RISK-BASED AND SITE-SPECIFIC INDUSTRIAL USE WATER QUALITY GUIDELINES
DEVELOPMENT OF A RISK-BASED APPROACH

P Moodley, C Pardesi, Y Vemblanathan, P Wille, G Singh, N Juggath, L Boyd and T Coleman

Volume 1: Decision Support System

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RISK-BASED AND SITE-SPECIFIC INDUSTRIAL USE WATER QUALITY GUIDELINES

Development of a Risk-based Approach

Volume 1: Decision Support System

A Report to the
Water Research Commission

by

P Moodley, C Pardesi, Y Vemblanathan, P Wille, G Singh, N Juggath, L Boyd and T Coleman

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EXECUTIVE SUMMARY

The current series of South African Water Quality Guidelines (SAWQGs) (DWAF, 1996) has been an extremely important contribution to water resource management in South Africa. It reflects the scientific thinking at the time it was produced. Subsequently, the decision support function of water quality guidance has grown and become more complex. With the evolvement of water resource management within South Africa, the SAWQGs have become decision support tools rather than a list with numbers. Both application and scope issues related to risk, site specificity and guidance on an expanded set of water quality constituents have become more apparent.

The need for a quantifiable assessment system to judge fitness for use and suitability of water quality that moves beyond simple numeric values has been identified. Such a system must provide an assessment in terms of the nature of the resource and the nature of the water user.

In 2008, a national review by then Department of Water Affairs and Forestry (DWAF) on the 1996 SAWQGs recognised the need for the development of South African risk-based Water Quality Guidelines. The following three phased approach has been undertaken:

Phase 1: Development of philosophy

Phase 2: Application of philosophy and development of prototype guidelines

Phase 3: Development of tools for higher-tier site-specific guidelines

Phase 1 was completed culminating in the compilation of a Needs Assessment and Philosophy document (DWS, 2008).

In light of the review and recommendations of the Phase 1 outcomes, the Water Research Commission (WRC) initiated an overarching project to address Phase 2. A series of projects to develop risk-based approaches for water quality guidelines per user group was commissioned.

This project is part of the Phase 2 series of projects and addresses the approach development for *Volume 3 – Industrial Water Use* as part of the South African Water Quality Guidelines series. It attempts to present new approaches that will expand the scope of water quality guidelines in terms of how they are presented, applied and decision support that is provided to the user.

The risk-based water quality guidelines need to be applied in a manner that support site specificity and be based on a risked philosophy, whilst providing for a tiered assessment approach presented as a software-based decision support tool. The proposed revision to the current guidelines lies in that the fitness for use assessment now relates to risk, which combines hazard and exposure, rather than the hazard predominantly, as applied in the 1996 guidelines. "Risk-based" guidelines simply allow the suitability of the water quality to be interpreted in terms of risk of specific adverse effects.

The new goal may thus be stated as ‘to adequately describe the outcome of a water use quality under a specific context in a manner which enables a more realistic decision to be reached regarding either accepting some degree of adverse outcomes or reducing the risk factors identified, to an acceptable level’.

OBJECTIVE AND AIMS OF THE PROJECT

The objective of this project was to develop a risk-based philosophy and site-specific methodology for assessing water quality requirements and fitness for use of water for industrial use. The specific aspects addressed include firstly the development of the basis of the risk approach and quantification methodology for the risk assessment; and secondly the development of the informatics for a technology demonstrator decision support system that addresses the main decision contexts for industrial water use.

SCOPE OF THE PROJECT

The project required that the revised water quality guidelines be risk based, support site specificity and be presented as a software decision support tool as aligned to the philosophy as defined in the Phase 1 document of 2008.

For purposes of the risk-based guideline development, the scope of this project has focused on the input (source) water into an industrial process (irrespective of the source), as the intention of the South African Water Quality Guideline Series (Volumes 1 to 7) is to support users make informed judgements about fitness for use and for other water quality management purposes. Due to the variation, differentiation and diversity in the sector types, the current approach has not focused on individual industries per se. It focuses on well-defined problems occurring in industry, *viz*. scaling, corrosion, fouling identified through stakeholder engagement; and considers the process applications in the larger manufacturing and processing industrial sectors in South Africa. By defining the context of the situation/site and the processing/manufacturing units a risk approach for assessing fitness for use and specifying water quality requirements has been developed.

While it is accepted that most industries use bulk water supplies as their source water or treat water to their requirements, there are some that rely on water extracted directly from the water resource. The tool however supports either type of user to assess fitness for use, irrespective of the water source. The tool easily lends itself to expansion in future to consider fitness for purpose in re-use applications.

GENERAL APPROACH

The determination of the risk and associated factors require that they are measurable to an extent and exhibit characteristics or outcomes that can be adequately described for the industrial use. At this point the limitation is related largely to the availability of this science and empirical data to support the risk based calculations related to industrial water quality use problems.

Unlike the other user water quality guidelines, for industrial use, no prior work or research has been undertaken since the 1996 edition. Thus the 1996, Volume 3 Industrial User Water Quality Guidelines remained the departure point for this undertaking, and which has required as the basis, the definition of risk approach fundamentals.

Fundamental to the basis of the guidelines is what constitutes risk to the industrial water use(r).

The core of the proposed approach requires accounting for the end point adverse effects (key water quality problems) posed by the water quality constituents and the manner and extent to which they express themselves, and further within site-specific scenarios of the water use. Water quality problems in industrial use and the constituents that cause them are largely known and well documented in literature.

The fitness for use assessment thus still forms the core technical requirement of the guidelines. The focus of this endeavour has therefore been to formulate a mathematical approach (modelling) to the fitness for use analysis as the basis for derivation of the risk-based guidelines. The ability of the user to provide some input to the risk assessment process and contextualising the scenario, supports the presentation of the guidelines as a software product rather than a static document.

For the industrial user the risk-based guidelines serve the purposes,

- in a generic context evaluating the fitness for use of the source water, and
- in a specific context as a screening tool to guide and support decision-making regarding industrial water related problems (e.g. scaling, corrosion, fouling, foaming, abrasion).

While the generic guidance of the DSS addresses fitness for use objectives of source water in industrial uses irrespective of whether it is treated or devoid of treatment (similar to the 1996 guidelines), the site-specific guidance defined by the risk factors associated with the industrial process (the processing application) and input water quality concentrations form the basis of risk based guidance. Based on the understanding of the chemistry and science associated with the commonly and most recurrent water quality end point adverse effects (e.g. scaling, corrosion), the probability of occurrence and extent of effect can be calculated for the industrial process in question. This is then reported as the water quality risk in the DSS tool.

The materials of construction of the processing units and the key water quality problems, *viz*. corrosion, and scaling were selected as the end points of the risk assessment quantification for the purposes of the methodology development to define the concept approach.

It is well accepted that water quality problems within an industrial process or operation can often be addressed through some form of engineered solution. Thus it is the intention that the decision support tool to also serve as a platform for industrial water users to account for potential water quality risks that could manifest and contribute towards improved and informed decision making regarding the timing, implementation and design options of the engineered solution or operational interventions.

The risk based guidance may also account for waters incorporated into processes as part of water use efficiency or re-use measures by varying the source water as the input variable in the risk assessment to the use scenario.

In defining a proposed risk-based approach for industrial water use, it has become apparent that greater site-specificity, particularly in respect of the nature of the characteristics of the material exposed to/contacting the water, and measured quality, make the risk-based water quality guidelines much more relevant and meaningful in terms of the guidance.

OVERVIEW OF THE DECISION SUPPORT SYSTEM (DSS)

The final product of the risk based approach was that the envisaged DSS should comprise a three-tiered system:

- Tier 1 is equivalent to 1996 generic guidelines;
- Tier 2 allows for site-specificity in generic specified contexts;
- Tier 3 allows for site-specificity in localised contexts, allowing the user to adjust the reference data in the coding modules. This would require significant expertise.

The DSS presents a functional tool for user application that can be extended as data becomes available. A user-friendly interface is presented providing water quality guidance outputs. The risk-based water quality guidelines are reported as water quality requirements or as a fitness for use assessment both of which incorporating the analysis of the risk and the mitigation guidance thereof. A simplified schematic representation of the industrial water use DSS structure is shown in Figure E1.

The Development Platform

The project design specification required the adoption of open-source software for the Decision Support System (DSS). Python was selected to develop the DSS since it is an open-source, cross-platform programming language well-suited for developing desktop applications. It has a valuable collection of frameworks, such as PyQt5, a graphical interface designer for quickly creating sophisticated graphical user interfaces. The database is built on the JSON framework, an open-source document database that operates on Linux, Windows, and several Unix platforms.

The software has been identified as being a robust calculation and graphic programming tool. The graphical interface is user friendly and provides results that can be exported to an Adobe PDF. The application introduces custom dialog boxes, dropdown list boxes and message boxes that prompt user errors or instructions.

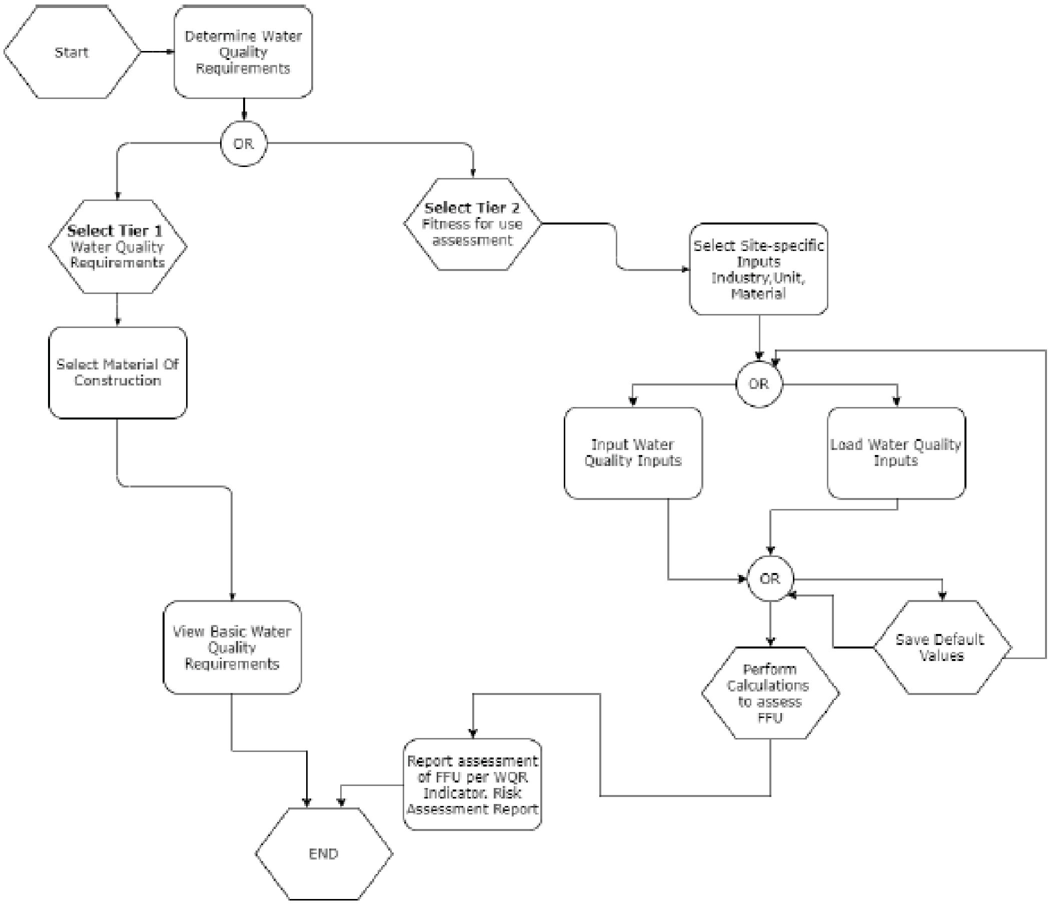

Figure E1: Architectural overview of the DSS Application

Reporting in the Decision Support System

The risk-based water quality guidelines are reported at two levels, as follows:

- ***Water Quality Requirements***: a report of all threshold criteria and associated fitness for use levels for associated water quality adverse effect, for the specific industrial process unit material selected (ideal OR acceptable OR tolerable OR unacceptable). This would guide the user on the requirements of the quality of water needed for the intended industrial water use scenario.

- ***Fitness for Use***: the fitness for use category of the input water quality composition presenting the acceptability and implied risk (ideal OR acceptable OR tolerable OR unacceptable) together with the likelihood and description of the associated adverse effects and proposed mitigation measure.

The water quality guidance reporting in the DSS is categorised visually in a colour-coded manner that the user is able to immediately assess suitability and the potential risk posed. The reporting system includes a four-category system which has been based on the classification system adopted by the DWS to categorise fitness for use ranges. In order to ensure that all the risk-based guidelines of the different South Africa Water Quality Guideline Freshwater Series Water User groups are consistent and aligned, this system has been applied. The four-category reporting system is in harmony with a risk-based assessment of water quality in that the 'Ideal' category represents a no risk scenario (safe level), while the 'Unacceptable' category represents a high-risk scenario (most likely occurrence/ significant consequence of the adverse effect).

The generic categorization is shown below.

A generic description of the fitness for use categories used for reporting

Reported Category	Description
Ideal	A water quality fit for a lifetime of use.
Acceptable	A water quality that would exhibit minimal impairment to the fitness of the water for its intended use. Minor risk of adverse effects.
Tolerable	A water quality that would exhibit some impairment to the fitness of the water for its intended use. Moderate risk of adverse effects presenting themselves.
Unacceptable	A water quality that would exhibit unacceptable impairment to the fitness of the water for its intended use. Significant risk of adverse effects, presenting themselves.

Modelling Aspects

The DSS tool has been designed at three levels specified to cater for a range of target audiences (novice, intermediate and expert user) based on the availability of the measured water quality data and site-specific detail. Transition between Tiers 1 and Tier 2 is the primary focus of the tool, with Tier 3 representing a higher degree of user defined input and updates to the risk methodology. The transition to Tier 2 and 3 aligns with the objective of determining an acceptable risk level as new data captured, for example, specific material of construction detail, chemistry or exposure conditions, could lead to a significant change in the risk posed under the specific site-conditions applicable.

These tiers are flexible with increasing variations of site-specific detail use as the user moves from one Tier to the next, with a general migration from reference documentation used in the calculations performed, to user-defined site-specific input.

The DSS has been designed to present:

- Generic risk-based water quality requirements for industrial related water quality problems; and
- Site-specific assessment of the fitness for use of input water quality and the operational conditions.

The tool is designed to cater for the exposure scenarios of the particular industrial water use situation. By assessing the specific aspects built into the modelling approach of the tool *viz.* processing unit and material of construction, water quality data inputs of the sample composition and exposure conditions, a potential risk is calculated. At this point the risk-based guidance has focused on predicting the likelihood of occurrence of corrosion, scaling and fouling as the major water quality problems (adverse effects) of relevance to industrial water use.

Fitness for use of the water quality is determined by selecting the material of construction of the mechanical/civil infrastructure of the industrial process in question, which is then assessed on the basis of the input water quality composition that is entered. Using the built-in reference data and the calculation algorithms coded in the DSS for corrosion, scaling and fouling, the probability of risk of the water quality problem is presented based on the assessment of the interaction of the water quality relative to the material of construction. This predictive quantitative output is presented as indices or ranges linked to the scientific literature based reference data. The tool reports on the significance of the adverse effect and if it is feasible to take remedial/mitigation action or not. The results are output as a PDF report which incorporates mitigation measures in instances where a risk has been noted.

The components and data flow relating to the modelling aspects in the DSS tool, at the 3 tiers is provided below.

Tier 3

Tier 3 calculations cater for the site-specific scenarios, exposure conditions and detailed assessments not covered by Tier 2 and is targeted at an expert user. This tier allows for more site specificity in other *ad-hoc* contexts. In addition to the hazard-based assessment of water quality composition entered and material of construction, the user will apply additional protocols to assess detail site data such as water pressure, density, material thickness, etc. The Tier 3 functionality is still to be developed further with the protocols and modules to be applied.

Tier 2

Tier 2 is seen as the more widely used applicability and functionality of the DSS tool. Tier 2 allows for site-specificity by selection of default-based site-specific factors provided for in the DSS and for the input of water quality composition of source. The exposure scenario is defined by the material of construction and exposure conditions.

The calculations are run in the model to generate the fitness for use report of quantitative outputs (calculated indices and ranges for scaling, fouling and corrosion related to the water quality hazards of relevance). This allows the user to assess if the risk is an acceptable one in the specific context or to reduce the risk factors identified to an acceptable level.

Tier 1

Tier 1 requires very little input from the user and presents the water quality requirements for industrial water use with an account of associated risk to the material construction of the processing/manufacturing infrastructure in reference to the water quality problem of concern. It can be considered somewhat equivalent to 1996 generic guidelines. Tier 1 assessment does not involve any calculation methodology and contains specific literature-based information about water quality constituents of relevance to hazard characterisation and potential adverse effects. Ranges of threshold limits are presented in terms of the four-level categorisation from an ideal water quality (safe level) to an unacceptable level (highest risk level). Tier 1 however does allow for an input to be made by the user to indicate the material of construction of the processing/manufacturing infrastructure if this is known.

CONCLUSION

As the intention of the Industrial Water Use Water Quality Guidelines (Volume 3) is focused on the assessing risk associated with the use of ‘freshwater’ sources, as with the rest of the South African water quality guideline series, the scope of the DSS tool functionality has been defined to meet that purpose. The fitness for use assessment still forms the core technical requirement of the guidelines. However, in the design of the tool any input water quality composition (treated, not treated, from any source) maybe assessed to determine fitness for purpose relative to the industrial infrastructure. The ability for a user to input a user-defined water quality composition and site-specific detail to derive a computated risk output is a paradigm shift in how water quality guidelines are presented, for South Africa and internationally as well. The DSS improves the accuracy with which water quality adverse effects are predicted and assessed. This adds significant value in terms of applicability and relevance of the revised water quality guidelines.

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LIST OF ABBREVIATIONS

Al	Aluminium
C	Carbon
Ca	Calcium
$CaCO_3$	Calcium Carbonate
Cl	Chloride
COD	Chemical Oxygen Demand
Cr	Chromium
CSMR	Chloride to Sulphate Mass Ratio
Cu	Copper
DSS	Decision Support System
DWA	Department of Water Affairs
DWAF	Department of Water Affairs and Forestry
DWS	Department of Water and Sanitation
EC	Electrical Conductivity
HI	Hazard Index
HP	High Pressure
LP	Low Pressure
LSI	Langelier Saturation Index
Mg	Magnesium
Mn	Manganese
Mo	Molybdenum
MOC	Materials of Construction
Na	Sodium
Ni	Nickel
NWA	National Water Act
Pb	Lead
PGM	Platinum and other Platinum group metals
PO_4	Phosphate
PREN	Pitting Resistance Equivalent
PTFE	Polytetrafluoroethylene
PVC	Poly-Vinyl Chloride

PVFD	Polyvinylidene Fluoride
RO	Reverse Osmosis
SAWQG	South African Water Quality Guidelines
SDI	Silt Density Index
Si	Silica
SO_4	Sulphate
TDS	Total Dissolved Salts
Ti	Titanium
TSS	Total Suspended Solids
TWQR	Target Water Quality Range
UDC	Under Deposit Corrosion
WRC	Water Research Commission

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1.0 INTRODUCTION

1.1 Background

The Department of Water and Sanitation's (DWS) South African Water Quality Guidelines (SAWQGs) for Fresh Water (Second Edition) published in 1996 have been an extremely important contribution to water resource management in South Africa. The guidelines reflected the scientific thinking at the time and are still widely used.

Subsequently, the decision support function of water quality guidance has grown and become more complex. Increased scientific understanding of the complexity of water resource systems and adaptive management processes have led to new ways of managing water quality, where water quality is defined as physical, chemical and microbiological properties of the water. Since the evolvement of water resource management within South Africa, the SAWQGs have become decision support tools rather than just a list with limits, and traditional scientific and management approaches may not be adequate to deal with contemporary water quality issues. In parallel water treatment technologies have been optimised and new technology developments continue to enter the market.

Both application and scope issues made it necessary to re-examine the philosophical basis used for determining and applying water quality guidelines, which included the concept of risk as a potential common basis for decision making in various contexts, site specificity and advancements in guideline determination internationally, amongst other legal requirements under the National Water Act (Act No. 36 of 1998) (NWA).

The need for a quantifiable assessment system to judge fitness for use and suitability of water quality that moves beyond simple numeric values, that provides an assessment in terms of the nature of the resource and the nature of the water user, was identified by the DWS in 2008, through a project commissioned to critically investigate the need for a review of these guidelines, and the principles that govern them.

The outcomes of the Phase 1 investigation highlighted the necessity to extend the application of the 1996 version of the South African water quality guidelines. The project concluded that the new envisaged guidelines would be different in the following ways:

- They would be risked-based,
- They would allow for greater site specificity, and
- They would be made available primarily as a software decision tool to support decision making.

A key fundamental change in philosophy from the 1996 guideline series has been the concept of "acceptable risk" that now needs to be adopted by the user audience of the risk-based guidelines, from water resource managers to the water users, in order to allow for informed decisions to be made concerning water use. This is a paradigm shift in thinking and arguably the most important concept to adopt, as it represents a significant departure from the previous versions of the South African Water

Quality Guidelines (DWAF, 1996) in which a “desired state” of a Target Water Quality Range was the goal and generally construed to imply a “no adverse effect” state.

The new goal may thus be stated as to adequately describe the outcome of a water use under a specific context in a manner which enables a more realistic decision to be reached regarding either accepting some degree of adverse outcome or reducing the risk factors identified to an acceptable level. The decision support provided by the guidelines would need to relate to the assessment of fitness for use and water quality requirements in, primarily, freshwater resources

In light of the recommendations of the Phase 1 outcomes, the Water Research Commission (WRC) initiated an overarching project that has seen the commissioning of a series of projects to develop risk-based approaches and decision support tools for water quality guidelines per user group, encompassing Phase 2 of the process.

This project addresses the Volume 3-Industrial Water User Guidelines as part of the 1996 SAWQGs series. It attempts to present new approaches that will expand the scope of water quality guidelines in terms of how they are presented and applied, including decision support that is provided to the user.

1.2 Project Objective

The objective of this project was to develop a risk-based philosophy and site-specific methodology for assessing water quality requirements and fitness for use of water for industrial use. The specific aspects addressed included the development of the basis of the risk approach and quantification methodology for the risk assessment; and secondly the development of the informatics for a technology demonstrator decision support system that addresses the main decision contexts for industrial water use.

The intention with the risk-based guidelines is that the final product provides a series of tiered assessment levels that supports a greater diversity of guideline use and facilitates the decision making (DWAF, 2008). A three-tiered set of guidelines is to be defined. The Tier 1 and Tier 2 facility must be as easy to use as possible. Each tier provides an output that has to comply with the concept of categorisation. The difference between the tiers lies primarily in the degree of site-specificity required to produce an output. All tiers must be categorised in terms of risk objectives (categories).

The methodology for this project has been designed to achieve the general aim of developing a software-based tool able to provide both generic and site-specific risk-based water quality guidance for industrial water use scenarios. The current undertaking must also achieve the maximum possible synergy and compatibility with the approaches related to the revision of the other use volumes of the 1996 South African Water Quality Guidelines Series (*viz*. Recreation, Irrigation, Domestic, Aquaculture, Livestock and Aquatic Ecosystems) recently completed or which are currently underway.

Ultimately, once the all the user group DSS tools are developed to full scale application, an online database would be adopted for the programming software. This is a requirement for the DSS tools of all the respective user groups of the South African Water Quality Guidelines series which would eventually be accessible via an integrated online platform.

1.3 Risk-based Product

The proposed revision to the current guidelines lies in that the fitness for use assessment now relates to risk, which combines hazard and exposure, rather than the hazard predominantly, as applied in the 1996 guidelines. "Risk-based" guidelines simply allow the suitability of the water to be interpreted in terms of risk of specific adverse effects. The guidelines are intended to differ in a fundamental way from the existing 1996 guidelines by adopting a risk and site-specific approach that accounts for exposure conditions although still being concentration-based. In addition, the structure of the guidelines is to include a tiered assessment level system that is presented and operated through a software decision support system (DSS). Guidelines reflect the scientific environment.

Risk is a statistical concept defined as the expected likelihood or probability of undesirable effects resulting from a specified exposure to a known or potential environmental concentrations of a material or contaminant. A material/contaminant is considered safe if the risks associated with its exposure are judged to be acceptable (EPA Victoria, 2004).

A risk is posed when there is a source, an exposure pathway and a receptor (receiving environment, the so-called "population at risk"). It is important to note that risk is not a concentration, dose, other value-based point, or even non-value-based levels. Risk is the probability that a particular adverse effect occurs during a stated period of time (DWAF, 2005). Risk-based can therefore be defined as recognising the risk factors in giving effect to risk objectives.

In the course of deriving the guidelines risk refers to the probability of specific adverse or undesired effects to the industrial process application using water containing a potential hazard, including the severity of the consequences.

Hazard in this context refers to a range of water quality constituents and physical properties that may be present in the water that renders it less fit for use, and its consequences is based on how the water is used or how it is contacted. Thus, risk is a function of hazard and exposure, where,

- *hazard* = biological, chemical or physical agent that has the potential to cause harm to a receptor ,
- *hazard effect* = adverse impact on process/equipment/output that can result from exposure to the contaminant/ substance/property, and
- *exposure* = contact between a substance/contaminant and a "population" (industrial water use process/unit/material/product).

The threat caused by a hazard depends not only on the severity of its effect but also on whether or not the effect is reversible (Leiss and Chociolko, 1994) or in the case of industrial water use, whether it is recoverable. Description of the risk therefore requires an assessment that provides answers to the following three questions:

- What can happen (the scenario and effect) (dependent on the way/circumstances the water is experienced);
- How likely is this to happen (probability); and
- If it does happen, what are the consequences (effects of the hazard, in this case to the industrial use, process and product).

In the development of the risk-based water quality guidelines, the adoption of the risk approach is that it can provide a common philosophical basis for decision-making in different contexts. This risk approach generalises the basis for decision-making by incorporating as much of the relevant situational evidence as possible. It is generally accepted that a risk-based approach can assist with decision-making and is a useful management tool. It is particularly useful in that it helps to set priorities on a comparative basis and can assist in allocating expenditure of capital and resources.

The ability of the user to provide some input to the risk assessment process and contextualising the scenario, supports the proposal of presenting the guidelines as a software product rather than a static document.

Acceptable Risk

Risk is generally taken to be the probability of adverse effect, injury, disease, or death under specific circumstances. Acceptable risk decisions are rarely easy. The subject of what constitutes an acceptable risk is an extremely complex issue. In determining acceptability, it is however largely the perceived risk that determines the basis of what can be tolerated. Acceptable risk is highly location and scenario specific. For this reason, it plays an important role in adapting guidelines to suit local circumstances, where the user situation and available data is vital. In the context of industrial water use, and in the development of the risk based approach, the concept of acceptable risk is seen to relate to the likelihood of specific adverse/undesired effects manifesting within the industrial processing units based on an input water quality (treated or untreated or re-used), and based on a calculation methodology that accounts for site-specific factors to enable a more realistic decision to be reached regarding either accepting some degree of adverse outcomes or reducing the risk factors identified to an acceptable level. In industrial water use processes the risks versus benefits while primarily assessed on the basis of costs (capex and opex), other considerations such as optimal operation, product quality and aesthetics are also important.

Site specificity

While not explicitly related to the concept of risk, a significant deficiency of the 1996 water quality guidelines is that they are generic and uniformly applied. Fitness for use water is dependent on its composition in relation to its intended use. This therefore implies that site specificity is necessary so that decision making on water fitness for use can be assessed accurately based on its character and context of the intended use. A further specification of the guidelines is that assessment should ensure that the experience of different users is the same, wherever they may be.

The risk-based guidelines aims to this by allowing the fitness for use assessments to be done for more specific scenarios. If the water quality guidance has been derived from an unrealistic base, then it could well mean that significant socio-economic impact will be attributable to scientifically tenuous factors, which in turn, could have an impact on the water user operations. These considerations place a responsibility on the scientific integrity of the data and processes used in deriving the water quality assessment guidance (S Jooste, 2015, unpublished).

The inclusion of this functionality into the decision support system will overcome the shortcoming of the generic nature of the 1996 guidelines, will expand its use to support the industrial user to a greater degree as well as facilitate more informed decision making related to water resource use and management (DWAF, 2008).

While site location is a major factor, the new guidelines would need to handle different scenarios or contexts at the same site. The site-/ scenario specificity of the new guidelines will relate primarily to the nature of the source water and the nature of the industrial use context (sector/sub-sector/processes).

1.4 Volume 3: Industrial Use Guideline

Water quality guideline development for Industrial water use in South Africa having received little attention over the recent decade has been limited. The Phase 1 Philosophy and Needs Assessment report (DWAF, 2008) of the project also did not address industrial use as a user to any extent. The 1996, Volume 3: Industrial Use Water Quality Guidelines thus was the departure point for this undertaking, and therefore required the definition of approach fundamentals, a risk concept for industrial water use and the basis of a proposed approach, prior to the development of the decision support methodology.

The 1996 guidelines, published as Volume 3 (DWAF, 1996) were an improvement on the previous 1993 edition which did not account for the inherent differences between industries and included only a limited number of industry types. The second edition of 1996 saw the revision of the approach to focus on the description of general and specific industrial processes, and by doing so water quality guidelines could be specified for any industry based on the building block approach. By assigning industrial processes to categories, water related problems and related constituents could be identified. Based on an understanding of fitness for use water quality guidelines were then developed.

In the DWAF 1996 Industrial Use water quality guidelines, industries have been defined as systems of water-using processes, in which fitness for use of water is defined by the following norms which are used as yardsticks for defining the basis of the effects of water quality constituents (Table 1):

- impacts on equipment and structures

- interference with processes
- product quality and
- complexity of waste handling.

Table 1: Norms and corresponding water quality effect applicable

Norm	Effect
Damage equipment and structures	Corrosion Abrasion Scaling Blockages Resin films Fouling Resin poison Embrittlement Discolouration
Interference with processes	Precipitates Colour changes Foaming Sediments Gas production Contamination Interference Resin impairment Odours HE impairment
Product quality	Taste Discolouration Inadequate treatment Foam Sediment Tarnish Odour Turbidity Coagulation Blemishes Contamination Health hazards
Complexity of waste handling	pH Salts Suspended Solids Iron/Manganese Chemical Oxygen Demand

The risk to the industrial water user in the 1996 guidelines was accounted for in terms of process categories to account for water 'purity' required:

- process type (4 categories defined based on degree of purity of water required or stringency);
- water use such as evaporative cooling, solvent and utility, and
- long term and short term effects.

Process types include cooling, steam production, process water (solvent, diluent, carrier), product water (as in beverages), utilities (domestic, fire protection) and wash water (DWAF, 1996).

Water quality problems were then identified with the water quality constituents that contribute to them, in terms of the norms defined (Table 1). Water quality guidelines for the four categories of industrial processes have been compiled in terms of eleven constituents, which comprise the Volume 3 Industrial Use Guidelines as it currently exists.

Table 2: Potential water-related problems associated with various industrial processes

Process Type	Equipment Damage	Process Problems	Product Problems	Waste Disposal
Cooling Water	Corrosion Scaling Fouling Blockages	Foaming Sediments Gas production Odours Heat Exchanger impairment		pH Total dissolved salts Chemical oxygen demand Suspended solids
Water for steam generation	Resin film Resin poison Corrosion Scaling	Resin impairment Competition	Inadequate treatment	pH Total dissolved salts
Process Water	Corrosion Scaling Fouling Blockages Embrittlement Discolouration	Precipitates Foaming Colour effects Gas production Interference	Sediment Foam Colour Taste/odour Tarnish	Suspended solids Iron Manganese Total dissolved salts
Product water	Corrosion Scaling Fouling Blockages	Precipitates Foaming Gas production Interference	Sediment Turbidity Foam Colour Taste/odour Coagulation	
Utility water	Corrosion Scaling Fouling Blockages Abrasion		Sediment Turbidity Foam Colour Taste/odour Intestinal irritation Health hazard	pH Total dissolved salts Chemical oxygen demand Suspended solids Iron/Manganese
Wash water	Corrosion Scaling Fouling Blockages Abrasion solutions	Contamination	Contamination Blemishes Sediment Process	pH Total dissolved salts Chemical oxygen demand Suspended solids Iron/Manganese

The definition of the categories, process types and associated effects in the 1996 guidelines, for its time represented a progressive approach to guideline development that does to an extent account for risk (potential adverse effect based on a hazard). This approach provided a basis to the development of a risk-based philosophy.

For the other user groups developed as part of the South African Water Quality Guideline Series, it was possible to define a No Effect Range. This is the range of concentrations or levels at which the presence of a particular constituent would have no known or anticipated adverse effects on the fitness of water for use. The purpose of defining such a range is for water resource managers to use it as guidance for setting water quality management objectives (DWAF, 1996).

With respect to industrial water use however, some processes, e.g. steam generation, have such stringent and unique water quality requirements that it would not be practical or possible to manage the quality of a water resource to meet such requirements. For such processes, pre-treatment of intake water is a necessity as a standard requirement. Therefore, in the case of industrial water use, from a water resource management perspective, it serves no purpose to define a No Effect Range. Instead, in the 1996 guideline, a Desired Water Quality Range was defined which is the range of concentrations or levels at which the presence of that particular constituent would not result in any extraordinary requirements, in terms of cost or any other requirements, in order to use water from a particular resource for a particular industrial process category (DWAF, 1996).

This difference in approach to the 1996 guideline development for Industrial use, resulted in misapplication and incorrect use of the guidelines with respect to water quality objective setting, where desired ranges for industrial use where compared to the no effect ranges of the other guidelines (used in direct comparison, with the consequences not understood).

The water quality guidelines for Industrial Use, as it exists do provide a comprehensive set of generic guidance, however a concentration-based statement on fitness for use is no longer considered to be adequate. Site-specific risk assessment is needed to address the decision contexts that water users are faced with, especially as water becomes a scarce commodity.

1.5 Framework for guideline development

The majority of water resources utilised for industrial applications in South Africa do not comply with local or international recommended water quality requirements. Based on the nature of the varied and stringent processes that require some form of pre-treatment, a risk-based approach to guideline development for industrial water use is necessary to achieve the objective of efficient, optimal utilisation of water on site and ultimately of South Africa's limited water resources. Environmental changes, increasing demands, lack of regulator enforcement and over utilisation over the past few decades have had an impact on water availability for all water use sectors.

The principles of site-specific risk assessment are well understood and is not new to the industrial sector. Industries have been involved in risk management since before the industrial revolution − each generation has brought new challenges and new opportunities (Deloitte and MAPI, 2015).

Today, there is an increased awareness of the diverse ways in which water use can pose substantial threats to businesses in certain regions and sectors. As a result, several businesses have become involved in water risk assessment studies and have begun taking initiatives on designing tools which would help them understand how to mitigate such risks. It was found that owing to the pressing need for judicious water management, businesses have been conducting water audits regularly to understand the complete water use pattern in their operations and to find avenues for water saving and efficiency (FICCI and CWC, 2012). However, such assessments are based largely on water usage (quantity) and very rarely account for quality.

Water is an input constraint in industrial production. Risk from insufficient water and the consequences of its scarcity and lack thereof as a business risk is well understood, whether it be physical, financial or regulatory (WWF, 2009). However, a clear understanding of the risks and consequences associated with water quality within an industrial application's water use pattern and operation is limited to the types of effects. The need for a risk-based approach to determine an estimation of the degree of effects, when they occur and the conditions under which they will present themselves following exposure, will add to the water risk assessment picture for an industrial operation or application.

It is equally important to follow a risk-based approach as in many cases the required water treatment costs to arrive at "ideal/required" concentrations are expensive, requiring huge investment. Risk-reduction measures aimed at arriving at an "acceptable risk level" may not only be more economically feasible, but also practical, for water use and also for wastewater disposal which is becoming complex and prohibitive.

The environment in which an industrial sector operates would be amenable to the implementation of risk-reduction measures to a process or water use if the water quality risks are understood and quantified to an adequate degree, where identified factors can be manipulated to a meaningful extent. A site-specific risk-based approach would present this opportunity.

Additionally, many industrial production operations or applications do not rely on a single water source, but use multiple sources, including surface water resources, groundwater sources, municipal water supply and increasingly are re-using water from within the industrial process where permissible.

Demonstrating the current recognition that water quality is a key input to performance for an industrial use, many users have their own in-house stringent water quality requirements as part of the comprehensive management guidelines for the technology applied and in terms of the specifications of quality and standards of their products or application.

A challenge with the guidelines in the form they currently exist is that they are largely generic and lack the extent of water qualities faced locally and within the site-specific context, to be meaningful to the extent needed by the local industrial user. The guidelines are largely beneficial from a water resource management perspective in setting instream objectives to cater for industrial abstractions from a water resource, in order to maintain the fitness-for-use of water on a sustained basis (which in recent years is on the decline for many water resources in South Africa). It does however not cater for the industrial user, where pre-treatment of intake water for many processes is a standard requirement. Water quality guidelines as they are prescribed in terms of the category of use and norms thus have little application in this context. It is a given that providing water quality guidelines to cater for all types of industries, operations, processes and situations would be nearly impossible, but with a risk-based site-specific approach it does however present a more practical and useful application for an industrial user within the context of the operation and scenario, beyond just as an input.

As it exists, for industrial use applications, many users are often unaware of the benefit that water quality can be manipulated to achieve optimal production through the process to its disposal, as opposed to simply being made “compliant/safe”, as an input variable only. Managing water quality on a risk basis presents an opportunity for improving performance as opposed to only enabling it. This performance-based approach is seen to be part of a higher level tier within the risk-based guideline system.

As per the risk-based approach philosophy prescribed in terms of the guideline revision, a key aspect includes a tiered-approach wherein a generic assessment is progressively moved towards a site-specific assessment in which increased accuracy of source, pathway and receptor components allow for the identification, and thus mitigation option formulation, of key risk factors.

This shift in thinking and departure from only ensuring the ‘required or standard water quality concentration’ of input water, to one which considers the scenario and local conditions within the broader industrial application, that incorporates risk-reduction measures aimed at arriving at an “acceptable risk level”, is not only scientifically more defensible, but also more practical and cost-effective.

Various guidelines for water use exist in different parts of the world; but none of these include a risk-based approach to industrial use. In fact, very little guidance is available for industrial water use *per se*. Most of the selected water quality instruments ultimately aim to protect public health or have a public health component. Guidelines related to industrial use for the large part are concerned with the impact of pollutant concentrations on receiving water resources and the environment, guidance on water re-use and limitations on effluent discharge.

The guidelines or water quality regulations specified internationally, could be divided into two major groups (UN Water, 2015):

- Instruments with prescribed standards (e.g. EPA reuse guidelines, or EU Directives) including numerical standards (e.g. maximum concentration of pollutants), treatment standards (specified treatment processes) or standards for materials used for water treatment and distribution.
- Instruments based on risk assessment and risk management (e.g. WHO 2006 reuse guidelines and the WHO Drinking Water Guidelines 2011; Australian Drinking Water Guidelines 2011 or Canadian Drinking Water Guidelines 2014). This is a holistic approach that addresses the risk to water quality from source to user.

The former is relevant to a greater extent to industrial water use and wastewater generation and the latter specifically to drinking water.

Water quality guidance for industrial use, as to the extent provided for in the South African Water Quality Guidelines, Volume 3 is almost non-existent, internationally:

- Canadian water quality guidelines for industrial use (1987 to 1999) specified guidance on water quality requirements for a number of Canadian industries. The guidelines provided information concerning the major effects that specific water quality parameters have on various industrial processes; and recommended water quality guidelines applicable at the point of use for generic processes and specific industries types (Canadian Council of Ministers of the Environment, 2008). However, these guidelines have been superseded by the Canadian Environmental Quality Guidelines (CEQGs) since 1999 to date (through continuous evolvement). Industrial water use requirements are however not addressed in the CEQGs.
- India has water quality standards and the methods of chemical treatment for attaining them for different types of industrial water-cooling systems (Bureau of Indian Standards, 1999).

The lack of quality guidelines is largely based on the premise that water use for industry can be treated to the standard required and thus prescription of fitness for use is not required. Thus, there is no known precedent internationally for a risk-based approach to water quality in industrial applications.

1.6 Generic and Specific Guidance

Review of international practice has highlighted that very little water quality requirements guidance is provided for industrial sector in terms of fitness for use, largely for two reasons, (1) industrial use is so varied and diversified that it's not possible to cater for all types of uses and (2) the water required for a particular use can be easily treated to the required desired standard based on the water purity needed. South Africa could be considered progressive in its approach, in the development of industrial use water quality guidelines of 1996, focusing on the description of general and specific industrial processes, and by doing so water quality guidelines could be specified for any industry based on the building block approach. Although this has related primarily to fitness for use, guiding management largely from a water resource perspective.

The need for both generic and site-specific water quality guidance for industrial use is fundamental component of the risk-based philosophy proposed, the intention is that decision support focus on both fitness for use and on water quality requirements. The site specificity component manipulated through software decision support model is a paradigm shift for industrial water quality guidelines worldwide.

This initial generic approach adopted by the 1996 guidelines is no longer deemed sufficient, and a more detailed generic format focusing on the industrial use is required. This technically generic approach, as part of this project is referred to as Tier 1 concept as part of the guideline development. A generic guideline application, although implying an absence of site-specific information, has been improved in terms of a first tier approach in assessing risk, but also accounting for some industry specific factors on water quality requirements (e.g. types on industrial use; water sources and predominant problematic water quality constituents; existing supporting information).

The need for the guideline to move from a concentration-based statement on fitness for use to a site-specific risk assessment related to the specific industrial use scenarios, was required to be defined/determined in the course of guideline development. Within the significant variation in industry types and settings, a site-specific approach was a fundamental requirement to accurately assessing fitness for use and formulating sound decision support water quality guidance.

The risk-based tool presented here provides a data capturing model for industrial use scenarios. The water specific guidance has two main outputs:

- A risk assessment in which key risk factors are identified.
- A method of manipulating the inputs to arrive at an acceptable risk level.

1.7 Fitness for Use

The concept of fitness for use is well defined and in the context of water quality guidelines, 'is a judgement of how suitable the quality of water is for its intended purpose' (DWAF, 1996). The concept of fitness for use of water in industrial applications differs in some respects from other water user groups.

Most industries are comprised of various water-using processes, often each with its own specific water quality requirements. Some processes are highly sensitive to water quality changes, while others may be unaffected. Consequently, in a single industry, water that is ideally fit for one process may be totally unfit for another. Treatment technology also permits that any quality water can be used for a specific purpose provided it can be treated to the required specifications.

Therefore, in industrial applications, how fit a particular water source is for use depends on the design/technical specifications for the process and how much the user is prepared to invest in treating the water to comply with these specifications. Thus while it would seem that the fitness for use concept's relevance and applicability to industrial water uses might be irrelevant, this holds true if one only considers the hazard concentration in the input (source) water. However, the applicability of the risk-based guidelines extends beyond input water; by the incorporation of the exposure water use scenarios and site-specific risk factors within the process, the user is presented with added guidance on the probability of the risks that are likely to occur. This fitness for use concept is thus extended from a hazard basis to a risk basis accounting for the suitability of the water to be assessed and interpreted in terms of specific adverse effects.

The fitness for use assessment thus still forms the core technical requirement of the guidelines. The focus of this endeavour has therefore been to formulate a mathematical approach (modelling) to the fitness for use analysis as the basis for derivation of the risk-based guidelines. The ability of the user to provide some input to the risk assessment process and contextualising the scenario, supports the proposal of presenting the guidelines as a software product rather than a static document.

For the industrial user the risk-based guidelines would thus serve the purposes,

- in a generic context evaluating the fitness for use of the source water, and
- in a specific context as a screening tool to guide and support decision-making regarding processing aspects of specific industrial problems (e.g. effects such as scaling, corrosion, fouling, foaming, abrasion).

1.8 General Approach

The risk-based guidelines must still present to the water user a source of information which allows them to determine the water quality requirements for the applicable water use.

The core of the proposed approach required accounting for the end point adverse effects posed by the water quality constituents and the manner and extent to which they express themselves, and further within site-specific scenarios of the industrial water use. Water quality problems in industrial use and the constituents that cause them are largely known and well documented in literature. Identifying these key water quality problems/adverse effects specific to the South African industrial sector has formed the basis of the risk-based guideline development.

The development of the industrial use risked based guidelines approach and prototype DSS emanates from the key aspects highlighted as follows:

- A description of the project objectives and context, definition of the framework for the risk based approach development and associated concepts and outlined the process to be followed for the development of the industrial use risk-based water quality guidelines.
- A literature-review and sector engagement to obtain understanding of the industrial user group, the sub-sectors and the nature and manner of the water uses and specifically the key water quality problems. Sixteen sectors were engaged through the submission of a questionnaire that was circulated to representative companies.
- Identification and definition of the key concepts, fundamentals and components to be considered for determining the risk (on which the modelling approach could be based upon and a decision support system designed). This was fundamental to determining the risk factors that should be accounted for and whether the effect was measurable on a scientifically sound basis.
- An assessment of the water quality hazards focusing on understanding the interactions of water quality hazards and determination of the site scenarios and operating conditions, as a means to assess the effects. The key water quality problems identified by the sector, as well literature-based information directed this component;
- Definition risk calculation methodologies for determining the adverse effects for a range of industrial use scenarios. This component was fundamental to the modelling of the risk, requiring the identification of the mathematical formulae for the quantification of various water quality problems that could be applied as a measurement of the risk based on the site-scenario and water quality inputs. These were tried, tested and peer reviewed by a sector specialist to ensure scientific soundness and credibility.

- Development, design and programming of the prototype DSS. The risk calculation methodologies developed were used as the basis to define the informatics for the software application. The demonstrator tool programming was then undertaken, based on the best suited selected software application to develop the functionality and presentation as required. The definition of the levels of tiered assessment, the modelling of the generic and site-specific applications, collation of all the reference data and the development of graphic user interface were developed. Further to this an important aspect was the fitness for use assessment and reporting of the outputs that were required.

The determination of the risk and associated factors required that the effects are measurable to an extent and exhibit characteristics or outcomes that can be adequately described for the industrial use scenario. The availability of the scientific empirical data to support this 'measurability' of a water quality hazard (constituent) was found to be the major limitation to the number of water quality adverse effects that could be incorporated into the tool at this stage. However, the design of the tool and the associated modelling easily lends itself to the addition of further risk factors to industrial water use as the scientific evidence for these become available.

The generic first tier guidance of the DSS is seen to address water quality requirements of source water in industrial uses irrespective of whether it is treated or devoid of treatment (similar to the 1996 guidelines). The site-specific guidance defined by the risk factors associated with the industrial processing units and input water quality concentrations form the basis of the higher tier fitness for use assessment. Based on the understanding of the chemistry and science associated with the commonly and most recurrent water quality end point adverse effects (e.g. scaling, corrosion, fouling) and the site scenario, the probability of occurrence and extent of effect can be calculated which would then be reported as the risk.

The risk-based guidance may also account for waters incorporated into processes as part of water use efficiency or re-use measures by varying the source water concentrations as the input variables in the risk assessment to the use scenario.

It is well accepted that water quality problems within an industrial process or operation can often be addressed through some form of engineered solution. Thus it is the intention that this decision support tool serve as a platform for industrial water users to account for probability of the water quality risks that could manifest and contribute towards improved and informed decision making regarding the timing, implementation and design options of the engineered solution or operational interventions. In addition the tool does serve to guide the user on the water quality requirements to manage the key water quality problems. As a volume of the suite of the South African Water Quality Guideline Freshwater Series, the guideline is primarily intended to guide the fitness for use assessment for the more common adverse water quality effects associated with industrial water use.

This report presents the DSS and provides an overview of its development for the evaluation of fitness for use and water quality requirements for industrial water use. It provides an indication of what the system looks like from a user-interface perspective and explains the functionality and modelling aspects of the technology demonstrator tool. This report consists of two volumes, Volume 1: Description of the Decision Support System (this report) and Volume 2: Technical Support.

2.0 OVERVIEW OF THE DECISION SUPPORT SYSTEM

As the risk-based models are fundamentally an analysis of risk enabling the management thereof, the design may be considered to equate to data flow (decision tree analysis). The DSS thus provides a structured approach necessary for addressing the main decision contexts for the assessment of risk in industrial water use. The overall product will allow for a three-tiered system with increasing data flow noted with higher tiers. The difference between the tiers lies primarily in the degree of site-specificity required to produce an output. A DSS offers the advantage of improving the way in which the guidelines are used because the focus will be on supporting decisions in specific contexts. The definition of the assessment levels that inform the basis of design for the DSS informatics are aligned with the philosophy specifications of Phase 1 (Table 3). The three tiers are as follows:

- Tier 1 is largely equivalent to 1996 generic guidelines and is made available in the DSS. Tier 1 assessment does not involve any calculation methodology however it does bring in the site specificity in terms of industrial processing units and exposure scenarios at a generic level. It requires minimal user defined input, and it is intended to reflect the most conservative set of conditions, even if these do not occur together. This tier communicates the minimum requirements to the user, highlighting potential problems if these are not met and is conservative.
- Tier 2 is a specific application level with increasing data inputs to the model occurring, as more site-specific detail is provided. It largely uses pre-defined industrial water use scenarios and limited site characterisation choices with common field observation and or measurement input required from the user for the assessment. It allows for user access to deeper levels of guideline generation.
- Tier 3 is reliant on additional specialist input (in addition to the site-specific data) with additional calculation methodology. It allows for site specificity in other *ad-hoc* contexts, using modules of the DSS and possibly requiring significant expertise and additional methodology protocols and data.

Table 3: An overview of the Tiered Assessment System

Water Quality requirement	Fitness for Use	
Tier 1	**Tier 2**	**Tier 3**
Most generic (and by implication the most conservative) approach to risk guidance. Minimum user input required and simple output provided. Simplified generic conservative assumptions used and totally reliant on the default datasets (worst case exposure). Does not involve rigorous calculation methodology.	Moderately site-specific, requiring some skills, but largely uses pre-defined water use scenarios and limited site characterisation choices with common field observation and or measurement input required from the user for scenarios manipulation. Rule-based output interpretation.	The most site-specific guidance. A risk assessment protocol, requiring highly skilled input and output interpretation. Allows for the adjustment of the modelling and reference data. Default site-specific component options that can be changed to suit site-specific circumstances (more specific models and parameters).

Water Quality requirement	Fitness for Use	
Tier 1	**Tier 2**	**Tier 3**
Output: Descriptions and risk-based thresholds of levels of water quality requirements (most conservative and generic) per water quality problem, applicable water quality constituent of concern and related to the material on construction of the processing unit.	*Output:* Presentation of the risk assessment of the water quality problems and associated fitness for use based on the water quality input and selection of the pre-defined exposure scenarios	*Output:* Presentation of the risk assessment based on the adjustment of site-specific exposure scenarios and methodology

Whilst these descriptions conveniently demarcate tiers, these are in reality more flexible with increasing variations of site-specific detail use as the user moves from Tier 1 to Tier 3, with a general migration from reference documentation used in the calculations performed to user-defined site-specific input. In computing terms, this may be considered as moving from recursive algorithms to dynamic algorithms.

2.1 Water Quality Assessment

The DSS has been designed to assess two levels of functionality:

- Water quality requirements for industrial related water quality problems; and
- Site-specific assessment on the fitness for use of source water and the operational scenarios.

The overall product allows for a tiered system with increasing data flow noted with higher tiers. The difference between the levels lies primarily in the degree of site-specificity required to produce an output. The two-level assessment system accommodates for the needs of the novice, intermediate and expert user, dependant on the decision support required. The risk-based water quality guidelines are reported as water quality requirements or as a fitness for use assessment both of which incorporating the analysis of the risk and the mitigation guidance thereof. A simplified schematic representation of the industrial water use DSS structure is shown in Figure 1.

- **Water Quality Requirements:**

This tier yields a fast and "conservative" industrial water quality assessment. Water quality guideline requirements are acquired by selecting a processing unit material of construction generating Water Quality Guidelines related to the water quality problem. Alternatively the complete list of requirements maybe required if the user is unfamiliar with site-specific information.

- **Fitness for Use**

Fitness for use evaluations enable the user to select from a range of site-specific parameters, resulting in a risk assessment of how the specific input water quality composition and data about its site-specific exposure could produce an adverse effect. The assessment recommends the required treatment procedures to mitigate the undesirable effects. As a result, this risk-based assessment enables the user to determine how implementing various site-specific remedial actions (e.g. different building material or water type) may contribute to the alleviation of the risk of a given impact such as scaling, corrosion, or fouling. Numerous factors are utilized to determine the potential contribution to the likelihood of the adverse effect occurring. The tool modelling functionality compares the input parameters to several reference indices/ranges in order to calculate the potential risk posed by the water sample in question. Quantitative and qualitative risk assessments are modelled in the tool.

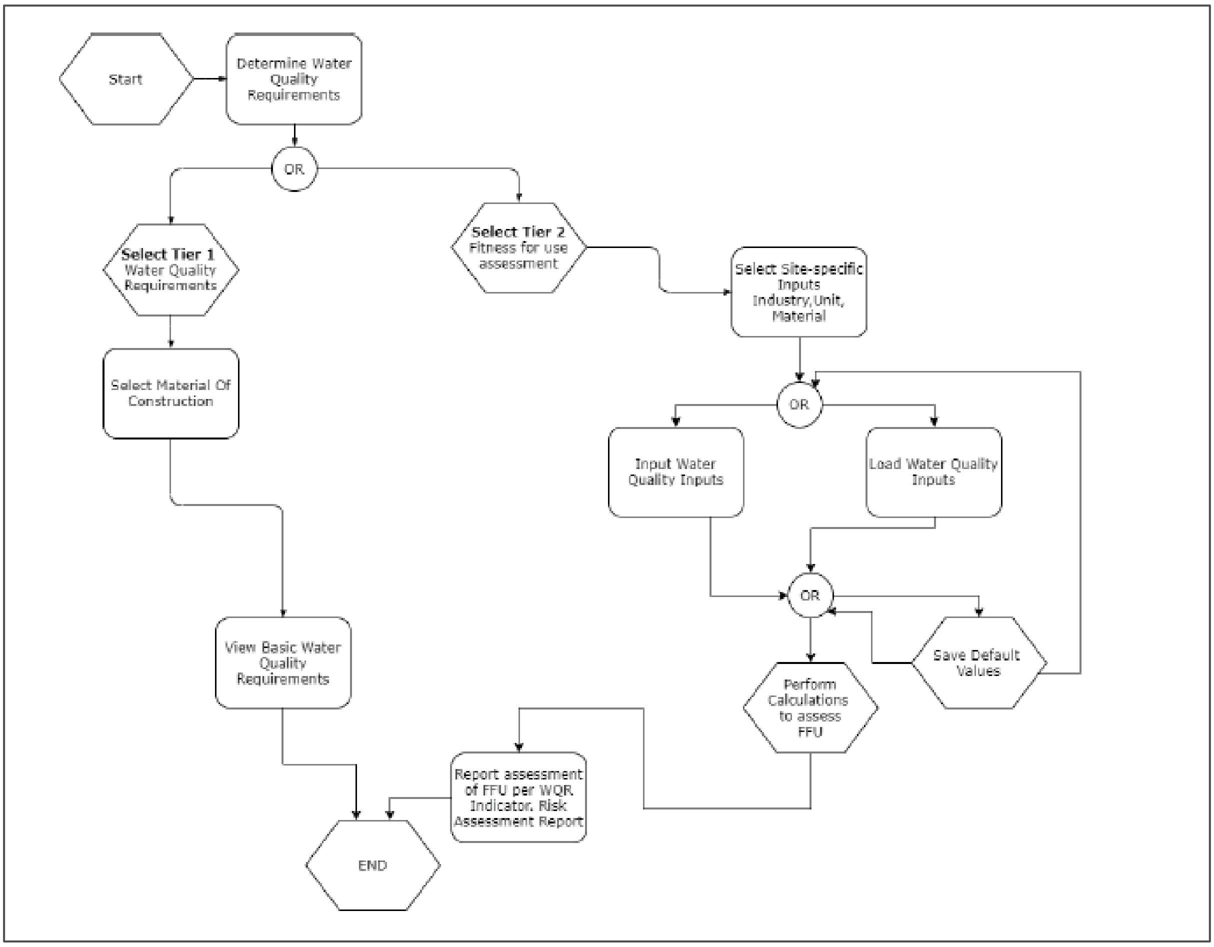


Figure 1: Overview of the DSS

2.2 Reporting in the Decision Support System

As described above the risk-based water quality guidelines are reported at two levels, as follows:

- ***Water Quality Requirements***: a report of all threshold criteria and associated fitness for use levels for associated water quality adverse effect, for the specific industrial process unit material selected (ideal OR acceptable OR tolerable OR unacceptable). This would guide the user on the requirements of the quality of water needed for the intended industrial water use scenario.

- ***Fitness for Use***: the fitness for use category of the input water quality composition presenting the acceptability and implied risk (ideal OR acceptable OR tolerable OR unacceptable) together with the likelihood and description of the associated adverse effects and proposed mitigation measure.

The water quality guidance reporting in the DSS is categorised visually in a colour-coded manner that the user is able to immediately assess suitability and the potential risk posed. The reporting system includes a four-category system which has been based on the classification system adopted by the DWS to categorise fitness for use ranges. In order to ensure that all the risk-based guidelines of the different South Africa Water Quality Guideline Freshwater Series Water User groups are consistent and aligned, this system has been applied. The four-category reporting system is in harmony with a risk-based assessment of water quality in that the 'Ideal' category represents a no risk scenario (safe level), while the 'Unacceptable' category represents a high-risk scenario (most likely occurrence/ significant consequence of the adverse effect).

The generic categorization is shown below.

A generic description of the fitness for use categories used for reporting

Reported Category	Description
Ideal	A water quality fit for a lifetime of use.
Acceptable	A water quality that would exhibit minimal impairment to the fitness of the water for its intended use. Minor risk of adverse effects.
Tolerable	A water quality that would exhibit some impairment to the fitness of the water for its intended use. Moderate risk of adverse effects presenting themselves.
Unacceptable	A water quality that would exhibit unacceptable impairment to the fitness of the water for its intended use. Significant risk of adverse effects, presenting themselves.

3.0 THE DEVELOPMENT PLATFORM

The prototype DSS is designed to present the graphical user interface of the modelling aspects that are assessed to determine the risk-based water quality guidance. The project design specification required the adoption of open-source software for the Decision Support System (DSS). Python was selected to develop the DSS since it is an open-source, cross-platform programming language well-suited for developing desktop applications. It has a valuable collection of frameworks for quickly creating sophisticated graphical user interfaces. The database is built on the JSON framework, an open-source document database that operates on Linux, Windows, and several Unix platforms.

The risk-based DSS has been developed using the visual methods application, Framework PyQt5, graphical interface designer in Python 3. The software has been identified as being a robust calculation and graphic programming tool. The graphical interface is user friendly and provides results that can be exported to an Adobe PDF. The application introduces custom dialog boxes, dropdown list boxes and message boxes that prompt user errors or instructions. tool. The tool is designed to guide users through a series of 'User Forms' at each assessment level to produce a relevant result based on the option selected.

The tool provides a predictive assessment of the likelihood of an adverse effect of the water quality intended for an industrial use in a specific use scenario to derive a fitness-for-use classification. The system is designed to visually communicate and offer guidance on the risk outcomes based on the input parameters.

General System Requirements

The minimum system requirements necessary to be able to use the tool effectively include:

Parameter	Minimum Requirement
Processor	64-bit CPU
Operating System	Windows Preferred
RAM	4 GB
Disk Space	5 GB
Software	Microsoft Excel, Adobe Reader

Installation Instructions

The tool is provided via a compressed folder. Within this folder there is an executable file with the EXE file extension. The files are extracted within the zip folder to a local file path on C-drive. From the extracted folder, an executable file titled "Industrial Water Quality Guidelines DSS.exe" is accessed. The installation guide as shown Figure 2 will be opened. The user is then able to follow the prompts from the installation guide to successfully install the tool. The user will be informed once the tool is installed and will be given the option to launch the tool.

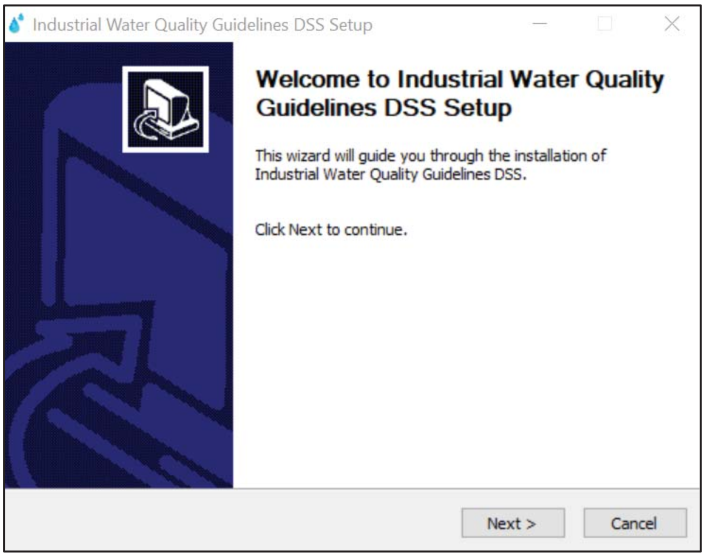


Figure 2: Industrial WQGs DSS Installation Guide

The software is suited for online application and would be able to support vast amounts of information. No separate database would be required, and it would be amenable to easy integration into a tool that incorporates all user groups of the water quality guideline series.

4.0 CALCULATION METHODOLOGIES

In defining a water quality risk-based guideline, the decision support outcome is a function of the intrinsic risk of the water quality constituents (the hazard present in the water) and the extrinsic risk presented by the site scenario, i.e. industrial process, unit and exposure conditions that is derived through a mathematical modelling approach (calculation methodology) that compromises the risk assessment. The DSS generates the results of this modelling as the output, which is presented as the “risk” (probability of the adverse effect).

Risk is a function of hazard and exposure. The threat caused by a hazard depends not only on the severity of its effect but also on whether or not the effect is reversible. The risk assessment methodology accounting for exposure and hazard forms the basis of the calculation methodology applied in the DSS to provide water quality guidance for.

The building blocks that defined the informatics applied in the development of the industrial user water quality guidelines DSS included:

- Definition and description of the scenarios/situation:
    - Description of the site-specificity risk factors for industrial water use (the exposure)
- Characterisation of the hazards
    - Hazard identification and characterisation (defining the concentrations of no effect and the full adverse effect, behaviour, characteristics, chemistry), and
    - Categories of adverse effects (key end points to direct the modelling approach).
- Risk assessment (evaluation of the hazard and exposure to determine probability of occurrence of the risk posed)
        - i.e. Calculation Methodology formulation.

4.1 Description of the Scenarios/Site-specific Situation

The definition of the exposure scenario/site-specific parameters as it pertains to industrial water use comprises the first building block to the risk analysis approach adopted for the decision support system, in that it defined the risk factors that were of consequence.

Through the developmental process, and in assessing the fundamentals of the what and where the risk presents itself in respect of industrial water use, the receptor and exposure site scenario for industrial applications in general were determined to pertain to:

- the manufacturing and processing units/components of the industry sector,
- the mechanical/civil infrastructure,
- the materials of construction.

The above receptors/ exposure site scenarios were selected as the factors for the basis of assessing risks as the water quality effects are measurable to an extent and exhibit characteristics or outcomes that can be adequately quantified and described for industrial water use. The exposure definition of the mechanical/civil infrastructure associated with the processing components/steps that are linked to some form of water usage in the major industrial use sectors is the initial consideration in the DSS data flow.

The materials of construction (MOC) of the infrastructure comprises the ultimate receptor of the water quality hazard and required identification and characterisation in order to define the risk relationships and scientific basis to the calculation methodology. The MOC forms the basis of the risk approach definition for industrial water use. While the MOC has been characterised for a number of processing sub-units/components for inclusion into the DSS, the reference DSS database can be easily expanded to include new MOCs and related data as they become available.

The typical materials of construction identified for processing units for the various industries and typical operating parameters are discussed in the following sub-sections. These MOCs form the basis of the exposure considerations for evaluating the risk.

4.1.1 Carbon Steel

Uses of carbon steel are most common in engineering material. It is an inexpensive material that is available in a range of standard forms and sizes. It also has a good tensile strength and ductility. Carbon steel is least resistant to corrosion in concentrated sulphuric acid and caustic alkali environments. They are more suited for applications with organic solvents. Carbon steel is used in most industrial boiler and feedwater systems. Carbon steel typically experiences uniform corrosion. This is because carbon steel has a lower corrosion resistance in aggressive environments and hence is corroded uniformly.

4.1.2 High Silicon Irons

High silicon irons (14-15% of Silicon) have a high resistance to mineral acids with the exception of hydrofluoric acid. They are particularly suitable for use with sulphuric acid at all concentrations.

4.1.3 Stainless steel

Stainless steel is a group of iron-based alloys that contain different concentrations of chromium. The higher chromium content within different grades of stainless steel prevents the susceptibility towards corrosion and other associated risks. To impart corrosion resistance the chromium content must be greater than 12%. A wide range of stainless steels are available, with compositions tailored to give the properties required for specific applications. They can be divided into three broad classes according to their microstructure;

- Ferritic:13-20% chromium, <0.1% carbon and no nickel
- Austenitic: 18-20% chromium, >7% nickel
- Martensitic: 12-14% chromium, 0.2-0.4% carbon and 0-5% nickel

The uniform structure of Austenitic stainless steel is the most desired structure for corrosion resistance and its grades are widely used in the chemical industry. The most common grades are 304/304L, 321,347, 316, 309 and 310.

The higher the alloy content of the austenitic grade, the better the corrosion resistance, cracking resistance and other common risks associated with the use of stainless steels. As a rough guide the ranking in order of increasing corrosion resistance is shown below (Table 4) using type 304 as a basis.

Table 4: Corrosion resistance ranking

Type	304	304L	321	316	316L	310
Ranking	1	1.1	1.1	1.25	1.3	1.6

Intergranular corrosion, also known as weld decay and stress corrosion cracking, are operational problems associated with the use of stainless steel. Stress corrosion and cracking in stainless steel is caused by chloride rich environments. Generally stainless steels are used for corrosion resistance when oxidizing conditions exist. Stainless steel is a component of boilers such as the superheated elements. Stainless steel has a higher corrosion resistance than carbon steel due to a higher chromium content as shown in Figure 3. This figure is adapted from (Prasath, Thirugnanan, & Lidhuveniya, 2020), and is based on the uniform atmospheric corrosion resistance. The stainless-steel grade is dependent on the extent of corrosion.

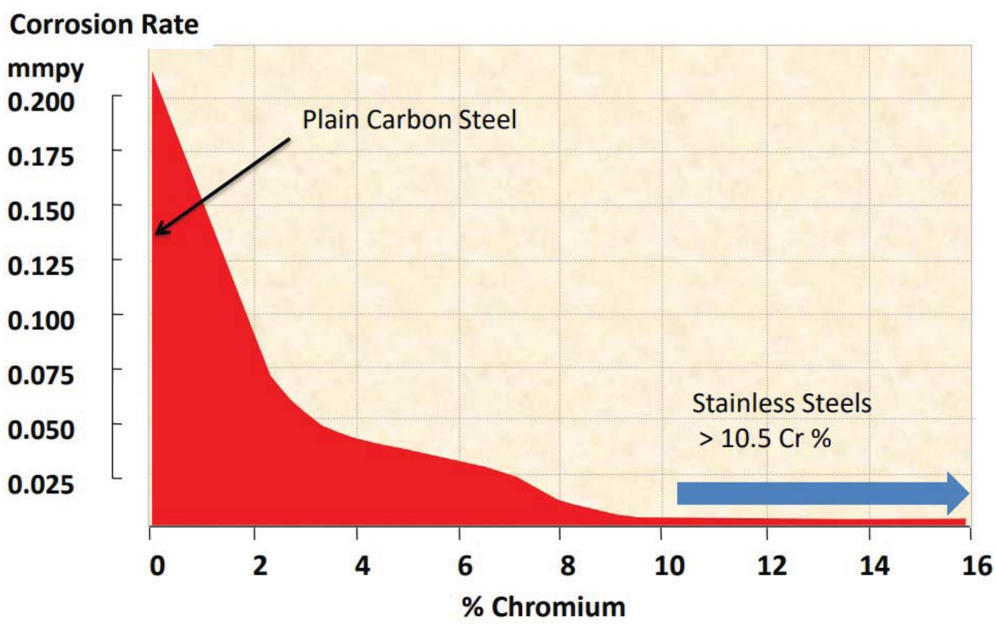


Figure 3: Corrosion Rate of Carbon Steel and Stainless Steel

The following section discusses the most common grades of stainless steel that can be used in local South African industries.

4.1.4 Stainless Steel 304/304L

Stainless steel 304 is an austenitic grade of steel and 304 L is the low carbon version of stainless steel 304. Both grades of steel have dominated the brewery, dairy, food and pharmaceutical industries. It has a relatively high resistance towards corrosion. Pitting and crevice corrosion can occur in environments containing chlorides. Stress corrosion cracking can occur at temperatures over 60°C. Stainless steel 304 has a good resistance towards oxidation for intermittent to continuous service. In instances where corrosion resistance, in water with temperatures within the ranges of 425-860°C, is required, the use of stainless steel 304L is preferred as it has a high resistance towards carbide precipitation. It is inexpensive and is best suited for applications that require low temperature performance. It is also resistant to scaling that may be caused from alkali solution, organic acids and inorganic acids. Although 304/304L is most commonly used in industrial applications. The short coming of this grade is its low mechanical strength (AZO, 2005).

4.1.4.1 Stainless Steel 321

Stainless steel 321 is a titanium settled austenitic stainless steel with a high overall corrosion resistance. It can withstand intergranular corrosion resistance at high temperatures of 427-816°C in chromium carbide precipitation. Whereas unstable alloys such as 304 are subjected to intergranular attack. Stainless steel 321 can be utilised in dilute organic acids at moderate temperatures and in pure phosphoric acid (>99% mw). It opposes polythionic acid stress corrosion in hydrocarbon service. It can also be used in environments with fluoride-free caustic solutions at moderate temperatures. As versatile and advantageous as the 321 grade is, it still does not perform well in chloride or sulphuric acid applications (Interalloy, 2021).

4.1.4.2 Stainless Steel 347

Stainless steel 347 is basis austenitic 18/8 grade 304 with added columbium. The addition of columbium stabilizes the steel and eliminates carbide precipitation which is the main cause of intergranular corrosion. Stainless steel grade 347 is beneficial for its higher creep stress and rupture properties as compared to 304. It can be used in high temperature services such as ASME Boilers and pressure vessels. This grade is typically used in heat exchangers, high temperature stream services as well as high temperature chemical process equipment (Masteel, 2021).

4.1.4.3 Stainless Steel 316/316L

Stainless steel grade 316 is a more reliable variation of 304 with the addition of molybdenum and a higher nickel content. This results in an increased corrosion resistance in aggressive environments. The molybdenum makes the steel more resistant to pitting and crevice corrosion in chloride-contaminated media, sea water and acetic acid vapours. The lower rate of general corrosion in mildly corrosive environments gives the steel good atmospheric corrosion resistance in polluted marine atmospheres. At higher temperatures 316 has a higher strength and better creep resistance. This grade of stainless steel has good mechanical properties and fabricability. Stainless steel 316 is used in tanks and storage vessels for corrosive liquids, as well as being widely applied in process equipment in the chemical, food, paper, pharmaceutical, petroleum and mining industries (SKZN, 2021).

4.1.4.4 Stainless Steel 309/309S

Alloys 309 and 309S are austenitic chromium-nickel stainless steels that are often used for higher temperature applications. Due to their high chromium and nickel content, Alloys 309 and 309S are highly corrosion resistant, have outstanding resistance to oxidation, and excellent heat resistance while providing good strength at room and elevated temperatures. This grade of stainless steel is exclusively known for is high temperature resistance and resistance to creep deformation in harsh environments. It is used in aircraft and jet engine parts, heat exchangers, heating elements, sulphite liquor handling equipment, Kiln liners, Boiler baffles, Refinery and chemical processing equipment. 309/309S is more corrosion resistant to marine atmospheres than 304. It also has a high resistance towards scaling (PSP, 2021).

4.1.4.5 Stainless Steel 310

These grades contain 25% chromium and 20% nickel, making them highly resistant to oxidation and corrosion. Grade 310S is a lower carbon version, less prone to embrittlement and sensitisation in service. The high chromium and medium nickel content make these steels suitable for applications in reducing sulphur atmospheres containing H_2S. They are widely used in moderately carburising atmospheres, as encountered in petrochemical environments. For more severe carburising atmospheres other heat resisting alloys should be selected. Grade 310 is not recommended for frequent liquid quenching as it is sensitive to thermal shock. The grade is often used in cryogenic applications, due to its toughness and low magnetic permeability. Typical applications of Grade 310/310S is used in fluidised bed combustors, kilns, radiant tubes, tube hangers for petroleum refining and steam boilers, coal gasifier internal components, lead pots, thermowells, refractory anchor bolts, burners and combustion chambers, retorts, muffles, annealing covers, food processing equipment, cryogenic structures (Materials, 2021).

4.1.4.6 High Alloy Stainless steel

Super austenitic, high-nickel stainless steels containing between 29-30% nickel and 20% chromium, have a good resistance towards acids and chlorides. Duplex and super-duplex stainless steels contain high percentages of chromium. They are called duplex because their structure is a mixture of austenitic and ferritic phases. They have a better corrosion resistance than austenitic stainless steel and have a reduced susceptibility to stress corrosion cracking. The super-duplex steels were developed for use in aggressive offshore applications. The principal applications for these steels are for chemical-processing and power-generating equipment involving corrosion service in aqueous or liquid-vapour environments at temperatures normally below 315°C. These alloys are also used for special services at temperatures of up to 650°C (Sinnot, 2011).

4.1.5 Nickel

Nickel has good mechanical properties. The pure metal (>99%) is generally not used in a chemical plant. Its nickel alloys are preferred for most applications. Its main use is for equipment handling for caustic alkalis. Nickel is not subject to corrosion cracking like stainless steel (Sinnot, 2011).

4.1.6 Monel

Monel the classic nickel-copper alloy (ratio of 2:1, two parts of nickel and 1 part of copper). It is commonly used in chemical plants and is more expensive than stainless steel. Monel has good corrosion resistance in dilute mineral acids. It can potentially be used in equipment handling of alkalis, organic acids, salts and sea water (Sinnot, 2011).

4.1.7 Inconel and Incoloy

Inconel is generally used for acid resistance at high temperatures. It maintains its strength at elevated temperatures and is resistant to sulphur free furnace gas. Nickle alloys with a higher chromium content such as Incoloy have a better oxidation resistance at higher temperatures (Sinnot, 2011).

4.1.8 Hastelloy's

Hastelloy's are made from a range of nickel, chromium, molybdenum and iron alloys that were developed for corrosion resistance to strong mineral acids, especially hydrochloric acid. Hastelloy B and C are the most common forms of Hastelloy (Sinnot, 2011).

4.1.9 Aluminium and its alloys

Pure aluminium lacks mechanical strength but has a higher resistance to corrosion than its alloys. The pure metal can be used for cladding on dural plates. The corrosion resistance of aluminium is due to the formation of a thin oxide film. It is most suitable for uses in strong oxidizing conditions. It is not suitable for environments that have mineral acids. Aluminium and its alloys are most commonly used in the textile and food industry (Sinnot, 2011).

4.1.10 Platinum and other Platinum group metals (PGMs)

The platinum group metals are very common with regards to the chemical structure. Platinum, Iridium and Osmium are the densest metals. Platinum and palladium are soft and ductile and resistant to oxidation and high temperature corrosion. They have widespread catalytic uses and are often used with the addition of other metals including platinum group metals. Rhodium and Iridium are difficult to work but are valuable alone as well as in alloys. Their chemical compounds have many uses and rhodium is a particularly good catalyst. Ruthenium and Osmium are hard, brittle and difficult to work with. These platinum group metals have a poor oxidation resistance but become valuable when they are added to other metals. PGM's are high in demand and are predominantly used in the electronic equipment and as a catalytic converter (Sinnot, 2011).

4.1.11 Copper

Copper is one of the oldest and most versatile materials that have been used mainly in engineering constructions. It also has a good resistance towards corrosion due to the protective patina that forms on its surfaces. It has a low thermal expansion and is stable and resistant to deterioration from movement. It is relatively light in comparison to lead and other metals. It requires minimal maintenance and has good bio-fouling resistance. It is commonly used to form pipes and tubing for potable water distribution and heating and cooling systems as it is malleable and can easily be soldered. It is recyclable and has relatively low life cycle impacts. It can also be used in boilers and has a high sensitivity to ammonia (Sinnot, 2011).

4.1.12 Brass

Brass is a common material of construction that is made from the combination or alloy of copper and zinc. It is a good conductor of heat and is corrosion resistant. It is typically used in the industry as pipes, tubes, radiators, etc. It has good strength and can be retained even when subjected to high temperatures usually up to 200°C. This material can be used in applications that require high tensile strengths. Brasses can resist corrosion as it does not rust and can resist salt water. When lead is combined with brass it gains a low wear and low friction properties that make them wear resistant (Sinnot, 2011).

4.1.13 Galvanised Steel

Galvanised steel is a steel/iron-based metal with protective zinc coating layer. The zinc layer acts as a corrosion protection layer. Galvanised steel is used in the automotive industry. It is also used as a replacement for plastic pipes in applications where they are not strong enough. Some of the benefits of galvanised steel is that they have a low initial cost, it has a relatively long-life cycle and can last for about 20-50 years in extremely harsh environments. Its zinc layer acts as a protective buffer between the steel/iron and the moisture or oxygen within the environment (Sinnot, 2011).

4.1.14 Plastics

Plastics are predominantly used in the food processing industry and biochemical plants. It is used as a corrosion resistant material and can be divided as being.

- Thermoplastic material – soften with increasing temperature, e.g. polyvinyl chloride and polyethylene.
- Thermosetting material – materials that have a rigid structure such as epoxy resins.

The biggest uses of plastics are for piping and plastic sheets for lining vessels. Plastics are considered to complement metals as corrosion resistant materials. They have a good resistance to dilute acid and inorganic salt attacks. Plastics absorb metals causing degradation, swelling and softening of the plastic structure. Plastics are also susceptible to solar embrittlement which is the impact of plastics with regards to solar degradation (Sinnot, 2011).

4.1.14.1 Poly-Vinyl Chloride (PVC)

PVC is the most common thermoplastic material in the chemical industry. It is resistant to most inorganic acids except for salt solutions, concentrated sulphuric and nitric acid. They are unsuitable when exposed to organic solvents as they are prone to swelling. The maximum operating temperature for PVC is 60°C. The main grade of PVC that is used is CPVC. It has a greater temperature resistance. CPVC also has an excellent chemical resistance and can transport hot fluids. It has been successful in the chemical processing piping systems, pulp and paper processing piping systems, food processing pipe systems and water and sewage treatment piping systems (Sinnot, 2011).

4.1.14.2 Polyolefins

Low-density polyethylene is inexpensive, tough and flexible. Its low softening points makes it not suitable for temperatures higher than 60°C. The solvent resistance to polyolefins is similar to that of PVC (Sinnot, 2011).

4.1.14.3 Polytetrafluoroethylene (PTFE)

PTFE is commonly referred to as Teflon and Fluon, it is resistant to all chemicals with the exceptions of molten alkalis and fluorine and can be used for temperatures up to 250°C. PTFE is used for gaskets, on valve stems and as coatings which acts as non-stick coating to surfaces such as filter pads. It is also used as vessel linings (Sinnot, 2011).

4.1.14.4 Polyvinylidene Difluoride (PVDF)

PVDF is similar to PTFE. It has a good resistance to inorganic acids, alkalis and organic solids. It has a maximum operating temperature at 140°C (Sinnot, 2011).

4.1.14.5 Glass Fibre Reinforced Plastics

Polyester resins, reinforced with glass fibre are the most common thermosetting plastics used in a chemical plant. They are relatively strong and have a resistance to a wide range of chemicals such as dilute mineral acids, inorganic salts and solvents. They are less resistant to alkalis. Reinforced glass fibres are wound on in the form of a continuous filament which results in a high strength material that can be used to make pressure vessels (Sinnot, 2011).

4.1.15 Rubber

Rubber is particularly used for linings of tanks and can be used as pipes. It has a good resistance to acids and alkalis but is not suitable for uses that include organic solvents (Sinnot, 2011).

4.1.16 Concrete

Concrete has a good corrosion resistance. It can have a limited pressure range and has the additional risk of corrosion of reinforcement beams/structures and spalding. It can degrade in soft water. It is typically used in a wide range of industries as storage tanks, raw water reactors and versatile equipment handling (Sinnot, 2011).

4.2 End Points (Adverse Effects) and Hazard Characterization

Industrial water using processes are affected in different ways by interaction with the water (containing the water quality hazard). Each of the adverse effects resulting from the exposure to the hazard are characterised by an end point which results in negative impact to the industrial processing unit use based on the water composition and interactions. For industrial use, the adverse effects formed the basis of the risk-based water quality guidelines calculation methodology development. The physical characteristics of and chemical and microbiological contaminants in water determine its properties and thus its potential to cause undesirable effects to industrial processes, i.e. the concentrations/presence of the contaminant or physical property of the water defines the hazard and resulting adverse effect.

It is important that the adverse effect description is categorised in a manner and range such that the user is able to adequately judge the acceptability of the risk. Representative constituents linked to the most common adverse effects (water quality problems) have been built into the DSS to present the risk-based methodology.

The three most common adverse effects (end points) of significant concern to industrial water have been included in the risk-based methodology presented in the decision support system, *viz:*

- Corrosion
- Scaling
- Fouling.

Based on the adverse effects selected above and associated hazards linked to them, the hazard function related to each required characterisation. The hazard characterisation is the process of determining whether exposure to a hazard (water quality constituent) can cause an increase in incidence of specific adverse effects (e.g. corrosion). This formed a fundamental component to the risk assessment quantification as one needed to determine what data would be used to formulate the hazard function for each hazard as it related to the occurrence of end point defined (the risk).

This is based on the site-specific conditions (the relationship between the contributing *in-situ* conditions and the input water quality composition) and the exposure assessment (examines what is known about the materials of construction). This defined the calculation procedures of the fitness for use assessments in the DSS in order to determine a risk and has defined the informatics and design of the DSS. The hazard characterisation also allows the determination of the uncertainties in terms of deriving the guidelines.

4.3 Hazard Characterization and Risk Assessment

The hazard characterisation and risk assessment calculation methodology for scaling, corrosion and fouling as applied in the DSS are described below. Both quantitative and qualitative approaches to assessing the likelihood of the risk (adverse effect) occurring are incorporated.

4.3.1 Corrosion

Corrosion is defined as the destruction of a metal by chemical or electrochemical reaction with its environment. Corrosion involves the oxidation of metal atoms to cations, which in turn can react to form oxides, hydroxides, and other species on the metal surface. In these scenarios, the metal cations may not directly be released into the water and could form precipitates or films. If corrosion occurs rapidly enough that the formation of these films is not possible or if the films that form are insufficiently protective, the release of metal cations into the water will occur. At this point, other chemical processes such as precipitation and dissolution of other metal compounds, such as carbonates, silicates, and other scales, then control the quantity and form of metal released into the water.

The extent, rate, and mechanisms of corrosion that occur all depend on numerous factors. Such factors include the pH, temperature, and chemistry of the water such as hardness and chloride content. Water quality analysis is complex and involves the interaction between multiple species and different chemical additions. Each of these factors plays a role in the corrosion mechanism which is also dependant on the material of construction with which the water is in contact.

In industry, corrosion can cause numerous problems. This includes the failure of equipment which has the added cost of replacement and plant downtime. Furthermore, in cooling or heating systems, this can lead to decreased plant efficiency as a loss of heat transfer is observed caused by the accumulation of corrosion products. Corrosion is specific to the water quality and material of construction as discussed below.

4.3.1.1 Factors (Water quality hazards) Affecting Corrosion

4.3.1.1.1 pH

pH is a major contributing factor to metal corrosion and release. The pH can have an effect on multiple factors that range from the rate of dissolution, the solubility and protectiveness of different films and scales, to the appearance and morphology of the corrosion observed. Low pH values (<4) tend to have a higher corrosion rate. At low pH values, acids release hydrogen ions, which oxidize the metals in pipes, accelerating corrosion. At pH values less than 5, rapid corrosion of iron, copper, and lead may occur. At more alkaline pH values greater than 9, corrosion of these metals is typically reduced due to the formation of protective films. However, at higher alkaline pH values, scale formation and the efficiency of certain corrosion inhibitors can be hindered and hence corrosion may increase again.

4.3.1.1.2 Temperature

Temperature does play a significant role in corrosion in water systems. A general rule with regards to the effect of temperature on the corrosion rate is that the corrosion rate will double for every 10°C increase in temperature. Furthermore, an increase in temperature influences both the rate of corrosion and the type or mode of corrosion (e.g. critical pitting temperature). Temperatures over 60˚C are not recommended for stainless steel grades 304 or 316 due to the risk of sudden failure from chloride stress corrosion cracking. Furthermore, oxygen degassing occurs at temperatures >60°C, which generates a higher level of corrosion. The effect of temperature is addressed in the indices calculation (See Section 4.3.3) as these calculations are dependent on the water temperature.

4.3.1.1.3 Hardness

Hardness refers to the concentration of dissolved calcium and magnesium in the water. Hard water has a high concentration of calcium and magnesium, which has a tendency to result in scaling. Consequently, this makes this water less corrosive due to the tendency to form protective films in the pipe. However, this is dependent on the alkalinity and pH. Soft water has a lower concentration of calcium and magnesium and thus is often more corrosive than hard water. Typically, water is considered soft if the total hardness is less than 50 mg/L $CaCO_3$ while values greater than 150 mg/L $CaCO_3$ are considered hard water. Galvanized piping, like steel and cast-iron piping, tends to experience its best performance in hard water compared to soft water due to scale formation. However, hard water is not always the most beneficial as in cases whereby copper piping is used, pitting corrosion in typically observed and occurs at low temperatures. However, if the hardness in the water is primarily non-carbonate, the chlorate and sulphate ions will tend to keep the calcium in solution and will prevent scale formation. Excessive scale formation is also not preferable as high amounts of scale deposition on the surface will limit the heat transfer efficiency of certain equipment.

Table 5: Hardness Indication

Hardness (mg $CaCO_3$/L)	Classification	Risk
0-50	Soft	Unacceptable
50-150	Moderately Hard	Acceptable
150-300	Hard	Ideal
>300	Very Hard	Tolerable

Based on the common materials on construction, the following guidelines are proposed with regards to water hardness –

- Concrete – Soft water is found to be detrimental to concrete. This is observed as, when the concrete is in contact with soft water, the calcium hydroxide in the hardened concrete matrix is leached out in order to establish an ion balance. This causes weakening of the concrete matrix and is referred to as a soft water attack. A study done by (Otieno, Alexander, & du Plessis, 2019) showed that a loss of 10 mm depth of concrete could take place over a period varying from less than 1 year to 22 years. This is accompanied by an increase in surface roughness. Moderately hard water is preferred and will lead to a lower corrosion rate as if the water contains more calcium, the likelihood of the leaching is reduced. However, very hard water will cause scale formation on the concrete surface also resulting in increased surface roughness.
- Carbon steel – It was found that soft water has a higher corrosion rate than hard water. This is due to scale formation in hard water that deposits on the surface. It was also found that soft water leads to uniform corrosion whereas hard water corrodes unevenly through hard deposits
- (Nallasivam & Perumal, 2016).
- Stainless steel – No significant difference between soft and hard water on the rate of corrosion has been found with regards to stainless steel (Munn, 1993). However, this is dependent on the chloride concentration.

As seen above, soft water is more corrosive, and corrosion is further enhanced when the water contains a low pH and low total dissolved salts (TDS). Although scale can be seen as a corrosion control mechanism, scale formation varies and can be porous or soft and irregular. Corrosion can still occur under conditions that are favourable to the formation of scale or even when scale is already present. This is referred to as under deposit corrosion and is discussed in Section 4.3.3.1.3.

4.3.1.1.4 Alkalinity

Alkalinity measures the buffering capacity of water and its ability to neutralize acids. Alkalinity is a good indicator of the total dissolved inorganic carbon (bicarbonate and carbonate anions) present. Alkalinity is a measure of how easily the pH of the water can be changed. Hence it is considered to be a mitigating influence with regards to extreme pH levels. Water with a high alkalinity is more likely to be scale-forming even at a relatively low pH. In contrast, low alkalinity waters lack the buffering capacity to deal with acids, so they can easily become more acidic and corrosive. High alkalinity is preferred as it helps control pH changes which reduces corrosion.

Table 6: Alkalinity Classification Levels and associated Risk

Alkalinity (mg $CaCO_3$/l)	Classification	Risk
<12	Very low	Unacceptable
25 41	Low	Tolerable
41-98	Medium	Tolerable
98-148	High	Acceptable
>148	Very high	Ideal

4.3.1.1.5 Chlorides

Chlorides are found to be the most aggressive ion regarding corrosion, specifically in the case of crevice and pitting corrosion typically used stainless steel grades with continuous exposure at neutral pH and ambient temperatures, the following chloride levels are proposed per grade as shown in Table 7.

Table 7: Chloride Levels for Stainless Steel at ambient temperature

Chloride Level	If Temperature >35°C and pH <7, Limits Decrease To:	Suitable Stainless-Steel Grades
<200 mg/L	50 mg/l	304, 304L
<300 mg/l	100 mg/l	316/316L
<400 mg/l	150 mg/l	Alloy 20
3000 mg/l	2000 mg/l	904L
>3600 mg/L and seawater	3000 mg/l	Duplex Stainless steel
<200 mg/L	50 mg/l	304, 304L

The maximum level guidelines allow for the presence of crevices (such as bolt heads, flanges or deposits) but assume that the surface has been passivated. In alkaline environments whereby the pH>7, higher chloride levels can be tolerated. Higher temperatures reduce the maximum tolerated chloride level. In general, if the temperature is greater than 35°C or the pH is lower than 7, the maximum chloride level should be lowered. For 304L, an upper limit of 50 mg/L should be adapted and 100 mg/L for 316L (Cutler, 2003). The combined action of environmental conditions (chlorides/elevated temperature) and stress – either applied through a load or residual causes stress corrosion cracking (SCC). Only austenite stainless steel is susceptible to this type of corrosion.

4.3.1.1.6 *Chloride to Sulphate Mass Ratio*

Increasing the chloride to sulphate mass ratio (CSMR) will accelerate corrosion in the presence of materials that contain lead or copper. (Edwards & Triantafyllidou, 2007) found that while sulphates tend to inhibit corrosion by forming passive protective film layers and reducing galvanic currents between dissimilar metals, chlorides prevent the formation of such passive layers and stimulate galvanic current. Thus, if the source water contains natural levels of chloride and the treatment process is designed to remove sulphate, this will increase the CSMR and potentially increase the rate and likelihood of corrosion.

The risk of CSMR is evident when pipes contain lead such as galvanized pipes, brass/bronze fittings, faucets or lead solder. If the CSMR >0.5, there is a significant risk of corrosion which may be difficult to control and will result in lead exposure. However, if the CSMR >0.5 coupled with alkalinity <50 mg/L as $CaCO_3$, there is a serious risk of corrosion and lead exposure. In such cases, treatment is recommended to remove or reduce the chloride and sulphate concentration.

4.3.1.1.7 *Sulphate Attack*

Sulphate attack is specific to concrete. It is a complex process, which includes physical salt attack due to salt crystallization and chemical sulphate attack by sulphates in the surrounding water. Sulphate attack can lead to expansion, cracking, strength loss, and disintegration of the concrete.

Table 8: Sulphate Concentrations and Risk of Sulphate Attack

Index	Description	Risk	Treatment Recommendations
>= 10 000 mg/l	Very severe risk of sulphate attack	Unacceptable	Treatment Recommended – Water treatment for sulphate removal
>=1 500-<10 000 mg/l	Severe risk of sulphate attack	Tolerable	Treatment Recommended – Water treatment for sulphate removal
>=150-<1500 mg/l	Moderate risk of sulphate attack	Acceptable	Treatment May Be Needed – Water treatment for sulphate removal
<150 mg/l	Low risk sulphate attack	Ideal	No Treatment

4.3.1.2 Corrosion Indices

4.3.1.2.1 Calculation 1: Langelier Saturation Index

Based on the factors discussed above which includes the pH, temperature, hardness and alkalinity, the Langelier index analysis is a combination of these parameters to determine the extent of corrosion on different materials of construction.

The Langelier Saturation Index (LSI) is an equilibrium model derived from the concept of saturation. It is purely an equilibrium index and deals only with the thermodynamic driving force for calcium carbonate scale formation and growth. The calcium carbonate saturation is useful in determining in a specific water quality is aggressive/corrosive, balanced, or scale-forming (high LSI). The LSI is given by the following formula –

$$LSI = pH - pH_s$$

Whereby pHs is given as follows –

$$pH_s = (9.3 + A + B) - (C + D)$$

Whereby the factors are given by –

$$A = \frac{Log_{10}[TDS] - 1}{10}$$

$$B = -13.12 \times Log_{10}(°C + 273) + 34.55$$

$$C = Log_{10}[Ca^{2+} as\ CaCO_3] - 0.4$$

$$D = Log_{10}[Alaklainity\ as\ CaCO_3]$$

The following conclusions can be derived by the value of the LSI –

- LSI is negative: Risk of corrosion.
- If LSI is positive: Low risk of corrosion
- If LSI is close to zero: Borderline corrosion potential. Water quality or changes in temperature, or evaporation could change the index.

Table 9: LSI Rankings

LSI	Description	Risk	Treatment Recommendations
>= -5	Severe Corrosion due to $CaCO_3$	Unacceptable	Chemical treatment recommended – Treatment through addition of corrosion inhibitors OR Consider an alternative material of construction OR Consider additional treatment of the water to more suitable feed quality
>= -2-<-5	Mild Corrosion due to $CaCO_3$	Tolerable	Treatment may be needed – Treatment through addition of corrosion inhibitors OR Consider an alternative material of construction OR Consider additional treatment of the water to more suitable feed quality
>0.5-<-2	Mild Corrosion due to $CaCO_3$	Acceptable	Treatment may be needed – Treatment through addition of corrosion inhibitors OR Consider an alternative material of construction OR Consider additional treatment of the water to more suitable feed quality
>= 0.5	Minimal to no risk of corrosion	Ideal	No treatment required
>= -5	Severe Corrosion due to $CaCO_3$	Unacceptable	Chemical treatment recommended – Treatment through addition of corrosion inhibitors OR Consider an alternative material of construction OR Consider additional treatment of the water to more suitable feed quality

4.3.1.2.2 Calculation 2: Ryznar Index

The Ryznar index (RI) is considered in conjunction with the LSI index as it affords greater protection against corrosion, than does the more familiar Langelier Index. It boosts the calcium hardness to a point, where scale begins to form, which actually helps protect the equipment, from corrosion. This index aims to quantify the relationship between the calcium carbonate saturation state and scale formation. The index was founded in 1944 (Ryznar, 1944).

The Ryznar index is calculated as follows, the pHs is as calculated above.

$$RI \ = 2 \ \times pH_s - pH$$

Table 10: Ryznar Index Rankings

RI	Indication/Description	Risk	Treatment Recommendations
>= 8,5	Severe Corrosion due to lack of $CaCO_3$ formation	Unacceptable	Chemical treatment recommended – Treatment through addition of corrosion inhibitors OR Consider an alternative material of construction OR Consider additional treatment of the water to more suitable feed quality
>=7,8-<8,5	Mild Corrosion due to lack of $CaCO_3$ formation	Tolerable	Treatment may be needed – Treatment through addition of corrosion inhibitors OR Consider an alternative material of construction OR Consider additional treatment of the water to more suitable feed quality
>=6,8-<7,8	Mild Corrosion due to lack of $CaCO_3$ formation	Acceptable	Treatment may be needed – Treatment through addition of corrosion inhibitors OR Consider an alternative material of construction OR Consider additional treatment of the water to more suitable feed quality

4.3.1.2.3 Calculation 3: Pitting Corrosion

Many alloys, such as stainless steels and Aluminium alloys, are useful only because of passive films, which are thin (nanometre-scale), oxide layers that form naturally on the metal surface and greatly reduce the rate of corrosion of these alloys. However, these passive films are often susceptible to localized breakdown resulting in the accelerated dissolution of the underlying metal (Frankel, 1998). Pitting corrosion is highly dependent on the chloride content, pH, temperature and the presence of an oxidizing agent.

This type of corrosion occurs when the passive film is damaged and becomes exposed. This can occur through chemical attack, mechanical damage, presence of microstructure irregularities such as non-metallic inclusions which is caused by machining. Stainless steel resistance to pitting corrosion is dependent on temperature, pH, aggressive anion concentration and on the alloy's composition. This is particularly important with regards to the chromium and molybdenum percentages in stainless steel. A particular steel's resistance to corrosion pitting can be evaluated as its chromium equivalent or PREN (pitting resistance equivalent) through the following equation:

$$PREN = \%Cr + (3.3 \times \% Mo) + (16 \times \%N)$$

The percentages must be expressed as mass percentages. The greater the PREN value, the better corrosion resistance. A PREN:

- >35 is required for pitting resistance in seawater,
- >40 in the case of hot and stagnating seawater,
- >45 for crevice corrosion resistance.

The PREN value is useful to compare stainless steel grades resistance against pitting. The PREN value cannot be used in isolation to determine whether a particular grade will be suitable for a given application.

The critical pitting temperature is an important parameter that determines the minimum temperature at which alloys start to corrode. Pitting corrosion is accelerated by temperature. According to the ASTM G48 standard, the critical pitting temperatures are shown in Table 11. Critical pitting temperatures determined by different methods should not be compared. The critical pitting temperatures are found to decrease with increasing chloride concentrations.

Table 11: Critical Pitting Temperatures

Grade	Typical PREN Value	Critical Pitting Temperature
304/304L	20	18°C
316/316L	25	20°C
Alloy 20	30	90°C
904L	36	40°C

4.3.1.2.4 Calculation 4: Larson Skold Index

The Larson-Skold index refers to an empirical scale used to measure the degree of corrosiveness of water relative to mild steel metal surfaces. This index looks at the potential corrosivity of iron and steel. The Larson-Skold index is the ratio of twice the number of moles per litre (mol/L) of sulphate (SO_4^{2-}) plus chlorides (Cl^-), to the moles per litre of alkalinity that is typically in the form of bicarbonate and/or carbonate. The Larson-Skold index scale presents the following outcomes of corrosion tendency –

$$Ratio = \frac{(Sulphate \times 2) + Chloride}{Alkalinity}$$

Table 12: Larson-Skold Index

Index	Tendency to Corrosion	Risk	Treatment Recommendations
>= 1,2	Severe pitting corrosion	Unacceptable	Treatment recommended – Water treatment to reduce the sulphate or chloride concentration OR Consider additional treatment of the water to more suitable feed quality
>= 1,0-<1,2	Significant pitting corrosion	Tolerable	Treatment may be needed – Water treatment to reduce the sulphate or chloride concentration OR Consider additional treatment of the water to more suitable feed quality
>=0.8-<1	Mild pitting corrosion	Acceptable	Treatment may be needed – Water treatment to reduce the sulphate or chloride concentration OR Consider additional treatment of the water to more suitable feed quality

4.3.1.3 Calculation 6: Aggressive Index

The aggressive index (AI) relates to the corrosive tendency of water. It is particularly important in pipes that contain cement and asbestos. It is given by the following equation –

$$AI = pH + log\ (A \times H)$$

Where –

A is the alkalinity in mg/L $CaCO_3$ and H is the hardness in mg/L $CaCO_3$. The relative risk rankings and limits for the aggressive index are shown in Table 13. The aggressive index relates to the corrosion of the concrete reinforced bars and hence would only be applied in specific cases.

Table 13: Aggressive Index Rankings

AI	Indication/Description	Risk	Treatment Recommendations
>= 12	Nonaggressive – Lack of pitting corrosion of the concrete reinforced bars	Ideal	No Treatment
>=11 to <12	Moderately aggressive – Moderate pitting corrosion of the concrete reinforced bars	Acceptable	Treatment may be needed – Chemical treatment through addition of Antiscalants OR Water treatment for softening
>=10 to <11	Mildly aggressive – Mild pitting corrosion of the concrete reinforced bars	Tolerable	Treatment may be needed – Chemical treatment through addition of Antiscalants OR Water treatment for softening
<10	Very aggressive – Severe pitting corrosion of the concrete reinforced bars	Unacceptable	Treatment recommended – Treatment recommended – Chemical treatment through addition of Antiscalants OR Water treatment for softening

4.3.1.4 Summary

There are various water properties that have an effect on the corrosivity of the material which it is in contact with. A general summary of each parameter and this effect can be seen in Table 14. These parameters determine the level of corrosion risk presented based on the water sample composition and are accounted for in the modelling.

Table 14: Water Properties and Effect on Corrosion

Water Properties	Corrosivity
Hardness	As hardness increases, corrosion decreases.
Alkalinity	Increase in alkalinity causes a decrease in corrosion.
pH	Corrosion depends on its value – Corrosive at low pHs, as pH increases up to 8.5, corrosion decreases.
Temperature	Increase in temperature, corrosion increases
Chloride	Higher chloride concentration increases water corrosivity
Sulphate	Higher sulphate concentration increases water corrosivity
Temperature	Pitting corrosion is accelerated by temperature

4.3.2 Calculation 7: Corrosion Rate

A study conducted by (Pisigan, 1985) predicted the expected corrosion rate of stainless steel based on an eight-variable empirical mode. The models suggest that increasing chloride, sulphate, alkalinity, and dissolved oxygen levels would accelerate corrosion, whereas increases in calcium, buffer capacity, saturation index, and exposure time would lead to decreasing corrosion rates. This index was used to predict the corrosion rate based on these variables. The calculation of the corrosion rate is shown below –

$$Corrosion\ Rate = \frac{(Cl^{-1})^{0.509} \times (SO_4^{2-})^{0.025} \times (Alkalinity)^{0.423} \times (DO)^{0.799}}{(Ca)^{0.676} \times \beta^{0.030} \times (10^{SI})^{0.107} \times Day^{0.381}}$$

Where: DO = dissolved oxygen (mg/l as O_2), Ca = calcium (mg/l as $Ca2^+$), β = buffer capacity (mg/l as $CaCO_3$), SI = Langelier Saturation Index, Day = days.

4.3.3 Scaling

The following parameters have used in the DSS to determine the extent of scale possible in industrial processing units.

4.3.3.1 Scaling Indices

4.3.3.1.1 Calculation 8: Langelier Saturation Index

The LSI can also be utilised to assess scaling risk. It is an equilibrium model derived from the concept of saturation. It is purely an equilibrium index and deals only with the thermodynamic driving force for calcium carbonate scale formation and growth. The calcium carbonate saturation is useful in determining in a specific water quality is aggressive/corrosive, balanced, or scale-forming (high LSI). Although the index is useful in determining whether the water quality is scale forming or corrosive, it provides no indication as to how much scale or calcium carbonate will actually precipitate in order to bring water to equilibrium. Furthermore, it does not consider film formation by phosphates and silicates The LSI is given by the formula as given in Section 4.3.1.2.1. The model was initially developed in 1936 (Langelier, 1936) as a qualitative test used primarily for potable water rather than cooling water. Furthermore, it was initially used for scaling prediction and has since been adapted to predict corrosion.

The following scale formation risk conclusions can be derived by the value of the LSI –

- LSI is negative: No potential to scale, the water will dissolve $CaCO_3$.
- If LSI is positive: Scale can form and $CaCO_3$ precipitation may occur.

- If LSI is close to zero: Borderline scale potential. Water quality or changes in temperature, or evaporation could change the index.

Table 15: LSI Rankings

LSI	Indication/Description	Risk	Treatment Recommendations
0	Balance – No scale	Ideal	No Treatment
0.5 to 2	Mild scale formation	Acceptable	Probably no treatment
3	Moderate Scale Formation	Tolerable	Treatment recommended
4	Severe Scale Formation	Unacceptable	Treatment recommended

4.3.3.1.2 Calculation 9: Puckorius Scaling Index

The Puckorius Scaling Index (PSI) is based on the buffering capacity of the feed water, and the maximum quantity of precipitate that can form in bringing the water to equilibrium (Puckorius, 1990). Water containing high concentrations of calcium, but low in alkalinity and buffering capacity can have a high calcite saturation level. The high calcium level increases the ion activity product. Such water might have a high tendency to form scale due to the driving force, but scale formed might be of such a small quantity as to be unobservable. The water has the driving force but not the capacity and ability to maintain pH as precipitate matter forms. The PSI index is calculated in a manner similar to the Ryznar stability index. Puckorius uses an equilibrium pH rather than the actual system pH to account for the buffering effects as shown in the equation below –

$$PSI = 2pH_s - pH_{eq}$$

Where –

$$pH_{eq} = 1.465 \times log_{10}[Alkalinity] + 4.54$$

Table 16 shows the Puckorius scaling index and the relevant risk and descriptions. The scale tendency increases as the index decreases and the corrosive nature to carbon steel increases as the index increased. Based on the typical industry uses, the Puckorius Scaling index was not used in the tool. The Ryznar index would provide a more accurate indication of scaling and hence that index was adapted.

Table 16: Puckorius Scaling Index

PSI	Indication/Description	Risk
4,5 >PSI	Optimal range	Tolerable/Acceptable
PSI <4,5	Water has tendency to limescale	Unacceptable

4.3.3.1.3 Calculation 10: Under Deposit Corrosion

Under deposit corrosion (UDC) is a form of localized corrosion that develops beneath or around deposits present on a metal surface. These deposits preferentially form at the bottom of pipes under stagnant or intermittent flow conditions (e.g. in dead legs or during plant shutdowns) or in areas where the flow velocity is at a minimum. (Although scale formation is a commonly implemented control method to prevent corrosion, under deposit corrosion may still occur. The main driving force behind UDC is the chemical and physical differences between the covered and uncovered areas, created by the formation of the deposit, which promotes corrosion attack. This includes pH differences, a higher or lower concentration of particular ions or molecules (i.e. oxygen or corrosive species) or the presence of microbial cultures underneath the deposits (Obot, 2021). The presence of other contaminants such as microbes, inorganic and organic scales like FeS, $FeCO_3$, $CaCO_3$, asphaltenes or waxes cause under deposit corrosion which results in pitting corrosion.

Similar limits apply as mentioned in the sections above for the predication of corrosion occur, however this type of corrosion will only occur if the surface has fouling or scaling. Furthermore, corrosion can be enhanced in the case of biological deposits. Certain bacteria release harmful by products which further enhance the rate of corrosion.

Under deposit corrosion occurs through multiple steps which include deposit formation, onset of primary corrosion, oxygen depletion, start of secondary corrosion and acceleration of acidic corrosion. In general, corrosion mechanisms deplete free oxygen. In steel piping systems, the primary corrosion mechanism depletes free oxygen and continues as long as free oxygen and moisture are in contact at the pipe wall. While this is the most common corrosion route, some systems do not include the oxygen depletion step. The secondary corrosion occurs after the galvanic cell is set up. Finally, if the correct ions are present, the pH decreases and the water trapped in the deposit becomes more acidic. The lower pH accelerates the corrosion rate.

4.3.3.1.4 Calculation 11: Calcium Phosphate Scaling

Calcium phosphate ($CaPO_4$) is less soluble in neutral and alkaline conditions and dissolve in acidic conditions. Aluminium and iron phosphates, however, are less soluble at moderately acidic conditions. Thus it is important to remove aluminium and iron in a pre-treatment step as well. Because of the complexity of phosphate chemistry, it is not easy to predict a threshold level of phosphate scaling. The calcium phosphate stability index (SI), however, was proposed by (Kubo, 1979).

The calcium phosphate stability index is determined by the levels of calcium and phosphate present, pH, as well as the temperature. A negative stability index (SI)I signifies a low potential for calcium phosphate scaling and a positive value indicates the potential for calcium phosphate scaling. SI is determined by the following equation –

$$SI = pH_a - pH_c$$

Where pHa is the actual pH of the water and pHc is the critical pH. The critical pH is calculated by –

$$pH_c = \frac{11.755 - \log(CaH) - \log(PO_4) - 2\log(t)}{0.65}$$

Where CaH is the calcium hardness (mg/l $CaCO_3$), PO_4 is the phosphate concentration (mg/l) and t is the temperature as °C.

Table 17: Calcium Phosphate Stability Index

SI	Indication/Description	Risk	Treatment Recommendations
=<0	Balance – Low potential for scale formation	Ideal	No treatment
>0	Potential of Scale Formation	Tolerable	Treatment recommended

4.3.3.2 Rules of Thumb

There are many simple rules of thumb and indices used to predict scale formation and, in many cases, to determine the maximum concentration ratio between two parameters for effective operation. The following rules of thumb were adapted from (Ferguson, 2004).

Magnesium silicate is a common scale produced in industry. Magnesium silicate can form in a cooling system via two distinct mechanisms, namely the formation of a stoichiometric $MgSiO_3$, and through interaction with precipitating magnesium hydroxide. If the ion product is greater than the specified limit, unacceptable magnesium silicate scaling is expected. However, if the ion product is below the limit, acceptable magnesium silicate scaling is expected. The ion product limit is shown in Table 18.

Table 18: Magnesium Silicate Scaling

pH	Ion Product Limit [Mg (mg/l)] x [SiO_2 (mg/l)]
>= 7.5	<= 12 000
<7.5-<8.5	>=6000-<12 000
>= 8.5	0 -<6000

Calcium sulphate is also another common scale produced in industry. Gypsum is the expected form of calcium sulphate scale in cooling systems whereas anhydrite is more prevalent at temperatures above those normally encountered in cooling water. The ion product limit is shown in Table 19.

Table 19: Calcium Sulphate Scaling

Water Treatment	Ion Product Limit [Ca (mg/l)] x [SO4 (mg/l)]
No water treatment with regards to antiscalants	0-<50 000 mg/l
With water treatment with regards to antiscalants	>=50 000-10 000 000 mg/l

4.3.3.3 Silica

Silica deposits are glass-like coatings that can form almost invisible deposits on metal surfaces. The solubility of silica increases with higher temperatures and pH. Consequently, this occurs in opposite operating regimes to $CaCO_3$ scale formation. Once formed, it is difficult to remove even with aggressive acid cleaners. The solubility of silica in steam increases with an increase in temperature. Thus, the solubility of silica increases as steam is superheated. In boiler water systems, as steam is cooled by expansion through the turbine, silica solubility is reduced and deposits are formed, usually in cases where the steam temperature is below that of the boiler water. To minimize this problem and prevent silica scale from forming, the concentration of silica in the steam must be controlled. The maximum limits of silica in the steam should be 0.02 mg/L (Suez Water Technologies and Solutions, 2021).

Table 20: Silica Rankings

Silica content (mg/L)	Indication/Description	Risk	Treatment Recommendations
>0,02	Severe scale forming	Unacceptable	Treatment recommended
<0,02	Limited to no silica scale formation	Acceptable	Treatment may be needed

4.3.4 Fouling

Fouling occurs when insoluble particulates suspended in a water system form deposits on a surface. Fouling mechanisms are dominated by particle-particle interactions that lead to the formation of agglomerates. Fouling is typically experienced in membrane systems through precipitation and deposition of molecules or particulates on the membrane surface or membrane pores. The consequences of membrane fouling are increased membrane separation resistances, reduced productivity, and/or altered membrane selectivity.

Particulate fouling is caused by suspended solids (foulants) such as mud, silt, sand or other particles in the water. Fouling can occur due to inorganic mechanisms such as silt deposition or organic mechanisms such as in the case of microbial sludge deposition. Biofouling occurs when living matter grows on the equipment. In many cases, re-circulating cooling systems are ideal for promoting the life of microorganisms thus promoting biofouling. In cases whereby fouling occurs, under deposit corrosion may be a concern as the deposits create a favourable environment for this type of corrosion. Fouling typically occurs in membranes as well as different types of equipment and in pipelines. Each is discussed separately as they occur differently.

Other types of fouling include corrosion fouling which occurs when corrosion products accumulate and adhere to the surface of the equipment. Biological fouling which occurs when living organisms such as macro-organisms and /or microorganism grow and are deposited onto the walls of the equipment. These deposited biofilms are of concern as they can accumulate debris that may impede or completely block flow through the equipment.

4.3.4.1 Fouling in Equipment and Pipelines

Fouling in equipment and pipelines occurs due to the accumulation and formation of unwanted materials on the surfaces of equipment or pipelines. This type of fouling is of concern in heat transfer equipment as fouling on the fouling of heat transfer surfaces drastically reduces the efficiency. Furthermore, as fouling deposition occurs, the cross sectional area is reduced, which causes an increase in pressure drop across the equipment.

4.3.4.1.1 Calculation 12: Suspended Solids

Suspended solids (SS) consist of inorganic and organic matter which includes silt, sand, clay, particles or any type of suspended matter. Particulate fouling occurs due to a high suspended solids in the feed which results in deposition of these suspended solids in the process streams due to gravity settling as well as other deposition mechanisms. Limits of the suspended solids concentration in a feed is shown in Table 21.

Table 21: Suspended Solids Risk

SS (mg/L)	Indication/Description	Risk	Treatment Recommendations
>= 30	High chance of fouling	Unacceptable	Treatment recommended – Upfront filtration pre-treatment
>=15-<30	Moderate fouling	Tolerable	Treatment may be needed – Upfront filtration pre-treatment OR Chemical treatment by addition of dispersants
>=5-<15	Mild fouling	Acceptable	Treatment may be needed – Upfront filtration pre-treatment OR Chemical treatment by addition of dispersants
0-<5	No fouling predicted	Ideal	No Treatment

4.3.4.2 Fouling in Membrane Systems

Membrane fouling occurs when a foulant is deposited on a membrane surface which causes a blockage of the membrane pores. This occurs in membrane bioreactors, reverse osmosis, forward osmosis, membrane distillation, ultrafiltration, microfiltration, or nanofiltration systems. Fouling in membrane systems decreases the performance of the membrane. The risk of scaling and corrosion of membrane systems is dependent on the LSI index. This is because the LSI index does not favour $CaCO_3$ precipitation. Any scale formation is not advisable in membrane systems as this can block the membrane pores.

4.3.4.2.1 Particle Size

The fouling tendency is dependent on the size of the particles requiring removal and the type of membrane technology. The fouling tendency of membranes is dependent on the size of the particles requiring removal and the type of membrane technology. In general, the fouling layer is formed by particles having a dimension up to 10 times the pore size. Table 22 shows the typical membrane operation and pore sizes. If the particle size is less than the pore size, it will pass through and generally not cause fouling.

Table 22: Fouling Particle Size Guideline

Particle Size	Indication/Description	Treatment Recommendations
>1000 µm	Pre-treatment required	If Particle size > Lower limit, Treatment Recommended – Consider use of microfiltration
0,1 to 1 µm	Microfiltration	If Particle size > Lower limit, Treatment Recommended. This technology is recommended for suspended solids and large colloids
0,1 to 0,001 µm	Ultrafiltration	If Particle size > Lower limit, Treatment Recommended. This technology is recommended for removal of proteins and large organics
0,001 µm	Nanofiltration	If Particle size > Lower limit, Treatment Recommended. This technology is recommended for organics and dissolved solids
<0,001 µm	Reverse Osmosis	If Particle size > Lower limit, Treatment Recommended. This technology is recommended for dissolved salts and organics

4.3.4.2.2 Calculation 13: Silt Density Index

Silt is composed by suspended particulates of all types that accumulate on the membrane surface. The silt density index (SDI) is a method for estimating the rate at which colloidal and particle fouling will occur in water purification systems, especially using Reverse Osmosis systems (RO) or Nanofiltration membranes systems. The SDI is purely a measurement of the fouling potential since each suspended particulate matter differs in size and shape. The test is dependent on the site-specific details and should be performed according to the standard test method (ASTM D4189, 2014).

Table 23 below shows the fouling potential based on the SDI in RO systems.

Table 23: Fouling SDI Risk

SDI	Indication/Description	Risk	Treatment Recommendations
<1	Several years without colloidal fouling	Ideal	Treatment not Recommended
>= 1-<3	Several months between cleaning	Acceptable	Treatment Recommended – Regular cleaning required
>= 3-<5	Particular fouling likely a problem, frequent cleaning	Tolerable	Treatment Recommended – Regular cleaning required
>5	Unacceptable, additional pre-treatment is needed	Unacceptable	Treatment Required – Additional upfront pre-treatment required

4.4 Materials of Construction

Based on the factors and manifestation of adverse effects discussed above, a summary of the various calculations methodologies applied in the DSS as they pertain to the materials of construction of industrial processing units is shown in Table 24. In the case of cooling water, the Puckorius index is used as opposed to the Ryznar index as it accounts for the buffering capacity of the water.

Table 24: Material of Construction Summary

Material of Construction	Adverse Effect	Applicable Risk Quantification Calculation
Concrete	Corrosion	Ryznar index Aggressive Index
	Scaling – Calcium Carbonate and silica	Ryznar index Silica concentration
	Sulphate attack	Sulphate concentration
	Fouling	Suspended solids
Stainless Steel	Corrosion	Ryznar index Temperature Chloride concentration Fluoride concentration PREN Value
	Scaling – Calcium Carbonate and silica	Ryznar index Silica concentration in Steam Magnesium and Silica concentration Calcium and sulphate concentration
	Fouling	Suspended solids
Carbon steel	Corrosion	Larson Skold Index

Material of Construction	Adverse Effect	Applicable Risk Quantification Calculation
		Ryner Index Pisigan and Shingley corrosion rate
	Scaling – Calcium Carbonate and silica	Ryznar index Silica concentration in Steam Magnesium and Silica concentration Calcium and sulphate concentration
	Fouling	Suspended solids
Alloys (With lead)	Corrosion	Ryznar index Larson index Chloride to sulphate mass ratio PREN value
	Scaling – Calcium Carbonate and silica	Ryznar index Silica concentration in Steam Magnesium and Silica concentration Calcium and sulphate concentration
	Fouling	Suspended solids
Plastic	Scaling	Ryznar index
	Fouling	Suspended solids
Equipment and piping	Fouling	Suspended solids
Membranes	Scaling	Langelier saturation index
	Fouling	Suspended solids Silt density index Particle size

4.5 Typical Water Qualities

The DSS tool is equipped with pre-loaded typical water qualities that the user may apply for the input water quality sample composition. The user has the option to choose these qualities should they want to test a generic water type. These qualities were estimated based on an average of literature sources as shown in Table 25. The potable water standard was adapted from the SANS 241:2015 drinking water standard (SANS241, 2015).The typical water types and associated qualities are shown in Table 25.

Table 25: Typical Water Types and Qualities

Parameter	Unit	Seawater	Brackish Water	Surface Water	Ultra-Pure Water	SANS 241 Potable Water Standard
Calcium (Ca)	mg/l	400	1 000	100	2	75
Magnesium (Mg)	mg/l	1 200	100	50	4	30
Sodium (Na)	mg/l	10 000	250	200	10	200
Sulphate (SO_4)	mg/l	3 000	500	130	14	250
Chloride (Cl)	mg/l	20 000	2 300	200	6	300
Fluoride (F)	mg/l	0	0.1	1	0	1.5
Alkalinity	mg/l $CaCO_3$	120	100	120	10	20
Temperature (C)	°C	25	25.00	25	25	25
pH		7	7	7	7	7
TDS	mg/l	35 000	4 500	700	50	1 200
EC	µS/cm	50 000	7 800	1 200	30	170

4.6 Modelling Aspects

The DSS tool has been designed at three levels specified to cater for a range of target audiences (novice, intermediate and expert user) based on the availability of the measured water quality data and site-specific detail. Transition between Tiers 1 and Tier 2 is the primary focus of the tool, with Tier 3 representing a higher degree of user defined input and updates to the risk methodology. The transition to Tier 3 aligns with the objective of determining an acceptable risk level as new data captured, for example, specific material of construction detail, chemistry or exposure conditions, could lead to a significant change in the risk posed under the specific site-conditions applicable.

These tiers are flexible with increasing variations of site-specific detail use as the user moves from one Tier to the next, with a general migration from reference documentation used in the calculations performed, to user-defined site-specific input.

The DSS has been designed to present:

- Generic risk-based water quality requirements for industrial related water quality problems; and
- Site-specific assessment of the fitness for use of input water quality and the operational conditions.

The tool is designed to cater for the exposure scenarios of the particular industrial water use situation (the risk-based functionality of the DSS). By assessing the specific aspects built into the modelling approach of the tool *viz.* processing unit and material of construction, water quality data inputs of the sample composition and exposure conditions, a potential risk is calculated. At this point the risk-based guidance has focused on the risk probability of the occurrence of corrosion, scaling and fouling as the major water quality problems to industrial water use.

Fitness for use of the water quality is determined by selecting the material of construction of the mechanical/civil infrastructure of the industrial process in question, which is then assessed on the basis of the input water quality composition that is entered. Using the built-in reference data and the calculation algorithms coded in the DSS for corrosion, scaling and fouling, the probability of risk of the water quality problem is presented based on the assessment of the water quality relative to the material of construction. This quantitative output is presented as indices or ranges linked to the scientific literature based reference data. The tool reports on the significance of the adverse effect and if it is feasible to take remedial/mitigation action or not. The results are output as a PDF report which incorporates mitigation measures in instances where a risk has been noted.

The components and data flow relating to the modelling aspects in the DSS tool, at the 3 tiers is provided below.

4.6.1 Tier 3

Tier 3 calculations cater for the site-specific scenarios, exposure conditions and detailed assessments not covered by Tier 2 and is targeted at an expert user. This tier allows for more site specificity in other *ad-hoc* contexts. In addition to the hazard-based assessment of water quality composition entered and material of construction, the user will apply additional protocols to assess detail site data such as water pressure, density, material thickness, etc. The Tier 3 functionality is still to be developed further with the protocols and modules to be applied.

4.6.2 Tier 2

Tier 2 is seen as the more widely used applicability and functionality of the DSS tool. Tier 2 allows for site-specificity by selection of default-based site-specific factors provided for in the DSS and for the input of water quality composition of source. The exposure scenario is defined by the material of construction and exposure conditions.

The calculations are run in the model to generate the fitness for use report of quantitative outputs (calculated indices and ranges for scaling, fouling and corrosion related to the water quality hazards of relevance). This allows the user to assess if the risk is an acceptable one in the specific context or to reduce the risk factors identified to an acceptable level.

4.6.3 Tier 1

Tier 1 requires very little input from the user and presents the water quality requirements for industrial water use with an account of associated risk to the material construction of the processing/manufacturing infrastructure in reference to the water quality problem of concern. It can be considered somewhat equivalent to 1996 generic guidelines. Tier 1 assessment does not involve any calculation methodology and contains specific literature-based information about water quality constituents of relevance to hazard characterisation and potential adverse effects. Ranges of threshold limits are presented in terms of the four-level categorisation from an ideal water quality (safe level) to an unacceptable level (highest risk level). Tier 1 however does allow for an input to be made by the user to indicate the material of construction of the processing/manufacturing infrastructure if this is known.

5.0 TECHNOLOGY DEMONSTRATOR TOOL

The prototype DSS design presented as the outcome of this project reflects the modelling and corresponding calculations discussed in the previous sections and supporting technical information document. Much of what has been presented is viewable in the User Interfaces of the DSS in a user-friendly manner. This is best viewed by engaging with the prototype DSS provided with this final report.

An overview of the system flow is provided in Section 2.0 with the figures below providing the core interfaces to the DSS functionality.

5.1 Use and Application

When the DSS Tool is launched, the user is presented with the tool's home interface. This landing page provides links that direct users to background information and project support. The DSS home page allows the user to connect to the relevant level of assessment they wish to access. Each level of assessment requires additional user inputs to assess the risk outcome involved. Input parameters for each tier is filled sequentially to generate a report. The Python software is linked to an internal database that it extracts data from. The Python software also has inbuilt calculations within its coding framework which is used to determine the outputs of the tool. A user interface is also developed within the Python framework through which the user can enter site-specific inputs and make a range of selections specific to their scenario of interest. The tools reporting takes place within the software as well as the option to export PDF files of the results.

5.2 The Home Page

The home page is illustrated in Figure 4. On this page, the user will have the option to choose between the two different assessments to obtain the required guidance on water quality for industrial use. The different assessments are (i) Water Quality Requirements and (ii) Fitness for Use Assessment. Each assessment tier requires additional information (User input) to assess the risk outcome involved in the industrial use of the water. The home page also provides the user with the following options a ‘Help’, ‘About’, ‘Background Information’ and ‘Quit’ button.

The functions of these buttons are listed below.

- ‘Help’ button – The help button option provides the user manual for this tool.
- ‘About’ button – The about button provides the user with information about the tool development such as the version number, developers and operating system.
- ‘Background Information’ button – The background information button provides supporting information of the risk-based approach and the calculation methodology applied to calculate the indices used to make quantifiable predictions.
- ‘Quit’ button – This button allows the user to exit the application.

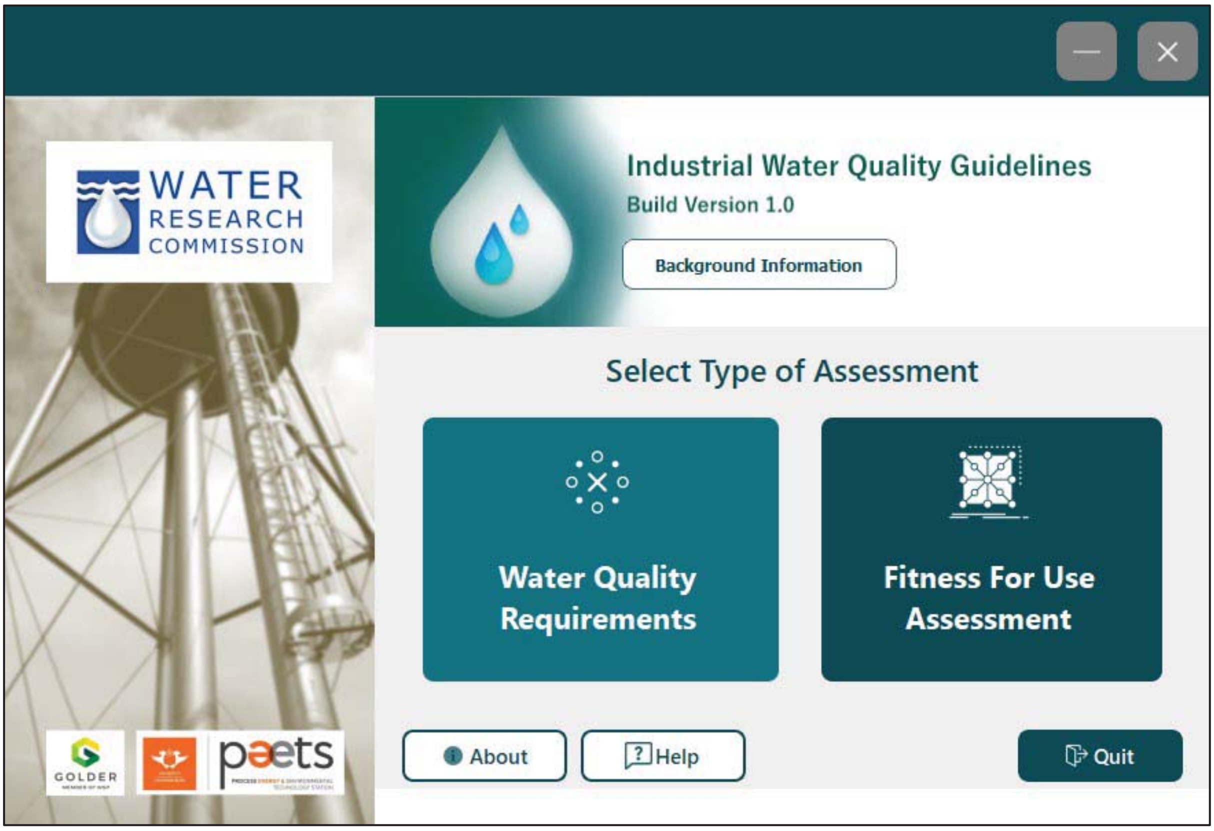


Figure 4: DSS Tool Home (Landing) Page

5.3 Water Quality Requirements Page

Upon the selection of the water quality requirements assessment analysis from the Home Page, the, the home page will automatically close, and another user interface will open allowing the user to set the material of construction of interest (Figure 5). Only one material of construction can be assessed at a time. However, should the user be unsure of this site-specificity detail, and the option of 'All' can be selected. The drop-down menu details the different materials of construction that can be analysed.

This tier is designed for a basic evaluation and considers minimal site-specific inputs. Due to the low level of complexity at this tier, the calculation's primary function is to sort the data into a clear format and export it to the report worksheet. This tier's calculation sheet matches the material of construction data selected by the user (one or all) to the constituent database in the reference sheets. The data is extracted and displayed in water quality requirements reporting worksheet. If the user wishes to return to the home page, the 'Back' button is clicked. This will close the water quality requirements assessment and return the user to the Home Page.

Once the material of construction is selected, the user selects the 'Proceed' button. The program will use the previous inputs to generate the Tier 1 report screen (Figure 6). Here the user can view the relevant material of construction, the guideline value for that specific material and the associated risk as well as the treatment recommendations to reduce or mitigate the risk. The user has the option to save the report as a PDF document by selecting the button ‘Export to PDF’ on the bottom left. The ‘Back’ button will direct the user to the previous page to select the material of construction.

If the user wishes to return to the home page, the ‘Back’ button is clicked. This will close the water quality requirements assessment and return the user to the home page. As with the Home Page, a ‘Help’ button is provided to assist the user. The functions of the ‘About’ and ‘Background Information’ tab will have the same information as explained in the home page.

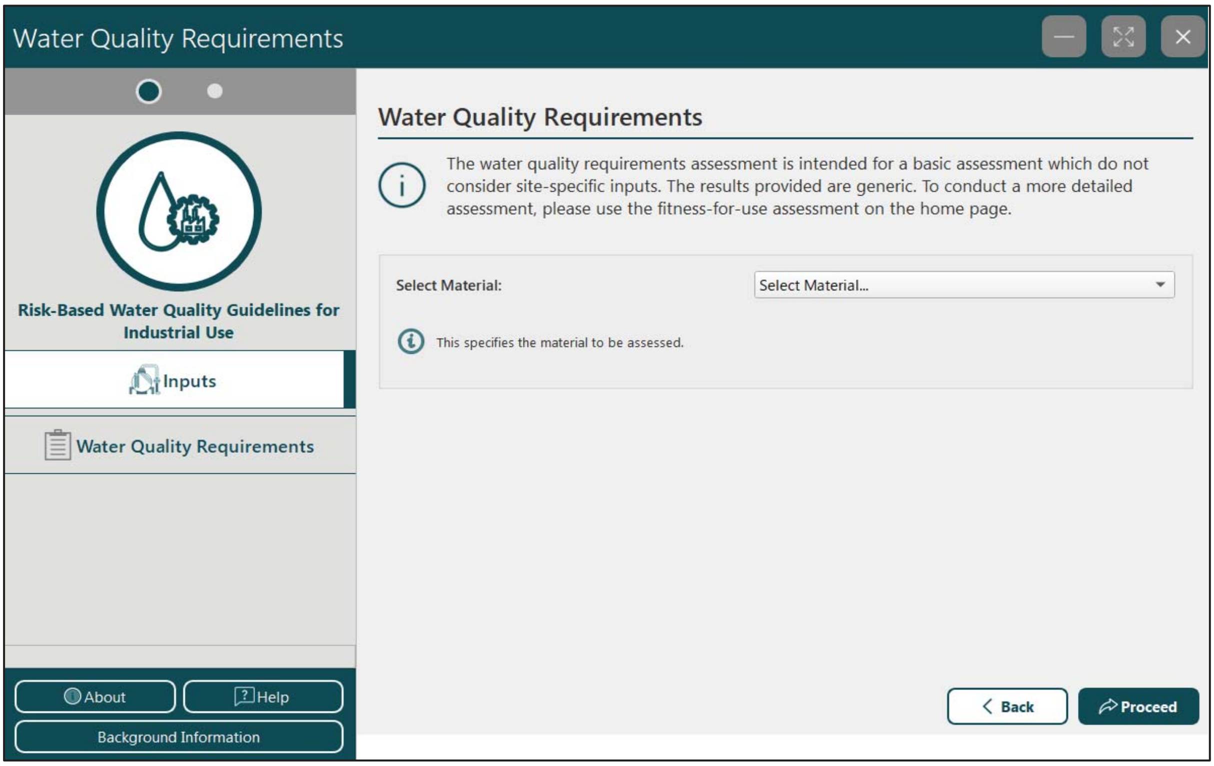


Figure 5: Water Quality Requirements Landing Page

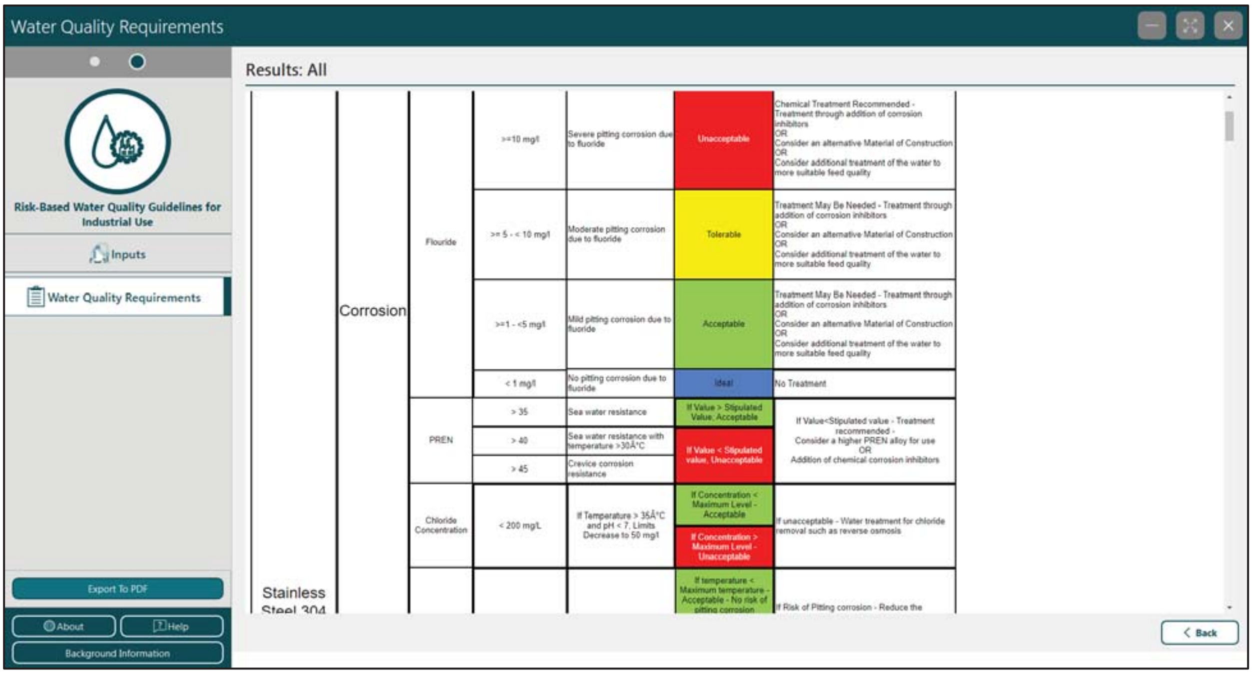


Figure 6: Water Quality Requirements reporting page

5.4 Fitness for Use Assessment

Should the user select the Fitness for use assessment from the home page (in Figure 4) the application will direct the user to the fitness for use site-specific input page (Figure 7).

This tier incorporates the user's input data, such as the user's information, water sample's composition, the concentration of constituents or operational conditions and material of construction. Thereafter, the risk is assessed and the probability of the effect is calculated using the respective calculation methodologies or rules of thumb. Here, the program differentiates between the different materials of construction and uses the appropriate equation to quantify the risk based on a site-specific water quality. For example, if concrete is selected as the material of construction, the parameters that would specially cause harm to concrete such as sulphate will be analysed. The risk of sulphate attack on concrete will be reported back to the user in the output report.

If the user selects stainless steel, the program will apply the inputted concentration to the risks of corrosion, scaling or fouling in stainless steel systems. As these risks are derived through different formulae, the output report sheet will deliver the risk of certain contaminants on different materials of construction. The information is collated under the fitness for use reporting worksheet with the risk probability and the risk level (defined as ideal, acceptable, tolerable and unacceptable).

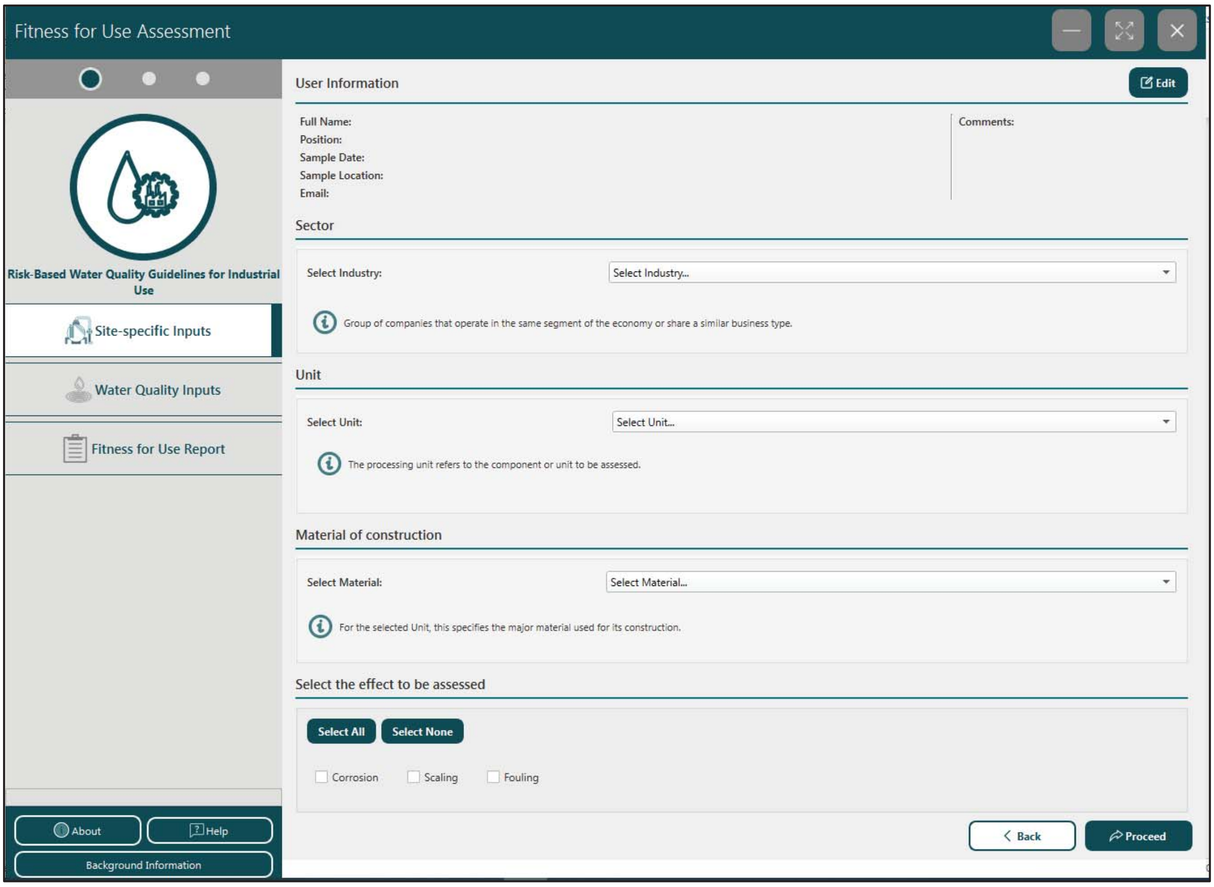


Figure 7: Fitness for Use Landing Page

Input and Edit User Information

The "Edit" button (shown in Figure 8) allows the user to edit and input information about the user. This includes information such as the user's name, position, sample date, sample location and email address. This field is optional and can be left blank depending on the user preferences. The comments section can be used to document any additional information that the user would like to input.

Site-specific inputs

The site-specific inputs section on the assessment page (displayed in Figure 9) includes three different categories which include the sector, unit and material of construction.

i. Sector – The Sector category allows the user to select (from a prepopulated drop down) an industry that the user wishes to assess. Information details are provided detailing the definition of an industry.

ii. Unit – Upon selection of the industry the user will be required to select a process unit for that specific industry (Figure 10). Should the user select any of the following process units – Dam, Reactor or Tank, the user will be prompted to select if these units are lined or unlined. By selecting the lined option, a prompt message will pop up instructing the user to contact the liner supplier as having a liner provides some sort of protection against harsh water qualities. The tool has not been designed to assess the impact on the lined infrastructure. Should the user tick the unlined option for these process units, this will allow the user to proceed with the water quality inputs assessment page.

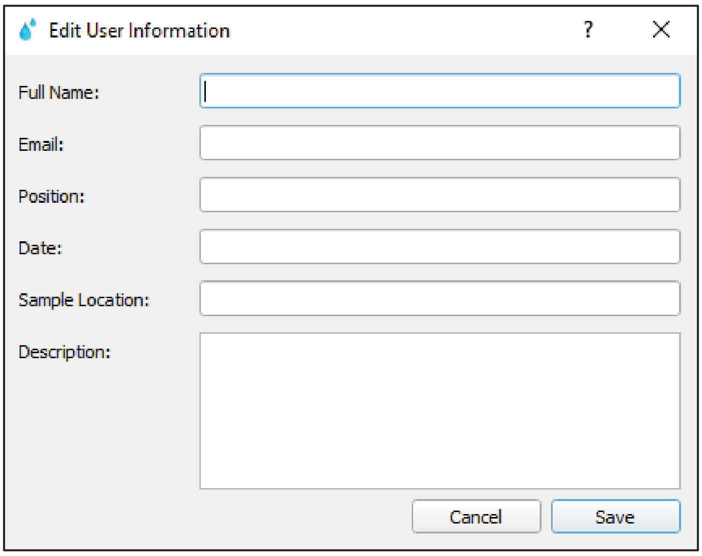


Figure 8: Edit User Information Input Screen

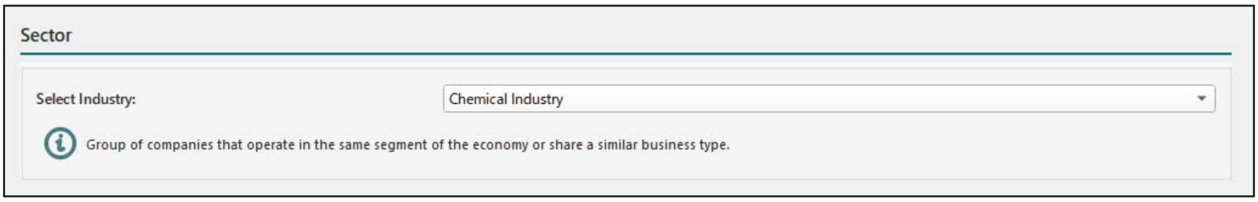


Figure 9: Sector drop down

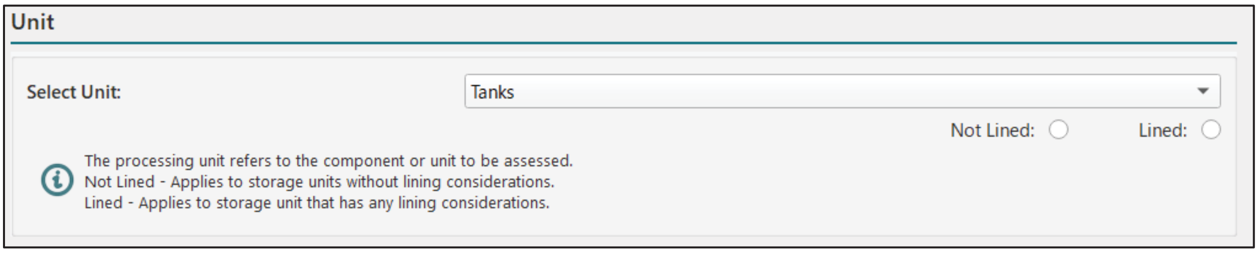


Figure 10: Process Unit Drop down

iii. Selection of Effects to be Assessed: The user will then be required to select an adverse effect (as shown in Figure 11. The adverse effects include corrosion, scaling or fouling. The user also has an option to assess all three adverse effects by clicking the “Select All” button. The user can select the “proceed” button to continue with the assessment or return to the home page by selecting the “back” button.

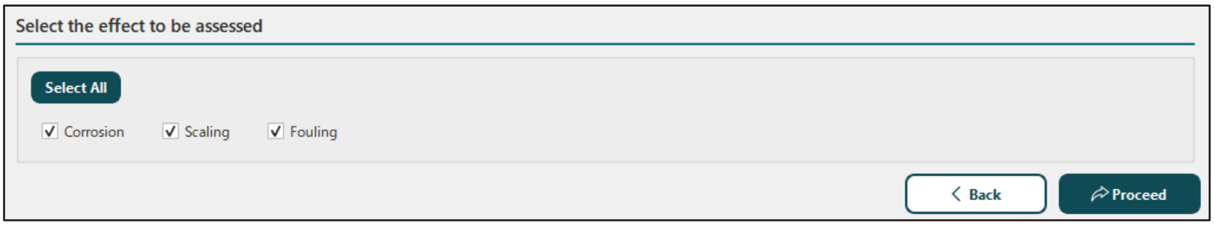


Figure 11: Selection of effects

The site-specific inputs mentioned above (i), (ii) and (iii) are required fields and will need to have populated fields to proceed to the water quality inputs page. If these fields are not specified various “pop up” messages will be displayed on the screen which will specify which field the user will need to fill in.

Water Quality Inputs

Once all the site-specific inputs are inserted, the water quality sample composition inputs need to be populated (Figure 12). The assessment details present a summary of the inputs on the previous page. The user will be required to input the water quality data that they wish to assess under the inputs category. These inputs can be site specific of pre-loaded from the default water type list. The water default types include brackish, sea, surface, ultrapure and potable water. Alternatively, the user can select a pre-loaded water type and edit specific values. Once the user has entered their input data, these values can be saved by selecting the ‘Save’ button at the bottom of the page. The required inputs will vary depending on the assessment type and material of construction.

Limits do exist for the inputs of certain parameters, i.e. the pH range is specified at 0-14. The tool will not allow insertion of a value outside of this range.

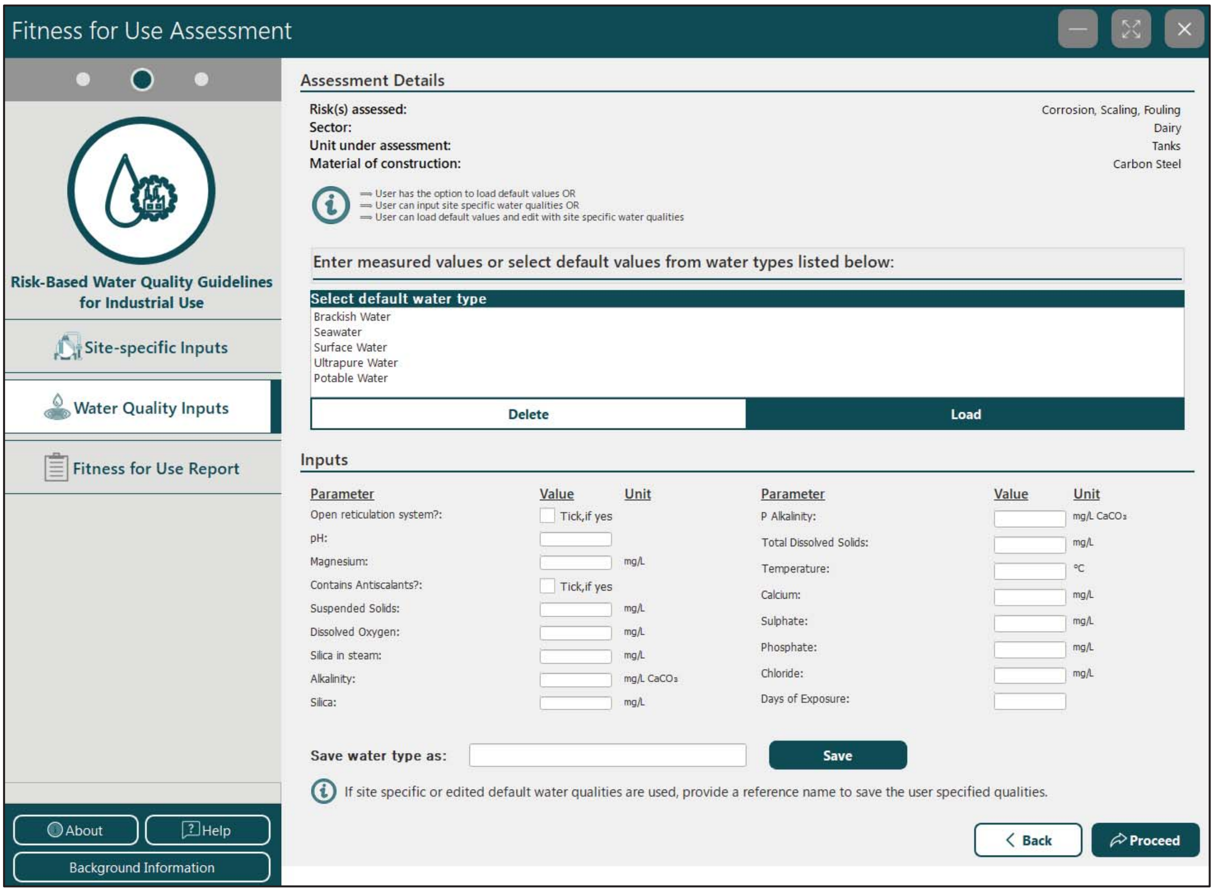


Figure 12: Water Quality Inputs

It is accepted that the user may not have values for all the required inputs. In this case, the assessment will still continue, however, the results will be limited. In the case whereby the assessment cannot continue, a 'pop up' message will appear prompting the user to insert a value under the required parameter. Such an example is shown in Figure 13. The user can then select 'OK' and return to the previous screen in order to input the missing values. In the case of the optional parameters, the user has the option to continue the limited assessment or return to the previous page in order to insert the missing value. The pop up in red indicates the required parameters whereas the pop up in orange indicates the optional parameters.

Once all the water qualities inputs are inserted, 'Proceed' will generate the fitness for use report (Figure 14). The results tab presents a summary of all the parameters inserted in the previous screens such as the site-specific assessment criteria, the water quality inputs as well as the user information.

The results for the corrosion, scaling and fouling are shown under the respective tabs. The parameters assessed, units and the value are displayed along with the description of the risk and the treatment recommendations. The fitness for use report can be exported as a PDF by selecting the appropriate button on the bottom left of the output screen (Figure 14).

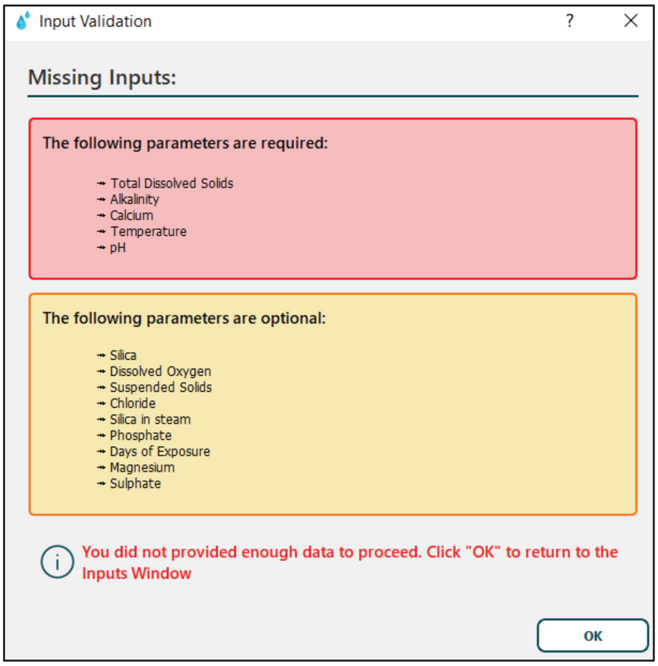


Figure 13: Input Validation Pop Up

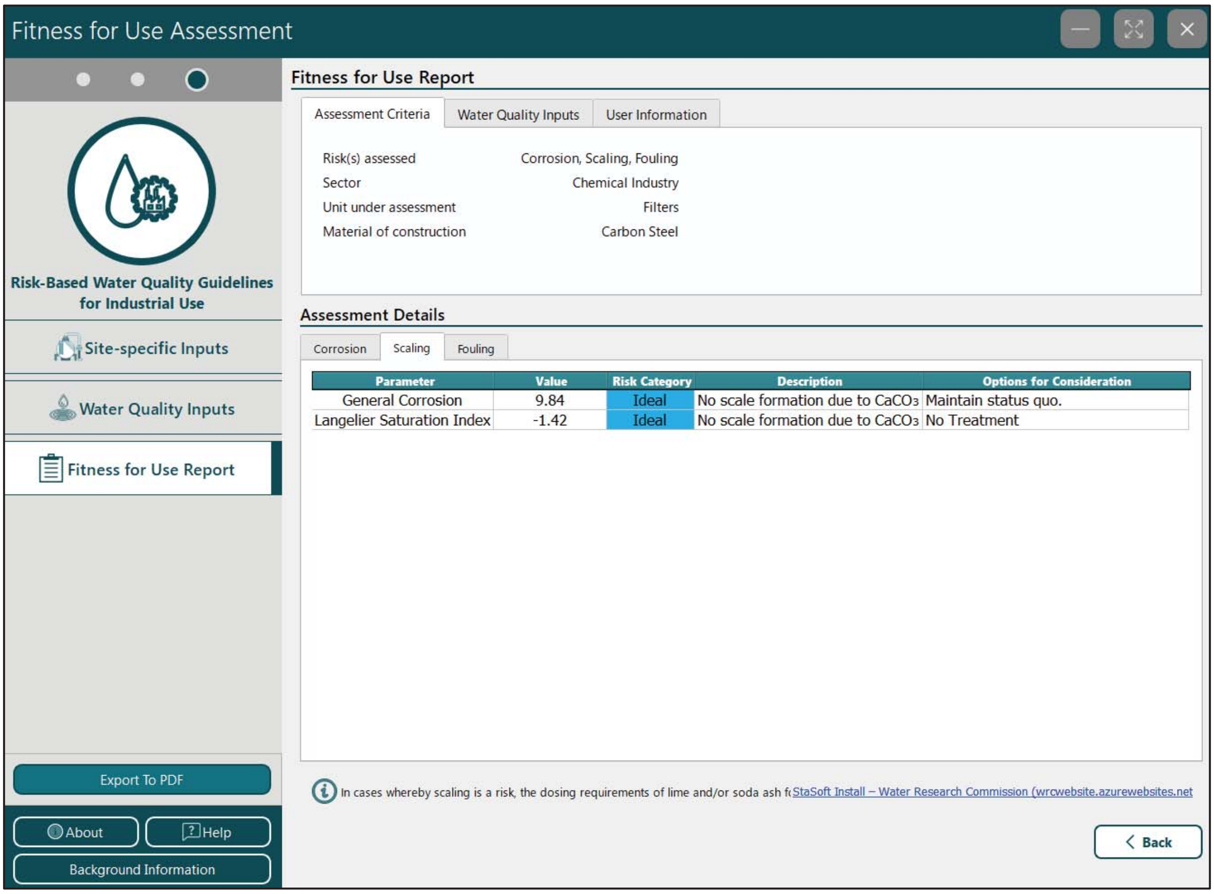


Figure 14: Fitness for Use Output Screen

5.5 Output Evaluations

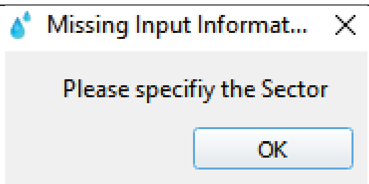
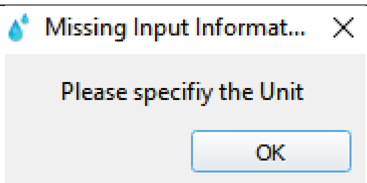
To conduct each computation, the DSS examines numerous datasheets. These reference sheets provide material-specific data, necessary computations, treatment recommendations, and adverse effect endpoint descriptions generated from literature-based scientific data and calculation methodologies. Each water quality constituent and adverse effects linked with industrial water use and material of construction usage has its reference sheet ad calculation methodology. End users cannot view these reference sheets because they are hidden. These will however be accessible to Tier 3 users and would be password protected.

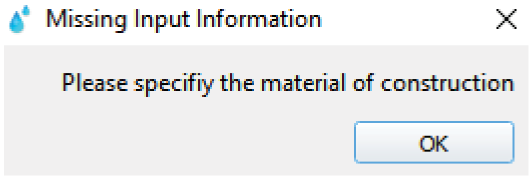
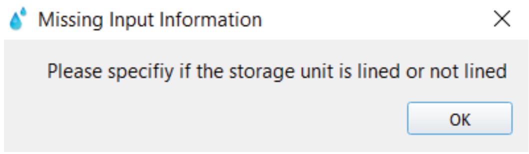
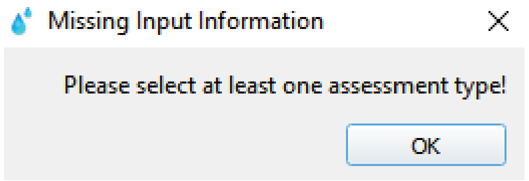
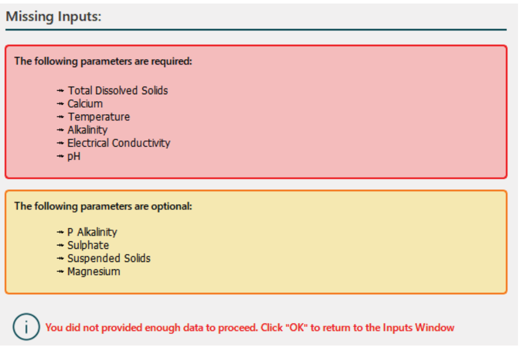
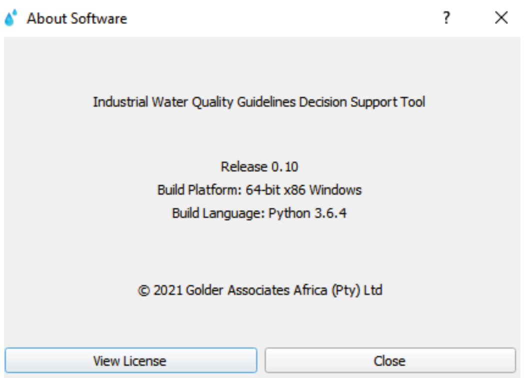
The reference sheets contain the range of threshold criteria for each index and/or variable for each material of construction and the factors used to evaluate exposure. When the user enters water quality and site-specific inputs, the DSS tool performs predictive calculations in respect of the likelihood of the adverse effect and presents the results of the assessment as a potential risk and recommendations as applicable.

5.6 Pop-Up Messages

The following table (Table 26) highlights the tools pop up messages, the explanation of these messages and how to proceed using the tool.

Table 26: Summary of pop-up messages

Pop Up message	Tool Display	Explanation	Troubleshooting
Missing Sector Input		The user has not specified an industry sector.	Select an industry from the “Select Industry” drop down list.
Missing Unit Input		The user has not specified a process unit for the specific industry sector.	Select an industry from the “Select Unit” drop down list.

Pop Up message	Tool Display	Explanation	Troubleshooting
Missing Material of Construction		The user has not specified a material of construction type for the specific unit.	Select a material of construction from the “Select material” drop down list.
Missing selection of lined units		The user has not specified if the units is lined or not lined.	Select “Lined” or “Not Lined”
Missing Adverse effect assessment		The user has not specified a type of adverse effect they wish to assess.	Tick either the corrosion, scaling or fouling adverse effects tick box or click the “select all” button.
Missing water quality input parameters		The user has not specified the input parameters that are required (red box) or optional (orange box) for the reporting assessment.	Input the required missing inputs for a limited reporting assessment or input all required and optional inputs for a full reporting assessment.
“About” button		Provides user with information about the tool.	User could view license or close the pop-up message.

6.0 CONCLUSION AND RECOMMENDATIONS

The intention of the guideline revision was to present a product that provides a series of tiered assessment levels to support a greater diversity of guideline use which facilitates risk-based assessments on the fitness for use of water for industrial applications. The fundamental objective is to assist decision making by improving the science behind the assessments. The objective has been achieved through this research project, by the development of a risk-based approach and site-specific methodology for assessing water quality requirements and fitness for use of water for industrial use within the scope of the intention of the SAWQGs series. The driving motivation behind the development of a DSS is to improve the accuracy with which water quality effects are predicted and assessed. The DSS is a user-friendly, self-contained system that incorporates the key features of risk and site specificity to provide risk-based guidance on water quality used for industrial use, using Python as the development platform.

For purposes of meeting the objective of this project, a risk-based concept presented for industrial water use has relied on available literature based scientific data, material of construction as the exposure scenario and the identified water quality adverse effects of significant concern to the sector in general.

- The tool assesses water quality risk related to scaling, corrosion and fouling as the key adverse effects related to industrial water users.
- The tool considered the most common types of material of constructions applicable to the major industrial water user sectors.
- The tool is set up in SI units.

This has sufficed in presenting a concept approach and technology demonstrator (prototype). The approach and functionality for similar hazards and effects can be added to the modelling approach as the DSS model is developed further.

The following must be noted as limitations of the tool –

- The tool has not been designed to assess the impact on lined infrastructure.
- The tool does not assess the impact or interaction of other chemicals in contact with the specified material of construction – i.e. the effect of other reagents.
- The corrosion rate is only predicted for carbon steel.
- The tool does not consider specific process operational conditions such as velocity or pressure amongst others.
- With regards to fouling, biological fouling has not been considered. Furthermore, the effect of the suspended solids particle densities and liquid viscosity has not been accounted for, i.e. the variables stated in Stokes Law.
- Guided mitigation and treatment recommendations are provided but not a definite solution and expert advice is recommended

The risk-based methodology and DSS may be built upon by further research and development work to consider other risk factors to the assessment as well other water quality adverse effects. The limitation is generically applicable literature based scientific data to support the risk analysis. This could possibly be addressed through more in depth detailed data mining and to carry out research to collect the necessary data.

It is well accepted that water quality problems within an industrial process or operation can often be addressed through some form of engineered solution. Thus it is the intention that this decision support tool serve as a platform for industrial water users to account for probability of the water quality risks that could manifest and contribute towards improved and informed decision making regarding the timing, implementation and design options of the engineered solution or operational interventions. In addition the tool does serve to guide the novice or intermediate user on the water quality requirements to manage the key water quality problems. As a volume of the suite of the South African Water Quality Guideline Freshwater Series, the guideline is primarily intended to guide the fitness for use assessment for the more common adverse water quality effects associated with industrial water use.

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