFC/GT hybrid power system has been demonstrated by Siemens Westinghouse, and FuelCell Energy has developed a Direct Fuel Cell/Turbine Hybrid System that is able to operate at atmospheric pressure by indirect transfer of heat to the turbine cycle through heat exchangers. The balance of characteristics between the fuel cell and the gas turbine combine in these hybrids to produce as close to ideal thermodynamic performance as is practical with current technology. High temperature fuel cell systems operating on coal gasifier product gas have also been studied extensively in past years. By integrating the fuel cell with a coal gasifier, it is possible to use waste heat from the fuel cell to generate steam required for the gasifier and generate additional power in a bottoming cycle. Studies have indicated that integration of BG/Lurgi Slagging Gasifier and MCFC could yield efficiencies up to 54% (HHV).

3.3 Proton Exchange Membrane (PEM) Fuel Cells

Solid polymer or PEM fuel cells are attractive for use in vehicles because of their low operating temperature (resulting in fast start-up time) and high power density (kW per litre). Development has reached the stage where most of the major auto-makers are building demonstration vehicles. Nevertheless, the cost of PEM systems is very high and an issue remains as to the most suitable fuel for fuel cell vehicles (FCV).

By 2010 it is expected that many fuel cell vehicles will be on the road and that hydrogen will be the fuel of choice. The issue then becomes how is the hydrogen to be produced, distributed and stored. Until this is addressed by energy companies, it could be some time before vehicle makers ramp up their level of production and bring down system costs.

There is an interest in using PEM technology in small scale stationary applications. The reasoning behind this is that if stack costs fall as a result of the development for vehicles, then the cost targets for stationary applications will be met before those for transportation. Thus, although the high temperature fuel cells are thermodynamically more suitable for natural gas fuelled power plants, if the stack costs of PEM systems can be made very low, then they will find application in stationary systems. Australia does not have any particular

advantage in terms of research and development or investment in PEM fuel cells, and may thus be consigned to the position of a “close-follower” in the race to produce PEM systems more economically.

4. DISCUSSION

It is apparent that, of all the hydrogen sources available for the production of hydrogen in Australia coal, NG, biomass and water offer the greatest potential. In terms of infrastructure, coal, water and NG have extensive distribution infrastructure already in place, while biomass has only minimal infrastructure. It remains to be determined whether it would be more economically efficient and environmentally acceptable to create hydrogen pipeline / transportation infrastructure from the source, or whether production would be best carried out in the vicinity of the end-user. In the Australian context, where the majority of the population is distributed within a few major centres, separated by vast distances, issues of transportation become very important, and may favour centralised or distributed production depending on economics.

Table 4 summarises some of the parameters and issues related to the hydrogen production technologies discussed above. Environmentally, the benefit or detriment of hydrogen generated from fossil fuels is highly dependent on the use of CO₂ sequestration. However, there is a gap in our knowledge regarding the overall efficiency of hydrogen production technologies in combination with CO₂ capture and sequestration. Capture and sequestration technologies are also energy intensive and an energy balance is required to verify the energy feasibility of each system. In addition, sequestration may be financially viable when CO₂ capture is not required or when oil recovery from exhausted oil wells or gas extraction from deep seam coal methane reserves provide an extra economic incentive. In terms of environmental benefit, it is essential to carry out Life Cycle Assessment of each process to determine which actually contributes the least damage over the entire lifetime of the process. At this stage, no analysis is available in terms of Australian production, although some work has been done on individual technologies in other parts of the world (Spath, 2001).

Table 4: Summary of Hydrogen Production Methods

Method	Fuels	Overall Efficiency (%)	H2 Cost (US\$/GJ)	TCI (US\$/GJ H ₂ Capacity)	Notes
Steam Reforming	NG, Oil	65-75 (LHV)	5-8	9-15	Well-established, Extensive infrastructure,
Partial Oxidation	NG, Oil	50 (LHV)	7-10	9-22	No infrastructure, Well-established, Variety of fuels
Auto-thermal Reforming	NG	N/A	N/A	N/A	No infrastructure,
Thermal Decomposition	NG	N/A	N/A	N/A	No infrastructure, Low emissions / easy waste handling, Potential for use with solar energy
Gasification	Biomass, Oil, Coal	42.5-46.5 (LHV)	10-12 9-13	33-34 20-42	Minimal infrastructure, Concentrated CO ₂ stream ideal for sequestration, Uses cheap fuels, Potential for use with solar energy
Pyrolysis	Biomass, Coal	47.9 (HHV)	9-13	15-19	No infrastructure, Uses cheap fuels, Concentrated CO ₂ stream ideal for sequestration
Electrolysis	Water, H ₂ S	35-42 (HHV) (Electricity source included) 70 (NG assisted)	20-25 (Large) 11-42 (Small)	3-30 (Large) 32-486 (Small)	Potential zero emissions with renewable electricity, Environmental / economic benefits depend on electricity supply, Water supply possibly unreliable
Biological Processes	Biomass	N/A	N/A	N/A	Undeveloped, Control and scale-up issues
Plasma Reforming	NG, Oil, Biomass	N/A	~10	N/A	Unproven commercially, Electricity source can affect environmental benefits

Notes: a) TCI = Specific Total Capital Investment (Padro and Putsche, 1999)

b) Some costs could not be converted to AU\$, so all values were left in US\$ for reasons of comparison

In terms of social and environmental issues, the use of biomass could be very attractive, in particular for farmers in Australia who are under intense economic pressure. Within a viable zone, biomass transport and pre-processing for hydrogen generation can be economically feasible. Provided that biomass production and consumption rates are maintained constant, a biomass utilisation cycle could be a sustainable option. In addition, tree plantations are an option that has three major environmental and social implications. Firstly, they are natural

carbon sinks that may help to reduce net carbon dioxide levels in the atmosphere. Tree plantations can also benefit those areas where land salinity is a problem as trees are natural pumps keeping the water table down. Further, financial incentives for tree plantations can have major social benefits for struggling farming communities. This could prove to be positive all round. Other important biomass resources for hydrogen generation that deserve attention are municipal waste and sugar cane bagasse, which are currently under-utilised.

Likewise, for electrolysis of water, the environmental benefit is dependent on the energy source – solar or wind could be more beneficial than fossil fuels without sequestration. Water has the disadvantage of being in scarce supply and high demand in some rural areas, where other sources may have an advantage. NG thermal decomposition using solar energy offers another option for reducing CO₂ emissions (producing only solid Carbon as the by-product), but is yet to become commercially viable, although it is currently being developed by the CSIRO. Biomass looks to be a possible winner in this category as the sustainable planting and harvesting of woody biomass offers a near-zero emissions alternative, whilst the use of municipal waste and other bio-waste products has the benefit of preventing methane escape, and producing a saleable product from waste. Co-gasification of coal and biomass may be one way of reducing coal-based emissions and enhancing the position of gasification processes in Australia. Utilising solar power to provide the energy required for gasification may also increase the efficiency and environmental benefit by avoiding or reducing the discharge of pollutants, not contaminating gaseous products with combustion by-products and upgrading the calorific value of the fuel (Zedtwitz and Steinfeld, 2003). The federal government's current project to increase the renewable energy production share of total electricity production may offer an opening for biomass projects to be funded in Australia. Although the current target is minimal (an extra 2% of the total by 2010 – compared to 22% for the EU), it may, if successful, lead to further similar measures.

The costs of hydrogen production are only one component of the price that the customer pays. To the figures given in Table 4 needs to be added that of transmission cost, and possibly storage. For pipeline transmission, depending on the transmission rate (GW) and distance of pipeline, the transmission costs are estimated by Padró and Putsche (Padro and Putsche, 1999) to be between US\$0.49 and US\$27/GJ of hydrogen. Most estimates, however, put the transmission costs between US\$2-3/GJ (Ogden, 1999). Transportation as liquid hydrogen is also relatively low cost, estimated to be between US\$0.75 and \$2.14/GJ via rail, and up to US\$15/GJ via ship. Other methods are invariably higher, ranging from

US\$3-42/GJ for truck transport in metal hydrides to US\$25/GJ for compressed gas transport via rail.

Estimates of the capital cost of hydrogen transmission pipelines range from US\$300,000 to \$1.4million per mile (Geiger, 2003) or US\$250,000 to \$1,000,000 (Ogden, 1999) as compared to NG pipelines, which cost from US\$200,000 to \$800,000 (Geiger, 2003). Costs vary according to the terrain and level of urbanisation – flat, relatively deserted areas costing less than highly urbanised or hilly regions. This cost tendency is beneficial in the Australian situation, where vast tracts of relatively uninterrupted flat terrain would have to be crossed if production was done at the fuel source. In the United States, it is estimated that 15-20% of these costs are due to labour, and a further 15-20% for engineering services for a flat-terrain pipeline (Ogden, 1999), these figures probably being similar to Australian figures.

Since the late 1980's there has been a growing interest in fuel cell technology which has been accompanied by multi-million dollar investments by companies such as DaimlerChrysler, Ford, Shell, General Motors, Toyota and many others. Five factors have brought about the growth of interest world-wide and also to Australia:

1. Political pressure arising from international commitments made by the major industrial powers at the Montreal and Kyoto summits on climate change. At the latter, pledges were made to reduce by 2010, emissions of major greenhouse gases by 8% relative to the level pertaining in 1990. This will only be achieved by making substantial reductions in the amount of CO₂ emitted by power stations and road vehicles and targets have been set with this in mind.
2. There are growing sociological pressures to improve air quality for inhabitants of major cities. Vehicle exhausts cause much of the smog affecting cities such as Rome, Mexico City, Los Angeles etc. and there an increasing awareness of the link between air quality and health.
3. Restructuring of the established power generation industry in many countries. At the same time, there has been greater interest in renewable forms of generation such as wind, wave and solar, and a decline in interest in nuclear power. De-regulation, the introduction of competition, rising transmission and distribution costs, increased social pressures against overhead power lines combined with difficulties in obtaining permits and other changes have seen the economics of distributed power generation become far more attractive.
4. Advances in science and technology have solved many of the materials problems that plagued early fuel cell work.

5. The upsurge in demand for electrical power particularly North America, has raised concerns about the security of supply from the grid. Local power generating plant offers users security of supply for essential users.

These factors have fundamentally changed the perceived benefits of using fuel cells:

- Fuel cells have higher efficiencies than other generation technologies, and their efficiency is not inherently tied to output power capacity.
- Fuel cells are modular. A 1-kW fuel cell module can be scaled up to 10-kW, 100-kW, or megawatt-scale with no fundamental change in design. Modular design creates the potential for volume production and low unit cost.
- Fuel cells have the lowest emissions of any hydrocarbon-fuelled generation technology, and therefore have positive environmental benefits.
- Fuel cell plants potentially need very little maintenance.

The SOFC and MCFC can deliver high concentration of CO₂ in their exhaust gases, avoiding the requirement of expensive gas capture technologies. As these are point source emissions, it will be much easier for power generation companies to set up sequestration programmes – the fuel cell itself acts as the gas separation or capture device.

5. CONCLUSIONS

From the process and fuel data reviewed, it is apparent that coal, NG, biomass and water could provide good sources of hydrogen for Australia in the future. Of these, NG steam reforming is a likely initial source of hydrogen, due mainly to being a highly established process and having both NG distribution infrastructure and large scale H₂ production facilities already in place. In the longer term however, coal, biomass and water are likely to come into play – especially with advances in wind, photovoltaics and other renewable electricity sources.

At this stage, it is difficult to say conclusively which technology will be the most successful, or even the most beneficial economically and environmentally. Life cycle assessment of the different technologies would provide a clearer picture of the actual lifetime impacts of the processes, and give a basis for informed future policy-making and industrial investment decisions.

Solar enhanced technologies such as solar thermal decomposition of NG and solar thermal gasification of coal and biomass are likely to be advantageous in terms of environmental

benefits, although this technology is not yet commercially available. This is especially relevant to Australia, with the highest average insolation value of any continent.

Whilst several engines and turbines may be successfully run on hydrogen, they all suffer from the disadvantage of conversion efficiencies limited by thermodynamic considerations (the Carnot cycle). In addition, steel used in such engines is subject to hydrogen embrittlement. The various fuel cell types are therefore preferred for converting hydrogen into electricity, since they operate at moderate temperatures and have much higher conversion efficiencies. Many millions of dollars are being spent on technology development and it is now clear that marketable products will be appearing in the coming months and years ahead. Of the various fuel cell types, the high temperature variants – solid oxide and molten carbonate fuel cells – are most suitable for hydrogen that is derived from hydrocarbon sources. Unlike low temperature cells such as the PEM, both the SOFC and MCFC can tolerate carbon oxides in the fuel and indeed are able to oxidise CO directly.

Studies have shown that fuel produced from coal gasifiers can be used in the MCFC and SOFC, which may be an important future application in Australia, which has expertise in this area.

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Appendix 2

Fuel Cycle Inventory

A2.1 Mining Equations

The mining and gas field emissions were determined via averaging from the literature, and from the National Pollutant Inventory Workbooks and the Queensland Department of Natural Resources and Mines (NRM, 2004; NPI, 2005; NPI, 2006). Other sources were used for the NG scenarios – e.g (Spath, 2001). Emission rates and fuel usage rates per tonne of product were the typical form of data used.

A2.2 Mining Emissions Results

Table 5: Emissions from Mining

Substance Emissions (kg/yr)	Gasification	Electrolysis
Ammonia (total)	0.66	1.34
Antimony & compounds	2.44	4.95
Arsenic & compounds	12.91	26.17
Benzene	27.68	56.10
Beryllium & compounds	4.30	8.71
Boron & compounds	113.22	229.48
Cadmium & compounds	0.90	1.82
Carbon monoxide	121560.72	246400.42
Chlorine	0.55	1.12
Chromium (III) compounds	34.35	69.64
Chromium (VI) compounds	86.10	174.53
Cobalt & compounds	20.22	40.99
Copper & compounds	87.22	176.79
Cumene (1-methylethylbenzene)	27.19	55.10
Ethylbenzene	4.97	10.08
Fluoride compounds	840.98	1704.65
Formaldehyde (methyl aldehyde)	232.07	470.40
n-Hexane	0.00	0.01
Hydrogen sulfide	0.07	0.15
Lead & compounds	44.99	91.20
Magnesium oxide fume	1.55	3.14
Manganese & compounds	944.89	1915.27
Mercury & compounds	0.50	1.01
Nickel & compounds	80.35	162.86
Oxides of Nitrogen	243121.43	492800.84
Particulate Matter 10.0 µm	950383.78	1926403.28
Polycyclic aromatic hydrocarbons	9.06	18.37
Selenium & compounds	1.91	3.86
Styrene (ethenylbenzene)	353.63	716.80
Sulfur dioxide	12156.07	24640.04
Toluene (methylbenzene)	28.07	56.90
Total Volatile Organic Compounds	33163.97	67222.51
Xylenes (individual or mixed isomers)	27.00	54.72
Zinc and compounds	287.38	582.50

Table 6: Fuel Usage and CO₂ emissions

Fuel Usage		
Diesel Use (kL / yr)	7151	14496
CO ₂ Emissions from Diesel Use (kg/yr)	19000	39081

Table 5 and Table 6 show emissions from coal-based electrolysis and coal gasification. No NPI workbook was available specifically for NG extraction, so the only emissions available, adapted from Spath (2001) are given in Table 7. Greenhouse gas emissions rates are determined from data in DEH (2006).

Table 7: Emissions from NG Extraction and Transport

Substance	Emissions (kg / yr)
NO _x	9378
SO _x	5478
PM ₁₀	426
Extraction - CH ₄	14,100
Transport - CH ₄	617,200
Transport - CO ₂	33,700

A2.3 Transportation Equations

The emissions rates given by Queensland Rail (Affleck, 2002) were used to determine the various emissions from the rail transport of coal from the mine to the plant. For NG, the emissions (listed above), were based on a variety of sources, including Encom (2000), Beer, Grant et al. (2001), AGA (2003) and SANTOS (2006). For the coal transport, the rates of emissions are given as g/NTK (grams per net tonne kilometre), which is multiplied by the mass of coal required and the kilometres travelled.

A2.4 Transportation Emissions Results

The results of emissions from the transport of coal for gasification and electrolysis are shown in Table 8.

Table 8: Emissions from Coal Transport

Substance emissions (kg/yr)	Gasification	Electrolysis
Acetaldehyde	3.6542	7.40
Antimony and compounds	0.0093	0.0188
Arsenic and compounds	0.0002	0.00041
Benzene	2.1296	4.32
1,3-Butadiene	1.9408	3.93
Cadmium and compounds	0.0045	0.0091
Carbon Monoxide	363.0000	735.79
Chromium (III) compounds	0.0004	0.00087
Chromium (VI) compounds	0.0002	0.00036
Cobalt and compounds	0.0004	0.00082
Copper and compounds	0.0020	0.0041
Ethylbenzene	0.0736	0.149
Formaldehyde	10.7932	21.88
Lead and compounds	0.0020	0.0041
Manganese and compounds	0.0015	0.0031
Mercury and compounds	0.0017	0.0034
n-Hexane	1.7327	3.51
Nickel and compounds	0.0010	0.002
Oxides of Nitrogen	2860.4400	5798.04
Particulate Matter <10.0 µm	67.2760	136.37
Polycyclic Aromatic Hydrocarbons	0.9099	1.84
Selenium and compounds	0.0003	0.00055
Sulphur Dioxide	125.3560	254.09
Toluene	2.1538	4.37
Total Volatile Organic Compounds	122.9360	249.19
Xylenes	0.3441	0.7
Zinc and compounds	0.0269	0.054
Fuel Usage and Emissions		
Fuel Usage (kL / yr)	48.4	98.1
CO2 Emissions (kg/yr)	130,680	264,880

A2.5 Hydrogen Plant Equations

The equations given here were utilised to determine the major emissions from a plant producing the required amount of Hydrogen (178 kt/yr) as described in Chapter 4.

A2.5.1 Coal Gasification Plant

The coal gasification plant, as the major plant of interest, was modelled in more detail than the Natural Gas Steam Reforming (NG-SR) plant and the electrolysis plant, which were both based on input-output calculations. The plant consisted of the units shown in Figure 3, and both the electricity and hydrogen production options were

modelled, although the hydrogen production option is the only one presented here. The underlying equations used to create the mass balance over each of the unit operations is described here.

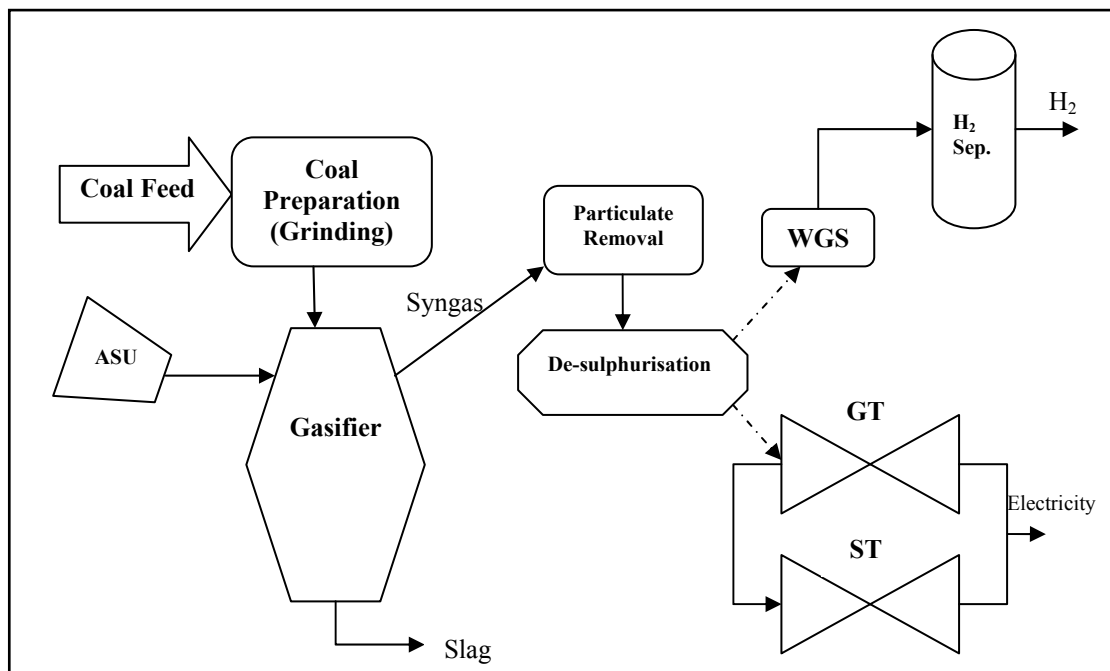


Figure 3: Coal Gasification (IGCC) Plant Diagram

The coal compositions utilised in the mass balance, in terms of the molar ratios of components, are given in Table 9. The results here are presented for the use of Callide coal in the gasification plant.

Table 9: Coal Compositions (molar ratio) for the FCI (Spero, 1997)

Component	Callide	Tarong
C	1	1
H	0.56	0.88
O	0.15	0.14
N	0.01	0.01
S	0.001	0.003
Ash %	16.0	28.0
H2O %	16.0	11.0

Ash composition used to determine the emissions rates is shown in Table 10, and the ash is assumed to be split 50% to fly ash and 50% to slag.

Table 10: Ash Composition (Tarong, 2006)

Ash Component	Weight %
SiO₂	38.1
Al₂O₃	33.8
Fe₂O₃	15.5
CaO	2.8
MgO	2

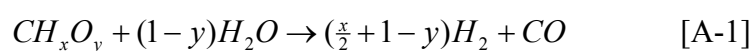
Operating parameters were sourced from existing plants. Some typical data is shown in Table 11.

Table 11: Operating Parameters of different Gasifiers (Innes, 1998)

Gasifier	Temp. (°C)	Press. (bar)	C Conversion	Ash Content	AFT Ash Fusion Temp.	Slag viscosity (Pa/s) at 1400°C
Fixed Bed	450 (top) – 2000 (bottom)	26	70-80			
Moving Bed				<15	<1400	<5
Fluid Bed	950-1100	20-30	95-98	<40	>1100	-
Entrained Flow	>1400	20-30	95-99	<25	<1500	<15 – 25

A2.5.1.1 Gasifier Unit

As described in Chapter 4, the gasifier utilised (based on the assessment of Patterson and Harris (1998), Innes (2003) and Do and Patterson (2004)) was the Shell Entrained flow Gasifier. Data on the performance of these units in operation worldwide was obtained from sources such as Shelton and Lyons (1998), Schellberg and Kuske (1999). Gasification was assumed to occur by Equation A-1 from Noyes (1967):



Gasifier conditions are given in Table 12.

Table 12: Gasifier Operating Conditions (Innes, 2003)

Condition	State	Units
Operating Temp.	1600	°C
Operating Pressure	31	bar
Exit Temp. (with Quench)	900	°C
Quench / Cooled Gas Temp.	250	°C
C/O Molar Ratio	3.3	
C Conversion	0.99	
CO Selectivity	0.84	

Figure 4 shows the basic flows entering and leaving the gasifier unit. The coal is considered to be dry fed, for although this leads to twice the feed power requirements of slurry feed (Innes, 1998), the slurry is typically 60-65% solids, with coal moisture lower than 10% required for efficiency reasons (Innes, 2003), and each 10% increase in water in the mixture decreasing the heating value by 1% (Thambimuthu, 1994). A quench configuration is adopted, which is predicted to decrease capital cost of the plant by 10% but reduce efficiency by 4% (Stoll and Todd, 1996). The selection of an entrained flow gasifiers, which has high conversion (98%), leads to the requirement of an air separation unit (ASU) to provide 95% pure oxygen to reduce flow volumes (Innes, 2003).

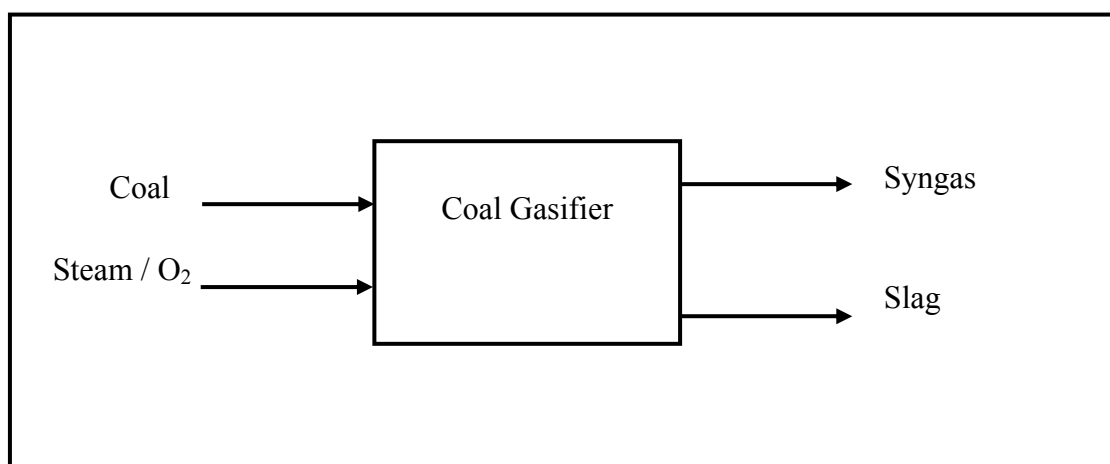


Figure 4: Gasifier Unit Flow Diagram

A2.5.1.2 Air Separation Unit (ASU)

The ASU was chosen to provide oxygen feed for the gasifier over the use of air, which increases flow volumes and therefore capital expenses, or production of oxygen via electrolysis. Electrolysis was examined as a method of co-production of O₂ and H₂, but the electrolysis energy usage of 209 (kWh / kmol O₂), was too high to be outweighed by the supplementary production of H₂ to be comparable with a standard Pressure Swing Adsorption (PSA) ASU (6.95 kWh / kmol O₂) (Innes, 2003).

A2.5.1.3 De-Sulphurisation Unit

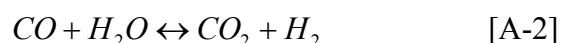
Desulphurisation was assumed to be based on amine (MDEA) removal. The various operational parameters were adapted from the US Department of Energy IGCC Base Cases (NETL/DOE, 2003) and are shown in Table 13.

Table 13: Desulphurisation Characteristic Assumptions (NETL/DOE, 2003)

Characteristic	Value
Steam Requirement	13.2 kg / kg S in feed
Removal Efficiency	99.3%
MDEA Loading Capacity	0.8 kmol S / kmol MDEA
Purge / Loss Rate	0.5%
Aqueous Concentration of MDEA	40% (Ullmann, 1986)

A2.5.1.4 Water-Gas Shift Reactor

The water gas shift (WGS) reactor is used to convert remaining CO and some hydrocarbons to further hydrogen via Equation A-2. Again, conversion over the WGS operation (typically including a number of reactors in series) is assumed to be 98% (Shoko, McLellan et al., 2006).



A2.5.1.5 Hydrogen Separation

Pressure Swing Adsorption is assumed to be the technique for hydrogen product purification, and modelled as per Walsh (2003). Hydrogen purity is assumed to be 99.95% as an industrial standard (Spath, 2001; Walsh, 2003) although “fuel grade” hydrogen is quoted as being as low as 93% pure (Kreutz, Williams et al., 2002). Hydrogen recovery is considered to be 90% as the highest economic recovery (Kreutz, Williams et al., 2002) Although 95% has been quoted as a possible recovery rate (Delallo, Klett et al., 1999).

A2.5.1.6 Coal Preparation

Feed preparation power was determined to be negligible – 5% (1.2-1.5MW) of 31MW auxiliary power requirement of the 250MW (net) Demkolec IGCC plant (Zon, 1996) and a rate of (1kWh / t) was used (ACPS, 1994). Water was not considered in this balance.

A2.5.1.7 Particulate Removal Unit

Particulate removal, based on the Buggenum plant (Innes, 2003), was assumed to be 99.8% effective.

A2.5.1.8 Auxiliary Power Requirements

The auxiliary power requirements are estimated, where possible, based on the individual units. Some of these requirements have been mentioned earlier for the individual unit operations, but further, general data is provided in Table 14.

Table 14: Auxiliary energy requirements of various IGCC demonstration plants (Mwe) (Innes, 1998)

IGCC Plant	Tampa Electric Polk County	Sierra Pacific Power Pinon Pine	Demkolec Buggenum	BGL (Design)	PSI Energy Wabash River
Gasifier	Texaco O ₂ Blown (Entr. Flow)	KRW Air Blown (Fluid Bed)	Shell (Entrained Flow)	BGL	Destec O ₂ Blown (Entr. Flow)
Gross Production	313	107.2	284	478.2	288
Auxiliary Requirements	64	7.5	31	39.1	32 ^a
ASU	54	-			~25
Net Generation	250	99.7	253	439.1	252
Aux. Req. (% Gross Production)	20.5	6.5	11		12.5
Plant Efficiency		40.7 (HHV)	43.2 (LHV)	44 (LHV)	38.5 (HHV)
Predicted Plant Efficiency			47		
Sulphur Removal			>98%		>99%
Capital Cost (US\$/kWe)	2040 (1996\$)	2330 (1996\$)	2000 (1993\$)	1660 (1995\$)	1590 (1996\$)
Predicted Cost (US\$/kWe)			1400		

^a Auxiliary power (Wabash Rr) 32MW = 12.5% of gross (25MW to ASU, 4MW to Combined Cycle, 3MW to mill & recycle in gasification plant)

A2.5.2 Natural Gas Steam Reforming Plant

The unit operations considered for the NG-SR plant are shown in Figure 5. Energy balances were not completed over this plant, as the desired emissions were available from a straightforward mass balance.

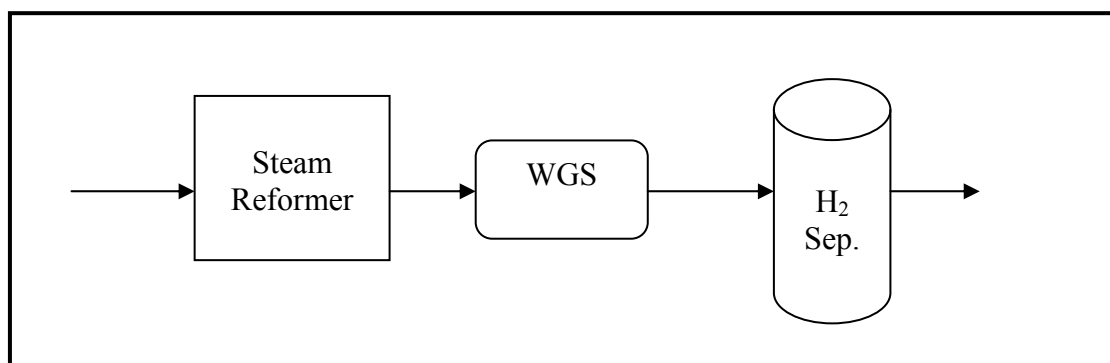


Figure 5: Steam Reforming Unit Operations

The NG supply was assumed to be pre-purified in preparation for the hydrogen production, and the gas composition was based on typical Australian NG (AGA, 2003) (see Table 15).

Table 15: Typical Natural Gas Composition (AGA, 2003)

Mole Fraction	Component
0.88	CH ₄
0.055	C ₂ H ₆
0.02	C ₃ H ₈
0.008	C ₄ H ₁₀
0	C ₅ H ₁₂
0.007	N ₂
0.03	CO ₂

Sample process data for existing steam reforming plants using different process conditions was available for comparison as shown in Table 16 - Table 18.

Table 16: Process 1 (S/C = 3.8, Quench) (Noyes, 1967)

Component	Input (mol/h)	Out (Stage 1)	Out (Stage 2)	Out (WGS)
N ₂ + Air	0.9	0.9	112.5	
CH ₄	94.3	28.9	1.5	
C ₂ H ₆	2.8	0	0	
C ₃ H ₈	1.0	0	0	
C ₄ H ₁₀	0.6	0	0	
C ₅ H ₁₂	0.4	0	0	
H ₂ O	407.7	286.6	498.0	
CO	0	36.0	59.8	<0.2% (dry mol)
CO ₂	0	42.3	45.9	
H ₂	0	269.1	295.3	

143 mol/h Air Input to Stage 2
CO/CO₂ Ratio: 1.3

Table 17: Process 2 (S/C = 3.8) (Noyes, 1967)

Component	Input (mol/h)	Out (Stage 1)	Out (Stage 2)	Out (WGS)
N ₂ + Air	0.9	0.9	112.5	
CH ₄	94.3	49.5	1.5	
C ₂ H ₆	2.8	0	0	
C ₃ H ₈	1.0	0	0	
C ₄ H ₁₀	0.6	0	0	
C ₅ H ₁₂	0.4	0	0	
H ₂ O	407.7	312.2	318.7	
CO	0	20.3	63.5	<0.2% (dry mol)
CO ₂	0	37.3	42.2	
H ₂	0	202.2	291.6	

143 mol/h Air Input to Stage 2

CO/CO₂ Ratio: 1.5

Table 18: Process 3 (S/C = 7.2, Quench) (Noyes, 1967)

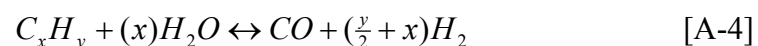
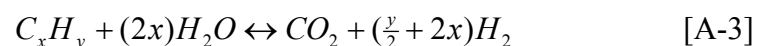
Component	Input (mol/h)	Out (Stage 1)	Out (Stage 2)	Out (WGS)
N ₂ + Air	0.9	0.9	113.8	
CH ₄	94.3	24.0	1.5	
C ₂ H ₆	2.8	0	0	
C ₃ H ₈	1.0	0	0	
C ₄ H ₁₀	0.6	0	0	
C ₅ H ₁₂	0.4	0	0	
H ₂ O	772.6	631.5	991.0	
CO	0	25.1	42.0	<0.2% (dry mol)
CO ₂	0	58.2	64.0	
H ₂	0	299.5	313.2	

143 mol/h Air Input to Stage 2

CO/CO₂ Ratio: 0.66

A2.5.2.1 Steam Reformer

The steam reformer unit converts hydrocarbon components to hydrogen, carbon monoxide and carbon dioxide predominately through reaction with steam through Equations A-3 and A-4 from Noyes (1967).



The conversion was assumed to be 98%, and the selectivity to be 95% towards CO₂.

A2.5.2.2 Water Gas Shift Reactor

The water gas shift (WGS) reactor is used to convert remaining CO and some hydrocarbons to further hydrogen via Equation A-2. The description of the WGS follows that provided in the section on coal gasification.

A2.5.2.3 Hydrogen Separation

Hydrogen is separated using cryogenic or PSA separation to a purity of 99.5% (Walsh, 2003), with a recovery of 90%. The balance over this unit splits the hydrogen, with the remaining impurities assumed to take up the remaining volume in a constant ratio to their content in the input.

A2.5.3 Electrolysis Plant

The electrolysis plant was to be provided with electricity from a scaled-down version of the Tarong power plant, such that emissions were determined based on a ratio of the power outputs of the modelled and Tarong plants.

A2.6 Hydrogen Plant Emissions Results

Table 19 shows the results of the FCI in terms of atmospheric emissions. Emissions from the Gasification plant are most comprehensive due to application of the NPI workbooks. For the sustainability assessment here, the most important emissions are SO_x, CO₂, H₂O and Coal / NG usage.

Table 19: Overall Emissions to Air from Hydrogen Production

Substance Emissions (t/yr)	Gasification	Electrolysis	NG-SR
PM ₁₀	30.73	4,193	
NO _x	561.58	33,944	
CO	34971.59	1,131	1,232
H ₂	2372.41		
CH ₄	232.61	120.5	91,844
H ₂ S	0.475		
SO ₂	88.43	22,631	
Antimony & Compounds	0.45	-	
Arsenic & Compounds	3.86	0.077	
Beryllium & compounds	0.16	0.034	
Boron & compounds	0.20	32.9	
Cadmium & compounds	2.16	0.02	
Chromium (III) compounds	18.62	0.32	
Chromium (VI) compounds	0.98	0.02	
Cobalt & compounds	5.16	0.02	
Copper & compounds	4.26	0.50	
Lead & compounds	9.74	0.49	
Manganese & compounds	123.38	0.81	
Mercury & compounds	0.01	0.11	
Nickel & compounds	27.13	0.31	
Zinc and compounds	55.63	0.61	
Special Emissions			
CO ₂	5,074,424	5,924,936	1,809,016
Usage Rates			
Coal (Mt / yr)	1.76	4.46	-
NG (bcm / yr)	-	-	0.744
Water (ML / yr)	4,176	470,384	1,514

The high rate of emissions shown in the gasification scenario for trace elements is due to the utilisation of general multipliers from the NPI Workbooks. The very high level in comparison with the more accurate estimates from Tarong, imply that the NPI workbooks are not the most accurate of measures (this agrees with the assessment of Tarong power staff in personal communications). However, as these minor compounds are not examined in the current work, it is deemed allowable to let these results stand.

A2.7 Mass Balance Tables – IGCC

The gasification process was modelled initially as a 300MW IGCC plant for electricity production, then adapted for the production of hydrogen. Tables giving the mass and energy balance results over the various units are given below. Such a

Figure 6: Mass Balance - Feed and Basis Conditions

A-39

Input					
Compare from Simbeck, et al. 1993 (mentioned in Williams, 2001)					
Input Coal	32.0	kg/s			
	22.24702718	kg/s (daf)			
MW	12	1	14	16	32
	C	H	N	O	S
Molar ratio	1	0.560	0.014	0.146	0.001
Wt %	79.3	3.7	1.26	15.45	0.29
kg/s	25.35	1.18	0.40	4.94	0.09
kmol/s	2.11	1.18	0.03	0.31	0.00
Solids Separation					
Fly Ash	50	%			
Slag	50	%			
Ash Mass Slag	2.301416605	kg/s			
Fly Ash Mass	2.301416605	kg/s			
Steam Feed	26.17622325	kg/s			
Q = MCdT	Quench				
Q1	102079.6458	kW			
Quench Flowrate	4.778184939	kmol/s			

Figure 7: Mass Balance - Gasifier Conditions

Heat Recovery						
Gasifier Exit Syngas						
Inlet T	1173	K				
Outlet T	523	K				
Q	214211.1718	kW				
Heat Recovery Efficiency	75	%				
Heat Recovered to Steam	160658.3788	kW				
Steam P	25	Mpa				
Steam T	839	K	hout	3387		kJ/kg
Boiler Water T	328	K	hin	251.4		kJ/kg
Mass of Steam HR	51.23688571	kg/s	dh	3135.6		kJ/kg
Gas Turbine Flue Gas						
Inlet T	548.0496401	K				
Outlet T	373	K				
Q	221313.3157	kW				
Heat Recovery Efficiency	75	%				
Heat Recovered to Steam	165984.9868	kW				
Steam P	25	Mpa				
Steam T	839	K	hout	3387		kJ/kg
Boiler Water T	328	K	hin	251.4		kJ/kg
Mass of Steam HR	52.93563809	kg/s	dh	3135.6		kJ/kg
Radiative Heat to Jacket						
Inlet T		K				
Outlet T		K				
Q	35189.21719	kW				
Heat Recovery Efficiency	75	%				
Heat Recovered to Steam	26391.91289	kW				
Steam P	25	Mpa				
Steam T	839	K	hout	3387		kJ/kg
Boiler Water T	328	K	hin	251.4		kJ/kg
Mass of Steam HR	8.41686213	kg/s	dh	3135.6		kJ/kg
Equivalent Combustion	35	%				

Figure 8: Mass Balance - Heat Recovery

	ASU			
O2 Purity	0.95			
O2 to Gasifier	0.4857628	kmol/s		
N2 to Gasifier	0.025566463	kmol/s		
Air to ASU (min)	2.313156192	kmol/s		
vol% O2 in Air	21	%		
Excess N2	1.801826929	kmol/s		
High O2 Rate Reduction factor	8	%		
Electricity Usage Rate	6.951689046	kWh/kmol	Target AVG Values 31.03250109 MW 10 %	
Power Required	12.15673898	MW		
Percentage of Gross Production	3.91742159	%		
	Gas Clean-up			
Acid Gas Removal T	40	C	313	K
Clean Gas T	40	C	313	K
Heat Capture Efficiency	75	%		
Reheat requirements	0	MWth		
	CO2 / Sulfur Removal			
	S			
Removal %	99.3	wt %		
Sulfur In Syngas	0.00	kmol/s	333.7054077	kg/h
Sulfur in Cleaned Gas	2.02772E-05	kmol/s	2.335937854	kg/h
Sulfur Product	0.00	kmol/s	331.3694698	kg/h
Steam Requirements	13.2	kg Steam / kg S in feed		
Steam In	0.001194909	kg/s	4.301671271	kg/h
Power Requirements	0.306	kWe / kg S/h in feed		
Power Use	0.102113855	Mwe		
Aqueous Conc. MDEA	40	wt %	9.146341463	mol %
Loading capacity	0.8	kmol S / kmol MDEA		
MDEA required	0.003620935	kmol/s	0.431615501	kg/s
MDEA solution circulated	0.039588894	kmol/s	1.079038753	kg/s
Purge / Loss rate	0.5	%		
Top-up MDEA	0.000197944	kmol/s		
MDEA Purge	0.000197944	kmol/s		
Water Purge	0.002164193	kmol/s		
Water Top-up	0.002164193	kmol/s		
	0.982799801	ML		6.8ML
	Secondary and Tertiary Comminution			
Feed Rate	31.96411951	kg/s	115.0708302	t/h
2ndary Power Rate	1	kWh/t		
Power 2 crush	0.11507083	MW	115.0708302	kWh/h
Tertiary Power Rate		kW/t		
Power 3 mill	5	MW		
Total Crushing Power	5.11507083	MW		

Figure 9: Mass Balance - Ancillary Units

Steam Turbine				
	Inlet	Outlet		
P	25	0.02	MPa	
T	839	333	K	
h	3387	2053	kJ/kg	
X	1	0.7639		
v	0.0131933	5.844	m ³ /kg	
Steam Rate	86.41196777	kg/s		
Power	115.273565	MW		
Thermal Efficiency	75	%		
Output Electricity	86.45517376	MW		
Steam % of Total Power	27.85955714	%		
Gas Turbine				
P _{in}	3.131	Mpa		
P _{loss over Combustor}	1	%		
P _{out}	0.15	Mpa		
O ₂ theoretical	1.768746939	kmol/s		
Excess air	150	%		
O ₂ actual	4.421867348	kmol/s		
N ₂ in air	16.62622123	kmol/s		
N ₂ NO _x control	1.705813494	kmol/s		
Flow POC	25.0048872	kmol/s		
T _{in}	1.29E+03	K	1.02E+03	
Thermal Efficiency	31	%		
dh (estimate)	28880.78476	kJ/kmol		
T _{out}	548.0496401	K	275.0496	
Power	223.8698372	MW		
Feed Compressor Power				
dP over Gas Cleaning	20	%		
P _{comp in}	2.5048	Mpa		
P _{comp out}	3.131	Mpa		
Efficiency	70	%		
Power	5.968730219	MW		
T _{comp out}	333.36114	K		

Figure 10: Mass Balance - Electricity Production from Turbines

Output							
H2	CO	CO2	H2O Used	CH4	H2S	N2 (Inert)	Total Gas Flow (kmol/s)
1.723459	1.756585	0.334587617	1.454235	0.021123	0.002897	0.12158	3.960231
86961.61	1240863	371414.7396	660394.7	8526.509	2484.77	42942.41	1753193 t/yr
	WGS	Conversion Rate	0.98				
178000	24817.26	2305322.517	800544.6	8355.979	2484.77	42942.41	3362467 t/yr
178	24.81726	2305.322517	800.5446	8.355979	kt/yr		
			1460.939	Reaction H2O			
			452.4805	Makeup H2O			
			1913.42	ML H2O			

Figure 11: Output of Syngas from Gasifier and Conversion to Hydrogen

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Appendix 3

Equations for the Emissions Transport Model

A3.1 Emissions Transport Model – Mathematical Underpinnings

The ETM was created in using a set of “fixed-box” model type “tanks” connected in series radially outward from a central emissions point. The mathematical derivation of the equations follows.

Using the innermost airshed as an example, a simple mass balance of the form:

$$\text{accumulation} = \text{in} - \text{out} + \text{generation}$$

we derive the following equation:

$$\frac{dM}{dt} = NF_i + E_i - NF_o - D \quad [A-5]$$

where:

$$NF_i = \text{Natural Flux In} = b.v.SA_1$$

$$E_i = \text{Emissions Rate}$$

$$NF_o = \text{Natural Flux Out} = c.v.SA_2$$

$$D = \text{Deposition} = u.c.FSA$$

$$M = \text{Total Mass of Compound}$$

$$b = \text{background concentration}$$

$$c = \text{concentration}$$

$$v = \text{wind velocity}$$

$$u = \text{deposition velocity}$$

$$FSA = \text{bottom surface area}$$

$$SA = \text{vertical surface area}$$

Under the assumption of steady state, this can be shown to lead to the concentration equation:

$$c = \frac{b.v.SA_1 + E_i}{v.SA_2 + u.FSA} \quad [A-6]$$

If however, we assume a dynamic system, with accumulation, then the subsequent derivation of the 1st order differential equation follows:

$$\begin{aligned}
\frac{dM}{dt} &= b.v.SA_1 + E_i - c.v.SA_2 - c.u.FSA \\
\frac{V.dc}{dt} &= [b.v.SA_1 + E_i] - [v.SA_2 - u.FSA].c \\
\frac{dc}{dt} &= \frac{[b.v.SA_1 + E_i]}{V} - \frac{[v.SA_2 - u.FSA]}{V}.c \\
\therefore \frac{dc}{dt} &= Q - P.c \\
\therefore c &= \frac{Q}{P} + \alpha.e^{-Pt}
\end{aligned}$$

for the known conditions ($t = 0$, $c = b$):

$$c = \frac{Q}{P} + \left[b - \frac{Q}{P} \right] e^{-Pt} \quad [A-7]$$

Likewise, if we follow the substitution and solution of the differential equations for each sub-airshed, we will be able to determine an equation giving the concentration assumed to be at the centre of each sub-airshed over time. The factor of distance can be left separate for the time being, in order to simplify the process, and is the simpler variable to incorporate, as it will depend on either a basic trigonometric or linear function in the radial direction. In the case of the current application, the distance is incorporated via the discretisation of the environment into sub-airshed tanks as described in Chapter 5.

$$\begin{aligned}
\frac{dc_2}{dt} &= \frac{c_1 vSA_2 - c_2 vSA_3 - c_2 uFSA_2}{V_2} \\
&= \frac{c_1 vSA_2}{V_2} - c_2 \frac{(vSA_3 + uFSA_2)}{V_2} \\
&= Q_2 + P_2 \\
\therefore c_2 e^{\int P_2 dt} &= \int Q_2 e^{\int P_2 dt} dt \\
e^{\int P_2 dt} &= e^{P_2 t} \\
\therefore \int Q_2 e^{\int P_2 dt} dt &= \int Q_2 e^{P_2 t} dt \\
&= \frac{vSA_2}{V_2} \int \left[\frac{Q}{P} + \left(b - \frac{Q}{P} \right) e^{-Pt} \right] e^{P_2 t} dt \\
&= \frac{vSA_2}{V_2} \int \left[\frac{Q}{P} e^{P_2 t} + \left(b - \frac{Q}{P} \right) e^{(P_2 - P)t} \right] dt \\
&= \frac{vSA_2}{V_2} \left[\frac{Q}{PP_2} + \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) e^{-Pt} \right] e^{P_2 t} + K \\
\therefore c_2 e^{P_2 t} &= \frac{vSA_2}{V_2} \left[\frac{Q}{PP_2} + \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) e^{-Pt} \right] e^{P_2 t} + K \\
c_2 &= \frac{vSA_2}{V_2} \left[\frac{Q}{PP_2} + \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) e^{-Pt} \right] + Ke^{-P_2 t}
\end{aligned}$$

For the known conditions, $t = 0$, $c_2 = b$, K is given by:

$$\begin{aligned}
b &= \frac{vSA_2}{V_2} \left[\frac{Q}{PP_2} + \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) \right] + K \\
\therefore K &= \frac{vSA_2}{V_2} \left[\frac{bV_2}{vSA_2} - \frac{Q}{PP_2} - \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) \right] \\
\therefore c_2 &= \frac{vSA_2}{V_2} \left[\frac{Q}{PP_2} + \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) e^{-P_1 t} \right] + \frac{vSA_2}{V_2} \left[\frac{bV_2}{vSA_2} - \frac{Q}{PP_2} - \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) \right] e^{-P_2 t}
\end{aligned}$$

Likewise, for the 3rd sub-airshed:

$$\begin{aligned}
\frac{dc_3}{dt} &= \frac{c_2 v S A_3 - c_3 v S A_4 - c_3 u F S A_3}{V_3} \\
&= \frac{c_2 v S A_3}{V_3} - c_3 \frac{(v S A_4 + u F S A_3)}{V_3} \\
&= Q_3 - P_3 c_3 \\
\therefore c_3 e^{\int P_3 dt} &= \int Q_3 e^{\int P_3 dt} dt \\
e^{\int P_3 dt} &= e^{P_3 t} \\
\therefore \int Q_3 e^{\int P_3 dt} dt &= \int Q_3 e^{P_3 t} dt \\
&= \frac{v S A_3}{V_3} \int \left[\frac{v S A_2}{V_2} \left[\frac{Q}{P P_2} + \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) e^{-P t} \right] + K e^{-P_2 t} \right] e^{P_3 t} dt \\
&= \frac{v^2 S A_2 S A_3}{V_2 V_3} \int \left\{ \left[\frac{Q}{P P_2} e^{P_3 t} + \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) e^{(P_3 - P)t} \right] + \frac{V_2}{v S A_2} K e^{(P_3 - P_2)t} \right\} dt \\
c_3 e^{P_3 t} &= \frac{v^2 S A_2 S A_3}{V_2 V_3} \left\{ \left[\frac{Q}{P P_2 P_3} e^{P_3 t} + \left(\frac{b - \frac{Q}{P}}{(P_2 - P)(P_3 - P)} \right) e^{(P_3 - P)t} \right] + \frac{V_2}{v S A_2} \frac{K}{(P_3 - P_2)} e^{(P_3 - P_2)t} \right\} + K_2 \\
\therefore c_3 &= \frac{v^2 S A_2 S A_3}{V_2 V_3} \left\{ \left[\frac{Q}{P P_2 P_3} + \left(\frac{b - \frac{Q}{P}}{(P_2 - P)(P_3 - P)} \right) e^{-P t} \right] + \left[\frac{b V_2}{v S A_2} - \frac{Q}{P P_2} - \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) \right] \frac{e^{-P_2 t}}{(P_3 - P_2)} \right\} + K_2 e^{-P_3 t}
\end{aligned}$$

For known conditions $t = 0$, $c_3 = b$, K_2 is given by:

$$\begin{aligned}
b &= \frac{v^2 S A_2 S A_3}{V_2 V_3} \left\{ \left[\frac{Q}{P P_2 P_3} + \left(\frac{b - \frac{Q}{P}}{(P_2 - P)(P_3 - P)} \right) \right] + \left[\frac{b V_2}{v S A_2} - \frac{Q}{P P_2} - \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) \right] \frac{1}{(P_3 - P_2)} \right\} + K_2 \\
K_2 &= \left\{ b - \left[\frac{v^2 S A_2 S A_3}{V_2 V_3} \left[\frac{Q}{P P_2 P_3} + \left(\frac{b - \frac{Q}{P}}{(P_2 - P)(P_3 - P)} \right) \right] - \left[\frac{b V_2}{v S A_2} - \frac{Q}{P P_2} - \left(\frac{b - \frac{Q}{P}}{P_2 - P} \right) \right] \frac{1}{(P_3 - P_2)} \right] \right\}
\end{aligned}$$

Likewise for the 4th sub-airshed:

$$\begin{aligned}
\frac{dc_4}{dt} &= \frac{c_3 vSA_4 - c_4 vSA_5 - c_4 uFSA_4}{V_4} \\
&= \frac{c_3 vSA_4}{V_4} - c_4 \frac{(vSA_5 + uFSA_4)}{V_4} \\
&= Q_4 - P_4 c_4 \\
\therefore c_4 e^{\int P_4 dt} &= \int Q_4 e^{\int P_4 dt} dt \\
e^{\int P_4 dt} &= e^{P_4 t} \\
\therefore \int Q_4 e^{\int P_4 dt} dt &= \int Q_4 e^{P_4 t} dt \\
&= \frac{vSA_4}{V_4} \int \left\{ \frac{v^2 SA_2 SA_3}{V_2 V_3} \left[\frac{Q}{PP_2 P_3} + \left(\frac{b - \frac{Q}{P}}{(P_2 - P)(P_3 - P)} \right) e^{-Pt} \right] + \frac{V_2}{vSA_2} \frac{Ke^{-P_2 t}}{(P_3 - P_2)} + K_2 e^{-P_3 t} \right\} e^{P_4 t} dt \\
&= \frac{vSA_4}{V_4} \int \left\{ \frac{v^2 SA_2 SA_3}{V_2 V_3} \left[\frac{Qe^{P_4 t}}{PP_2 P_3} + \left(\frac{b - \frac{Q}{P}}{(P_2 - P)(P_3 - P)} \right) e^{(P_4 - P)t} \right] + \frac{V_2}{vSA_2} \frac{Ke^{(P_4 - P_2)t}}{(P_3 - P_2)} + K_2 e^{(P_4 - P_3)t} \right\} dt \\
c_4 &= \frac{vSA_4}{V_4} \left\{ \frac{v^2 SA_2 SA_3}{V_2 V_3} \left[\left[\frac{Q}{PP_2 P_3 P_4} + \left(\frac{b - \frac{Q}{P}}{(P_2 - P)(P_3 - P)(P_4 - P)} \right) e^{-Pt} \right] + \frac{V_2}{vSA_2} \frac{Ke^{-P_2 t}}{(P_3 - P_2)(P_4 - P_2)} \right] + \frac{K_2}{(P_4 - P_3)} e^{-P_3 t} \right\} + K_3 e^{-P_4 t}
\end{aligned}$$

For the known conditions: $t = 0$, $c_4 = b$, K_3 is given by:

$$\begin{aligned}
b &= \frac{vSA_4}{V_4} \left\{ \frac{v^2 SA_2 SA_3}{V_2 V_3} \left[\left[\frac{Q}{PP_2 P_3 P_4} + \left(\frac{b - \frac{Q}{P}}{(P_2 - P)(P_3 - P)(P_4 - P)} \right) \right] + \frac{V_2}{vSA_2} \frac{K}{(P_3 - P_2)(P_4 - P_2)} \right] + \frac{K_2}{(P_4 - P_3)} \right\} + K_3 \\
K_3 &= b - \frac{vSA_4}{V_4} \left\{ \frac{v^2 SA_2 SA_3}{V_2 V_3} \left[\left[\frac{Q}{PP_2 P_3 P_4} + \left(\frac{b - \frac{Q}{P}}{(P_2 - P)(P_3 - P)(P_4 - P)} \right) \right] + \frac{V_2}{vSA_2} \frac{K}{(P_3 - P_2)(P_4 - P_2)} \right] + \frac{K_2}{(P_4 - P_3)} \right\}
\end{aligned}$$

Likewise again, for the 5th sub-airshed:

$$\begin{aligned}
\frac{dc_5}{dt} &= \frac{c_4 vSA_5 - c_5 vSA_6 - c_5 uFSA_5}{V_5} \\
&= \frac{c_4 vSA_5}{V_5} - c_5 \frac{(vSA_6 + uFSA_5)}{V_5} \\
&= Q_5 - P_5 c_5 \\
\therefore c_5 e^{\int P_5 dt} &= \int Q_5 e^{\int P_5 dt} dt \\
e^{\int P_5 dt} &= e^{P_5 t} \\
\therefore \int Q_5 e^{\int P_5 dt} dt &= \int Q_5 e^{P_5 t} dt \\
&= \frac{vSA_5}{V_5} \int \left\langle \frac{vSA_4}{V_4} \left\{ \frac{vSA_3}{V_3} \left[\frac{\frac{vSA_2}{V_2} \left[\frac{Q}{PP_2 P_3 P_4} + \left(\frac{b - \frac{Q}{P}}{(P_2 - P)(P_3 - P)(P_4 - P)} \right) e^{-P_1 t} \right] + \frac{K_2}{(P_4 - P_3)} e^{-P_3 t} \right\} + K_3 e^{-P_4 t} \right\} e^{P_5 t} dt \right. \\
&\quad \left. \therefore c_5 = \frac{vSA_5}{V_5} \left\langle \frac{vSA_4}{V_4} \left\{ \frac{vSA_3}{V_3} \left[\frac{\frac{vSA_2}{V_2} \left[\frac{Q}{PP_2 P_3 P_4 P_5} + \left(\frac{b - \frac{Q}{P}}{(P_2 - P)(P_3 - P)(P_4 - P)(P_5 - P)} \right) e^{-P_1 t} \right] + \frac{K_2}{(P_4 - P_3)(P_5 - P_3)} e^{-P_3 t} \right\} + \frac{K_3}{(P_5 - P_4)} e^{-P_4 t} \right\} + K_4 e^{-P_5 t} \right. \right.
\end{aligned}$$

From the 3rd sub-airshed, a pattern of expansion is obvious, by which any subsequent sub-airshed's concentration equation can be derived swiftly and simply (however, the page space does not allow us to proceed any further here). All the constants are known in the equations, hence the concentration curve can be estimated for any point in time, for any airshed.

Appendix 4

Representative Data for the Sustainability Assessment

A4.1 Australian Data Atlas Maps

One resource that is particularly useful in finding data on locally variable parameters is the Australian Data Atlas Online (DPI, 2006). The figures in this section are indicative of the full-scale availability of data, but the resource itself allows the user to zoom in to the level of interest.

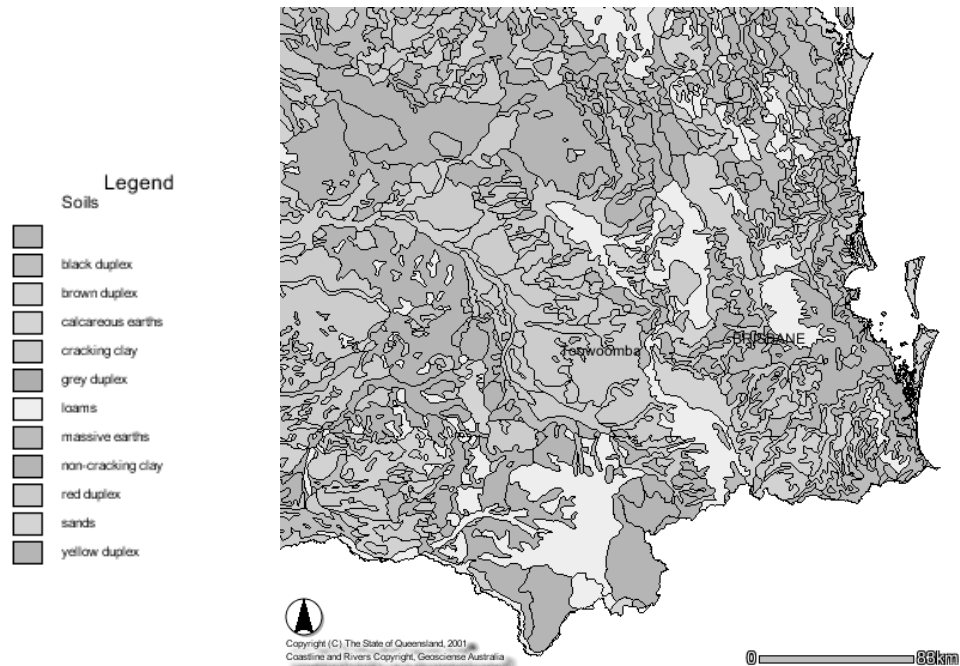


Figure 12: South-East Queensland Soil Types (DPI, 2006)

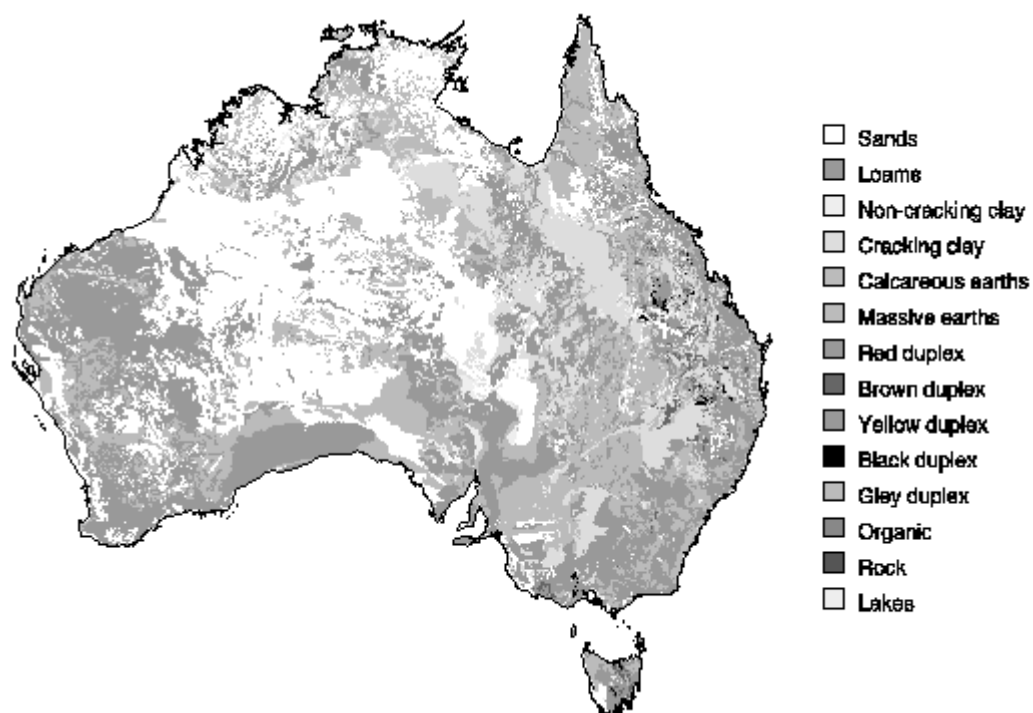


Figure 13: Australian Soil Types (DPI, 2006)

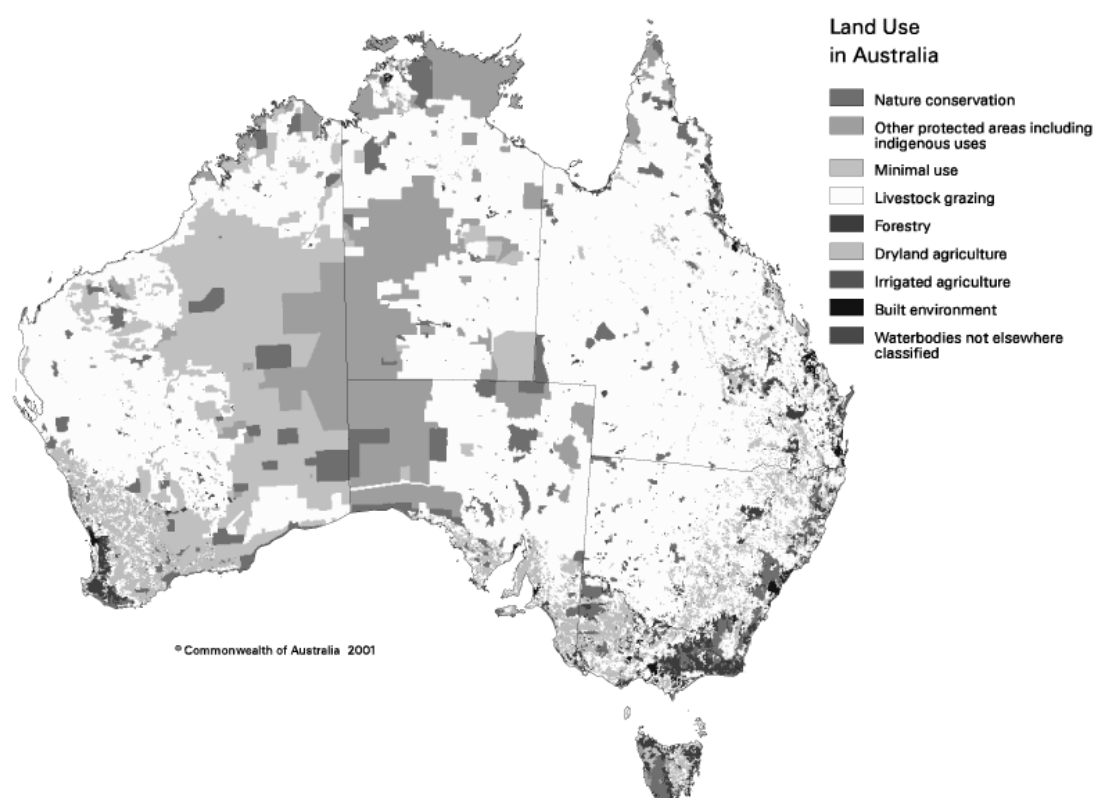


Figure 14: Australian Land Use (DPI, 2006)

A4.2 Australian Bureau of Meteorology

All relevant climatic data was found to be available through the Australian Bureau of Meteorology (BOM) website (BOM, 2006). In particular, the parameters of average annual rainfall and average days of rain, and the wind roses for the areas interest were readily available.

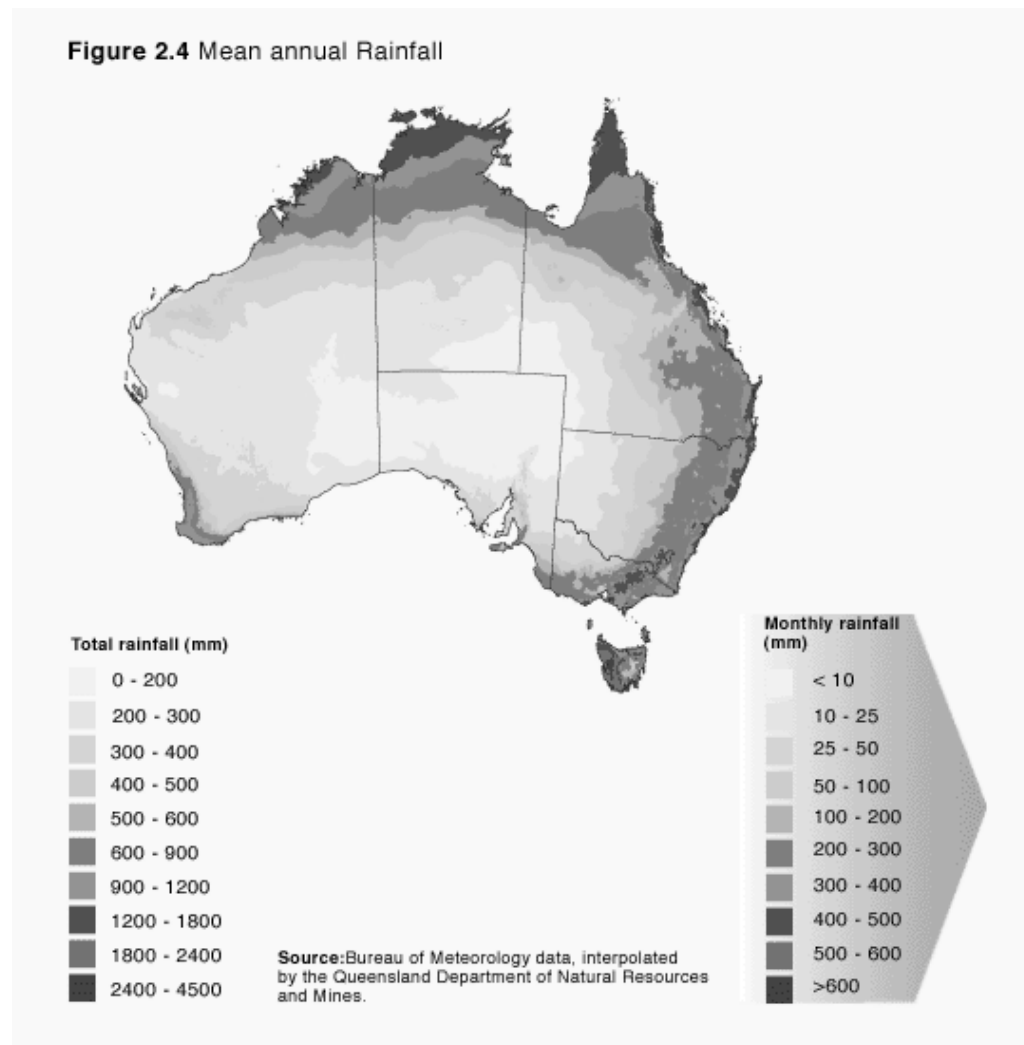


Figure 15: Mean Annual Rainfall (BOM, 2006)

Figure 2.13 Mean annual deep drainage.

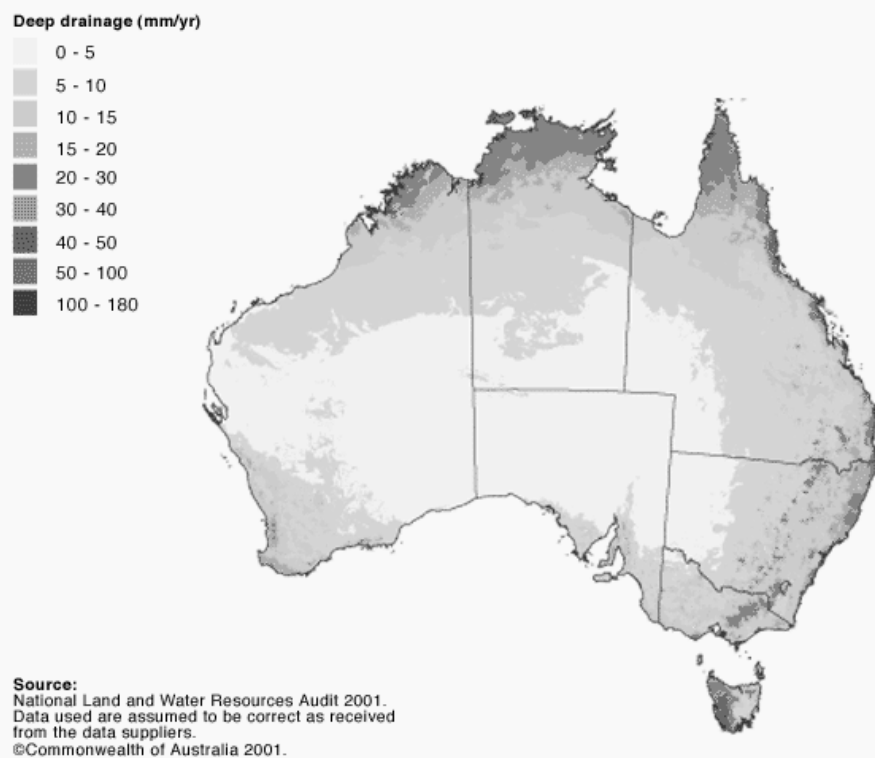


Figure 16: Average Annual Deep Drainage (BOM, 2006)

Figure 2.12 Mean annual total run-off (surface plus subsurface).

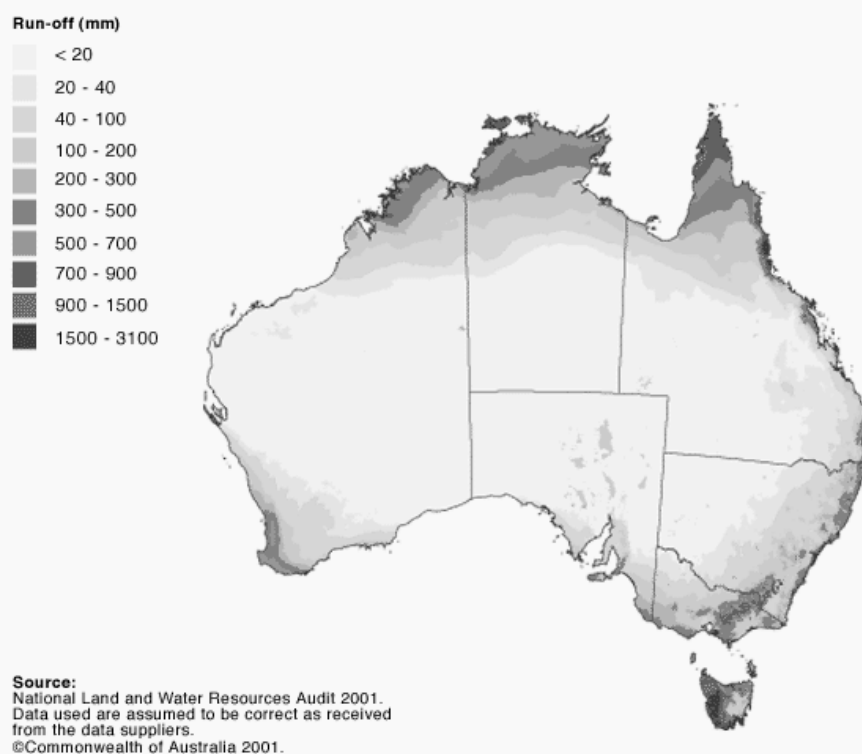


Figure 17: Average Annual Rainfall Run-off (BOM, 2006)

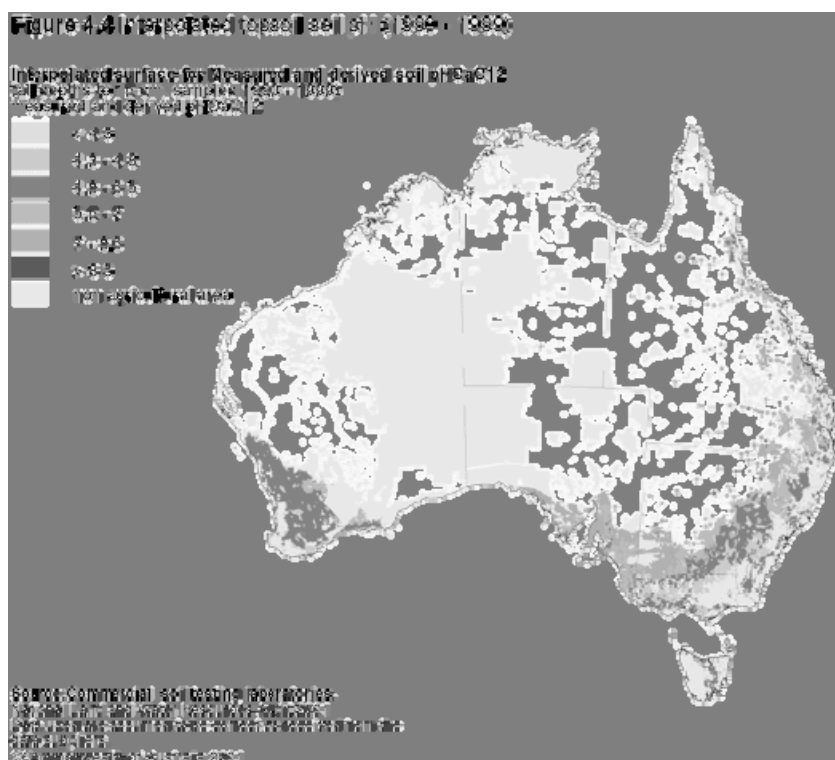


Figure 18: Topsoil pH (BOM, 2006)

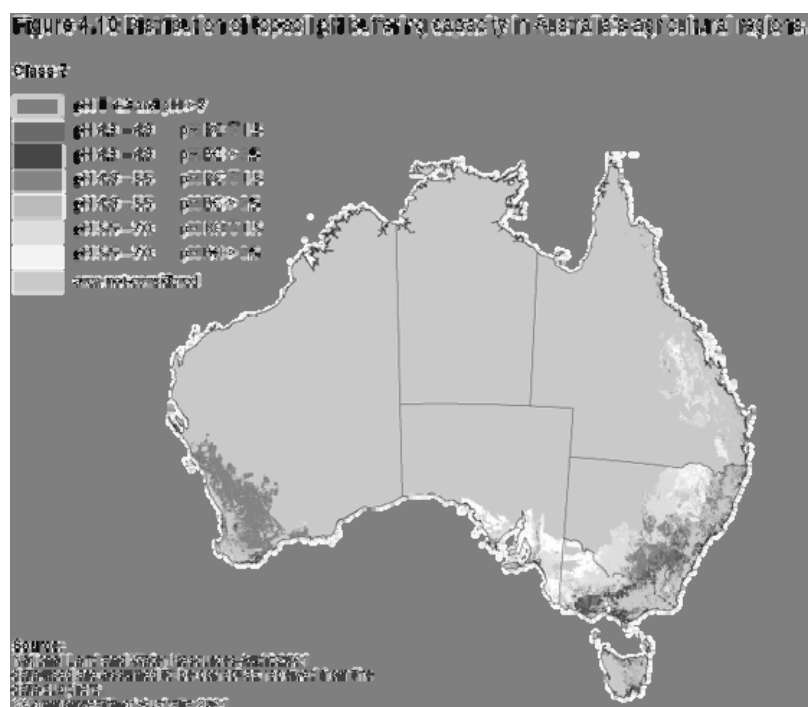


Figure 19: pH Buffering Capacity Estimates (BOM, 2006)

Particular data for Nanango – the closest monitoring site to Tarong, was obtained directly from the BOM, and is shown in graphic form in Figure 20.

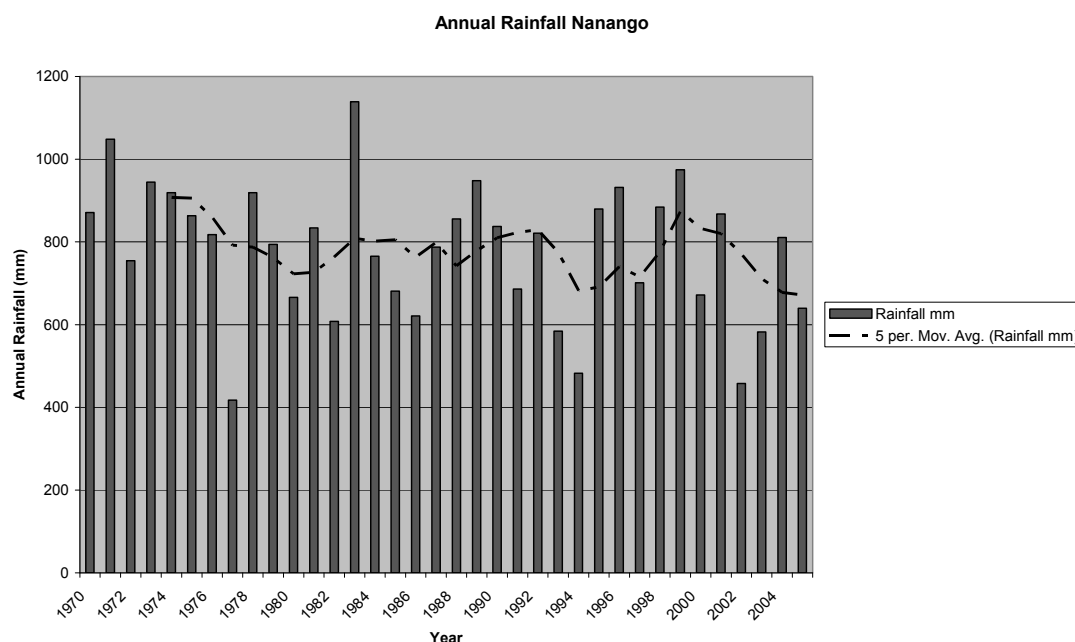


Figure 20: Annual Rainfall Data for Nanango (BOM, 2006)

A4.3 Resource Statistics

Data on available resources, production and utilisation statistics were acquired from various sources – e.g. (BP, 2002; EIA, 2004; ABARE, 2006; DPI, 2006; EIA, 2006). Emissions and greenhouse limitations can also be found (DEH, 2006; DEH, 2006).

References

- ABARE, Energy Update 2005 - Australian energy consumption and production, Australian Bureau of Agricultural and Resource Economics, <http://www.abareconomics.com/interactive/energy/excel.htm>, Canberra, 2005.
- BOM, Australian Bureau of Meteorology Website, Australian Bureau of Meteorology, www.bom.gov.au, 2005.
- BP, BP statistical review of world energy, 2002.
- DEH, National Greenhouse Gas Inventory 2004, Department of the Environment and heritage - Australian Greenhouse Office, Canberra, 2006.
- DEH, Queensland Greenhouse Gas Inventory 2004, Department of the Environment and heritage - Australian Greenhouse Office, Canberra, 2006.

- DPI, Queensland Node of The Australian Atlas, Queensland Department of Primary Industries,
http://chrisweb.dpi.qld.gov.au/website/ArcIMS_ACA/viewer.htm?Project=0,
Brisbane, 2006.
- EIA, Electric Power Annual 2003, Energy Information Administration, Washington, DC, USA, 2004.
- EIA, Energy Outlook 2006, Energy Information Administration - US Department of Energy, Washington, 2006.

Appendix 5

Tarong Power Station Data

A5.1 National Pollutant Inventory (NPI) Data on Tarong Emissions

Due to legal reporting requirements, emissions data is available from the NPI website for all major emissions sources in Queensland.

Table 20: Air Emissions Rates for Tarong Power Station 2001-05 (Adapted from NPI (2006))

Substance	Yearly Emissions to Air (kg)				
	2001	2002	2003	2004	2005
Arsenic & compounds	92	78	230	260	110
Beryllium & compounds		43	75	120	48
Boron & compounds		32000	32000	29000	43000
Cadmium & compounds	23	21	38	43	27
Carbon monoxide	1300000	1300000	1400000	1400000	1300000
Chlorine		5	4	2.7	2
Chromium (III) compounds		710	530	800	490
Chromium (VI) compounds	230	38	75	84	25
Cobalt & compounds	3	4	10	11	5
Copper & compounds		680	910	1200	720
Fluoride compounds	410000	390000	410000	410000	340000
Hydrochloric acid		3100000	740000	1000000	1400000
Lead & compounds	790	430	710	830	690
Magnesium oxide fume			0	0	0
Manganese & compounds		730	4200	5500	1100
Mercury & compounds	170	140	90	120	150
Nickel & compounds		440	590	630	420
Nickel carbonyl			0	0	0
Nickel subsulfide			0	0	0
Oxides of Nitrogen	43000000	41000000	44000000	48000000	43000000
Particulate Matter 10.0 um	6400000	6000000	7100000	9700000	6000000
Polychlorinated dioxins and furans		0		0.0011	0
Polycyclic aromatic hydrocarbons	52	57	66	67	61
Sulfur dioxide	27000000	27000000	24000000	27000000	24000000
Sulfuric acid		280000	270000	290000	250000
Total Volatile Organic Compounds		160000	160000	160000	150000
Zinc and compounds		870	1500	1500	800

A5.2 Tarong Soil Data

The Tarong Crop and Forestry Study (Plenderleith, 1989) provided data on the soil characteristics at each of the sites of interest, from which the buffering capacity was obtained in Appendix 7.

Table 21: Tarong Soil Characterisation Data (Plenderleith, 1989)

Site Number	14	15	16	17	18	19	20	21	22	23	24	25	27	28	29	30	31	32	33	34
Distance (km)	15.6	19.3	7	7	6.9	7.5	7.6	6	6	2.4	2.8	7.3	9.3	9.3	8.9	7.7	18.9	4.3	9.1	2.6
Bearing to Tarong	112	94	1	1	337	328	326	310	310	257	217	113	19	19	12	253	232	155	195	92
Bearing from Tarong	292	274	181	181	157	148	146	130	130	77	37	293	199	199	192	73	52	335	15	272
Elevation (m)	540	550	580	590	520	540	540	540	540	540	450	440	600	590	520	440	380	400	400	450
pH - B10	5.9	6.5	6.5	5.7	6.1	7.2	6.7	6.6	5.3	6.6	6.6	6.6	4.7	5.3	5.8	6.3	6.4	6.3	6	6
pH - 10	5.6	6.5	5.4	6.8	6.6	8	7.5	6.8	6	5.5	6.7	7.1	4.7	5	6.1	5.7	6.8	6	5.9	5.9
Cl % - B10	0.002	0.001	0.002	0.003	0.001	0.002	0.002	0.002	0.002	0.002	0.003	0.003	0.005	0.002	0.004	0.001	0.001	0.002	0.005	0.004
Cl % - 10	0.002	0.001	0.001	0.001	0.001	0.002	0.002	0.002	0.002	0.014	0.003	0.003	0.005	0.002	0.001	0.001	0.001	0.001	0.002	0.001
Silt	12	20	20	20	23	23	27	24	22	16	29	10	19	20	35	11	19	11	28	7
Clay	76	31	48	27	34	39	35	51	48	47	37	13	52	61	33	14	24	11	27	12
Exc - Total	8	16	7	18	11	27	24	18	18	6	26	17	18		19			6	13	3
Ca	5.7	8.5	5.6	15	7.2	22	21	15	14	5.1	21	13	16		10	4.3		3.4	5.8	1.8
Mg	2.3	6.1	1.5	1.9	2.2	3.6	2.4	2.9	3.4	0.91	3.5	3.5	2.1		6.5	0.6		1.9	5.2	0.7
Na	0.04	0.2	0.04	0.15	0.18	0.06	0.06	0.11	0.08	0.04	0.28	0.08	0.07		0.55	0.09		0.12	0.38	0.08
K	0.36	1.4	0.41	0.97	1.8	1.7	0.76	0.37	0.46	0.27	1.4	1	0.93		0.75	0.09		0.28	0.75	0.27
P %	0.099	0.286	0.16	0.156	0.182	0.225	0.19	0.119	0.126	0.249	0.228	0.01	0.19	0.031	0.179	0.074		0.01	0.04	0.01
K%	0.08	0.18	0.07	0.14	0.18	0.35	0.14	0.12	0.08	0.22	2.61	0.16	0.16	2.02	0.23	0.17		2.34	0.19	3.83
S %	0.056	0.045	0.067	0.051	0.052	0.043	0.067	0.072	0.08	0.065	0.106	0.058	0.1589	0.012	0.64	0.042		0.01	0.01	0.01
Org C% -10	3.3	3	3.7	3.4	2.1	2.7	4.8	3	5.9	3.3	5.1	4.1	9.4	3.6	5.5	3.4	3.4	2.1	3.7	1
Moisture % - B10	4.1	4.4	3.6	4.3	3.9	5.7	5.2	3.9	4.5	2.7	4.3	3.3								
Moisture % - 10	3.5	4	3.7	3.7	3.7	2.1	4	4	3.9	2.9	4.4	2.8	5	4.1	4	1.6	2.3	1.2	3.3	0.8
C %	3.3	3	3.7	3.4	2.7	2.7	4.8	3	5.9	3.3	5.1	4.1	9.4	3.6	5.5	3.4	3.4	2.1	3.7	1
N %	0.17	0.17	0.28	0.3	0.28	0.27	0.42	0.28	0.51	0.27	0.57	0.23	0.39	0.33	0.37	0.18	0.32	0.06	0.2	0.01
Fe	159	105	54	83	25	13	19	32	76	110	61	28	375		64	172	51	76	73	36
Mn	34	162	137	50	313	180	81	14	25	74	119	112	213		55	13	153	20	158	16
Cu	1	1.5	3.3	1.6	3.6	3.1	2	2.5	2.7	2.6	5.3	0.8	3.1		1.5	0.5	4	0.2	1.5	0.1
Zn	4.5	3.7	12	4.6	8.6	6.8	7.3	2.6	1.3	3.6	6.9	0.12	12		0.9	2.2	26	0.3	1.3	1.1
SO4 - B10	28	9	18	39	14	21	11	21	38	33	26	13	72	40	26	2	8	2	6	4
SO4 - 10	36	11	45	9	8	7	6	11	24	25	35	12	90	48	32	6	8	1	8	1
NO3 - B10	24	11	15	54	13	40	12	7	32	14	42	43	70	6	8		21	1	1	6
NO3 - 10	18	8	6	19	6	15	12	19	20	11	20	29	7	7	4		11	2	4	2
Alkali	0.2	0.04	0.29	0.15	0.01				0.04	0.16	0.05			2.4	0.1	0.55		0.05	0.05	0.06
Acid	0.28	0.07	0.39	0.16	0.03				0.15	0.28	0.35			2.6	0.1	0.63		0.08	0.12	0.1

A5.3 Tarong Ash Data

The data in Table 22 and Table 23 gives the coal sizing and ash composition for Tarong used in determining ash flows in the gasification mass balance.

Table 22: Tarong Power - Coal Size (Tarong, 2006)

ANALYSIS AND TESTING REPORT		
TARONG ENERGY - POWER STATION		
TARONG POWER STATION		
Primary Crusher		
Size Analysis		
Size Fraction	Fractional	Cumulative
(mm)	Mass %	Mass %
+12.5	0.2	0.2
- 12.5 + 6.30	6.5	6.7
- 6.30 + 3.35	20.6	27.3
- 3.35 + 0.500	57.3	84.6
-0.500	15.4	100.0
Raw Coal		
Mass:	17.1	kg
Size Analysis		
Size Fraction	Fractional	Cumulative
(mm)	Mass %	Mass %
+75.0	<0.01	<0.01
- 75.0 + 50.0	1.5	1.5
- 50.0 + 25.0	11.2	12.7
- 25.0 + 12.5	21.4	34.1
- 12.5 + 6.30	25.4	59.5
- 6.30 + 3.35	13.8	73.3
- 3.35 + 0.50	22.1	95.4
- 0.50	4.6	100.0

Table 23: Tarong Power - Ash Characteristics (Tarong, 2006)

	ANALYSIS AND TESTING REPORT		
	TARONG ENERGY - POWER STATION		
Proximate Analysis			
Air Dried %			
Moisture		4.1	
Ash		30.2	
Volatile Matter		27.5	
Fixed Carbon		38.2	
Proximate Analysis			
Dry Basis %			
Ash		31.4	
Volatile Matter		28.7	
Fixed Carbon		39.9	
	Air Dried %	Dry Basis%	Dry Ash Free Basis %
Specific Energy			
(MJ/kg)	21.58	22.50	32.82
Ultimate Analysis			
Moisture	4.1	-	-
Ash	30.2	31.4	-
Carbon	52.71	54.96	80.17
Hydrogen	3.79	3.95	5.76
Nitrogen	0.95	0.99	1.44
Sulphur	0.28	0.29	0.43
Oxygen(by difference)		8.4	12.2
Ash Analysis			
SiO ₂		69.7	
Al ₂ O ₃		27.0	
Fe ₂ O ₃		0.69	
CaO		0.07	
MgO		0.12	
Na ₂ O		<0.01	
K ₂ O		0.34	
TiO ₂		1.60	
Mn ₃ O ₄		<0.01	
SO ₃		<0.01	
P ₂ O ₅		0.06	
BaO		0.04	
SrO		<0.01	
ZnO		0.02	
Total		99.6	

References

- NPI, National Pollutant Inventory Emissions Data, National Pollutant Inventory, www.npi.gov.au, Canberra, 2006.
- Plenderleith, R. W., Tarong Crop and Forestry Study, ETM88/055, Queensland Electricity Commission - Generation Technology Department (Environmental Section), Brisbane, 1989.
- Tarong, Monthly Coal and Emissions Analysis, Tarong Power Corporation, Brisbane, 2006.

Appendix 6

Soil Sampling and Analysis Methods

A6.1 Tarong Crop and Forestry Study Surface Soil Sampling Methodology

Each 20 x 20m monitoring site was divided into four quarters, and one sample was collected from each quarter, with a fifth sample taken from the central area of the monitoring site. Samples were first collected from each site when the site was described by a soil surveyor, and thereafter in June of each year.

A bulk 0-10cm soil sample was formed by combining about 10 sub-samples in a plastic bucket, mixing them thoroughly with the sampling trowel, removing extraneous matter (bark, roots, stones, etc.), and retaining about 1.5kg in a sealed plastic bag. The remainder of the mixed composite sample was discarded.

Samples were delivered promptly to the Department of Primary Industries Agricultural Research Laboratories at Indooroopilly for drying and subsequent analysis.

A6.2 Tarong Crop and Forestry Study Soil Analysis Methodology

A6.2.1 pH, Electrical Conductivity, Chloride, Nitrate

These are measured sequentially on a 1:5, soil : deionised water suspension.

E.C. is measured in the supernatant of the suspension. Results are expressed in mS cm⁻¹ at 25°C.

pH is measured in the stirred soil : water suspension.

Chloride and nitrate are both determined by an autoanalyser to a colourimetric finish. Results are expressed as mg kg⁻¹ in both cases.

A6.2.2 Extractable Potassium

Potassium is determined in the centrifuged extract after four hours extraction with 0.05M HCl at a soil : solution ratio of 1:40. Results are expressed as milliequivalents per 100g.

A6.2.3 Acid Extractable Phosphorus

Acid extractable P is determined by autoanalyser after 16 hours shaking with 0.005M H₂SO₄ at a soil : solution ratio of 1:200. Results are expressed in mg kg⁻¹.

A6.2.4 Sulphur

Sulphate-sulphur is extracted with 0.01M Ca(H₂PO₄)₂.H₂O at pH 4.0 and 1:5 soil : solution ratio during 17 hours shaking. After determination by an autoanalyser distillation technique, results are expressed in mg kg⁻¹.

A6.3 Procedures Unlisted

Some other species of interest were also assessed, but the procedures for testing were not listed in the study. The relevant procedures were obtained from the University of Queensland School of Land and Food Sciences (SLAFS) Laboratories.

A6.3.1 Exchangeable Cations

Some techniques for the estimation of acid buffering capacity require the measurement of exchangeable cations. The background level of these was indicated in the Tarong Crop and Forestry Study (Plenderleith, 1989) but no ongoing measurements were taken, and no analysis technique was indicated.

The techniques described by the SLAFS¹ were:

- Exchangeable + Soluble bases – 1:5 extraction with ammonium chloride at pH7.5
- Exchangeable only – 1:50 extraction with 0.1M silver thiourea (total) while also sequentially extracting the free and bound basic cations using ethanol / glycerol and ammonium chloride.

A6.3.2 Extractable Metals

As per the exchangeable cations, no analysis technique was listed for extractable metals, and no ongoing measurements were taken. Extractable metals included Fe, Mn, Cu and Zn, and changes in levels of these metals may indicate an effect of fly ash deposition.

Measurement techniques described by SLAFS were:

- A 1:2 extraction with 0.005M DTPA using an ICPOES to determine elemental concentrations.

A6.4 Site Testing

34 sites were tested for Plenderleith (1989) including 14 crop sites and 20 forest sites (Table 24). Crop sites were immediately disregarded due to evidence that agricultural chemical applications affect the soil characteristics excessively, making trends impossible to quantify. Of the remaining sites, a set of 6 were selected based on the following criteria:

1. Can the site, in conjunction with at least one other site in a similar direction, assist in validating the ETM?
2. Can the site, based on its predicted buffering capacity, assist in validating the sustainability assessment methodology?

¹ Personal Communications with David Appleton (SLAFS)

Table 24: Forest Soil Testing Site Details (Plenderleith, 1989)

Site Number	Distance (km)	Bearing to Tarong	Bearing from Tarong	Elevation (m)
14	15.6	112	292	540
15	19.3	94	274	550
16	7	1	181	580
17	7	1	181	590
18	6.9	337	157	520
19	7.5	328	148	540
20	7.6	326	146	540
21	6	310	130	540
22	6	310	130	540
23	2.4	257	77	540
24	2.8	217	37	450
25	7.3	113	293	440
27	9.3	19	199	600
28	9.3	19	199	590
29	8.9	12	192	520
30	7.7	253	73	440
31	18.9	232	52	380
32	4.3	155	335	400
33	9.1	195	15	400
34	2.6	92	272	450

Based on the above criteria, sites 14, 15, 17, 25, 32 and 34 were selected as potentially appropriate for testing. Sites 15 and 34 were selected as a pair, given that they are at a similar bearing from the Tarong Power station, but at different distances, and were thus able to assist in validation of the ETM. Likewise, sites 14 and 25 were selected as a pair for validating the ETM. Site 17 was selected, as it is the site most likely to show a high deposition rate according to the modelling of Katestone (2005), whilst site 32 was predicted to have the highest deposition rate according to the initial model developed for this current work. Sites 32 and 34 unfortunately only have one initial data point (1987), which may make the data comparison slightly less reliable, but nonetheless allow some kind of comparison.

Soil from the selected sites was sampled on June 18th, 2006 using standard sampling methods under the regime used in the original study and confirmed in USDA (1972), SSSA (1990) and Tan (1995). Every effort was made to locate the exact sites, but vegetation and access difficulties meant that the exact 20m x 20m site was located in only 3 cases – sites 15, 17 and 32.



Figure 21: Photograph of Site 15



Figure 22: Photograph of Site 32

Site 14 was covered in thick, 2m high vegetation which made it impossible to pinpoint the exact site, but from the original aerial photographs and map grid references, the site was sampled within 50m of the actual site.



Figure 23: Photograph of Vegetation Covering Site 14

Sites 25 and 34 were inaccessible due to geographical and permission requirements. With the sites tested – in particular sites 15, 17 and 32, the model was able to be validated with some confidence, as the sites lie at different distances from the power station and have different pH buffering capacity. Data from the most recent samples is shown in Table 25, whilst the historical data may be found in Appendix 5.

Table 25: Soil Analysis from Samples taken July 2006

Sample	moisture	pH	EC	Ca	K	Mg	Na	CEC	S	NO3-N	Cl	Cu	Fe	Mn	Zn
	content %		ds/m ²	mg/kg	mg/kg	mg/kg	mg/kg	cmol(+)/kg	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg
14A	20.1	4.12	0.067	2642	641	797	34	1.80	156.0	3.5	24.0	0.15	7.0	4.7	0.28
14B	14.8	4.63	0.149	3594	773	736	38	6.87	54.8	28.2	29.6	1.76	55.5	161.0	6.53
14C	18.6	4.32	0.099	939	236	184	12	4.13	150.0	3.4	33.1	0.48	19.2	28.9	0.90
14	17.8	4.4	0.1	2391.5	549.9	572.5	28.2	4.3	120.3	11.7	28.9	0.8	27.2	64.9	2.6
15A	11.0	6.45	0.072	366	106	120	7	18.74	13.6	7.2	4.7	0.94	63.2	55.2	2.22
15B	13.3	6.50	0.143	1607	395	162	71	21.57	18.0	13.9	35.8	0.65	56.0	59.6	2.36
15C	12.1	6.23	0.091	749	333	164	8	19.00	16.6	12.1	13.4	0.68	67.8	69.0	1.86
15D	12.9	6.58	0.111	440	237	151	18	22.32	12.8	8.8	37.7	0.70	60.3	60.5	1.77
15E	12.4	6.26	0.162	444	114	139	12	27.31	22.0	22.0	35.1	0.74	77.4	56.0	2.36
15	12.3	6.4	0.1	721.4	236.9	147.0	23.3	21.8	16.6	12.8	25.3	0.7	64.9	60.1	2.1
17A	15.2	6.06	0.160	1192	295	90	28	18.43	32.8	23.3	19.0	1.58	63.2	52.1	6.09
17B	15.5	4.59	0.164	2183	354	852	38	7.58	50.3	33.4	34.1	1.41	139.1	117.7	3.97
17C	15.3	4.96	0.102	2332	515	680	36	5.98	77.3	13.7	11.0	4.18	63.0	110.5	1.93
17D	19.3	6.39	0.474	2815	529	339	48	26.17	72.4	42.2	82.5	1.49	46.0	76.3	11.28
17E	15.7	5.89	0.085	239	161	105	13	10.69	24.1	11.9	13.5	1.83	40.0	26.1	1.87
17	16.2	5.6	0.2	1752.3	371.0	413.2	32.5	13.8	51.4	24.9	32.0	2.1	70.3	76.6	5.0
32A	3.2	5.50	0.026	2588	606	927	46	3.13	3.9	1.6	10.8	0.07	87.9	8.0	0.21
32B	4.3	5.87	0.040	166	142	72	4	2.53	5.0	2.8	19.7	0.06	87.7	6.2	0.16
32C	3.5	5.40	0.026	305	102	126	11	2.87	3.5	2.0	11.2	0.08	123.8	7.8	0.17
32D	2.9	5.62	0.020	378	117	120	3	3.19	3.5	2.7	5.1	0.06	83.8	9.6	0.15
32E	3.5	5.78	0.036	3873	354	829	50	3.71	6.4	2.3	7.6	0.10	99.2	20.1	0.24
32	3.5	5.6	0.0	1461.8	264.0	414.8	23.0	3.1	4.5	2.3	10.9	0.1	96.5	10.3	0.2

References

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Appendix 7

Pre-calculations for Model Comparison

A7.1 Selection of Basis

The assumption of a basis of 1000MW production of hydrogen or equivalent electricity was based on a typical mid-size power plant. The following calculations were used to analyse the basis for a hydrogen production system, for comparison in the Australian, and particularly the Queensland context.

A.7.1.1 Predicted Hydrogen Usage per Car – Conversion from US to Australian Averages

The following calculations are a step by step conversion of the typical estimated hydrogen requirements for a future hydrogen fuel cell vehicle. The difference of driving patterns between Queensland and the USA were used to determine the equivalent number of cars that could be operated based on the produced hydrogen. A simple conversion has been used here, which does not take into account the different driving terrain and highway or city usage, however it should still provide a reasonable basis for comparison.

A7.1.1.1 Cars / Light Vehicles

Predicted H₂ usage per car (full tank) = 3.75 kg / 425miles (Ogden, Steinbugler et al., 1999)

$$\begin{aligned} &= 3.75\text{kg} / 680\text{km} \\ &= 0.0055 \text{ kg} / \text{km} \\ &= 0.00078 \text{ GJ} / \text{km} \\ &= 0.061 \text{ Nm}^3 / \text{km} \end{aligned}$$

1 Fuel Cell car (11,000 miles / yr) = 17,600 km / yr = 48.22 km / d
Car (0.038 GJ/d US driving – (Ogden, Steinbugler et al., 1999))

Australian Average (Gupta and Waikar) = 15,100 km / yr = 41.37 km/d
= 0.0323 GJ/d = 2.52 Nm³/d = 0.228 kg / d

Queensland Average (Table 27) = 15,770 km / yr = 43.21 km/d
= 0.0338 GJ/d = 2.64 Nm³/d = 0.238 kg/d

A7.1.1.2 Buses

1 Fuel Cell Bus (50,000 miles / yr) = 80,000km / yr = 219.18 km / d

Bus (2.7 GJ/d US driving – (Ogden, Steinbugler et al., 1999))
 = 0.0123 GJ / km
 = 0.962 Nm³ / km
 = 0.0868 kg / km

Australian Average (Table 26) = 34,300 km / yr = 93.97 km/d
 = 1.16 GJ/d = 90.4 Nm³/d = 8.16 kg / d

Queensland Average (Table 27) = 37,060 km / yr = 101.53 km/d
 = 1.24 GJ/d = 97.7 Nm³/d = 8.81 kg/d

(1 bus = 37 cars worth of hydrogen)

Table 26: Vehicle Use 2000-2001 (ABS, 2003)

BUSINESS AND PRIVATE VEHICLE USE - Year ended 31 October 2001(a)						
Type of vehicle	Business			To and from work	Private	Total
	Laden	Unladen	Total(b)			
TOTAL KILOMETRES TRAVELLED (million)						
Passenger vehicles	-	-	36,357	37,261	70,307	143,925
Motor cycles	-	-	250	452	745	1,448
Light commercial vehicles	13,889	5,413	19,301	4,962	6,466	30,728
Rigid trucks	4,690	1,773	6,463	101	63	6,627
Articulated trucks	3,933	1,384	5,317	*3	*2	5,321
Non-freight carrying trucks	-	-	265	*1	**	267
Buses	-	-	1,759	27	49	1,835
Total	22,512	8,569	69,713	42,807	77,632	190,152
AVERAGE KILOMETRES TRAVELLED(c) ('000)						
Passenger vehicles	-	-	11.4	7.7	8.4	15.1
Motor cycles	-	-	4.8	4.3	3.4	5.2
Light commercial vehicles	15.3	8.6	19.5	7.7	7.5	18.8
Rigid trucks	16.3	8.2	22.3	4.5	3.2	21.9
Articulated trucks	69.6	29.9	93.6	2.3	*1.7	92.1
Non-freight carrying trucks	-	-	15.3	*2.3	**1.5	15.4
Buses	-	-	35.9	7.5	8.0	34.3
Total	18.0	9.6	15.0	7.6	8.2	16.0
(a) Because of changes to methodology, caution should be used when comparing these data with data from earlier surveys presented in previous editions of Year Book Australia.						
(b) Includes business travel of non-freight carrying vehicles.						
(c) Average distance travelled for registered vehicles which were used.						
Source: Survey of Motor Vehicle Use, Australia, 12 Months ended 31 October 2001 (9208.0).						

Table 27: Motor Vehicle Use Queensland 2000-2001(ABS, 2003)

MOTOR VEHICLE USE, By state/territory of registration - 2001			
	Passenger vehicles	Motor cycles	Buses
TOTAL KILOMETRES TRAVELLED (million)			
New South Wales	44,480	389	492
Victoria	39,643	352	364
Queensland	28,051	387	468
South Australia	11,977	118	121
Western Australia	13,539	132	259
Tasmania	2,708	25	43
Northern Territory	953	16	55
Australian Capital Territory	2,575	27	34
Australia	143,925	1,448	1,835
NUMBER OF VEHICLES(a) (no.)			
New South Wales	3,041,251	91,753	14,407
Victoria	2,637,201	93,780	12,686
Queensland	1,778,871	73,758	12,628
South Australia	865,419	27,234	3,519
Western Australia	1,051,496	44,599	7,279
Tasmania	244,631	8,422	1,735
Northern Territory	67,215	3,537	1,965
Australian Capital Territory	175,723	6,383	859
Australia	9,861,807	349,465	55,078
(a) The average number of vehicles registered for the 12 months. Includes registered vehicles that did not travel during the reference period.			
Source: Survey of Motor Vehicle Use, Australia, 12 months ended 31 October 2001 (9208.0).			

A7.1.2 Number of Vehicles

Having calculated the average use of hydrogen per vehicle, the next step was to determine the number of vehicles that could be fuelled.

$$[178 \text{ (kt/yr)} \times 1000000 \text{ (kg/kt)}] / [0.238 \text{ (kg/d/car)} \times 365 \text{ (d/yr)}]$$

$$= 2.05 \text{ million cars based on Ogden, Steinbugler et al. (1999)}$$

The later work of Ogden (2003) indicates a higher usage rate of H₂ per car, which leads to a calculation of 1.57 million cars. This lower value is assumed to be more conservative, and thus is the one used in this work.

A7.2 Buffering Capacity at Tarong Sites

The data from the Tarong Crop and Forestry Study shown in Appendix 5 was used to determine the buffering capacity of the soils for the sustainability assessment, using the equation from Noble (2002) as described in Chapter 7.

Table 28: pH Buffering Capacity from Tarong Data

Site Number	Distance (km)	Bearing from Tarong	Elevation (m)	pH - B10	pH BC (2) (mmolH+/kg.pHunit)	mgSO4/kg
14	15.6	292	540	5.9	35.603	569.648
15	19.3	274	550	6.5	29.4	470.4
16	7	181	580	6.5	40.327	645.232
17	7	181	590	5.7	28.924	462.784
18	6.9	157	520	6.1	30.111	481.776
19	7.5	148	540	7.2	35.237	563.792
20	7.6	146	540	6.7	44.268	708.288
21	6	130	540	6.6	44.68	714.88
22	6	130	540	5.3	51.049	816.784
23	2.4	77	540	6.6	33.353	533.648
24	2.8	37	450	6.6	48.681	778.896
25	7.3	293	440	6.6	22.361	357.776
27	9.3	199	600	4.7	62.034	992.544
28	9.3	199	590	5.3	46.326	741.216
29	8.9	192	520	5.8	52.105	833.68
30	7.7	73	440	6.3	20.214	323.424
31	18.9	52	380	6.4	26.894	430.304
32	4.3	335	400	6.3	14.731	235.696
33	9.1	15	400	6	35.237	563.792
34	2.6	272	450	6	10.07	161.12

A7.3 Air Monitoring Sites

Appendix 3. Monitoring site locations

Figure 157. EPA and industry ambient air quality monitoring site locations.

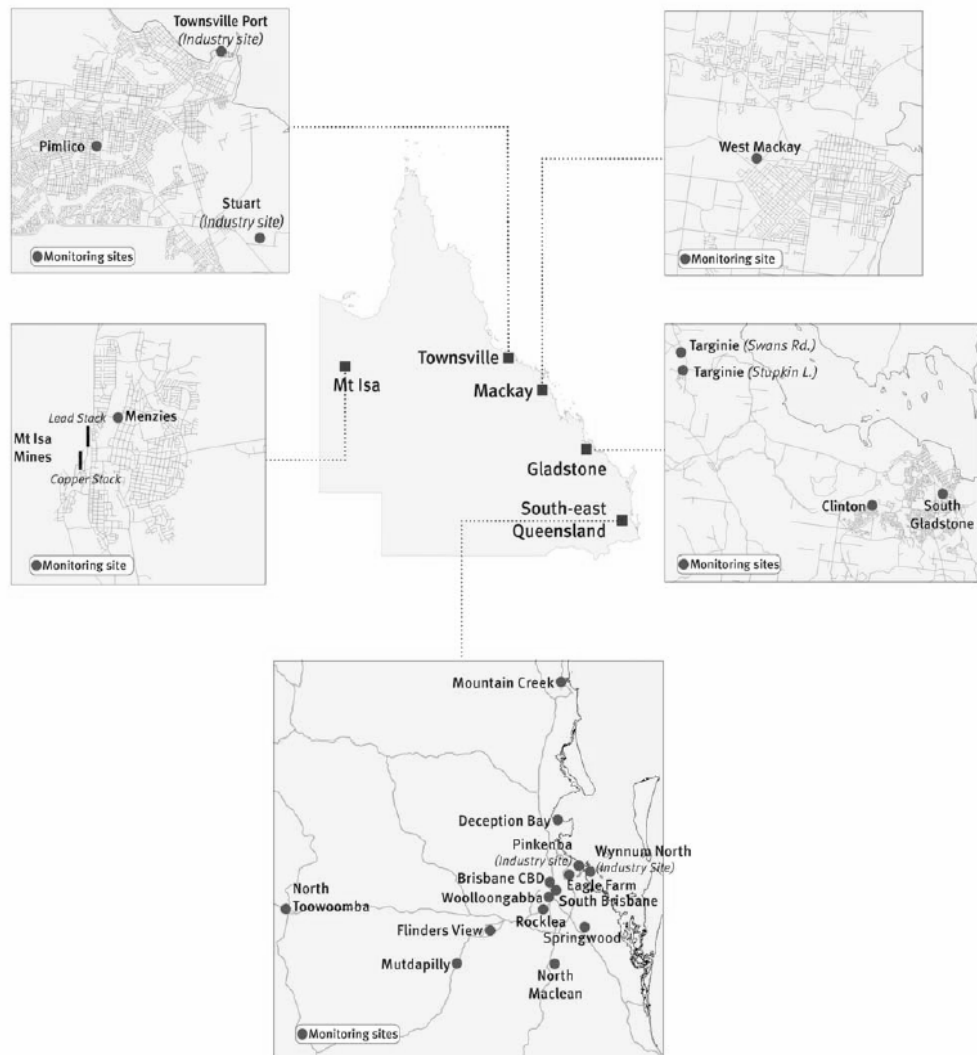


Figure 24: Queensland EPA Air Quality Monitoring Sites (Neale, 2005)

References

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Appendix 8

AUSPLUME Data for Comparison

A8.1 Concentration, Gravitational Settling, No Terrain

Concentration or deposition	Concentration
Emission rate units	kg/hour
Concentration units	micrograms/cub.metre
Units conversion factor	2.78E+05
Background concentration	1.00E+00
Terrain effects	None
Smooth stability class changes?	No
Other stability class adjustments ("urban modes")	None
Ignore building wake effects?	Yes
Decay coefficient (unless overridden by met. file)	0.000
Anemometer height	10 m
Averaging time for sigma-theta values	60 min.
Roughness height at the wind vane site	0.030 m

DISPERSION CURVES

Horizontal dispersion curves for sources <100m high	Sigma-theta
Vertical dispersion curves for sources <100m high	Pasquill-Gifford
Horizontal dispersion curves for sources >100m high	Briggs Rural
Vertical dispersion curves for sources >100m high	Briggs Rural
Enhance horizontal plume spreads for buoyancy?	No
Enhance vertical plume spreads for buoyancy?	No
Adjust horizontal P-G formulae for roughness height?	No
Adjust vertical P-G formulae for roughness height?	No
Adjustment for wind directional shear	None

PLUME RISE OPTIONS

Gradual plume rise?	Yes
Stack-tip downwash included?	Yes
Building downwash algorithm:	Schulman-Scire method.
Entrainment coeff. for neutral & stable lapse rates	0.60,0.60
Partial penetration of elevated inversions?	No
Disregard temp. gradients in the hourly met. file?	No

and in the absence of boundary-layer potential temperature gradients given by the hourly met. file, a value from the following table (in K/m) is used:

Wind Speed	Stability Class					
Category	A	B	C	D	E	F
-----+						
1	0.000	0.000	0.000	0.000	0.020	0.035
2	0.000	0.000	0.000	0.000	0.020	0.035
3	0.000	0.000	0.000	0.000	0.020	0.035
4	0.000	0.000	0.000	0.000	0.020	0.035
5	0.000	0.000	0.000	0.000	0.020	0.035
6	0.000	0.000	0.000	0.000	0.020	0.035

WIND SPEED CATEGORIES

Boundaries between categories (in m/s) are: 1.54, 3.09, 5.14, 8.23, 10.80

WIND PROFILE EXPONENTS: "Irwin Rural" values (unless overridden by met. file)

AVERAGING TIMES

average over all hours

1

+	-----	+
	SOURCE CHARACTERISTICS	
+	-----	+

STACK SOURCE: 1

X(m)	Y(m)	Ground Elev.	Stack Height	Diameter	Temperature	Speed
0	0	450m	210m	5.00m	408K	3.6m/s

No building wake effects.
(Constant) emission rate = 3.08E+03 kg/hour

Mass fraction	Settling Speed (m/s)	Reflection coefficient
-----	-----	-----
1.0000	0.005	0.300

1

+	-----	+
	RECEPTOR LOCATIONS	
+	-----	+

The polar receptor grid has the following radii:
0.m 3600.m 7200.m 14900.m 30900.m

and these bearings (in degrees):
0.0 45.0 90.0 135.0 180.0 225.0 270.0 315.0

DISCRETE RECEPTOR LOCATIONS

No.	RADIUS (m)	BEARING	No.	RADIUS (m)	BEARING	No.	RADIUS (m)	BEARING
1	15600.	292.	2	19300.	274.	3	7000.	181.
4	4300.	335.						

METEOROLOGICAL DATA : Ausplume Meteorological database for brisbane

AVERAGE OVER ALL HOURS AND FOR ALL SOURCES
in micrograms/cub.metre

R (km): 0.000 3.600 7.200 14.900 30.900

Bearing|

0.0	1.00E+00	5.65E+00	3.01E+00	1.95E+00	1.65E+00
45.0	1.00E+00	4.54E+00	2.56E+00	1.86E+00	1.60E+00
90.0	1.00E+00	4.00E+00	2.31E+00	1.71E+00	1.50E+00
135.0	1.00E+00	2.80E+00	1.77E+00	1.41E+00	1.30E+00
180.0	1.00E+00	3.17E+00	1.96E+00	1.49E+00	1.32E+00
225.0	1.00E+00	4.12E+00	2.34E+00	1.79E+00	1.51E+00
270.0	1.00E+00	8.75E+00	4.42E+00	2.83E+00	2.27E+00
315.0	1.00E+00	8.85E+00	4.45E+00	2.56E+00	2.07E+00

Concentrations at the discrete receptors (No. : Value):

1:3.31E+00 2:2.40E+00 3:2.00E+00 4:5.73E+00

A8.2 Concentration, Gravitational Settling, Terrain

Concentration or deposition	Concentration
Emission rate units	kg/hour
Concentration units	micrograms/cub.metre
Units conversion factor	2.78E+05
Background concentration	1.00E+00
Terrain effects	Egan method
Smooth stability class changes?	No
Other stability class adjustments ("urban modes")	None
Ignore building wake effects?	Yes
Decay coefficient (unless overridden by met. file)	0.000
Anemometer height	10 m
Averaging time for sigma-theta values	60 min.
Roughness height at the wind vane site	0.030 m

DISPERSION CURVES

Horizontal dispersion curves for sources <100m high	Sigma-theta
Vertical dispersion curves for sources <100m high	Pasquill-Gifford
Horizontal dispersion curves for sources >100m high	Briggs Rural
Vertical dispersion curves for sources >100m high	Briggs Rural
Enhance horizontal plume spreads for buoyancy?	No

Enhance vertical plume spreads for buoyancy? No
 Adjust horizontal P-G formulae for roughness height? No
 Adjust vertical P-G formulae for roughness height? No
 Adjustment for wind directional shear None

PLUME RISE OPTIONS

Gradual plume rise? Yes
 Stack-tip downwash included? Yes
 Building downwash algorithm: Schulman-Scire method.
 Entrainment coeff. for neutral & stable lapse rates 0.60,0.60
 Partial penetration of elevated inversions? No
 Disregard temp. gradients in the hourly met. file? No

and in the absence of boundary-layer potential temperature gradients
 given by the hourly met. file, a value from the following table
 (in K/m) is used:

Wind Speed		Stability Class					
Category	A	B	C	D	E	F	
-----+-----							
1	0.000	0.000	0.000	0.000	0.020	0.035	
2	0.000	0.000	0.000	0.000	0.020	0.035	
3	0.000	0.000	0.000	0.000	0.020	0.035	
4	0.000	0.000	0.000	0.000	0.020	0.035	
5	0.000	0.000	0.000	0.000	0.020	0.035	
6	0.000	0.000	0.000	0.000	0.020	0.035	

WIND SPEED CATEGORIES

Boundaries between categories (in m/s) are: 1.54, 3.09, 5.14, 8.23, 10.80

WIND PROFILE EXPONENTS: "Irwin Rural" values (unless overridden by met.
 file)

AVERAGING TIMES

average over all hours

```

-----
1      +-----+
      |           |
      | SOURCE CHARACTERISTICS |
      |           |
      +-----+
  
```

STACK SOURCE: 1

X(m)	Y(m)	Ground Elev.	Stack Height	Diameter	Temperature	Speed
0	0	450m	210m	5.00m	408K	3.6m/s

No building wake effects.
 (Constant) emission rate = 3.08E+03 kg/hour

Mass fraction	Settling Speed (m/s)	Reflection coefficient
1.0000	0.005	0.300

1

```

+-----+
|               |
| RECEPTOR LOCATIONS |
|               |
+-----+
```

The polar receptor grid has the following radii:
 0.m 3600.m 7200.m 14900.m 30900.m

and these bearings (in degrees):
 0.0 45.0 90.0 135.0 180.0 225.0 270.0 315.0

DISCRETE RECEPTOR LOCATIONS

No.	RADIUS (m)	BEARING	No.	RADIUS (m)	BEARING	No.	RADIUS (m)	BEARING
1	15600.	292.	2	19300.	274.	3	7000.	181.
4	4300.	335.						

METEOROLOGICAL DATA : Ausplume Meteorological database for brisbane

AVERAGE OVER ALL HOURS AND FOR ALL SOURCES in micrograms/cub.metre

R (km): 0.000 3.600 7.200 14.900 30.900

Bearing\	0.0	45.0	90.0	135.0	180.0	225.0	270.0	315.0
0.0	1.00E+00	5.65E+00	2.98E+00	1.90E+00	1.60E+00			
45.0	1.00E+00	4.05E+00	2.44E+00	1.75E+00	1.39E+00			
90.0	1.00E+00	4.00E+00	2.24E+00	1.52E+00	1.30E+00			
135.0	1.00E+00	2.71E+00	1.74E+00	1.47E+00	1.25E+00			
180.0	1.00E+00	3.38E+00	2.15E+00	1.49E+00	1.29E+00			
225.0	1.00E+00	3.02E+00	2.45E+00	1.88E+00	1.89E+00			
270.0	1.00E+00	8.75E+00	4.65E+00	2.83E+00	2.72E+00			
315.0	1.00E+00	8.85E+00	4.51E+00	2.56E+00	2.26E+00			

Concentrations at the discrete receptors (No. : Value):

1:3.85E+00 2:2.73E+00 3:2.18E+00 4:5.62E+00

A8.3 Concentration, No Gravitational Settling, Terrain

Concentration or deposition	Concentration
Emission rate units	kg/hour
Concentration units	micrograms/cub.metre
Units conversion factor	2.78E+05
Background concentration	1.00E+00
Terrain effects	Egan method
Smooth stability class changes?	No
Other stability class adjustments ("urban modes")	None
Ignore building wake effects?	Yes
Decay coefficient (unless overridden by met. file)	0.000
Anemometer height	10 m
Averaging time for sigma-theta values	60 min.
Roughness height at the wind vane site	0.030 m

DISPERSION CURVES

Horizontal dispersion curves for sources <100m high	Sigma-theta
Vertical dispersion curves for sources <100m high	Pasquill-Gifford
Horizontal dispersion curves for sources >100m high	Briggs Rural
Vertical dispersion curves for sources >100m high	Briggs Rural
Enhance horizontal plume spreads for buoyancy?	No
Enhance vertical plume spreads for buoyancy?	No
Adjust horizontal P-G formulae for roughness height?	No
Adjust vertical P-G formulae for roughness height?	No
Adjustment for wind directional shear	None

PLUME RISE OPTIONS

Gradual plume rise?	Yes
Stack-tip downwash included?	Yes
Building downwash algorithm:	Schulman-Scire method.
Entrainment coeff. for neutral & stable lapse rates	0.60,0.60
Partial penetration of elevated inversions?	No
Disregard temp. gradients in the hourly met. file?	No

and in the absence of boundary-layer potential temperature gradients given by the hourly met. file, a value from the following table (in K/m) is used:

Wind Speed	Stability Class					
Category	A	B	C	D	E	F
-----+-----						
1	0.000	0.000	0.000	0.000	0.020	0.035
2	0.000	0.000	0.000	0.000	0.020	0.035
3	0.000	0.000	0.000	0.000	0.020	0.035
4	0.000	0.000	0.000	0.000	0.020	0.035
5	0.000	0.000	0.000	0.000	0.020	0.035

6 | 0.000 0.000 0.000 0.000 0.020 0.035

WIND SPEED CATEGORIES

Boundaries between categories (in m/s) are: 1.54, 3.09, 5.14, 8.23, 10.80

WIND PROFILE EXPONENTS: "Irwin Rural" values (unless overridden by met. file)

AVERAGING TIMES

average over all hours

1 +-----+

 | |

 | SOURCE CHARACTERISTICS |

 | |

 +-----+

STACK SOURCE: 1

X(m)	Y(m)	Ground Elev.	Stack Height	Diameter	Temperature	Speed
0	0	0m	210m	5.00m	408K	3.6m/s

No building wake effects.
(Constant) emission rate = 3.08E+03 kg/hour
No gravitational settling or scavenging.

1 +-----+

 | |

 | RECEPTOR LOCATIONS |

 | |

 +-----+

The polar receptor grid has the following radii:

0.m 3600.m 7200.m 14900.m 30900.m

and these bearings (in degrees):

0.0 45.0 90.0 135.0 180.0 225.0 270.0 315.0

DISCRETE RECEPTOR LOCATIONS

No.	RADIUS (m)	BEARING	No.	RADIUS (m)	BEARING	No.	RADIUS (m)	BEARING
1	15600.	292.	2	19300.	274.	3	7000.	181.
4	4300.	335.						

METEOROLOGICAL DATA : Ausplume Meteorological database for brisbane

AVERAGE OVER ALL HOURS AND FOR ALL SOURCES
in micrograms/cub.metre

R (km): 0.000 3.600 7.200 14.900 30.900

Bearing|

0.0	1.00E+00	1.26E+01	6.81E+00	4.91E+00	3.54E+00
45.0	1.00E+00	1.10E+01	6.53E+00	4.49E+00	2.98E+00
90.0	1.00E+00	9.26E+00	5.39E+00	3.22E+00	2.40E+00
135.0	1.00E+00	5.68E+00	3.52E+00	2.91E+00	2.00E+00
180.0	1.00E+00	6.50E+00	4.19E+00	2.98E+00	2.14E+00
225.0	1.00E+00	6.49E+00	6.43E+00	4.15E+00	2.77E+00
270.0	1.00E+00	2.16E+01	1.32E+01	8.32E+00	5.60E+00
315.0	1.00E+00	1.88E+01	1.16E+01	7.78E+00	6.03E+00

Concentrations at the discrete receptors (No. : Value):

1:1.21E+01 2:6.39E+00 3:4.25E+00 4:1.08E+01

A8.4 Concentration, No Gravitational Settling, No Terrain

Concentration or deposition	Concentration
Emission rate units	kg/hour
Concentration units	micrograms/cub.metre
Units conversion factor	2.78E+05
Background concentration	1.00E+00
Terrain effects	None
Smooth stability class changes?	No
Other stability class adjustments ("urban modes")	None
Ignore building wake effects?	Yes
Decay coefficient (unless overridden by met. file)	0.000
Anemometer height	10 m
Averaging time for sigma-theta values	60 min.
Roughness height at the wind vane site	0.030 m

DISPERSION CURVES

Horizontal dispersion curves for sources <100m high	Sigma-theta
Vertical dispersion curves for sources <100m high	Pasquill-Gifford
Horizontal dispersion curves for sources >100m high	Briggs Rural
Vertical dispersion curves for sources >100m high	Briggs Rural
Enhance horizontal plume spreads for buoyancy?	No

Enhance vertical plume spreads for buoyancy? No
 Adjust horizontal P-G formulae for roughness height? No
 Adjust vertical P-G formulae for roughness height? No
 Adjustment for wind directional shear None

PLUME RISE OPTIONS

Gradual plume rise? Yes
 Stack-tip downwash included? Yes
 Building downwash algorithm: Schulman-Scire method.
 Entrainment coeff. for neutral & stable lapse rates 0.60,0.60
 Partial penetration of elevated inversions? No
 Disregard temp. gradients in the hourly met. file? No

and in the absence of boundary-layer potential temperature gradients
 given by the hourly met. file, a value from the following table
 (in K/m) is used:

Wind Speed		Stability Class					
Category	A	B	C	D	E	F	
-----+-----							
1	0.000	0.000	0.000	0.000	0.020	0.035	
2	0.000	0.000	0.000	0.000	0.020	0.035	
3	0.000	0.000	0.000	0.000	0.020	0.035	
4	0.000	0.000	0.000	0.000	0.020	0.035	
5	0.000	0.000	0.000	0.000	0.020	0.035	
6	0.000	0.000	0.000	0.000	0.020	0.035	

WIND SPEED CATEGORIES

Boundaries between categories (in m/s) are: 1.54, 3.09, 5.14, 8.23, 10.80

WIND PROFILE EXPONENTS: "Irwin Rural" values (unless overridden by met.
 file)

AVERAGING TIMES

average over all hours

```

-----
1      +-----+
      |           |
      | SOURCE CHARACTERISTICS |
      |           |
      +-----+
  
```

STACK SOURCE: 1

X(m)	Y(m)	Ground Elev.	Stack Height	Diameter	Temperature	Speed
0	0	0m	210m	5.00m	408K	3.6m/s

No building wake effects.
 (Constant) emission rate = 3.08E+03 kg/hour
 No gravitational settling or scavenging.



The polar receptor grid has the following radii:
 0.m 3600.m 7200.m 14900.m 30900.m

and these bearings (in degrees):
 0.0 45.0 90.0 135.0 180.0 225.0 270.0 315.0

DISCRETE RECEPTOR LOCATIONS

No.	RADIUS (m)	BEARING	No.	RADIUS (m)	BEARING	No.	RADIUS (m)
BEARING 1	15600.	292.	2	19300.	274.	3	7000.
4	4300.	335.					

METEOROLOGICAL DATA : Ausplume Meteorological database for brisbane

AVERAGE OVER ALL HOURS AND FOR ALL SOURCES in micrograms/cub.metre

R (km): 0.000 3.600 7.200 14.900 30.900

Bearing\	0.0	45.0	90.0	135.0	180.0	225.0	270.0	315.0
0.000	1.00E+00	8.06E+00	4.20E+00	2.75E+00	2.19E+00			
3.600	1.00E+00	6.39E+00	3.49E+00	2.51E+00	2.07E+00			
7.200	1.00E+00	5.56E+00	3.07E+00	2.23E+00	1.88E+00			
14.900	1.00E+00	3.74E+00	2.24E+00	1.72E+00	1.52E+00			
30.900	1.00E+00	4.29E+00	2.54E+00	1.89E+00	1.61E+00			
	1.00E+00	5.75E+00	3.12E+00	2.34E+00	1.93E+00			
	1.00E+00	1.28E+01	6.44E+00	4.21E+00	3.21E+00			
	1.00E+00	1.29E+01	6.55E+00	3.96E+00	2.98E+00			

Concentrations at the discrete receptors (No. : Value):

1:5.21E+00 2:3.65E+00 3:2.60E+00 4:8.22E+00

A8.5 Graphs Comparing Atmospheric Concentrations between AUSPLUME and the Current Model

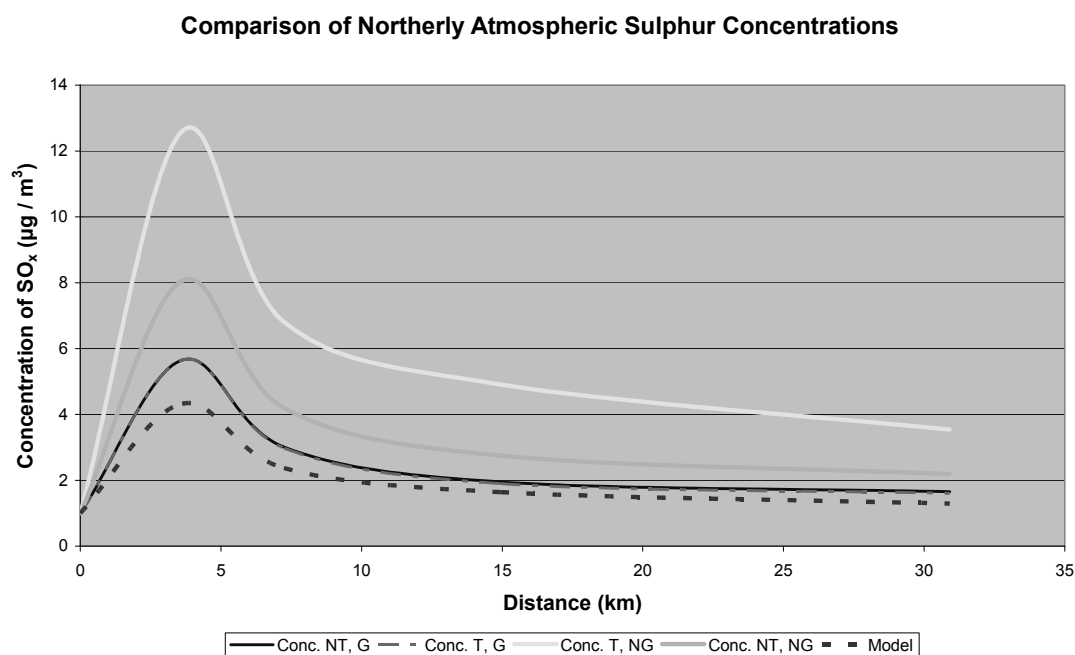


Figure 25: Comparison of Atmospheric Sulphur Concentrations - North

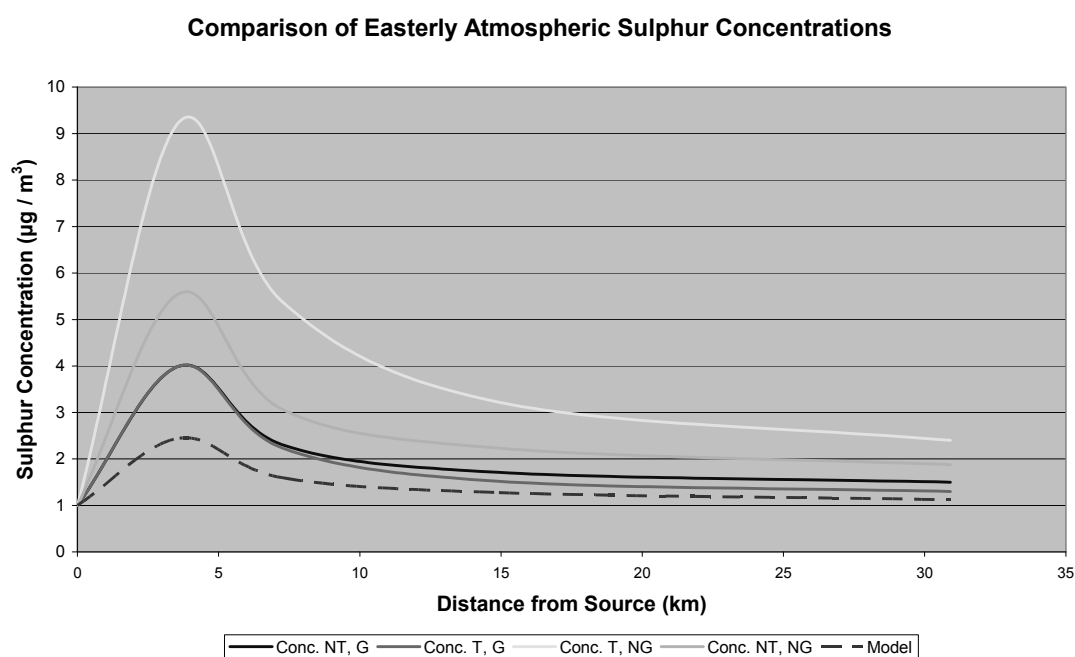


Figure 26: Comparison of Atmospheric Concentrations - East

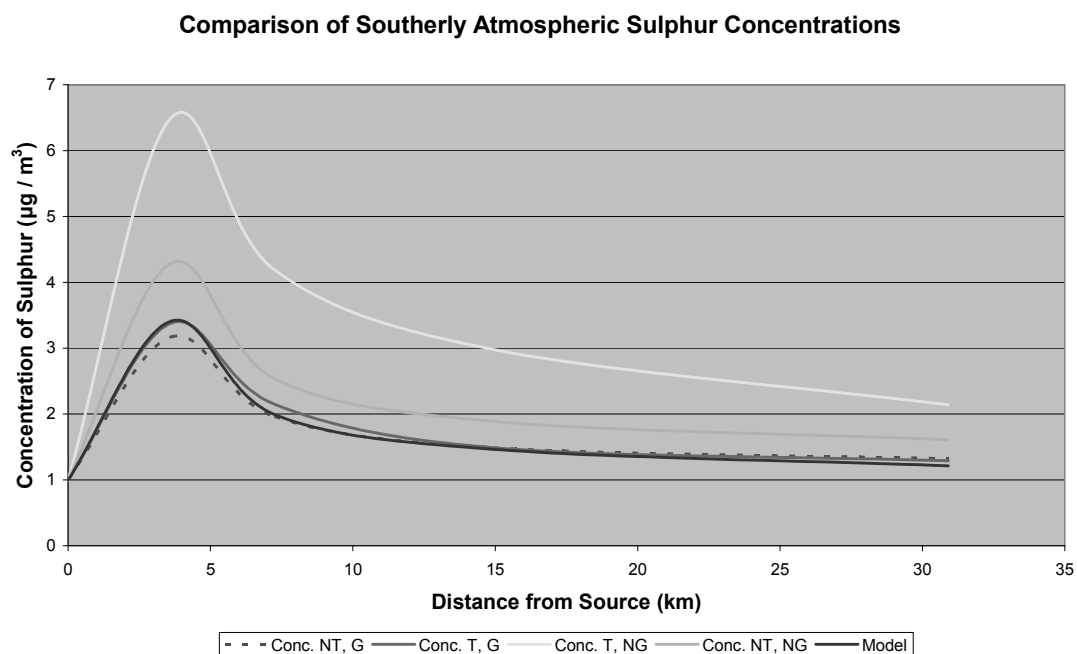


Figure 27: Comparison of Atmospheric Concentrations - South

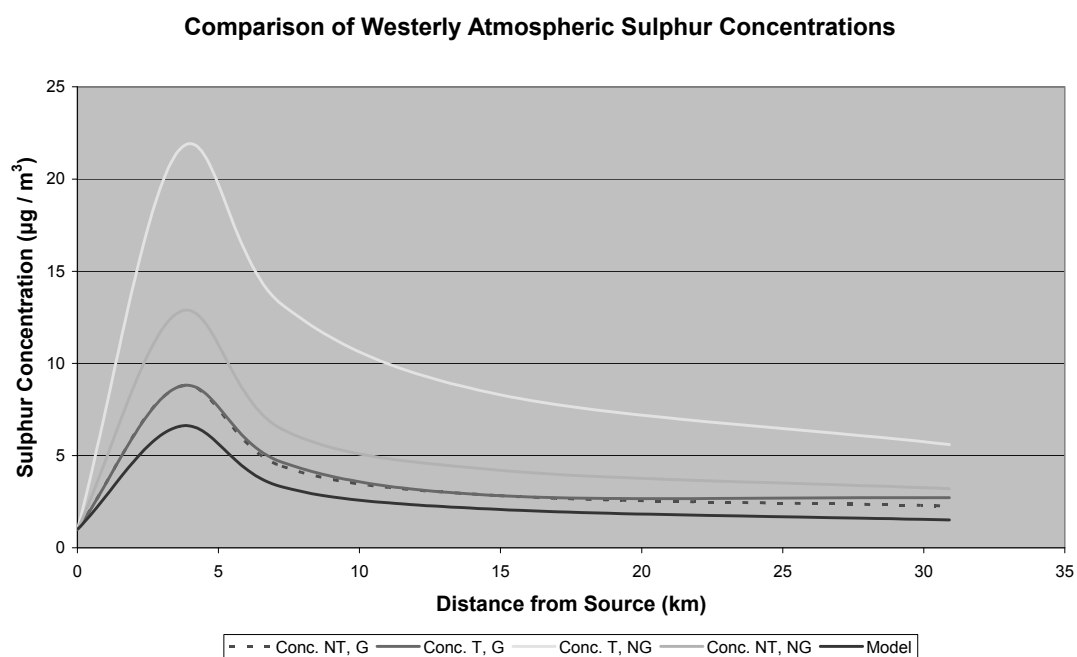


Figure 28: Comparison of Atmospheric Concentrations - West

Comparison of North-Easterly Atmospheric Sulphur Concentrations

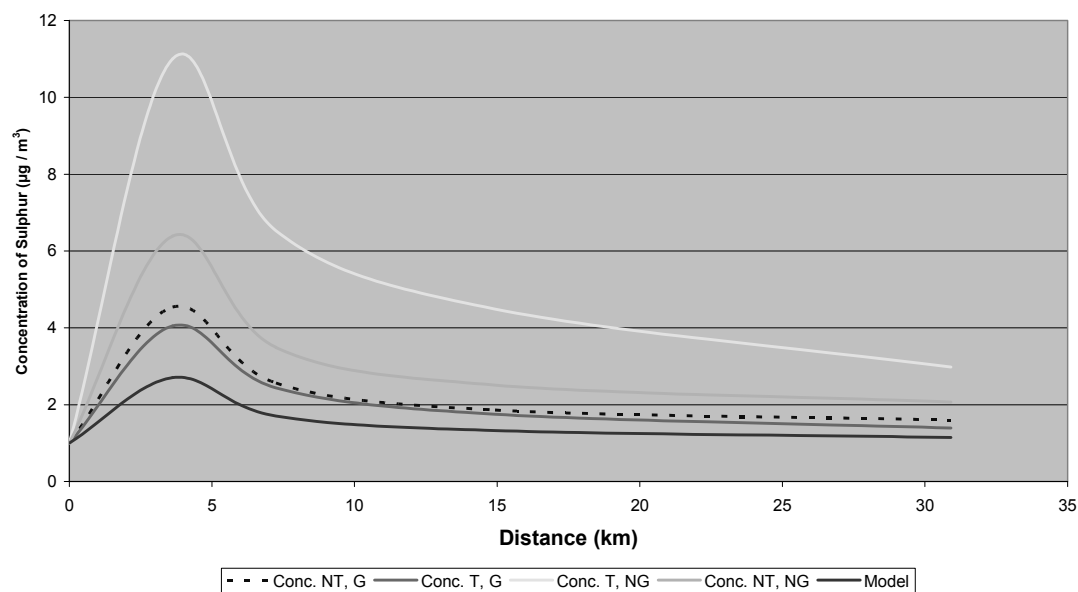


Figure 29: Comparison of Atmospheric Concentrations - North East

Comparison of South-Easterly Atmospheric Sulphur Concentrations

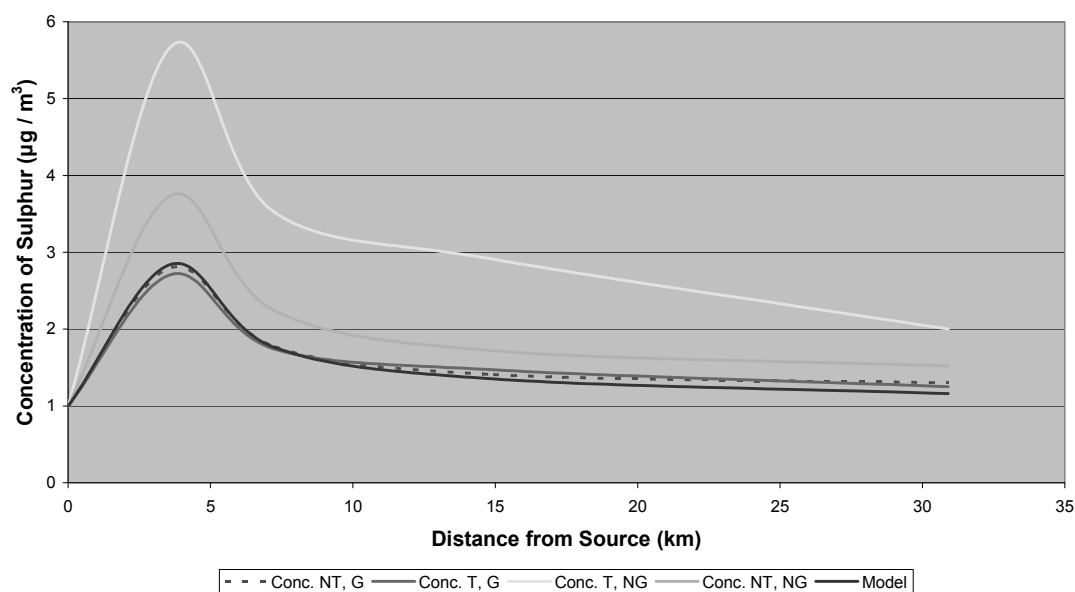


Figure 30: Comparison of Atmospheric Sulphur Concentrations - South East

Comparison of South-Westerly Atmospheric Sulphur Concentrations

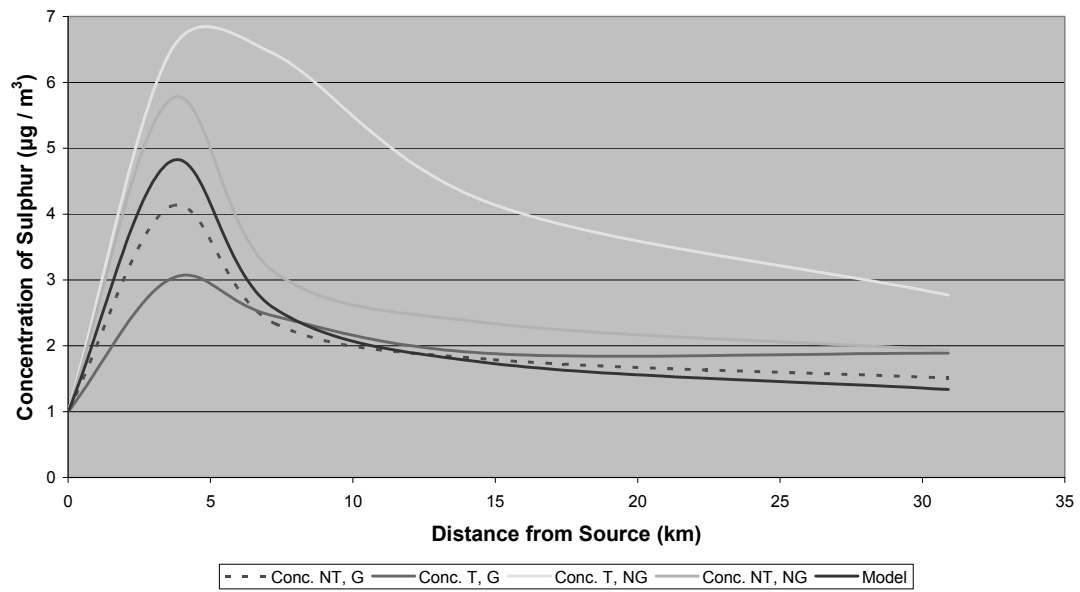


Figure 31: Comparison of Atmospheric Sulphur Concentrations - South West

Comparison of North-Westerly Atmospheric Sulphur Concentration

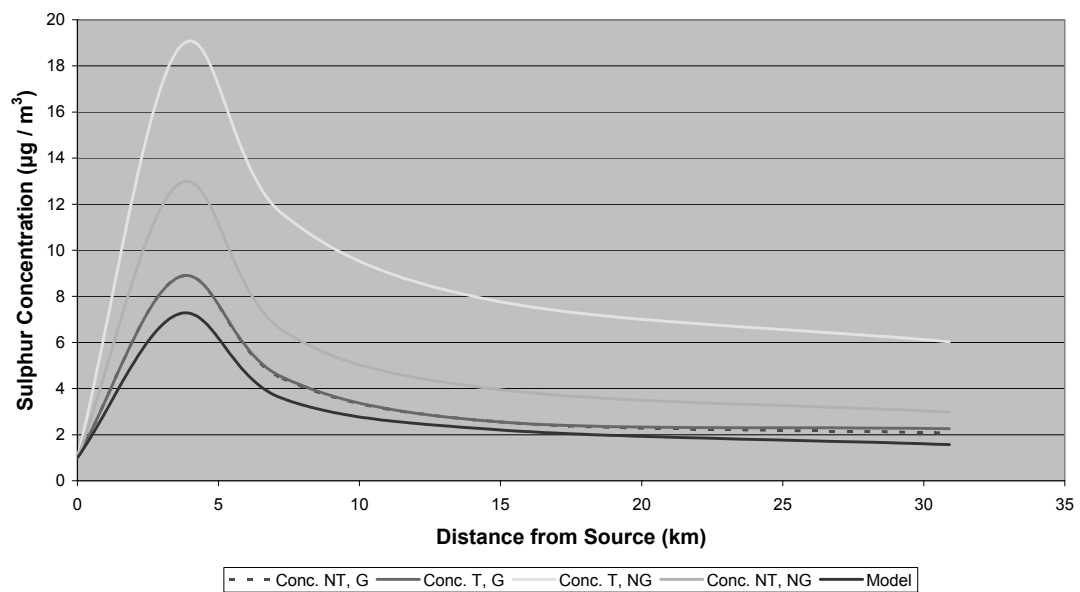


Figure 32: Comparison of Atmospheric Sulphur Concentrations - North West

Appendix 9

Sensitivity Analysis of Emissions Transport Model

A9.1 Graphs of Individual Parameter Variation in the ETM

The following graphs show the variability of parameters in response to a change in single parameters for all sites – this was not shown in Chapter 6 for fear of monotony and excessive repetition. Assessment of the relative behaviour of the parameters is given in Chapter 6. Error bars in the following graphs represent a 20% variation from the standard model.

Comparison of Sensitivity to Neutral Rainfall Value

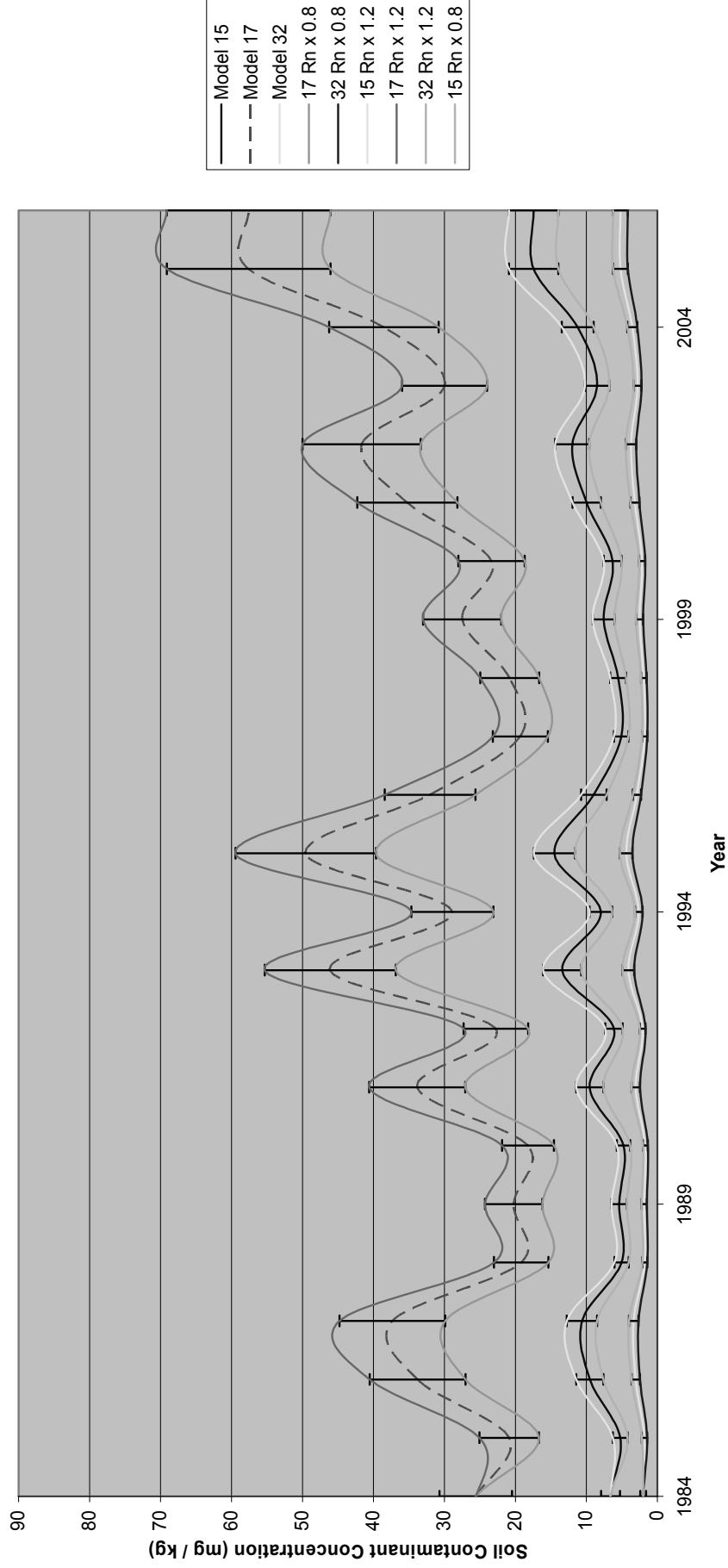


Figure 33: Sensitivity of All Sites to Neutral Rainfall

Comparison of Sensitivity to Variation in Permeability Factor (G)

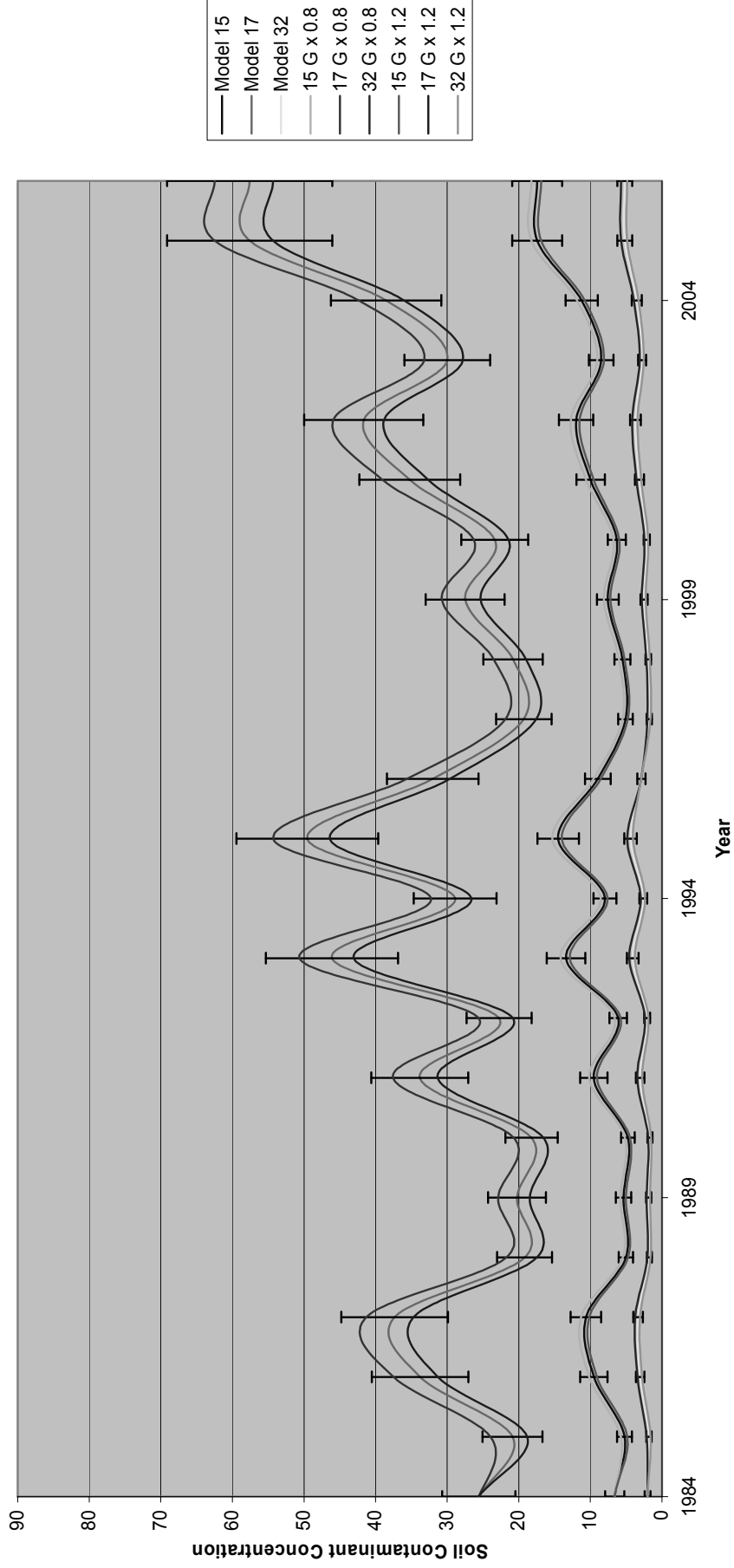


Figure 34: Sensitivity of All Sites to Permeability Factor (G)

Comparison of Sensitivity to Run-off Factor (F)

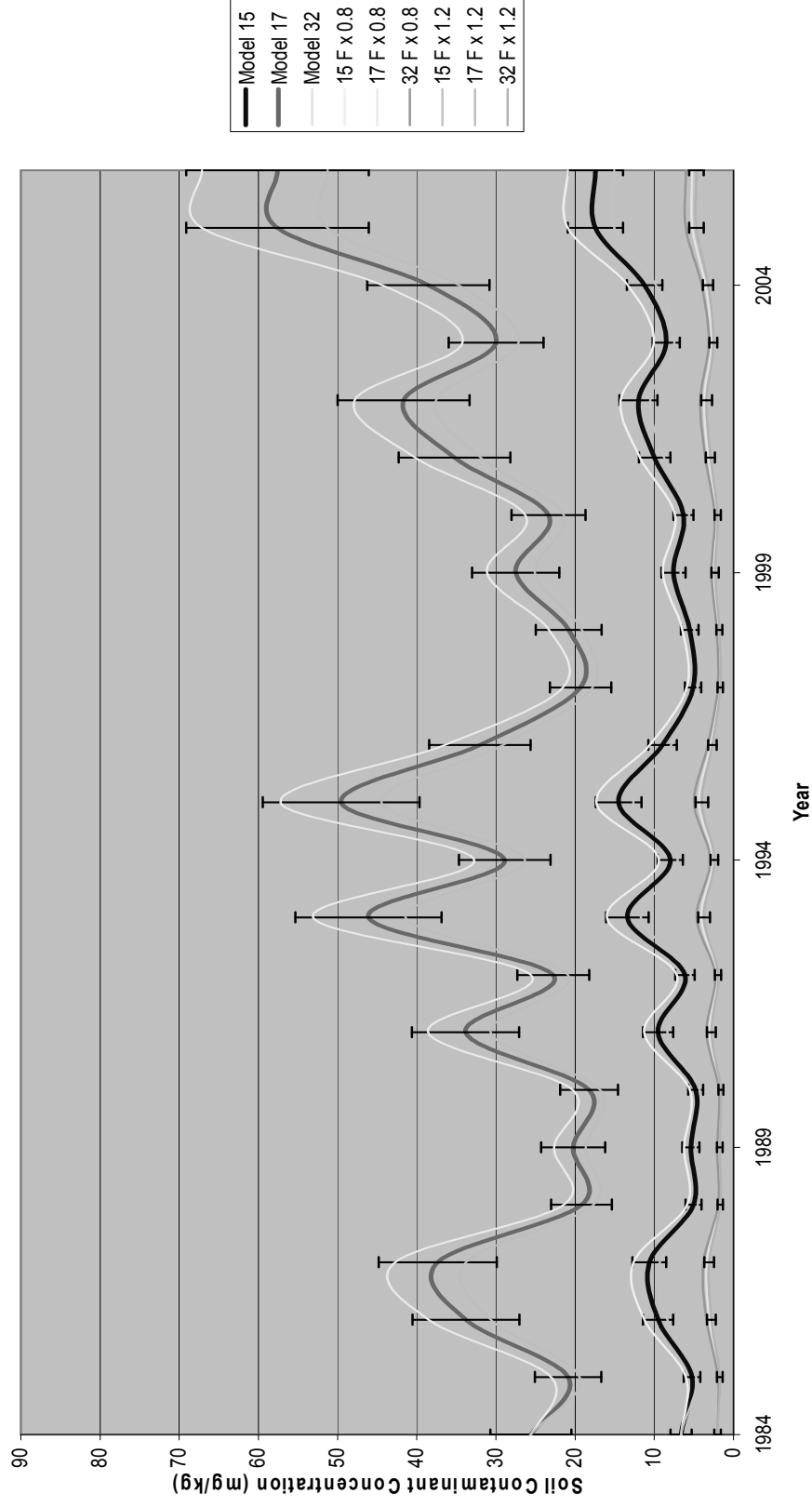


Figure 35: Sensitivity of All Sites to Run-off Factor (F)

Comparison of Sensitivity to Change in Rainfall

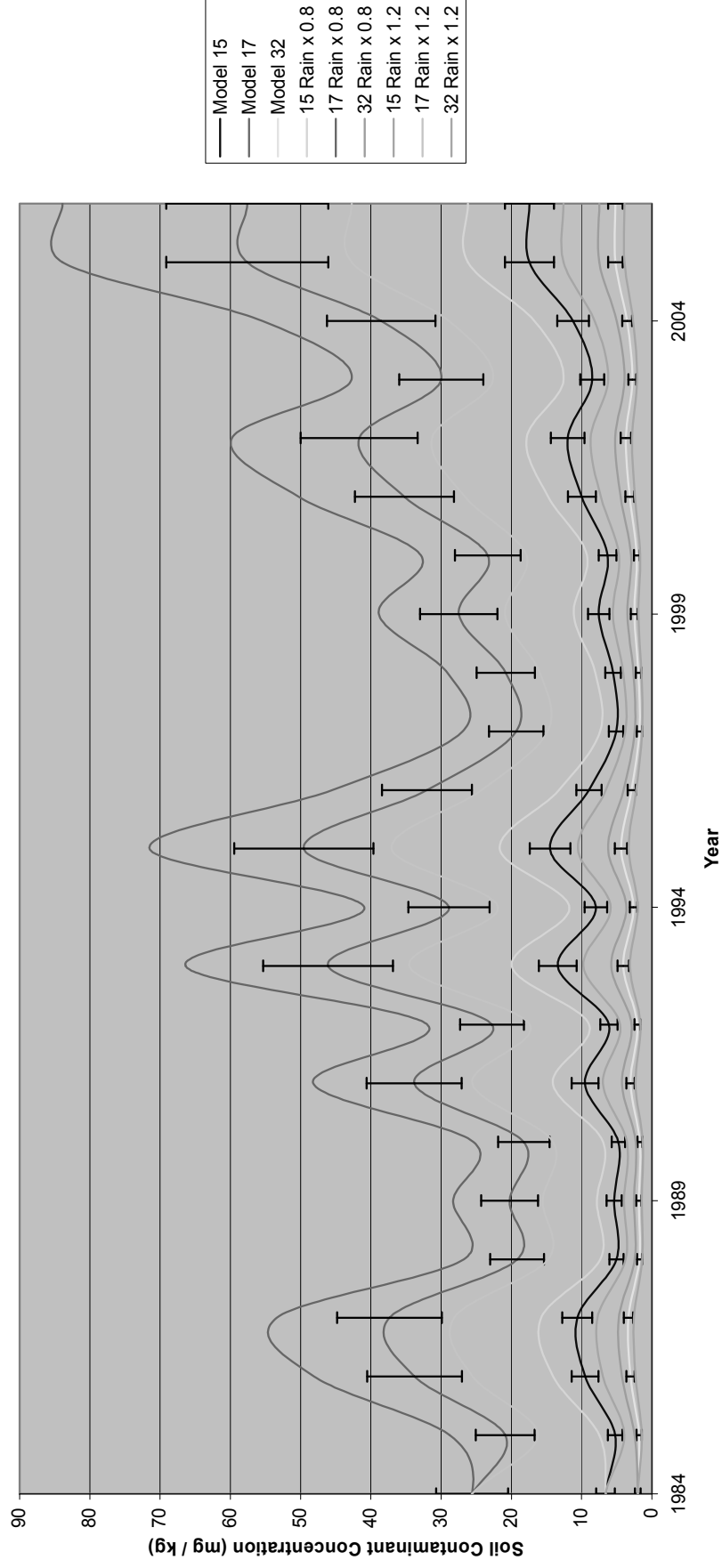


Figure 36: Sensitivity of All Sites to Rainfall

Comparison of Sensitivity to Dry Deposition Velocity

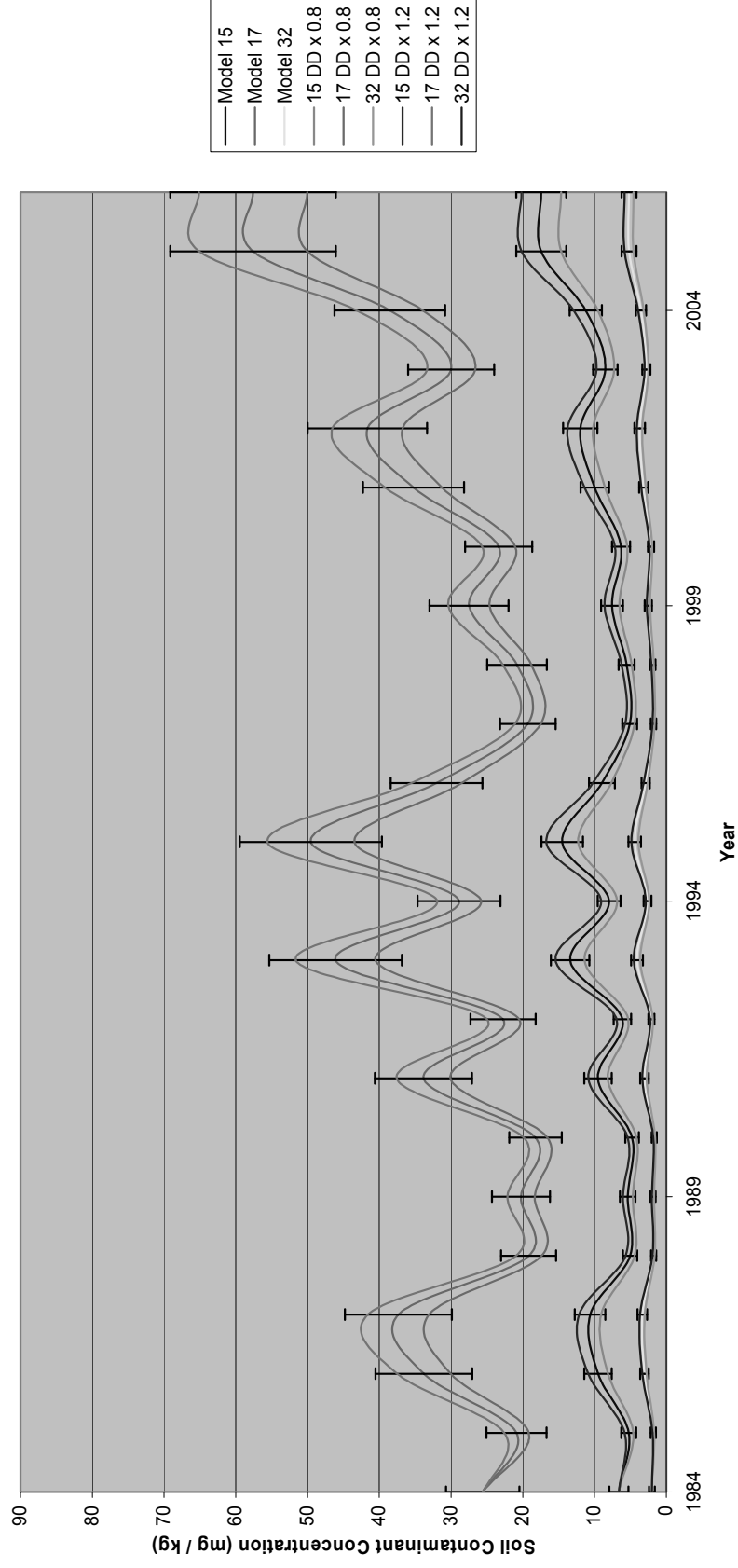


Figure 37: Sensitivity of All Sites to Dry Deposition Velocity

Comparison of Sensitivity to Emission Rate

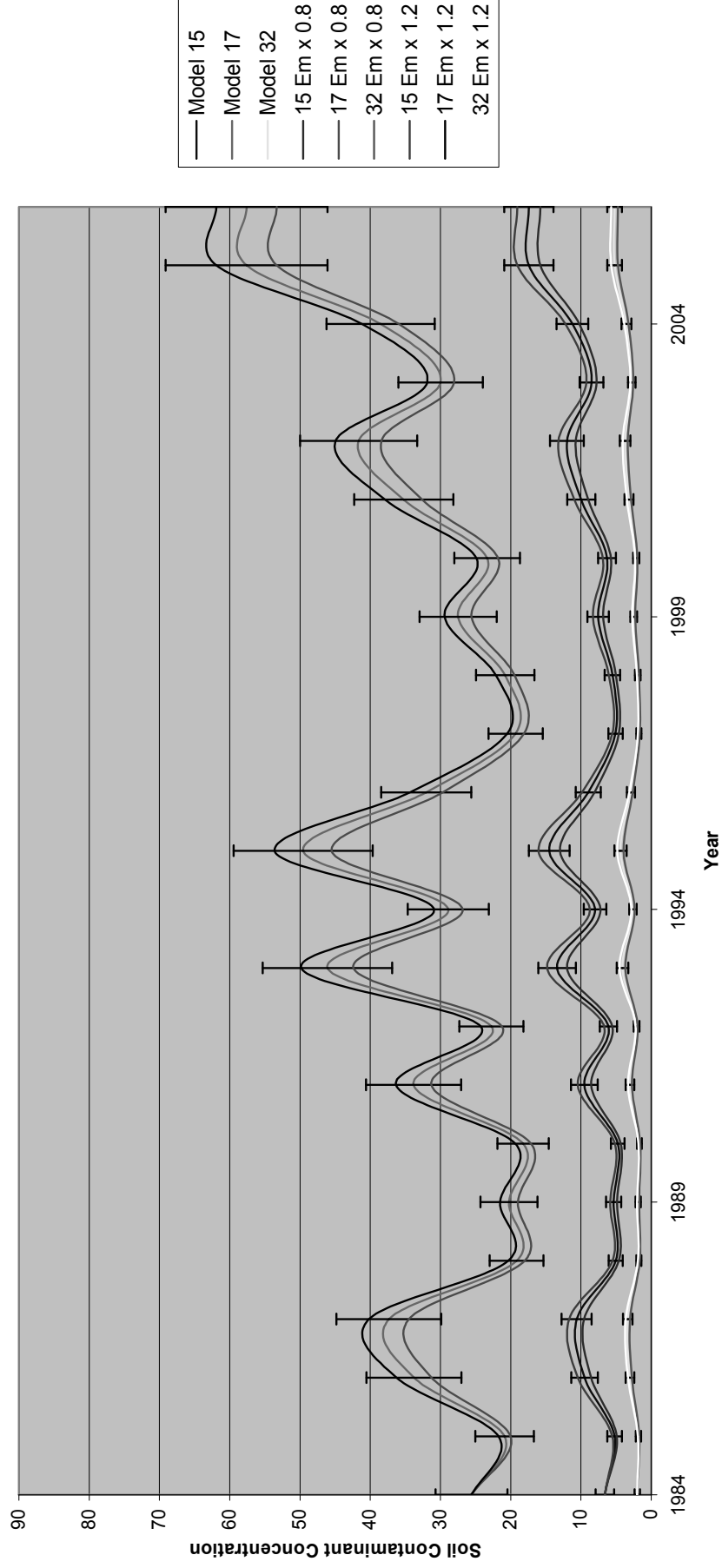


Figure 38: Sensitivity of All Sites to Process Emissions Rate

A9.2 Worst Case Scenarios

In order to obtain further information on the performance of the model, 4 “worst case” scenarios were examined. These scenarios tested the model performance assuming an error of 20% in each of the parameters of interest – thus examining the cumulative effect of moderate errors in parameters. To achieve the worst “Extreme Case” scenario, it was important to vary the parameters in the direction that would cause the highest increase (decrease) in contaminant concentration. The “All Factors” scenario gives the effect of all parameters being varied in the same direction. The direction of parameter variation is shown in Table 29.

Table 29: Direction of Change of Parameters for Worst Case Scenarios

Scenario	All Factors (-20%)	All Factors (+20%)	Extreme Case (Low)	Extreme Case (High)
Neutral Rainfall	⬇	⬆	⬇	⬆
Process Emissions	⬇	⬆	⬇	⬆
Dry Deposition Rate	⬇	⬆	⬇	⬆
Yearly Rainfall	⬇	⬆	⬆	⬇
Run-off Factor	⬇	⬆	⬆	⬇
Permeability Factor	⬇	⬆	⬆	⬇

The following graphs show the variability of soil sulphur concentration in response to the changes indicated in Table 29 for the “All Factors” and “Extreme Case” situations.

In the legends in Figure 39-Figure 41, “Half H” indicates the increase in all factors by 20%, while “Half L” indicates the decrease in all factors by 20 %.

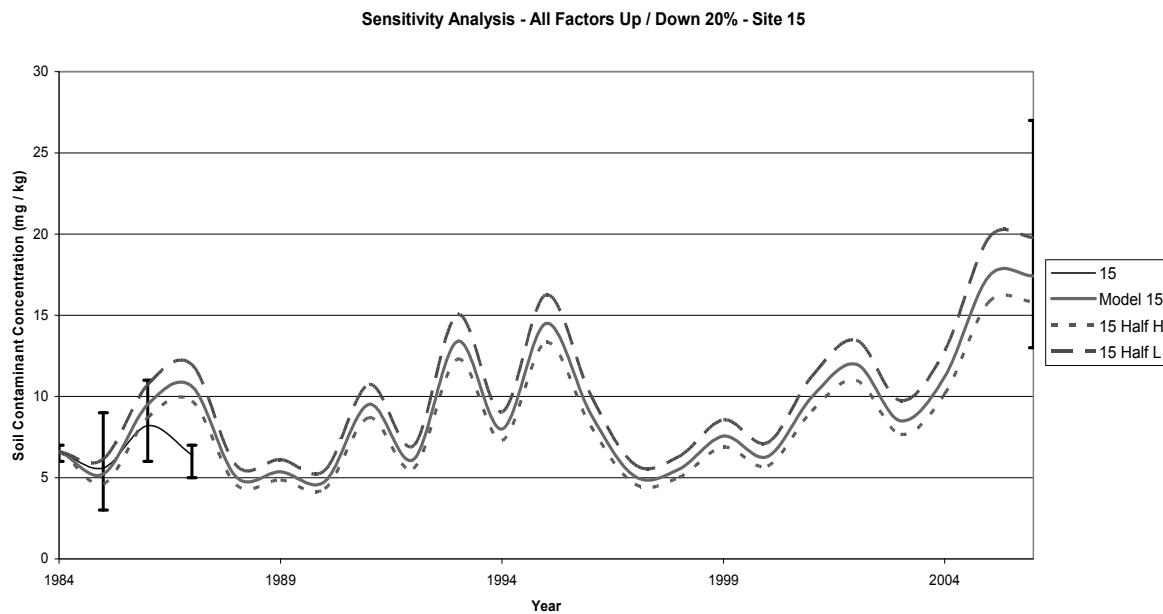


Figure 39: Sensitivity to All Factors Variation - Site 15

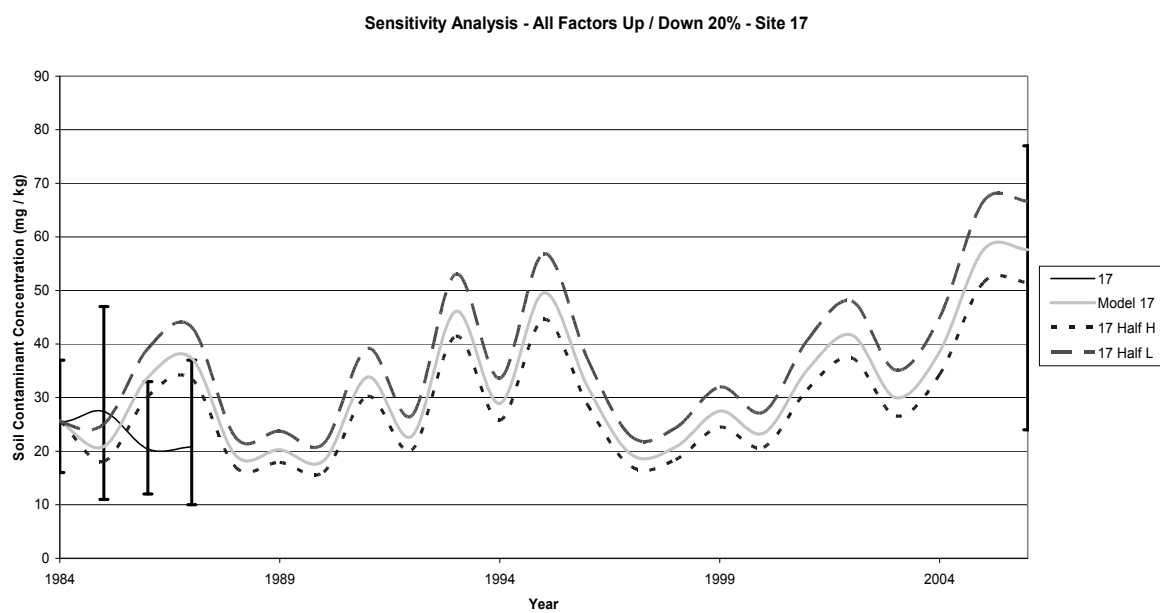


Figure 40: Sensitivity to All Factors Variation - Site 17

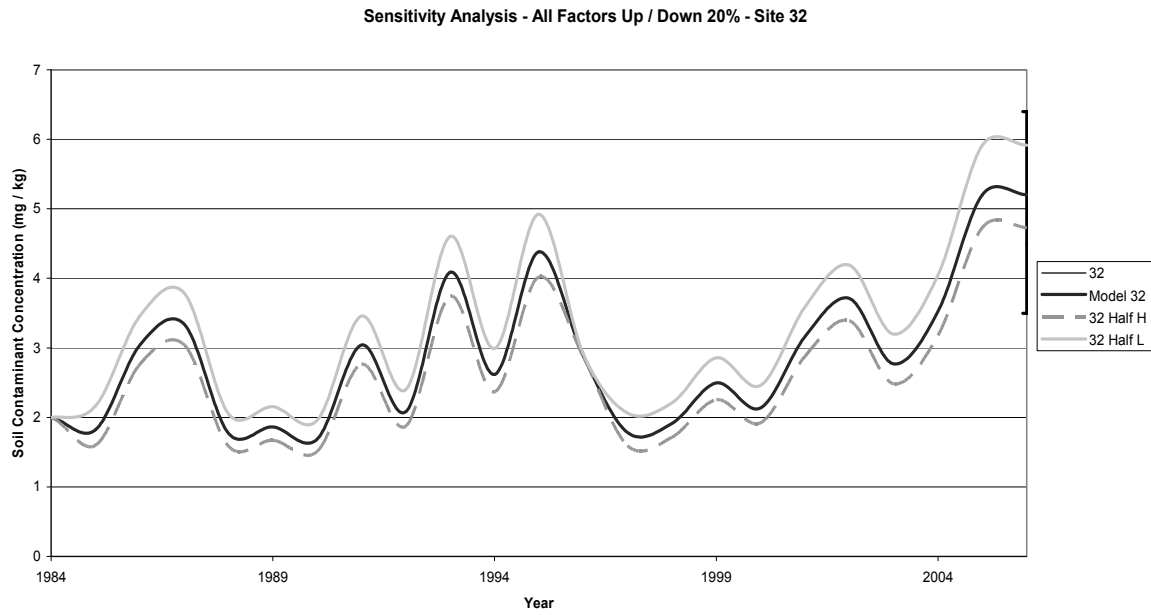


Figure 41: Sensitivity to All Factors Variation - Site 32

“High” and “Low” in the legend, indicate the highest and lowest possible values in the “Extreme Case” scenarios given in Figure 42-Figure 44.

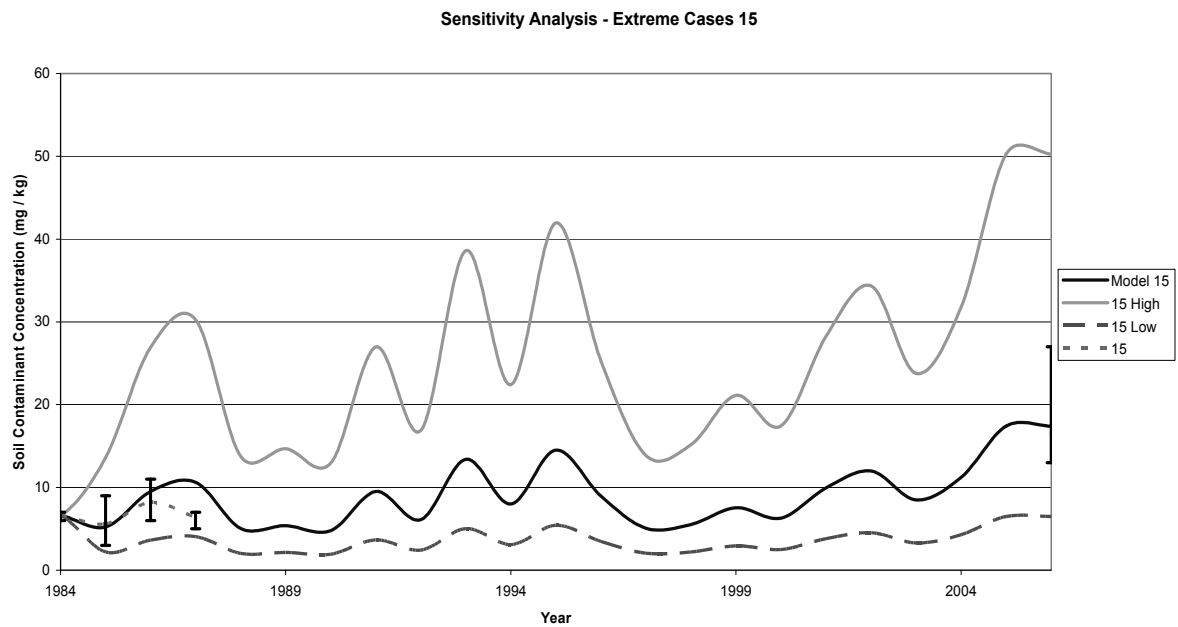


Figure 42: Sensitivity to Extreme Cases - Site 15

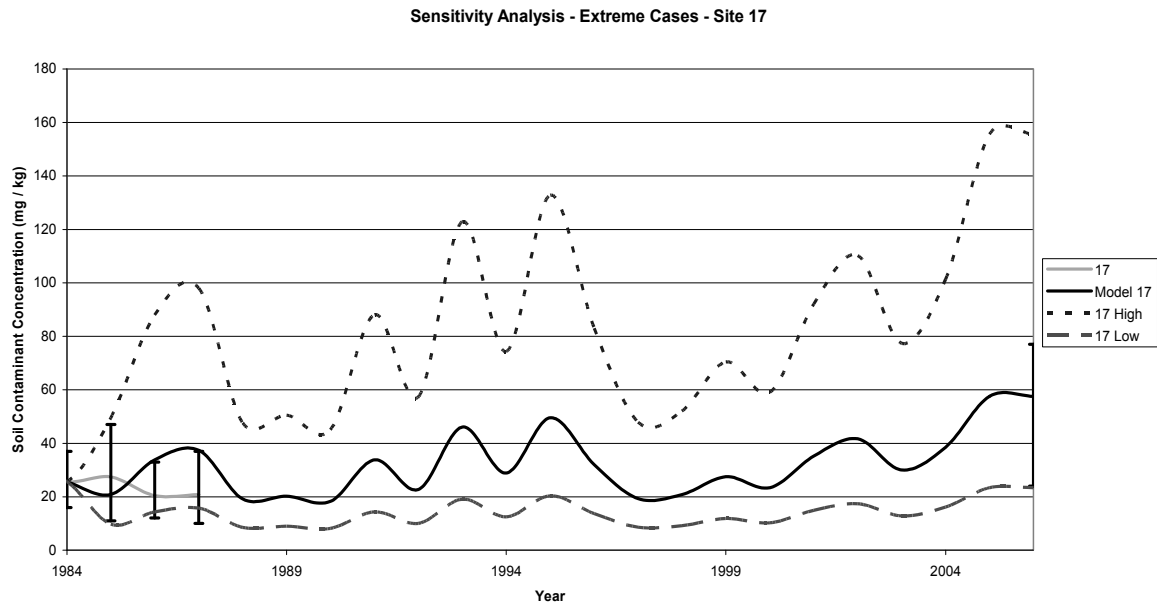


Figure 43: Sensitivity to Extreme Cases - Site 17

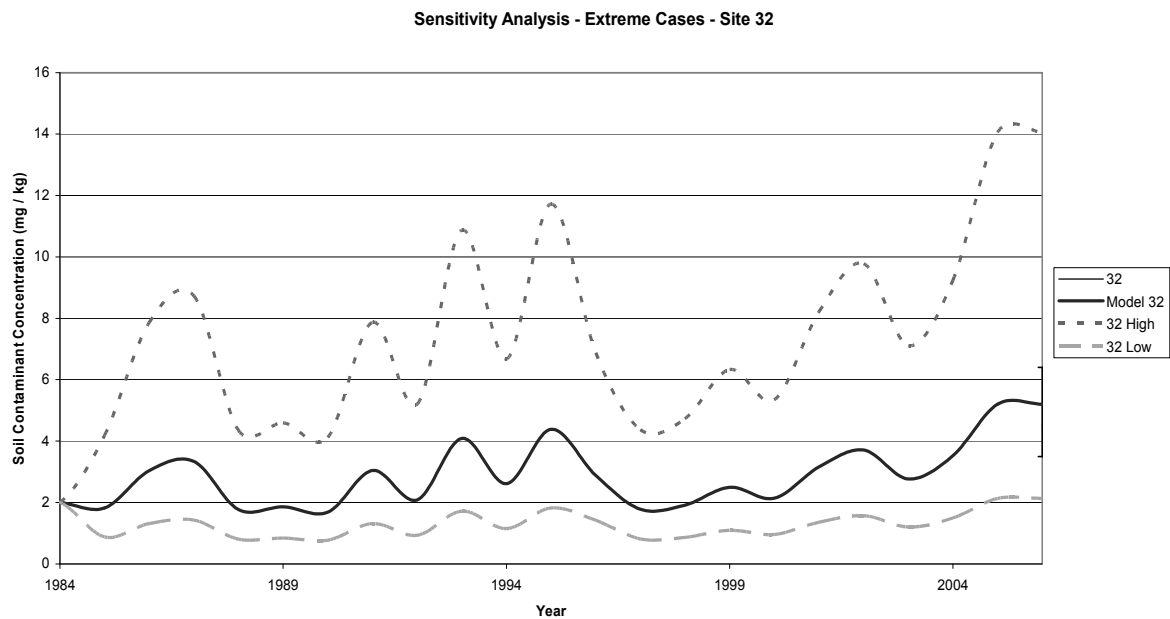


Figure 44: Sensitivity to Extreme Cases - Site 32

The assessment of the behaviour shown in Figure 39-Figure 44 is shown in Table 30, which gives a comparison between the single-parameter variation due to a 20% variation in each parameter and the 4 worst case scenarios. Response of each site to individual parameter variation is given in Appendix 10.

Table 30: Percentage Variation from the Base Model in Response to 20% Parameter Variation

Parameter	Percentage Response to Variation (%)					
	Site 15 (-20%)	Site 17 (-20%)	Site 32 (-20%)	Site 15 (+20%)	Site 17 (+20%)	Site 32 (+20%)
Neutral Rainfall	-20	-20	-20	+20	+20	+20
Process Emissions	-9.36	-6.9	-8.37	+9.36	+6.9	+8.37
Dry Deposition Rate	-14.09	-10.77	-9.45	+13.99	+10.73	+9.43
Yearly Rainfall	+47.32	+41.93	+39.80	-26.59	-24.19	-23.24
Run-off Factor (F)	+17.86	+13.55	+11.84	-11.91	-9.03	-7.89
Permeability Factor (G)	+7.14	+11.45	+12.57	-4.76	-7.63	-8.38
Extreme Cases	+180.0	+157.43	+154.44	-61.06	-57.01	-56.04
All Factors	-9.10	-11.0	-9.33	+13.57	+16.47	+13.98

The cases of most concern from the results in Table 30 are the “Extreme Cases” and “yearly rainfall” variation trials. Varying rainfall by 20% creates a change of greater than 20% in the soil concentration due to the effects of wash-out and run-off. Importantly, in the context of Australia, which is in the grip of a drought, and with the prospect of reduced rainfall in the future due to global warming, a reduction of rainfall by 20% causes greater than 39% increase in soil concentration. This could lead to a substantial increase in topsoil acidification. The “Extreme Cases” indicate that an error or unusual change in every factor in the worst possible direction simultaneously could cause large errors in the model results.

It is apparent from the results in Table 30 that the response of the model to the majority of parameters is non-linear. This is to be expected from the equations utilised, and from understanding of environmental processes, but is particularly significant when we consider the existing methodologies of sustainability. Existing sustainability indicators assume a directly proportional relationship between variation of process emissions and all subsequent environmental impacts. The current model indicates a linear relationship if the process emissions are the only variable (i.e. loading model only), but when other environmental parameters such as run-off rate, permeability and annual rainfall are included, the impacts become highly non-linear.

Thus the local environmental differences are of utmost importance in assessing sustainability.

Appendix 10

Sustainability Metrics Calculations and Global Metrics

A10.1 Greenhouse Gas Metrics

The major apparent globally important impact of fossil fuel processes is the emission of greenhouse gases (GHG). The results of the FCI for each of the scenarios for Greenhouse Gas Emissions is shown in Appendix 2. To compare GHG emissions from a single process to the total global emissions would diminish the value of the metric due to the many orders of magnitude difference. Comparison can be made with the total Australian GHG emissions allowed under the Kyoto Protocol (UNFCCC,2006; DEH, 2006), which may still be a vast difference in orders of magnitude, but could also be useful in the context of a carbon trading scheme.

Table 31: Baseline and Carrying Capacity Options for Greenhouse Gas Emissions

Emissions Limit	Mt CO₂-eq
Australian Kyoto Target (DEH, 2006)	596.1
Australian Current Emissions (2004) (DEH, 2006)	564.7
Queensland Current Emissions (2004) (DEH, 2006)	158.5
Queensland Stationary Power Generation Emissions (2004) (DEH, 2006)	52.2
Australian Stationary Power Generation Emissions (2004) (DEH, 2006)	279.9

The Kyoto target for Australia of increase in 1990 level emissions by 8% is used to determine the Kyoto limits for use as carrying capacities for the Queensland emissions as per Table 32.

Table 32: Carrying Capacity Limits for Greenhouse Gases

	Kyoto Limits	Current Emissions
	Mt CO₂-eq	Mt CO₂-eq
Australian Limits on Emissions Growth	31.4	564.7
QLD Stat. Power Emissions	4.2	52.2
QLD Emissions	12.7	158.5

Sustainability metrics using the equation of the form of Equation 8, the resulting metrics for each of the scenarios is shown in Table 33. The emissions of CH₄ are weighted 21 times that of carbon dioxide as per the standard methodologies.

$$SM = \left[1 - \frac{(CO_2 + 21 \times CH_4)}{CC} \right] \times 100\% \quad [8]$$

Table 33: Results - Sustainability Metrics for Greenhouse Gases

Scenario	Carrying Capacity	Kyoto Limits (Mt CO2-eq)	Current Emissions (Mt CO2-eq)
1	Australian Limits on Emissions Growth	87.90	99.33
	QLD Stat. Power Emissions	9.50	92.72
	QLD Emissions	70.07	97.60
2	Australian Limits on Emissions Growth	83.82	99.10
	QLD Stat. Power Emissions	-20.96	90.27
	QLD Emissions	60.00	96.79
3	Australian Limits on Emissions Growth	81.13	98.95
	QLD Stat. Power Emissions	-41.11	88.65
	QLD Emissions	53.33	96.26

The results of the sustainability metrics assessment using the Australian Kyoto emissions carrying capacity are shown in Figure 45.

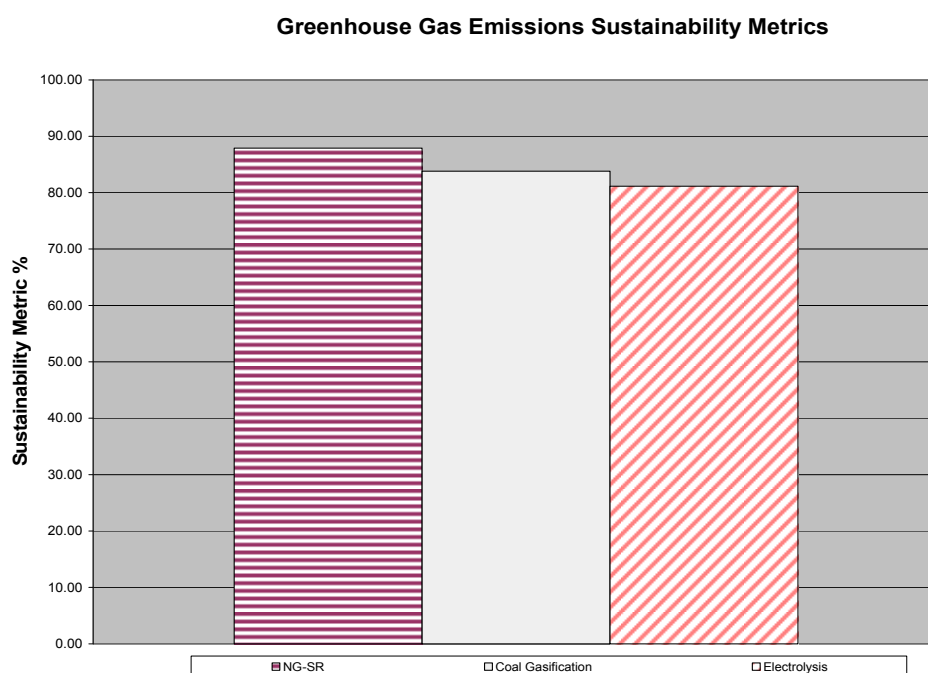


Figure 45: Comparison of Scenarios – Greenhouse Sustainability Metrics – Australian Limits on Growth Carrying Capacity

From Figure 45 it is apparent that Electrolysis option is significantly worse than the NG option, which in turn is slightly less sustainable than the coal gasification option. The fugitive emissions of NG in the extraction and transport stages of the fuel cycle reduce the sustainability of this scenario.

When the higher carrying capacities are utilized, the differentiation between scenarios is less, and the sustainability is higher, but the lower limits are not sustainable at all in some options, so for the sake of comparison the Australian Kyoto limits are utilized here.

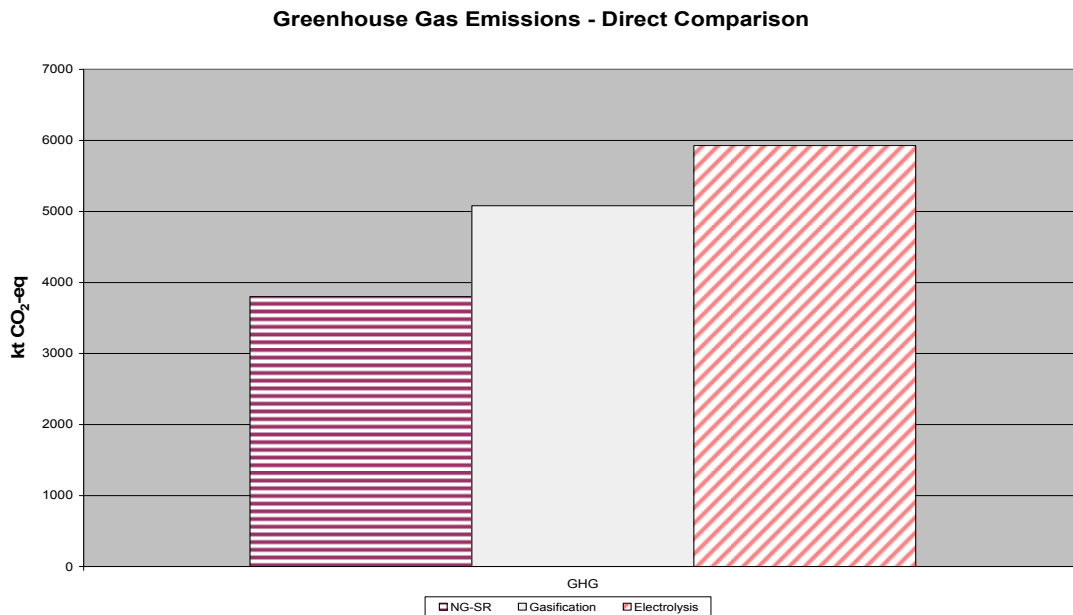


Figure 46: Direct Comparison of GHG Emissions

From the direct comparison in Figure 46, the emissions from the electrolysis scenario is shown to be approximately 2-3 times worse than the other scenarios. This can be converted to a sustainability comparison in Figure 47, where the percentage of sustainability is given by:

$$\%S = \left[1 - \frac{CO_{2-i}}{CO_{2-max}} \right] \times 100\%$$

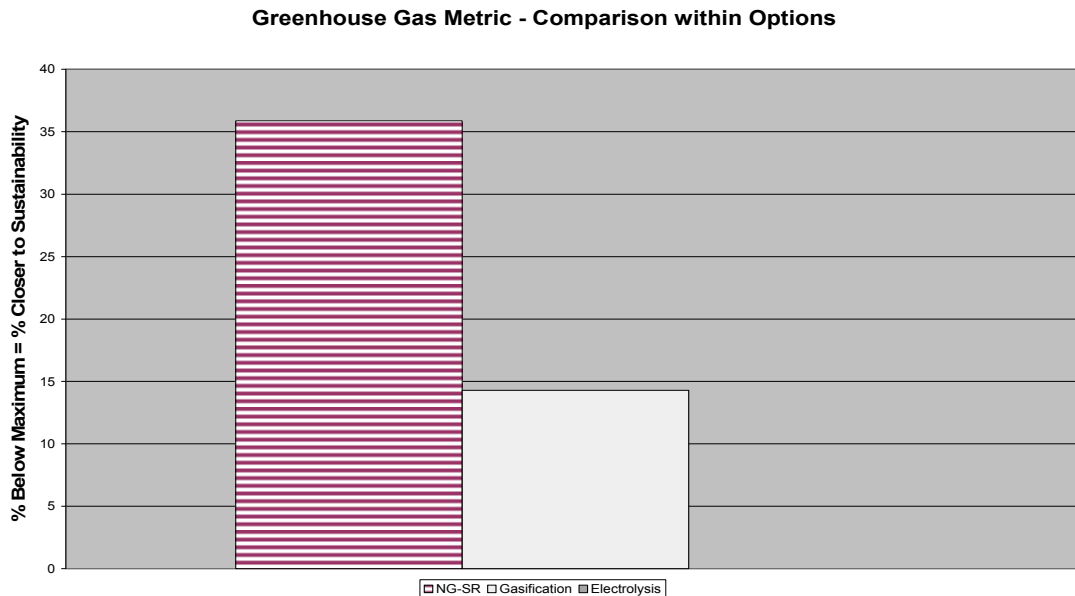


Figure 47: Conventional Sustainability Assessment for Greenhouse Gases - Comparison of Emissions to Maximum

Comparing the conventional methodology with the current methodology, there is no limitation incorporated in the direct comparison, which makes the comparison in terms of sustainability an arbitrary concept, in which any level of emissions can be compared, and the maximum will always be the least sustainable, but lower emissions will diminish in comparison to an increase in the highest emissions scenario. If no limitation is specified as the sustainability limit, then there can be no true sustainability assessment except as an indicator of relative sustainability of a variety of options.

A10.2 Contaminant Increase – Local Impacts – Atmospheric Contaminants

Many of the gaseous and particulate emissions from fossil fuel processes may be detrimental to human and environmental health. Examined here are the small particulate (PM₁₀) and major gaseous pollutants (SO_x and NO_x), which are selected as the major local impact emissions from Hydrogen energy processes. A more detailed process design may indicate emissions of other minor substances, but the National Pollutant Inventory (NPI) emissions workbooks do not cover processes such as gasification and steam reforming, so estimates are not feasible for the current work.

The carrying capacity of the emissions is determined from the local legal (Neale 2005) and international recommended limits (WHO 2005). It may be argued that these limits are artificial, in that the required background studies are not universal in scope, and the environment other than human health is typically not considered in their development, however their use can be justified as a pseudo-carrying capacity where more detailed studies are not feasible or available, as they represent real limits that industry must conform to. Table 34 shows the limits given by the World Health Organisation (WHO) and Queensland Environmental Protection Agency (EPA) which are used in the current work as carrying capacity limits.

Table 34: Annual Average Limits used as Carrying Capacities

Contaminant	WHO Limit (WHO 2005)	EPA Limit (Neale 2005)
NO ₂	40 µg/m ³	0.03ppm (30 µg/m ³)
SO ₂	50 µg/m ³	0.02ppm (60 µg/m ³)
PM ₁₀	-	50 µg/m ³

The limits for PM₁₀ were not available from the WHO. Rather, they refer to population risk factors, due to the complexity of dose-response relationships, and the variety of different potential particle compositions (WHO 2005).

The baseline values of contaminant concentrations from different sites are shown in Table 35. The baselines for Tarong is taken from the Mutdapilly or Toowoomba monitoring data in Neale (2005) as similar remote environmental locations. For SO₂, neither of these sites had available data, so the average remote ambient level was sourced from Gilmour, Mayhew et al. (2001). Brisbane has a number of monitoring sites, but the baseline data here was selected from the Pinkenba or South Brisbane monitoring sites, or an average over all inner-city sites, depending on data availability. Maps of the air quality monitoring sites are shown in Appendix 7.

Table 35: Baseline Annual Average Contaminant Concentrations

	Tarong	Brisbane
NO ₂	0.004ppm (4 µg/m ³)	0.018ppm (18 µg/m ³)
SO ₂	0.001ppm (3 µg/m ³)	0.002ppm (6 µg/m ³)
PM ₁₀	15.2 µg/m ³	19 µg/m ³

A10.3 Resource Depletion – Water Use

Of growing concern in many countries – and especially in Australia – is the efficiency of use of water. In hydrogen energy processes, water is often used in cooling processes, as well the important Steam Reforming (SR), gasification and “Water Gas Shift” (WGS) reactions. The carrying capacity of the recipient environment to provide water can be based on the rainfall within the locality of the process or the total flowrate of water into the source waterbody for the process.

For the rainfall case, the rainfall statistics are summarised in Table 36, with the historical average and the average over the past 5 years, which have been exceptionally dry.

Table 36: Rainfall at the Sites of Interest for Carrying Capacity

Location	Average Annual Rainfall (mm)	Last 5 years (mm)
Roma	596	511
Tarong	766	672
Brisbane	1136	881

Assuming the land area available as a catchment would be 1km radius (similar to the dimensions of the current Tarong power station). Assuming a 50% capture rate of rainfall, the carrying capacity of each site is given in Table 37.

Table 37: Carrying Capacity for Water Usage – 1km Radius Catchment

Location	Carrying Capacity
Roma	935 ML
Tarong	1202 ML

The sustainability of the water resource usage, judged by the area of the catchment available on the plant grounds, is shown to be 0 for each of the scenarios, due to the excessively high use of water. The measure of carrying capacity in this way is reflective of drought conditions in Australia, which have caused severe water restrictions and an increased awareness and competition between water users. Capture and storage of rainfall on the plant premises can secure at least part of the water resource requirements in a manner that is beyond the reach of competition from outside sources.

The concern for long term sustainability is that global climate change may permanently reduce rainfall, causing the sustainability to continue to decrease, as per the last 5 years.

A10.4 Resource Depletion – Hydrogen Source Use

When fossil fuels or other non-renewable resources are used to produce hydrogen, there is naturally depletion of the total available resource. In the particular cases being examined in the current work, coal and NG are the sources of interest. The Australian resources of these substances are very high when compared to global available resources. The carrying capacity can be judged as the total Australian available resource, the total production rate or the total resource in the source mine or gas field. Available data for deriving the carrying capacity is shown in Table 38 and Table 39.

Table 38: Natural Gas Statistics for Carrying Capacity Estimation

	Production (bcm)	Reserves (bcm)	Consumption (bcm)
Roma (SANTOS 2006)	0.0075	-	-
Queensland (NRW 2006)	5.205	-	-
Australia (ABARE 2006)	37.1	2520	25.7

Table 39: Coal Statistics for Carrying Capacity Estimation

	Production (Mt)	Reserves (Mt)	Consumption (Mt)
Tarong (Rio-Tinto 2006)	6.7	86.4	6.7
Queensland (NRW 2006)	172.7	32,729	28.4
Australia (ABARE 2006)	300.7	78,500	73.7

Many authors (e.g. ABARE (2002), BP (2002)) use a Reserves-to-Production ratio (R/P) to determine the number of years of available resources. However, this method can be adapted slightly to give a sustainability metric in the form of Equation 9, where P is the production rate per year, and the reserves are reduced by current pre-plant resource production rates each year, so that the carrying capacity varies over time as per Figure 48. Where the resource usage exceeds the available resource, the sustainability is assumed to be 0 rather than negative, as unsustainability can be said to be a quality that does not require measurement.

$$SM = \left[1 - \left(\frac{P \times t}{R} \right) \right] \times 100\% \quad [9]$$

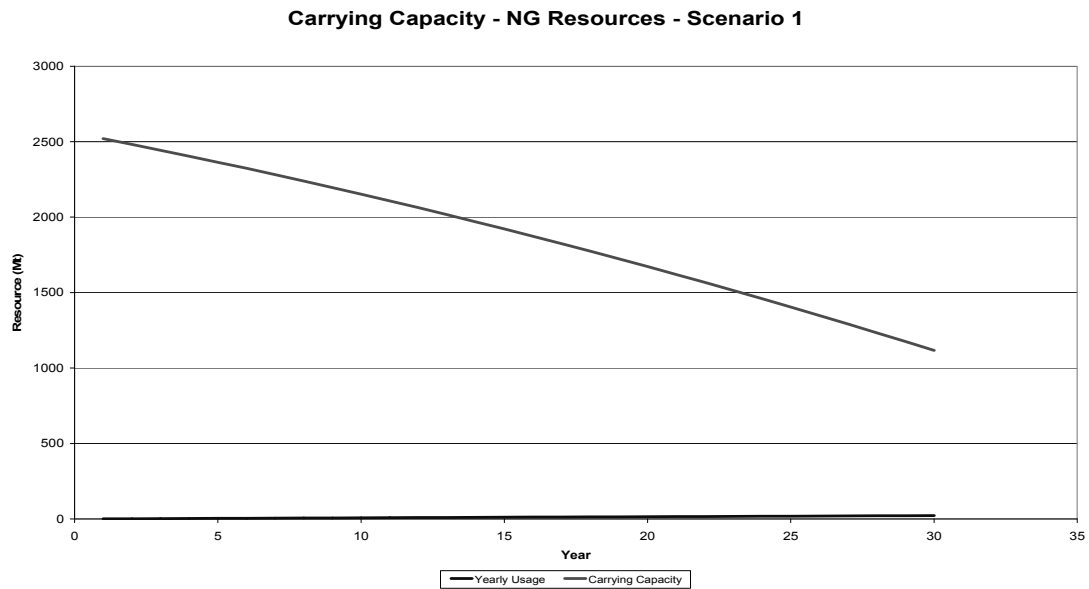


Figure 48: Variable Carrying Capacity in Resource Depletion

Applying the standard fossil fuel statistical metrics to the standard scenarios gives the results in Table 40.

Table 40: Results of Sustainability Assessment with Fossil Fuel Statistic Carrying Capacity

Scenario		Metrics based on Ratio to Current:			Metrics as per Equation 9
		Production	Reserves	Consumption	
1	Roma	(0) -9919			
	QLD	85.56			
	Australia	97.97	99.11	97.08	99.36
2	Tarong	67.00	23.23	67.00	0
	QLD	98.72	99.80	92.21	99.89
	Australia	99.26	99.92	97.00	99.95
3	Tarong	33.43	-54.86	33.43	0
	QLD	97.42	99.59	84.30	99.77
	Australia	98.52	99.83	93.95	99.91

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