FINAL REPORT

FAILURE ANALYSIS SIMULATION MODEL FOR THE APMRD–II
(Phase 1)

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Failure Analysis Simulation Model for the APMRD-II

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Executive Summary

Context. The Nuclear Waste Management Organization (NWMO) was formed with the mandate to provide recommendations for the long-term management of used nuclear fuel. Given the current state of Canadian technology, the construction of a deep geological repository to contain and isolate waste fuel has been retained as the best management option.

The success of this structure is critical, but it obviously cannot be tested as a whole before being in use, and it cannot be maintained once built. A number of technical issues must also be considered by the designers in order to minimize the associated risks (since all physical systems fail, given a long-enough horizon): in particular, the environment and materials involved are volatile and behaviours are difficult to predict.

Due diligence requires more than the belief that the repository structure will not fail: quantitative information about the failure aspects of the structure must be provided, in order to understand the necessary and sufficient conditions for failure or non-failure within a certain time range. This requires examining various scenarios (involving interactions between various processes) in order to obtain associated failure time probability.

Objectives and Problems. In the absence of an ideal testing scenario, we take the position that understanding and quantifying the failure of the system as a whole can be carried out by

- understanding and quantifying the failure circumstances of the system components
- understanding the causal relationships between these components
- creating models of the system as a whole based on these relationships
- determining the failure circumstances and probabilities of the constructed structure level models
- transferring these findings over to the structure itself.

In theory, this results in estimates of the failure circumstances and probabilities of the actual engineered structure as a whole. In practice, even if failure parameters can be simulated using a combination of physical testing and modeling, the system's complexity may play havoc with the ability to stitch back together too high a number of system components to obtain sufficiently accurate insights into the behaviour of the structure at large. Efforts to create high detail system models, such as the US model of Yucca Mountain, have run into challenges for this reason (see Lu and Mohanty 2001, and the Third Interim Report Total System Performance Assessment Peer Review Panel, 1998).

One of the stated objectives of this project was to gain a deeper understanding of the repository system, its major components and processes. Another crucial goal is to introduce the study of interactions between various processes. Causal network models can shed some light on the topology of components' interactions and on emergent system properties (that is, system properties which can not be derived on theoretical grounds from the isolated study of each component).

For instance, it is possible to study the effects of corrosion or load transfer on the UFC separately (e.g. Smart 2009, Nasira et al. 2013) – but what effect might the presence of a through-wall or thin-wall defect have on the corrosion process on the UFC's surface in the presence of various such as glaciation profiles? In any system with a sizeable number of such components, there will necessarily be a large number of causal chains to identify and study; in this report, we will attempt to build a methodology to study such interactions using a single prototype chain.

Since the state in which UFC are found in the repository is also likely to play a determining role in the interaction effects, we will also develop a stochastic model to help predict the likelihood of through-wall and thin-wall defects (among others). However, due to the a dearth of concrete data concerning the manufacturing process (probability of failure at various stages, distributions, etc.), we focus on a simplified model for which inputs can eventually be collected by the NWMO.

As a final objective, we will also attempt to locate where potential technical bottlenecks arise, such as:

- what time step length should be used (1 year, 10 years, 100 years, 1000 years, logarithmic time scale, etc.)?
- how to rein-in model complexity in relation to system complexity (modeling states instead of actions, using blackbox process rates instead of complicated physical models, etc.)?
- what simplification assumptions must be made in order to strike a balance between manageability (small number of parameters) and obtaining valuable insight from the prototype (applicability)?
- are there any technical issues which could prohibit the extension and generalization of the prototype to the entire system (running time required to generate enough simulations when exploring parameter spaces or when building marginal distributions, etc)?

Results and Analyses. Further details can be found in the report itself, in Sections 2, 3, and 4.

Data Collection and System Complexity. A number of NWMO documents were parsed to construct a structured database of components, leading to the identification of relevant items:

- chemical processes – galvanic corrosion, anaerobic corrosion, steel wall reduction, material transfer through bentonite buffer box, placement room environment evolution, bentonite material structure transformation, copper wall reduction
- mechanical processes– glacial loading process, UFC deformation process
- social/ecological + mechanical processes – manufacturing process, transportation process, placement room creation process.

Any serious study of the failure conditions of the system should at least consider those processes.

Prototype UFC Manufacturing Model. The used fuel container (UFC) manufacturing chain explores the relationship between various UFC states (such as poor tensile strength of the steel making up the UFC's components, or the adhesion properties of the copper coating which is electrodeposited onto UFC segments, to name but two) and the likelihood of unidentified flaws at a one stage introducing subsequent flaws in later stages, and whether these subsequent flaws remain masked, eventually leading to through-wall or thin-wall copper coating defects.

Our modeling approach incorporates three mechanisms:

1. Generating values for the state variables (container dimensions, surface finish roughness, copper coating minimal depth, etc.), whether with flawed or acceptable parent states. This step requires some approximate knowledge of the essential variable distributions (target copper coating depth, spread in weld material brittleness from UFC to UFC, etc.), as well as of the effect that undetected flaws can have on those parameters.
2. Determining whether the variables generated by the previous mechanism fall within their acceptable range. This step requires a good understanding of what the various acceptable ranges (smaller than some value, between two values, above some value) for each of the state and variables, but are not affected by undetected defective parent states.
3. Determining whether an acceptable UFC is correctly allowed to ultimately move on to the next stage or is incorrectly removed from the manufacturing process, or more significantly for the problem at hand, if a defective UFC is incorrectly allowed to move on to the next stage or correctly removed from the manufacturing process.

In an idealized setting, each UFC would be a True Positive at each stage, until defects appear at which point it would automatically become a True Negative. While we could accept that the classification scheme could produce False Negatives (at least, from a modeling standpoint), imperfections leading to False Positives are more worrisome.

This step requires estimates for the tolerance of the various measurement apparatus, as well as approximate probability values for ultimately correctly or incorrectly rejecting or accepting a UFC at each stage.

Both the distribution parameters and threshold values are expected to ultimately be derived from experimental data and theoretical models, while the probability values could conceivably be estimated using various quality control experimental design strategies. For the prototype, however, most of the values of the 70 or so model parameters were selected arbitrarily, yet somewhat reasonably.

A number of scenarios were simulated and analyzed, leading to two main conclusions (more details can be found in Sections 3.3 and 3.4).

- It is mainly the ratios of a certain small subset of parameters (the spread in the distribution of the variables, the length of the acceptable threshold region, and the tolerance of the appropriate measurement), together with three probability values of incorrectly accepting flawed UFCs (in the acceptable region, in the tolerance region, and in the rest) which seem to play a crucial role in the appearance of False Positives at various stages. Other parameters may also be significant, of course.
- It is not difficult to find reasonable parameter sets giving rise to non-zero probabilities of through-wall or thin-wall defects going undetected.

Granted, the conclusions cannot be made too strongly at this point since the current manufacturing model is still very much a prototype, but they are both derived from a structural form which would be preserved in any next phase model: the number of states, variables, and parameters may eventually change, as may the values used in the underlying distributions, or the parent/child links – but the basic principles would still be in place.

Prototype Modeling of Repository Interactions. The prototype model of repository interactions considered interactions between corrosion of the UFC steel wall and pressure exerted on the UFC by the surrounding environment, as well as key factors and events involved in determining corrosion rates and amount of exerted system pressure. Four model elements were used to represent relevant aspects of the barrier system: processes (e.g. galvanic corrosion), events (e.g. repository sealed) states (e.g. glacier exerting pressure on system) and properties (e.g. thickness of UFC steel wall).

Both expected and unexpected (counterfactual) scenarios were explored. The effects of varying levels of certainty associated with particular scenarios were also incorporated into the probability estimates for each scenario.

It quickly became evident that in the event of a through wall defect (assumed as a starting condition) corrosion would play a dominant role in system behaviour, interacting with, but largely eclipsing pressure effects, and, in essentially all scenarios, resulting in exposure of UFC contents. However, interactions between corrosion rate and probability (and certainty of occurrence) of key events were also significant determiners of system behavior and the resulting probability of UFC contents exposure over time. These results highlighted the need to thoroughly explore interactions under both expected and counterfactual scenarios, as well as the need to include certainty estimates in scenario exploration.

Evaluation and Recommendations Due to the nature of the time horizons under consideration, it is not entirely clear at this point how we would validate the prototype repository interaction model.

It may turn out that the best that can be hoped for in that regard is the appearance of emergent properties of the causal network, which could lead the NWMO to recognize certain correlations that were not originally on the radar, or certain interactions that radically alter the failure propagation mechanisms.

Another proxy may be to apply this causal modeling approach to a system of similar complexity, also with interacting components, but for which evaluation and verification are more easily available.

At the same time, failure curves do not live in a vacuum. In any modeling endeavour, we necessarily introduce a large number of simplifying assumptions. Different interaction scenarios give rise to different failure curves; it may be the differences between those curves that end up providing insightful sparks.

On the other hand, evaluating the manufacturing process model should prove significantly easier, if only because the process it models takes place over a shorter-term horizon.

The prototype has shown promise, and it has a structure which can be expanded in a fairly straightforward manner, but the question of what constitute reasonable parameter values still looms large at this stage. Future experiments may provide more information.

The ultimate goal for an exercise of this nature is to provide NWMO stakeholders with a detailed idea of the risks associated with the construction of the proposed repository structure; possible failure circumstances and probability estimates involving system component interactions (instead of a simple yes/no statement such as “No, the structure will not fail”) would go a long way towards providing the necessary information.

While this endgame is still out of reach at the current stage, we have established a causal network methodology that could, in theory, be used in combination with appropriate access to subject matter expert resources and sufficient computing power to explore various complex scenarios in an insightful manner.

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1 Introduction

Canada has a long history with nuclear power: the first self-sustained Canadian nuclear reaction was achieved at Chalk River's ZEEP reactor in 1945. Over the years, numerous research reactors and power reactors have been built and decommissioned – as of 2014, electricity is currently being produced by 19 CANDU reactors in Ontario and New Brunswick. Given that the existence of high energy nuclear waste in Canada is a *fait accompli* – we have already chosen, as a society, to use nuclear power and create nuclear waste – it is paramount that we find ways to safely dispose of this waste.

In 2002, the Nuclear Fuel Waste Act (NFWA) was enacted to study possible strategies for the management of Canada's used nuclear fuel. As a result, the Nuclear Waste Management Organization (NWMO) was formed by the Canadian nuclear power companies, with the mandate to provide recommendations to the Canadian Government for the long-term management of used nuclear fuel. One such recommendation, which was accepted in 2007, was the establishment of Adaptive Phased Management (APM) as both a social and technical approach to permanently manage Canada's used nuclear fuel. Canadian citizens determined that the optimal strategy, given the current state of technology in Canada, is the construction of a deep geological repository to contain and isolate the fuel.

This decision puts the NWMO in a unique and demanding position, as it is the first group in Canada to design and build a unique but extremely performance-critical engineering structure: a long term Canadian repository for high energy nuclear waste. By its very nature, this structure as a whole cannot be tested in advance of use and essentially cannot be maintained once it is built. Furthermore, the environment and materials involved are themselves volatile and their long term behaviour is difficult to predict.

Under such challenging circumstances, engineers must do their best to use all of the expertise at their disposal to create as perfect a design as possible for the required structure. Despite the uniqueness of the structure, they need to produce a design that will meet the requirements that have been set out, and then, once built, function exactly as predicted on the first try. Such a design process is necessarily a lengthy one, involving many designers with high levels of expertise. Many designs would be proposed and rejected before a final design is selected, based on all the evidence and expertise the design team have at their disposal.

At the end of the process the engineering team will have high confidence in the final design that is put forward. The success of the structure in question is critical, and, as responsible, professional engineers, they would not put forward a design for such a structure without being entirely certain, to the best of their collective ability, that this structure will not fail.

Despite this confidence, due diligence requires more than the simple assurance (and belief) from the design team that the structure will not fail. It is not enough, from a societal perspective, for the team to simply provide a "vote of confidence:" it also requires the provision of more quantitative information about the failure aspects of the structure. Those responsible for the structure need to be able to determine (and to help the stakeholders understand) what are the structure's necessary and sufficient conditions for failure (and by extension, the conditions for non-failure). To produce these answers they need to be able to quantitatively examine what circumstances the structure might encounter, and under these circumstances, what the probability of failure is.

From an ideal testing point of view, the entire proposed structure would be built many times over to run trials relating to each of the foreseen circumstances. Data would then be gathered and analyzed to determine the failure tolerance of the structure. Failure probabilities would be calculated based on this data, along with an understanding of possible failure circumstances – the structure might even be redesigned to take into account the results of the testing.

However, as we have already noted, this idealistic testing scenario is simply not an option in this case. The structure as a whole cannot be directly tested even once, let alone multiple times. And on top of this, even were many replications of the structure itself available for testing, not all failure circumstances (in particular those involving major geological forces and long time spans) would be possible to re-create in a test environment.

An alternative strategy is centered around a combination of physical testing and modeling of the behaviour of the structure and environment. More specifically, a larger structure is built up of many component parts, which themselves may be built up of many components. The failure parameters of these component parts may be tested, even if the structure as a whole cannot.

Similarly, while the structure itself, and perhaps even in some cases the components themselves, cannot be tested repeatedly, there remains the option of creating models of the structure and components in question, and then using the behaviour of these models to predict the behaviour of the components and, in turn, of the structure at large.

In the absence of the ideal testing scenario, understanding and quantifying the failure of the system as a whole can be carried out by understanding and quantifying the failure circumstances of the components of the system, understanding the causal relationships between these components, creating models of the system as a whole based on these relationships, determining the failure circumstances and probabilities of the constructed structure level models and then transferring these findings over to the structure itself. This results in an estimate of the failure circumstances and probabilities of the actual engineered structure as a whole.

The end result of this exercise will thus be, rather than a simple yes/no statement (such as “No, the structure will not fail”, for instance), a list of the possible failure circumstances and an estimate of the failure probabilities for both the structure components and the structure itself, along with a confidence measure indicating a level of confidence in the failure probabilities calculated for each failure circumstance.

Such a table of failure circumstances, probabilities, and confidence measures will allow those building the structure to open a legitimate dialogue with those responsible for, and those being affected by, the resulting structure. In essence, this deliverable will allow the designers of the structure to provide their stakeholders with a clearer and more detailed picture of the risks they are likely to encounter when undertaking the construction of such a structure.

1.1 General Objectives

The general objective of this Failure Analysis project as a whole is to estimate the failure probability of the Mark II canister and engineered barrier system immediately surrounding the canister. In order to achieve that larger objective, we anticipate that we will be using a combination of statistical analysis, mathematical modeling, and simulations, much as in this prototype.

More specifically, we will take the approach that our model is meant to answer a specific question, as well as to provide outputs that can be fed into other models, as may be required by already-developed NWMO models.

In this prototype phase, however, the objective is to develop a methodology and implementation framework to confirm that interactions (both planned and emergent) can in principle be captured by the modeling process, both at the repository and the manufacturing level.

For both the manufacturing process and the interactions models, a specific selection of a small number of sub-components of the entire system will be considered in this phase, in order to maintain focus on the development and testability of the methodology itself.

1.2 Report Outline

The rest of this report consists of 4 sections.

- In **Section 2** (pp. 13–18), we discuss some of the strategies that could be used to extract information and knowledge about the engineered barrier system, which could then be incorporated in any interaction model of its components. A structured database of system component facts was produced (cf. Figures 1, 2, 3, and accompanying files for details).

  A discussion of system complexity and the effect it had on our choice of modeling approach is also provided.

- In **Section 3** (pp. 18–62), we present a prototype UFC manufacturing process model: potential states, actions and variables are introduced, as well as the underlying modeling assumptions and families of parameters. The model is illustrated *via* a specific parameter set; a series of 8 scenarios showcase the effect of various parameter combinations.

  It should be noted that due to the uncertainty relating the manufacturing process parameters, the numbers presented in this section mostly play the roles of placeholders: reasonable estimates for a large number of these parameters will be required before the model can output meaningful failure estimates.

- In **Section 4** (pp. 63–91), we present a prototype causal chain modeling the interactions of pressure transfer and corrosion processes **in the case of a UFC with at least 1 through-wall defect**. Various deterministic and stochastic scenarios are discussed in order to illustrate interactions between corrosion rates, system pressure and the probabilities associated with system event and states. Estimates of the probability of exposure of the UFC contents within a given timespan are presented for each of the scenarios.

- Finally, a list of recommendations is provided in **Section 5** (pp. 91–92). These recommendations are based on our (outsiders') experience learning about the proposed engineered barrier system and designing the quantitative models of Sections 3 and 4. **In particular, they are not based on physical or engineering calculations, but on stochastic models of interactions between various system components.**

2 Methodology Considerations

The NWMO has a number of highly detailed models of specific components or aspects of the barrier system (e.g. models of the stability of the rock surrounding the placement rooms, models of the rates of corrosion). However, interactions between components and processes can have significant causal effects on the behaviour of the system over all. If existing models are largely single component focused, these interaction effects may not be fully take into account.

Although, in principle, the creation of a highly detailed full system model, possibly via the amalgamation and expansion of existing component models, might allow for the most comprehensive exploration of unanticipated interactions between system components, the level of detail in a such model must be properly managed to avoid the model become both unwieldy and inaccurate. Rather than resulting in a highly detailed, highly accurate model, acceptable inaccuracies in individual model components may be magnified in an amalgamated system model, resulting in a model that has behaviours which do not realistically reflect the behaviour of the modeled system as a whole. As well, pragmatically speaking, the creation, validation and management of such a highly detailed, large scope model can quickly become infeasible. In these ways model inaccuracy, invalidity and poor-functionality become introduced into the model.

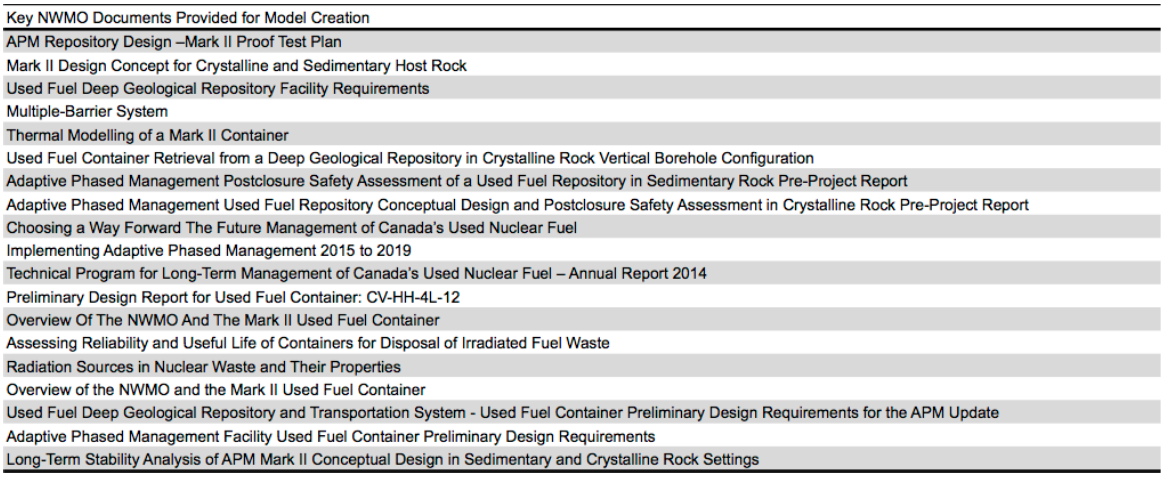
Failure Mode and Effects and Criticality Analysis (FMECA) seeks to take into account interactions between system components by eliciting possible sources and pathways towards failures of the system from subject matter experts (SMEs) via a structured interview process. Experts are also asked to estimate the possibility or likelihood of each of these pathways or failure modes. These estimates may then be used to generate a semi-quantitative failure model for the system.

Although this approach avoids both the issues that can arise from narrowly-scoped models, as well as those that may occur when attempting to create highly detailed full-system models, it also lacks one of the recognized advantages of such models- their ability to produce previously unanticipated results, emergent from the structure of the model. Given this, it would seem a hybrid approach combining the advantages of both of these strategies would be a useful step forward. A number of hybrid approaches have already been proposed (e.g. Baldwin et al. 1995, Eusgeld et al. 2011).

In order to develop a system-wide model of the engineered barrier system that can take into account relevant but possibly unanticipated interactions into account, we have also taken a hybrid approach. The resulting modeling framework incorporates process behaviours of system components (which may be modeled by outputs from existing detailed system component models) within a higher level causal framework that incorporates system event probability. The framework itself is created based on a combination of input from system experts and an analysis of documented system information.

2.1 Data Collection and System Analysis

One goal of the prototype project was to explore strategies for methodically and, when possible, automatically, extracting information about system components and component interactions, from documentation, and then systematically incorporating this extracted knowledge into the model of the system in such a way that previously implicit interactions would be captured and



Key NWMO Documents Provided for Model Creation
APM Repository Design –Mark II Proof Test Plan
Mark II Design Concept for Crystalline and Sedimentary Host Rock
Used Fuel Deep Geological Repository Facility Requirements
Multiple-Barrier System
Thermal Modelling of a Mark II Container
Used Fuel Container Retrieval from a Deep Geological Repository in Crystalline Rock Vertical Borehole Configuration
Adaptive Phased Management Postclosure Safety Assessment of a Used Fuel Repository in Sedimentary Rock Pre-Project Report
Adaptive Phased Management Used Fuel Repository Conceptual Design and Postclosure Safety Assessment in Crystalline Rock Pre-Project Report
Choosing a Way Forward The Future Management of Canada's Used Nuclear Fuel
Implementing Adaptive Phased Management 2015 to 2019
Technical Program for Long-Term Management of Canada's Used Nuclear Fuel – Annual Report 2014
Preliminary Design Report for Used Fuel Container: CV-HH-4L-12
Overview Of The NWMO And The Mark II Used Fuel Container
Assessing Reliability and Useful Life of Containers for Disposal of Irradiated Fuel Waste
Radiation Sources in Nuclear Waste and Their Properties
Overview of the NWMO and the Mark II Used Fuel Container
Used Fuel Deep Geological Repository and Transportation System - Used Fuel Container Preliminary Design Requirements for the APM Update
Adaptive Phased Management Facility Used Fuel Container Preliminary Design Requirements
Long-Term Stability Analysis of APM Mark II Conceptual Design in Sedimentary and Crystalline Rock Settings

Table 1: Barrier system documentation provided by NWMO and used as a basis for the prototype phase models

incorporated into the model behaviour. This structured knowledge would then be further supplemented and verified by system expert knowledge.

Knowledge extraction began by a preliminary pass through the system overview documents provided by NWMO (see Table 1). A high level system component schematic was created based on this review (see Figure 1), with a preliminary review by system experts to confirm that no significant system components had been neglected. The goal behind generating this system component model was to develop an understanding of parts of the system which might possibly interact with each other during system operation.

This system component model was then used to methodically extract and structure information contained in the provided documents. Specifically, facts about the system were tagged with system component labels if they provided information about these system components (see Figure 2). Facts tagged with multiple component labels could then provide support for hypotheses that these system components would potentially interact during operation of the system (see Figure 3). Information was extracted from the documents both manually and automatically, and the results of these two extractions compared. The goal of the automatic extraction was both to validate the manual extraction process and also to provide a test of feasibility of data extraction on a larger scale. The results of the data extraction were then used to generate a conceptual model of the engineered barrier system. Construction of model schematics and implemented models was supported by the structured system data.

Two stand alone models were constructed – the **barrier system component interaction** (causal chain) **model** (selected components) and a detailed model of the **manufacturing process** (see Sections 4 and 3, respectively). The manufacturing process model can also be viewed as a process that provides inputs into the system level model relating to the properties of the UFC.

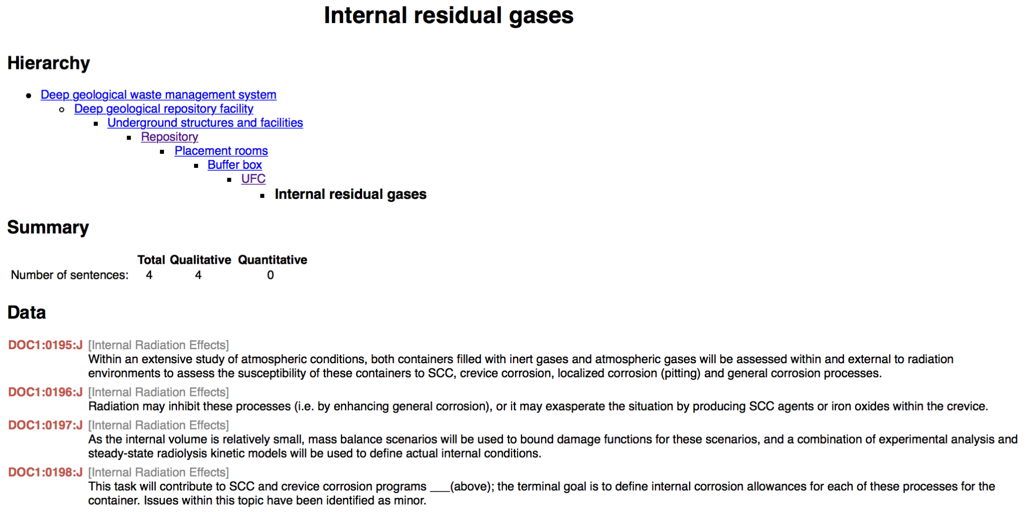
Simulations provided a relatively straightforward approach to programmatically represent the system, including complex interactions between system components. This came at the expense, however, of requiring exploration of a relatively large parameter space in order to determine system behaviour. The resulting simulation was a discrete time simulation, with the behaviour of

Figure 1: High level schematic of system components and their relationships (see accompanying file for larger figure)

each model element determined at each time step based on the states of elements in the preceding time step. Basic output of the models consisted of the system states and properties at each time-step of the model.

2.2 System Complexity

During the model development phase of this project, research was undertaken to determine which approach would be most suitable for the modeling of the engineered barrier system, generated from the conceptual model of the system that had been developed during the conceptual modeling phase. Broadly speaking, the research involved determining which combination of the two major branches of modeling – simulation models (which for greater clarity we will also refer to as programmatic models) and mathematical models – should be used. It is worth noting here that this distinction can be confusing and imprecise, as both types of models frequently employ computer code and mathematical equations. As well, it is possible for a given model to combine both methods. Nonetheless, there are some key differences in these methods.



Internal residual gases

Hierarchy

- Deep geological waste management system
    - Deep geological repository facility
        - Underground structures and facilities
            - Repository
                - Placement rooms
                    - Buffer box
                        - UFC
                            - **Internal residual gases**

Summary

	Total	Qualitative	Quantitative
Number of sentences:	4	4	0

Data

DOC1:0195:J [Internal Radiation Effects]
Within an extensive study of atmospheric conditions, both containers filled with inert gases and atmospheric gases will be assessed within and external to radiation environments to assess the susceptibility of these containers to SCC, crevice corrosion, localized corrosion (pitting) and general corrosion processes.

DOC1:0196:J [Internal Radiation Effects]
Radiation may inhibit these processes (i.e. by enhancing general corrosion), or it may exasperate the situation by producing SCC agents or iron oxides within the crevice.

DOC1:0197:J [Internal Radiation Effects]
As the internal volume is relatively small, mass balance scenarios will be used to bound damage functions for these scenarios, and a combination of experimental analysis and steady-state radiolysis kinetic models will be used to define actual internal conditions.

DOC1:0198:J [Internal Radiation Effects]
This task will contribute to SCC and crevice corrosion programs ___(above); the terminal goal is to define internal corrosion allowances for each of these processes for the container. Issues within this topic have been identified as minor.

Figure 2: Screenshot of structured database of system component facts (see accompanying files for complete database).

In the case of mathematical modeling, sets of equations are developed to describe the system, and then these sets are solved to find, effectively, all (or any) possible solutions, which then define all possible behaviours of the system. In the case of programmatic models, the behaviour of the system cannot be deduced by 'solving' the system. Rather system behaviour must be simulated, piecemeal, by setting up specific initial conditions in the system, simulating the behaviour of the system at each moment in time over a defined period of time and then reading off the results of the simulation at the end point to determine the state of the system at that end point, given those starting conditions and that passage of time.

Both approaches have strengths and weaknesses. Representing a system mathematically allows for highly generalizable conclusions to be drawn about the system. However as the mathematical representation of the system becomes more complicated, as perhaps is necessitated by the underlying complexity of the system itself, solving the mathematical system may become impractical or no more efficient than the simulation approach.

Simulations provide a relatively straightforward approach to programmatically representing the system, including complex interactions between system components, but analysis of the behaviour of the simulation is often challenging and only inductive conclusions about the system as a whole can be drawn based on the behaviour of system under specified circumstances. As well, running the system over a lengthy period of time in order to generate outcomes may be prohibitive from a computational cost point of view.

The overall conclusion from research carried out during the prototype project was that the simulation approach was most suitable for modeling the engineered barrier system, due to the fact that a major emphasis of this model was incorporating interaction effects between system components. The resulting simulation was a discrete time simulation, with the behaviour of each model element determined at each time step based on the states of elements in the preceding time step. Outputs of the model consisted of the model element states at each time step.

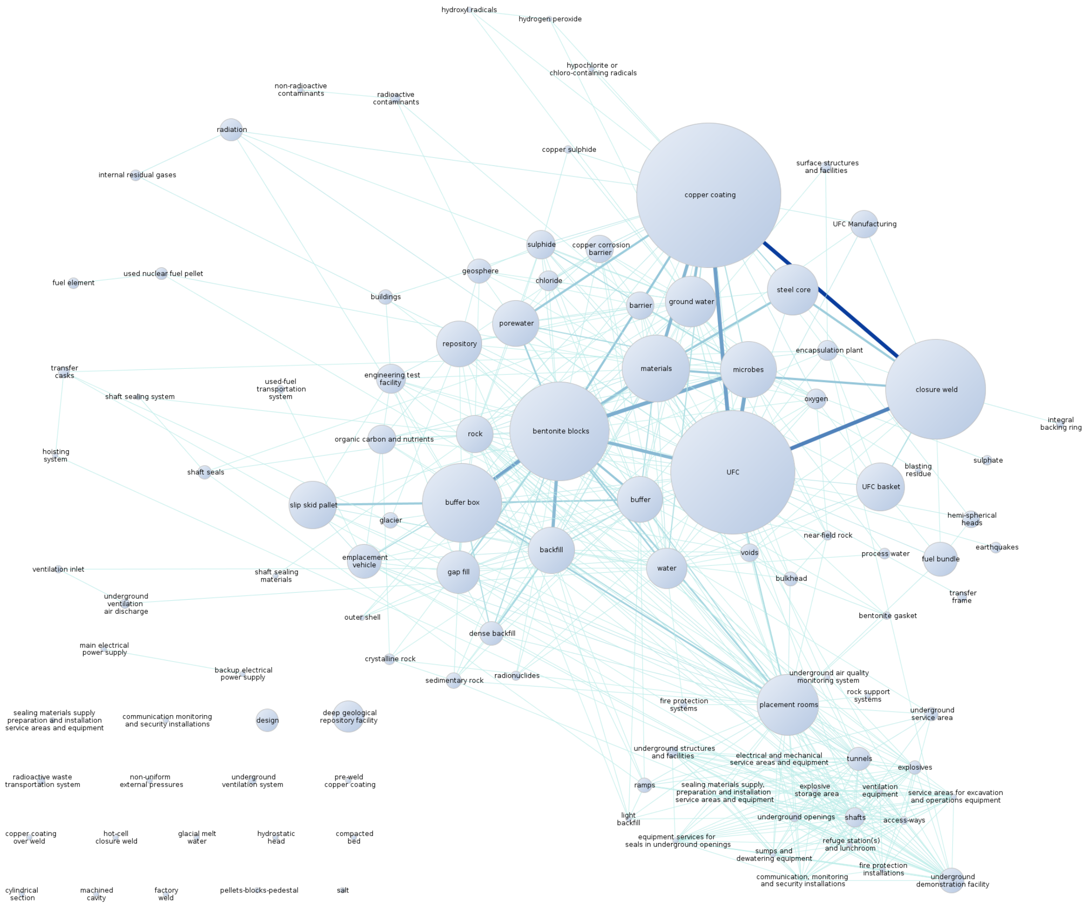


Figure 3: Bubble graph showing objects that were connected based on structured information extraction (see accompanying file for larger figure)

To deal appropriately with the complexity of the system while maintaining a manageable model, the model framework allowed for the ability to vary the level of detail of implementation, allowing for a very high abstraction representation of system, moving all the way to possible incorporation of very highly detailed models, all within the same implemented structure. Detail could be added or subtracted if it were determined that representing interactions required either a greater level of detail, or if components of the model could realistically be further simplified. Some structural elements were also incorporated in order to allow for the exploration of counterfactual scenarios- (i.e. in the absence of knowledge about what could cause a particular event to happen, it is still possible to consider the effects if it were to happen at a chosen point in time, and determine the potential consequences to the system).

References

- Baldwin, James F., Martin, Trevor P. and Athena Tocatlidou (1995). Uncertainty management in radioactive waste repository site assessment. Fuzzy Sets and Systems Volume 74(1), pp. 81-91.
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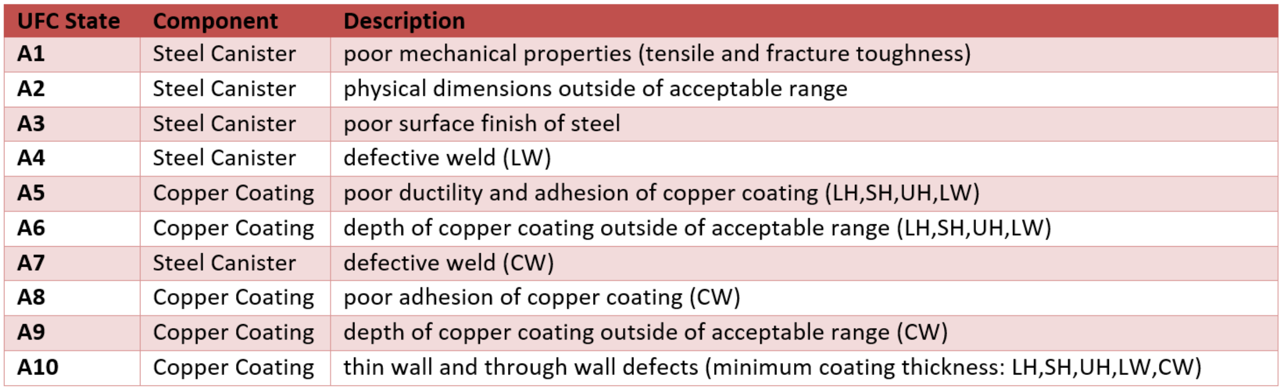


UFC State	Component	Description
A1	Steel Canister	poor mechanical properties (tensile and fracture toughness)
A2	Steel Canister	physical dimensions outside of acceptable range
A3	Steel Canister	poor surface finish of steel
A4	Steel Canister	defective weld (LW)
A5	Copper Coating	poor ductility and adhesion of copper coating (LH,SH,UH,LW)
A6	Copper Coating	depth of copper coating outside of acceptable range (LH,SH,UH,LW)
A7	Steel Canister	defective weld (CW)
A8	Copper Coating	poor adhesion of copper coating (CW)
A9	Copper Coating	depth of copper coating outside of acceptable range (CW)
A10	Copper Coating	thin wall and through wall defects (minimum coating thickness: LH,SH,UH,LW,CW)

Table 2: Manufacturing process model – States

3 Prototype Modeling of the UFC Manufacturing Process

Throughout, we assume that N containers are taken through the manufacturing process, independently of one another.

The UFC Manufacturing Process model requires inputs in four categories:

- **Model structure**: states, actions, essential variables, parent/child links
- V **parameters**: parameter values and ranges to determine the essential variable output values for each state
- A **parameters**: threshold values which determine the state value for each state
- R **parameters**: parameter values and ranges which determine whether unacceptable state values are accepted or rejected by the various tests.

There are 2 main applications for the prototype's use: exploring the parameter space, and running multiple simulations with a single set of parameters to determine intrinsic variability (which could be used to indicate the absence of crucial variables). In this report, we will mostly focus on the second application.

3.1 Manufacturing States, Actions, and Variables

The prototype model consists of 10 states (see Table 2), characterized by 50 variables (see Table 4), and linked according to the schematics shown in Figure 4. The UFC is assembled state-by-state (and step-by-step), following a series of manufacturing actions (both external and internal); after certain specific actions, some non-destructive examinations of the UFC components are conducted and non-compliant components are re-sent up the chain for repairs or, presumably, to be removed from the process if they have suffered irreparable damage at a prior stage (see Table 3 for a list and Figure 5 for a visual representation).

Actual state values (denoted by A_i throughout) are given **as of the last time a given state is tested during the manufacturing process**. Consequently, the value of A_i may be recorded after any number of times the UFC has been re-sent for repairs; this number includes the possibility that the UFC is never sent for repair at a given stage.

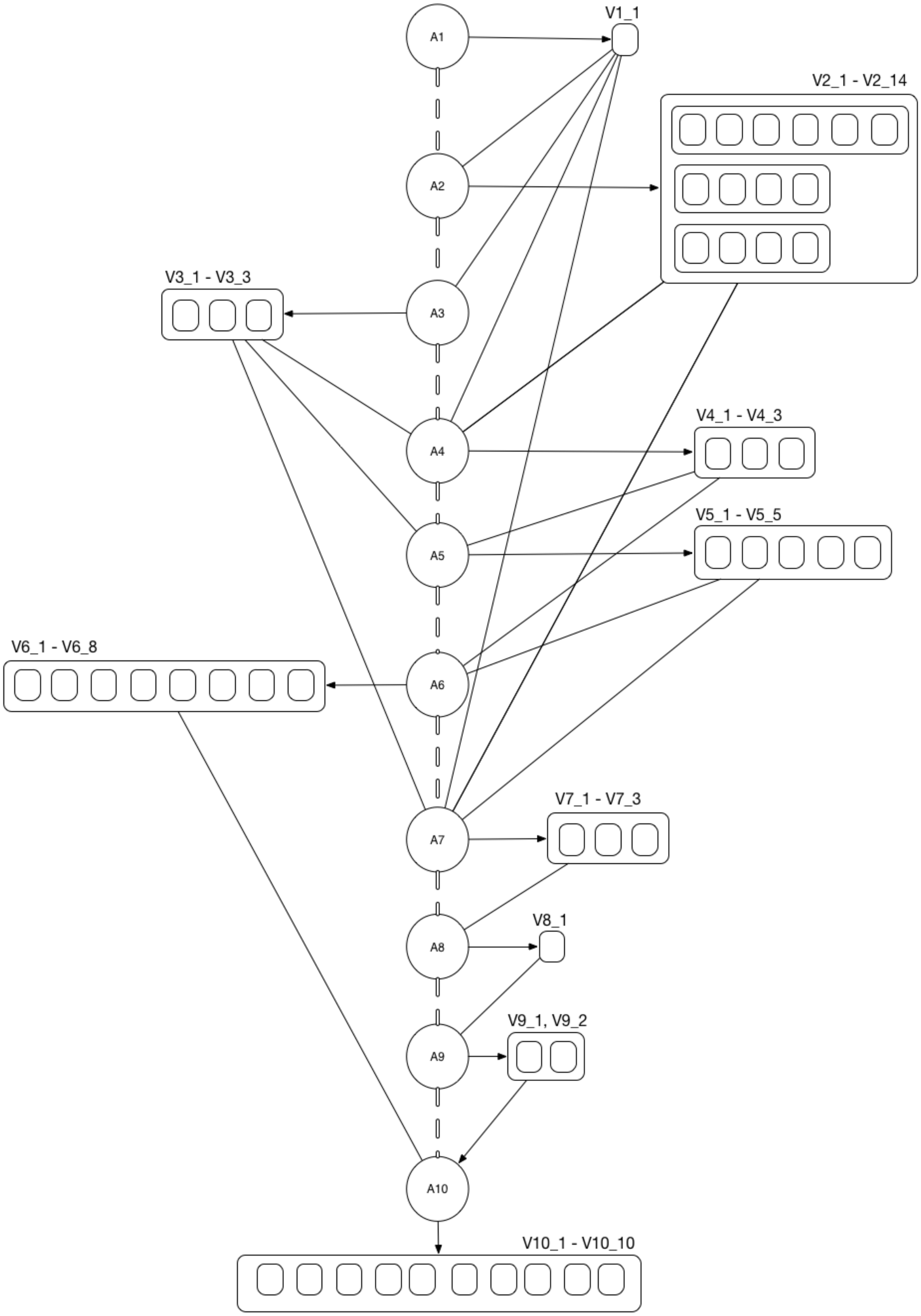
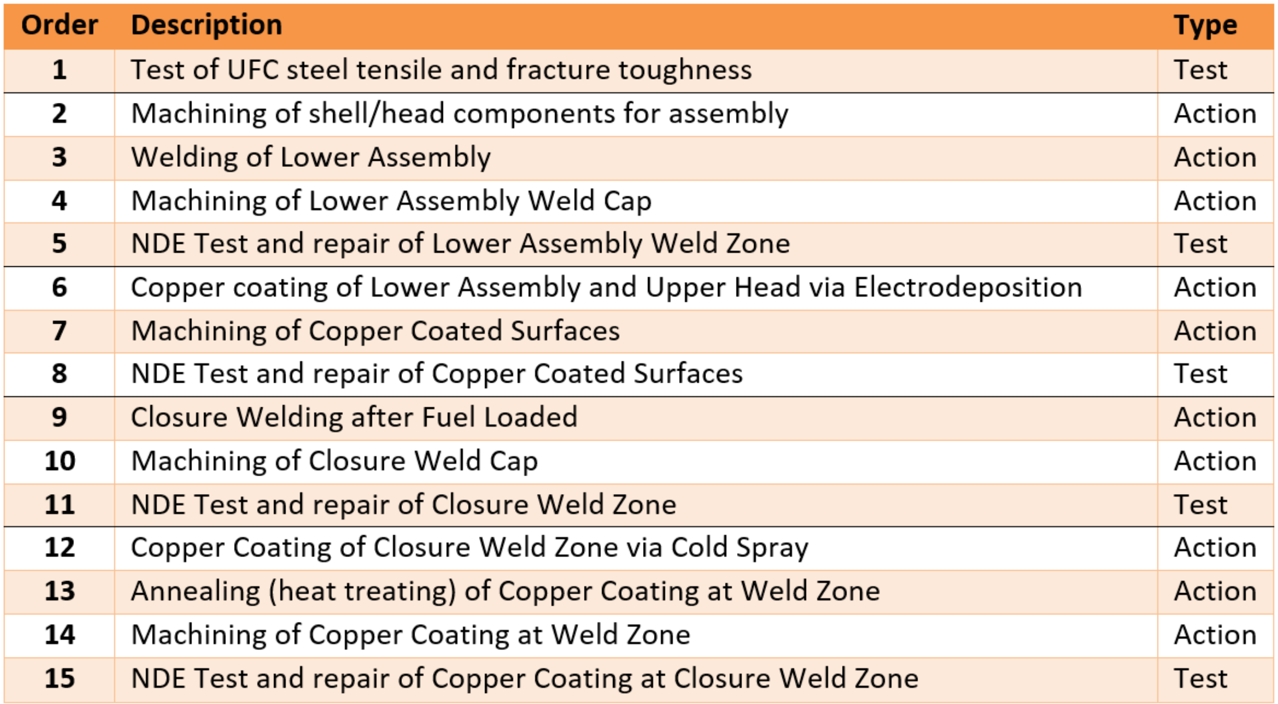


Figure 4: Manufacturing process model – Parent/child schematic links



Order	Description	Type
1	Test of UFC steel tensile and fracture toughness	Test
2	Machining of shell/head components for assembly	Action
3	Welding of Lower Assembly	Action
4	Machining of Lower Assembly Weld Cap	Action
5	NDE Test and repair of Lower Assembly Weld Zone	Test
6	Copper coating of Lower Assembly and Upper Head via Electrodeposition	Action
7	Machining of Copper Coated Surfaces	Action
8	NDE Test and repair of Copper Coated Surfaces	Test
9	Closure Welding after Fuel Loaded	Action
10	Machining of Closure Weld Cap	Action
11	NDE Test and repair of Closure Weld Zone	Test
12	Copper Coating of Closure Weld Zone via Cold Spray	Action
13	Annealing (heat treating) of Copper Coating at Weld Zone	Action
14	Machining of Copper Coating at Weld Zone	Action
15	NDE Test and repair of Copper Coating at Closure Weld Zone	Test

Table 3: Manufacturing process model – Actions and tests

A value of 1 corresponds to a “bad” state outcome (that is, at least one of the state’s essential variables falls outside its acceptable range), a value of 0 corresponds to a “good” state outcome (all of the state’s essential variable falls within their acceptable ranges). Recorded state values (R_i) follow the same valuation scheme.

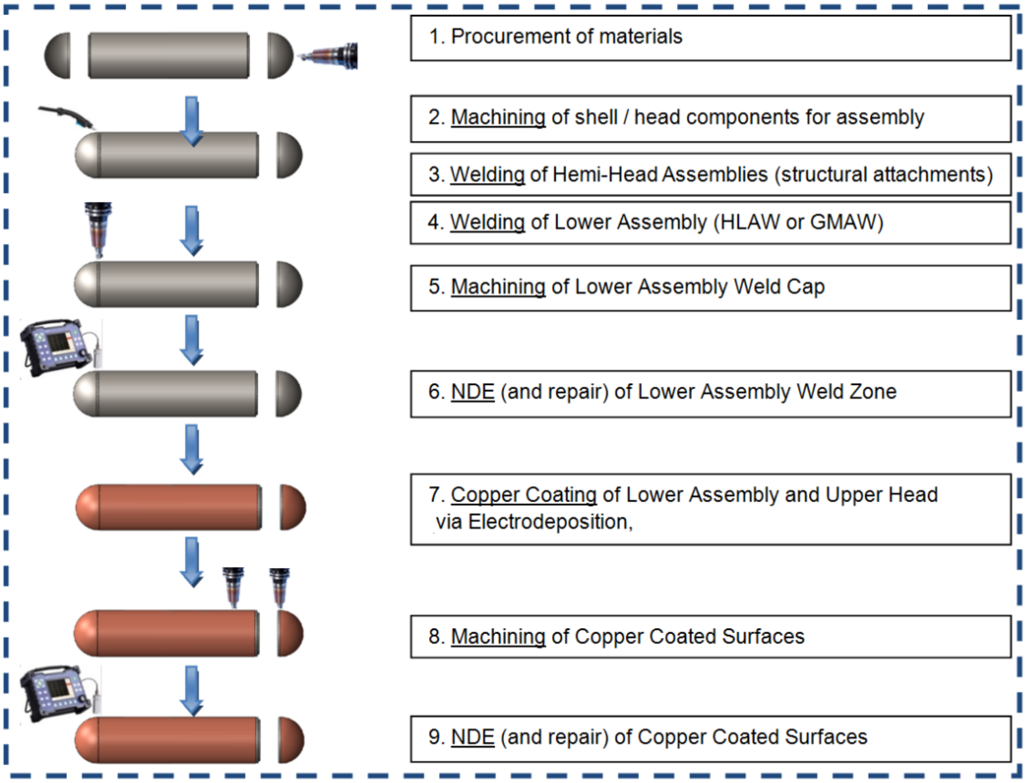
Each container state, then, belongs to one of 4 categories:

- $A = 0$ and $R = 0$ represent UFCs which were correctly retained
- $A = 0$ and $R = 1$ represent UFCs which were incorrectly removed from the process
- $A = 1$ and $R = 0$ represent UFCs which were incorrectly retained
- $A = 1$ and $R = 1$ represent UFCs which were correctly removed from the process

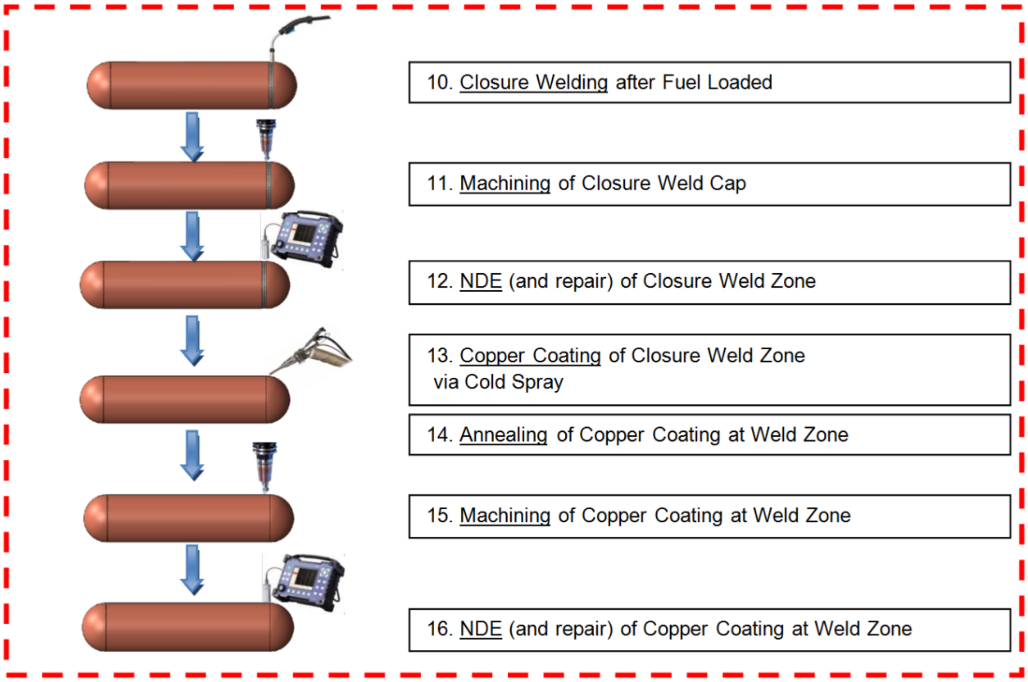
The number of UFCs which are removed from the process (whether correctly or incorrectly) may be important to the NWMO (after all, manufacturing a UFC is both financially and temporally costly), but from the point of view of the failure analysis, that figure is not relevant; the emphasis is devoted to estimating conditional probabilities

$$P(A = 1|R = 0) = \frac{P(A = 1, R = 0)}{P(R = 0)},$$

where A and R correspond to any pair of actual and recorded states in the manufacturing process. Of special interest will be the state 10 probabilities of sending a UFC to the repository with a **through-wall** or a **thinwall** defect.



(a) Off-site operations



(b) Radiological operations

Figure 5: Manufacturing process model – Visual representation (from *Overview of the NWMO and the Mark II Used Fuel Container*, C. Boyle)

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Label	Description	Variable Type	Target Values	Distribution
V1	tensile and fracture toughness	Strength	Unknown, but presumably exists	Normal
V2_1	minimal length of shell (SH) component	Length	Given by specs	Normal
V2_2	maximal length of SH component	Length	Given by specs	Normal
V2_3	minimal thickness of SH component	Length	Given by specs	Normal
V2_4	maximal thickness of SH component	Length	Given by specs	Normal
V2_5	minimal radius of SH component	Length	Given by specs	Normal
V2_6	maximal radius of SH component	Length	Given by specs	Normal
V2_7	minimal thickness of lower head (LH) component	Length	Given by specs	Normal
V2_8	maximal thickness of LH component	Length	Given by specs	Normal
V2_9	minimal radius of LH component (at the SH joint)	Length	Given by specs	Normal
V2_10	maximal radius of LH component (at the SH joint)	Length	Given by specs	Normal
V2_11	minimal thickness of upper head (UH) component	Length	Given by specs	Normal
V2_12	maximal thickness of UH component	Length	Given by specs	Normal
V2_13	minimal radius of UH component (at the SH joint)	Length	Given by specs	Normal
V2_14	maximal radius of UH component (at the SH joint)	Length	Given by specs	Normal
V3_1	surface finish variable for LH	Roughness	Unknown	Normal
V3_2	surface finish variable for SH	Roughness	Unknown	Normal
V3_3	surface finish variable for UH	Roughness	Unknown	Normal
V4_1	minimal thickness of lower assembly weld (LW)	Length	Given by specs	Normal
V4_2	minimal thickness of LW	Length	Given by specs	Normal
V4_3	brittleness of LW material	Brittleness	Unknown, but presumably exists	Normal
V5_1	ductility of copper used in coating	Ductility	Unknown, but presumably exists	Normal
V5_2	adhesion strength of LH copper coating	Unknown	Unknown	Normal
V5_3	adhesion strength of SH copper coating	Unknown	Unknown	Normal
V5_4	adhesion strength of UH copper coating	Unknown	Unknown	Normal
V5_5	adhesion strength of LW copper coating	Unknown	Unknown	Normal
V6_1	minimal depth of LH copper coating	Length	Given by specs	Folded Normal?
V6_2	maximal depth of LH copper coating	Length	Given by specs	Folded Normal?
V6_3	minimal depth of SH copper coating	Length	Given by specs	Folded Normal?
V6_4	maximal depth of SH copper coating	Length	Given by specs	Folded Normal?
V6_5	minimal depth of UH copper coating	Length	Given by specs	Folded Normal?
V6_6	maximal depth of UH copper coating	Length	Given by specs	Folded Normal?
V6_7	minimal depth of LW copper coating	Length	Given by specs	Folded Normal?
V6_8	maximal depth of LW copper coating	Length	Given by specs	Folded Normal?
V7_1	minimal thickness of closure weld (CW)	Length	Given by specs	Normal
V7_2	minimal thickness of CW	Length	Given by specs	Normal
V7_3	brittleness of CW material	Brittleness	Unknown, but presumably exists	Normal
V8	adhesion strength of CW copper coating	Unknown	Unknown	Normal
V9_1	minimal depth of CW copper coating	Length	Given by specs	Folded Normal
V9_2	maximal depth of CW copper coating	Length	Given by specs	Folded Normal
V10_1	number of through wall spots on the LH	Number	Unknown, but presumably exists	Poisson?
V10_2	number of thin wall spots on the LH	Number	Unknown, but presumably exists	Poisson?
V10_3	number of through wall spots on the SH	Number	Unknown, but presumably exists	Poisson?
V10_4	number of thin wall spots on the SH	Number	Unknown, but presumably exists	Poisson?
V10_5	number of through wall spots on the UH	Number	Unknown, but presumably exists	Poisson?
V10_6	number of thin wall spots on the UH	Number	Unknown, but presumably exists	Poisson?
V10_7	number of throughwall spots on the LW	Number	Unknown, but presumably exists	Poisson?
V10_8	number of thinwall spots on the LW	Number	Unknown, but presumably exists	Poisson?
V10_9	number of throughwall spots on the CW	Number	Unknown, but presumably exists	Poisson?
V10_10	number of thinwall spots on the CW	Number	Unknown, but presumably exists	Poisson?

Table 4: Manufacturing process model – Variables

A number of simplifying assumptions have been made regarding the distributions from which the various values are drawn; these may need to be changed once better information becomes available to the modelers or to the NWMO.

3.2 Modeling Assumptions and Parameters

Our approach is to model the statess stochastically rather than modeling them physically after each of the actions. We also assume that states are only affected by a subset of the actions and tests, and so the various state parameters have to reflect those. The dependencies are listed below:

UFC STATE 1 – poor mechanical properties of UFC steel (tensile and fracture toughness)

- Action: None
- Test: UFC steel tensile and fracture toughness

UFC STATE 2 – dimensions of UFC components outside of acceptable ranges

- Action: Machining of shell/head components for assembly
- Test: NDE and repair of Lower Assembly Weld Zone

UFC STATE 3 – poor surface finish of UFC steel

- Action: Machining of shell/head components for assembly
- Test: NDE and repair of Lower Assembly Weld Zone

UFC STATE 4 – defective weld of UFC Lower Assembly

- Actions: Welding of Lower Assembly; Machining of Lower Assembly Weld Cap
- Test: NDE and repair of Lower Assembly Weld Zone

UFC STATE 5 – poor ductility and adhesion of UFC copper coating (LH,SH,UH,LW)

- Action: Copper coating of Lower Assembly and Upper Head via Electrodeposition
- Test: NDE and repair of Copper Coated Surfaces

UFC STATE 6 – depth of copper coating outside of acceptable range (LH,SH,UH,LW)

- Action: Machining of Copper Coated Surfaces
- Test: NDE and repair of Copper Coated Surfaces

UFC STATE 7 – defective weld of UFC closure zone (CW)

- Actions: Closure Welding after Fuel Loaded; Machining of Closure Weld Cap
- Test: NDE and repair of Closure Weld Zone

UFC STATE 8 – poor adhesion of UFC copper coating (CW)

- Actions: Copper Coating of Closure Weld Zone via Cold Spray; Annealing (heat treating) of Copper Coating at Weld Zone
- Test: NDE and repair of Copper Coating at Closure Weld Zone

UFC STATE 9 – depth of copper coating outside of acceptable range (CW)

- Action: Machining of Copper Coating at Weld Zone
- Test: NDE and repair of Copper Coating at Closure Weld Zone

UFC STATE 10 – thin-wall and through-wall defect (minimum coating thickness)

- Action: None
- Test: None

3.2.1 Modeling Procedure

The modeling procedure for each state follows the same steps:

1. the state variables V_i are generated according to the appropriate parameters, the parent states A_j and essential variables V_j;
2. the actual state A_i (and its sub-states, corresponding to each of the variables) are updated according to the appropriate parameters, and
3. the recorded state R_i (and its sub-states) are generated according to the appropriate parameters.

The specifics of the parent/child relationships are listed in the last 2 columns of Table 5.

3.2.2 Effect of Undetected Flaws in Parent States

In the prototype, an undetected flaw at a parent stage **can only affect the process used to generate state variable values** – it does not affect the process by which the state is recorded.

For UFCs which were deemed acceptable at a given state ($R_i = 0$), we distinguish between 2 cases:

- UFCs which were correctly recorded as acceptable ($A_i = 0$ and $R_i = 0$), and
- UFCs which were incorrectly recorded as acceptable ($A_i = 1$ and $R_i = 0$).

Recall that the UFCs for which the recorded state were not deemed acceptable ($R_i = 1$) have been removed from the manufacturing process; what follows does not apply to them.

Assume that, when the parent states are such that $A = 0$ and $R = 0$, the variable V follows a distribution $\mathscr{D}(\mu, \sigma)$ (not necessarily normal) with mean μ and standard deviation σ (see leftmost target illustration in Figure 6).

How should the distribution of values be affected, however, if the parent states incorrectly identified the UFC as acceptable? For $k, \ell > 0$, we answer the question with the help of the distribution $\mathscr{D}(k\mu, \ell\sigma)$. If the flaw at the parent state is:

- unlikely to change the accuracy while changing the precision, we use $k = 1, \ell \neq 1$ (see third target diagram);
- likely to change the accuracy while preserving the precision, we use $k \neq 1, \ell = 1$ (see second target diagram);
- likely to change both the accuracy and the precision, use $k, \ell \neq 1$(see fourth target diagram).

State	Affected	Child Mean	Child SD	Child V			Parent A, R											
1				V1														
2	mean	mu2_i	sigma2	V2_1	...	V2_14	A1	R1										
3	mean	mu3	sigma3	V3_1	V3_2	V3_3	A1	R2										
4	sd	mu4_12	sigma4_12	V4_1	V4_2		A1	A2_1	...	A2_6	A2_7	...	A2_10	A3_1	A3_2	R3		
		mu4_3	sigma4_3	V4_3														
5	sd	mu5_1	sigma5_1	V5_1			A3_1	A3_2	A3_3	A4_1	A4_2	A4_3	R4					
		mu5_2345	sigma5_2345	V5_2	...	V5_5												
6	mean	mu6	sigma6_135	V6_1			A5_1	A5_2	R5									
				V6_3			A5_1	A5_3	R5									
				V6_5			A5_1	A5_4	R5									
			sigma6_7	V6_7			A4_1	A4_2	A4_3	A5_1	A5_5	R5						
7	sd	mu4_12	sigma4_12	V7_1	V7_2		A1	A2_1	...	A2_6	A2_11	...	A2_14	A3_1	A3_2	A5_3	A5_4	R6
		mu4_3	sigma4_3	V7_3														
8	sd	mu5_2345	sigma5_2345	V8			A7_1	A7_2	A7_3	R7								
9	mean	mu6	sigma6_7	V9			A5_1	A7_1	A7_2	A7_3	A8	R8						
10				A10_1			R9	V6_1										
				A10_2			R9	A6_1	A10_1									
				A10_3			R9	V6_3										
				A10_4			R9	A6_3	A10_3									
				A10_5			R9	V6_5										
				A10_6			R9	A6_5	A10_5									
				A10_7			R9	V6_7										
				A10_8			R9	A6_7	A10_7									
				A10_9			R9	V9_1										
				A10_10			R9	A9	A10_9									

Table 5: Manufacturing process model – Specifics of parent/child relationship.

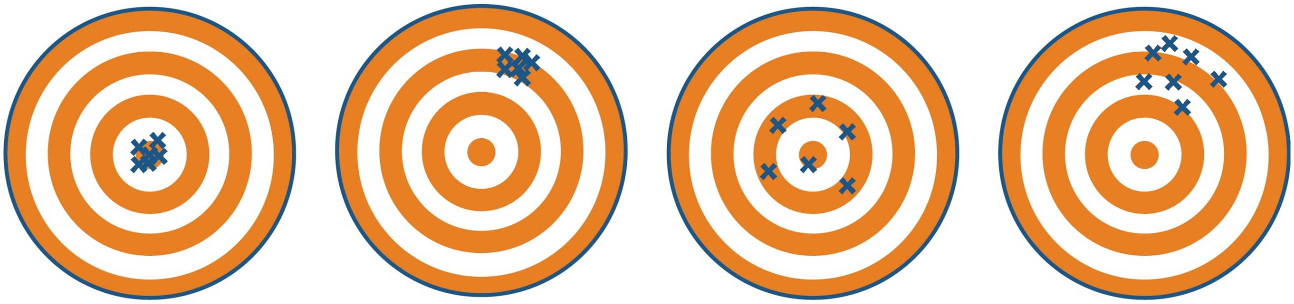


Figure 6: Illustration of the effect of flaw in parent state on a generic variable in a children state for the prototype. From left to right: no effect; mean only; variance only; both mean and variance.

Of course, the parent flaw could affect the variable V in different ways, such as changing the distribution type altogether, instead of simply modifying the distribution parameters), or being dependent on the “strength” with which a parent state fails. While other options can be implemented, we only consider situations given by the first, second or third diagram in this prototype model.

While this has the added benefit of not increasing the number of required input parameters, the main reason we are not considering cases described by the fourth diagram is that we have as yet very little information as to how exactly k, ℓ would be derived in each case. This state of affairs is surely temporary, however, and we have left some place holder parameters in the prototype to be able to make modifications simply in future iterations of the model.

The states for which only the mean is affected by defective parent states are labeled ‘mean’ in the second column of Table 5, while those for which it is the standard deviation that is affected are labeled ‘sd’.

3.3 Illustration of the Method

We illustrate the model with the help of a step-by-step interpretation of the input parameters. In the tables of this section, yellow rows correspond to parameters that are used to generate variable values, orange rows to parameters that are used to determine actual states, and green rows to parameters that are used to determine whether a UFC is removed from the chain, or accepted and passed along to the next stage.

As discussed above, the process is fairly similar from one step to the next; there are, however, various technical details which vary with each state. We shall only present these details when they are unique.

Furthermore, the level of certainty is not the same for each parameter and variable combination. For instance, the specs for the UFC dimensions are known, but the standard deviation of the lengths of the various component are unknown; the mean of the steel tensile strength is not currently known but could be easily estimated; same goes for the tolerance of the various tests, and so forth. **The parameter values listed in this section are thus not to be taken as realistic values in general; their sole purpose is to illustrate how the model works.**

State 1

The parameter values (with descriptions) for state 1 are shown in Table 6.

V Parameters

- Inputs: μ_1, σ_1
- Output: $V_1 \sim N(\mu_1, \sigma_1^2)$

A Parameters

- Input: ρ_1
- Output: $A_1 = \begin{cases} 0 & \text{if } V_1 > \rho_1 \\ 1 & \text{else} \end{cases}$

R Parameters

- Inputs: tol_1, prot_1, $p_{1,1}$, $p_{1,2}$
- Temporary:
  - acceptable region AcReg_1: (ρ_1, ∞)
  - tolerance region TolReg_1: $(\rho_1 - \text{tol}_1, \rho_1)$
  - probabilities: $P(R_1 = 1|V_1) = \begin{cases} 1 - \text{prot}_1 & \text{if } V_1 \in \text{AcReg}_1 \\ (1 - p_{1,2}) \times \text{prot}_1 & \text{if } V_1 \in \text{TolReg}_1 \\ (1 - p_{1,1}) \times \text{prot}_1 & \text{else} \end{cases}$
- Output: R_1

Notes

- ρ_1 is known with certainty. The other parmater values are assumed to be reasonable, but experiments will have to be conducted to determine valid estimates.

State 2

The parameter values (with descriptions) for state 2 are shown in Table 7.

V Parameters

- Inputs: outer radius, head thickness, shell length, shell thickness, σ_2, f_2
- Transition:
  - $\mu_1 =$ shell length
  - $\mu_3 =$ shell thickness
  - $\mu_5 =$ head outer radius
  - $\mu_7 =$ head thickness

  - $\mu_9 =$ outer radius
  - $\mu_{11} =$ head thickness
  - $\mu_{13} =$ outer radius
- Outputs: $V_{2,2j-1:2j} \sim (1-A_1)N(\mu_{2j-1}, \sigma_2^2) + A_1 N(\mu_{2j-1}/f_2, \sigma_2^2)$

A Parameters

- Input: threshold_2
- Outputs:
  - $A_{2,2j-1} = \begin{cases} 0 & \text{if } V_{2,2j-1} < \mu_{2,2j-1} - \text{threshold}_2 \\ 1 & \text{else} \end{cases}$
  - $A_{2,2j} = \begin{cases} 0 & \text{if } V_{2,2j} > \mu_{2,2j-1} + \text{threshold}_2 \\ 1 & \text{else} \end{cases}$
  - $A_2 = 0$ unless at least one of $A_{2,i} = 1$

R Parameters

- Inputs: tol_2, prot_2, $p_{2,1} = p_{2,\text{small}}$, $p_{2,2} = p_{2,\text{big}}$
- Transition:
  - acceptable region AcReg_2: $(\mu_{2j-1} - \text{threshold}_2, \mu_{2j-1} + \text{threshold}_2)$
  - tolerance region TolReg_2: $(\mu_{2j-1} - \text{threshold}_2 - \text{tol}_2, \mu_{2j-1} - \text{threshold}_2) \cup (\mu_{2j-1} + \text{threshold}_2, \mu_{2j-1} + \text{threshold}_2 + \text{tol}_2)$
  - probabilities: $P(R_{2,i} = 1 | V_{2,i}) = \begin{cases} 1 - \text{prot}_2 & \text{if } V_{2,i} \in \text{AcReg}_2 \\ (1 - p_{2,2}) \times \text{prot}_2 & \text{if } V_{2,i} \in \text{TolReg}_2 \\ (1 - p_{2,1}) \times \text{prot}_2 & \text{else} \end{cases}$
- Output: $R_2 = 0$ unless of one of $R_{2,i} = 1$

Notes

- The mean of the variables is divided by f_2 in cases where the parent state was defective: f_2 values smaller than 1 increase the mean, values greater than 1 decrease it. If defective parent states have no effect on the mean, set $f_2 = 1$.

State 3

The parameter values (with descriptions) for state 3 are shown in Table 8. The parameters are as in States 1 and 2, with the distinction that the acceptable and tolerance regions for surface roughness point in the other direction (by comparison with State 1):

- acceptable region AcReg_3: $(0, \mu_3 + \text{threshold}_3)$
- tolerance region TolReg_3: $(\mu_3 + \text{threshold}_3, \mu_3 + \text{threshold}_3 + \text{tol}_3)$

State 4

The parameter values (with descriptions) for state 4 are shown in Table 9. The parameters are as in States 1, 2, and 3, with the distinction that a defective parent state affects only the standard deviation in a child, and that the various sub-states have different test tolerances and region types:

- $V_{4,1:2} \sim (1-A_1)(1-A_2)(1-A_3)N(\mu_{4,1:2},\sigma^2_{4,1:2})+A_1(1-A_2)(1-A_3)N(\mu_{4,1:2},(f_{4,1,1:2}\sigma_{4,1:2})^2)+\cdots+A_1A_2A_3N(\mu_{4,1:2},(f_{4,1,1:2}f_{4,2,1:2}f_{4,3,1:2}\sigma_{4,1:2})^2)$
- $V_{4,3} \sim (1-A_1)(1-A_2)(1-A_3)N(\mu_{4,3},\sigma^2_{4,3})+A_1(1-A_2)(1-A_3)N(\mu_{4,3},(f_{4,1,3}\sigma_{4,3})^2)+\cdots+A_1A_2A_3N(\mu_{4,3},(f_{4,1,3}f_{4,2,3}f_{4,3,3}\sigma_{4,3})^2)$
- $\text{AcReg}_{4,1:2}$ and $\text{TolReg}_{4,1:2}$ are as in State 2, $\text{AcReg}_{4,3}$ and $\text{TolReg}_{4,3}$ as in State 1.

Notes

- The standard deviation of the variables is multiplied by products of f in cases where the parent state were defective: f_4 values smaller than 1 decrease the standard deviation, values greater than 1 increase it. If a defective parent state have no effect on the mean, set its factor to 1.
- The factors affect the standard deviations by combinatorial multiplication: the more parent states are defective, the more terms enter the final factor.
- The values used for $\mu_{4,1:2}$ are close to the expected depth of the welding substrate; but the values for brittleness $V_{4,3}$ have been arbitrarily selected – reasonable values will need to be provided in future iterations of the model.

State 5

The parameter values (with descriptions) for state 5 are shown in Table 10. The parameters are as in States 1 – 4, with no major difference.

Notes

- $A_{5,1}$ is independent of previous states, whereas States $A_{5,2}$ to $A_{5,4}$ depend on the previous states.

State 6

The parameter values (with descriptions) for state 6 are shown in Table 12. The parameters are as in previous states, with a number of major differences:

- copper coating thicknesses are drawn from a folded normal with mean 3 and standard deviations depending on the UFC component of interest (weld vs. non-weld)
- the parameter strength_6 is used to increase the likelihood of pinhole through-wall defects in the copper coating (large values increase the likelihood)

- the parameter $p_{6,0}$ is the probability of detecting a pinhole through-wall defect (as opposed to detecting a thin-wall defect).

- the parameter threshold_6 can be used to determine what constitutes a thin-wall defect

- the tolerance region recognizes 0 as a copper coating thickness of special importance:

$$P(R_{6,i} = 1|V_{6,i}) = \begin{cases} 1 - \text{prot}_6 & \text{if } V_{6,i} \in \text{AcReg}_6 \\ (1 - p_{6,2}) \times \text{prot}_6 & \text{if } V_{6,i} \in \text{TolReg}_6 \\ (1 - p_{6,0}) \times \text{prot}_6 & \text{if } V_{6,i} = 0 \\ (1 - p_{6,1}) \times \text{prot}_6 & \text{else} \end{cases}$$

State 7

The parameter values (with descriptions) for state 7 are shown in Tables 9 and 11. The parameters are exactly those of State 4, but extra parameters have been provided in case it turns out that the copper coating on the shell and on the upper head have an effect on the closure weld.

State 8

The parameter values (with descriptions) for state 8 are shown in Table 10. The parameters are exactly those of State 5.

State 9

The parameter values (with descriptions) for state 9 are shown in Table 12. The parameters are exactly those of State 6.

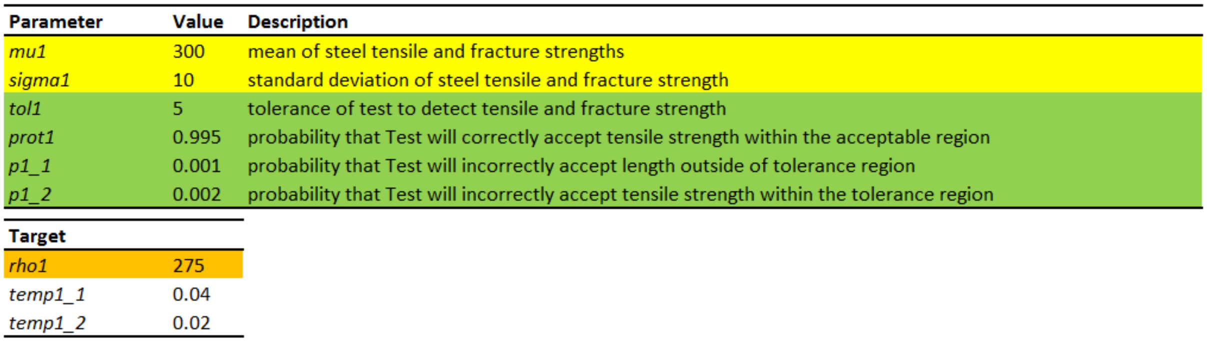
State 10

A Parameters

- Odd csub-states represent the presence of a through-wall defect on each of the 5 UFC components; even sub-states represent the presence of thin-walls on each of the 5 UFC components.
- The thin-wall level is controlled by the value of threshold_6.

R Parameters

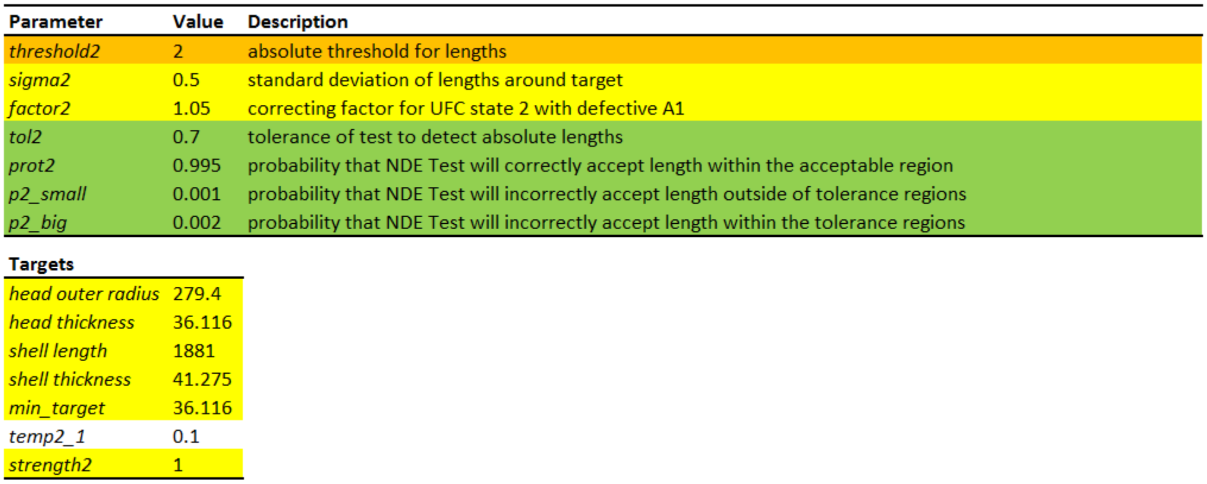
- All containers getting to this point are assumed to be without defect, thus $R_{10,j} = 0$, independently of the actual state of the container.



Parameter	Value	Description
mu1	300	mean of steel tensile and fracture strengths
sigma1	10	standard deviation of steel tensile and fracture strength
tol1	5	tolerance of test to detect tensile and fracture strength
prot1	0.995	probability that Test will correctly accept tensile strength within the acceptable region
p1_1	0.001	probability that Test will incorrectly accept length outside of tolerance region
p1_2	0.002	probability that Test will incorrectly accept tensile strength within the tolerance region

Target	
rho1	275
temp1_1	0.04
temp1_2	0.02

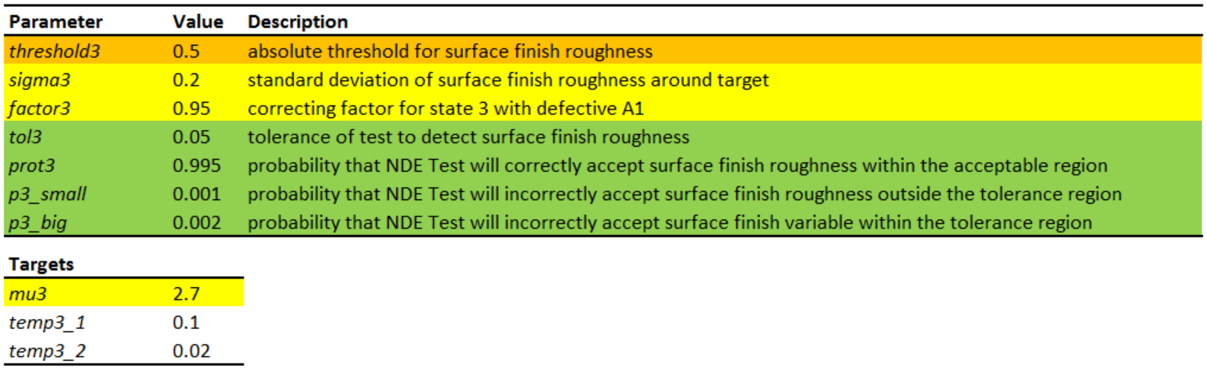
Table 6: Parameters for State 1 (yellow – V; orange – A; green – R; white – unused)



Parameter	Value	Description
threshold2	2	absolute threshold for lengths
sigma2	0.5	standard deviation of lengths around target
factor2	1.05	correcting factor for UFC state 2 with defective A1
tol2	0.7	tolerance of test to detect absolute lengths
prot2	0.995	probability that NDE Test will correctly accept length within the acceptable region
p2_small	0.001	probability that NDE Test will incorrectly accept length outside of tolerance regions
p2_big	0.002	probability that NDE Test will incorrectly accept length within the tolerance regions

Targets	
head outer radius	279.4
head thickness	36.116
shell length	1881
shell thickness	41.275
min_target	36.116
temp2_1	0.1
strength2	1

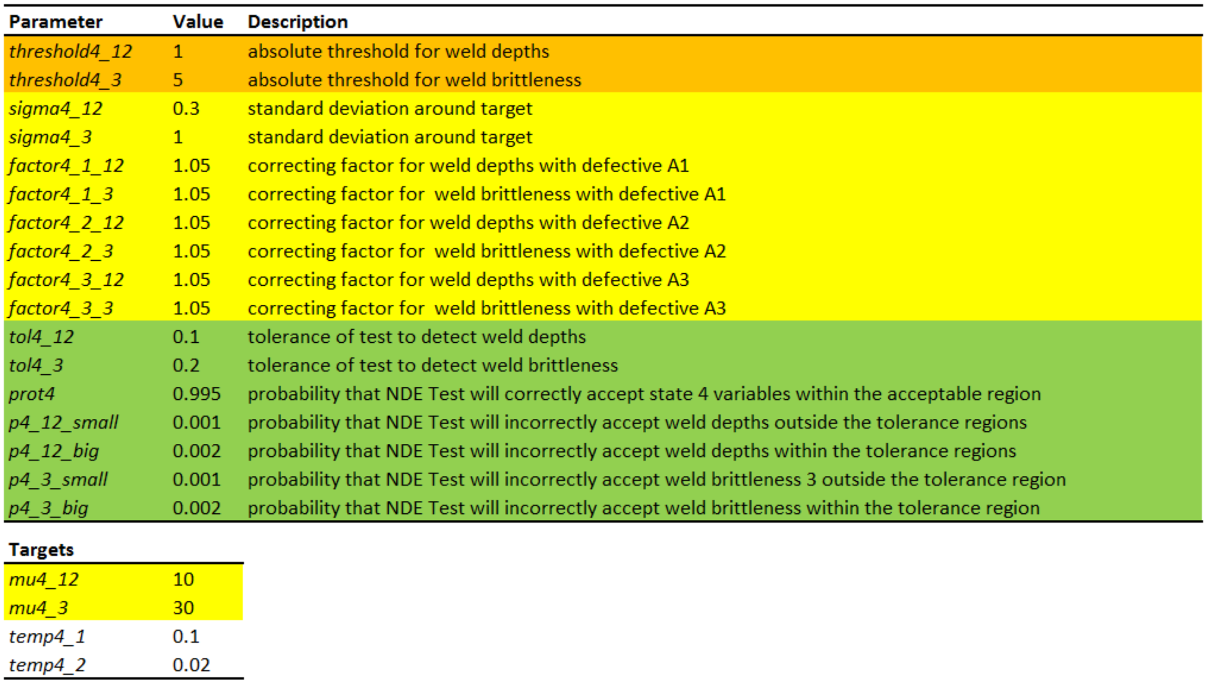
Table 7: Parameters for State 2 (yellow – V; orange – A; green – R; white – unused)



Parameter	Value	Description
threshold3	0.5	absolute threshold for surface finish roughness
sigma3	0.2	standard deviation of surface finish roughness around target
factor3	0.95	correcting factor for state 3 with defective A1
tol3	0.05	tolerance of test to detect surface finish roughness
prot3	0.995	probability that NDE Test will correctly accept surface finish roughness within the acceptable region
p3_small	0.001	probability that NDE Test will incorrectly accept surface finish roughness outside the tolerance region
p3_big	0.002	probability that NDE Test will incorrectly accept surface finish variable within the tolerance region

Targets	
mu3	2.7
temp3_1	0.1
temp3_2	0.02

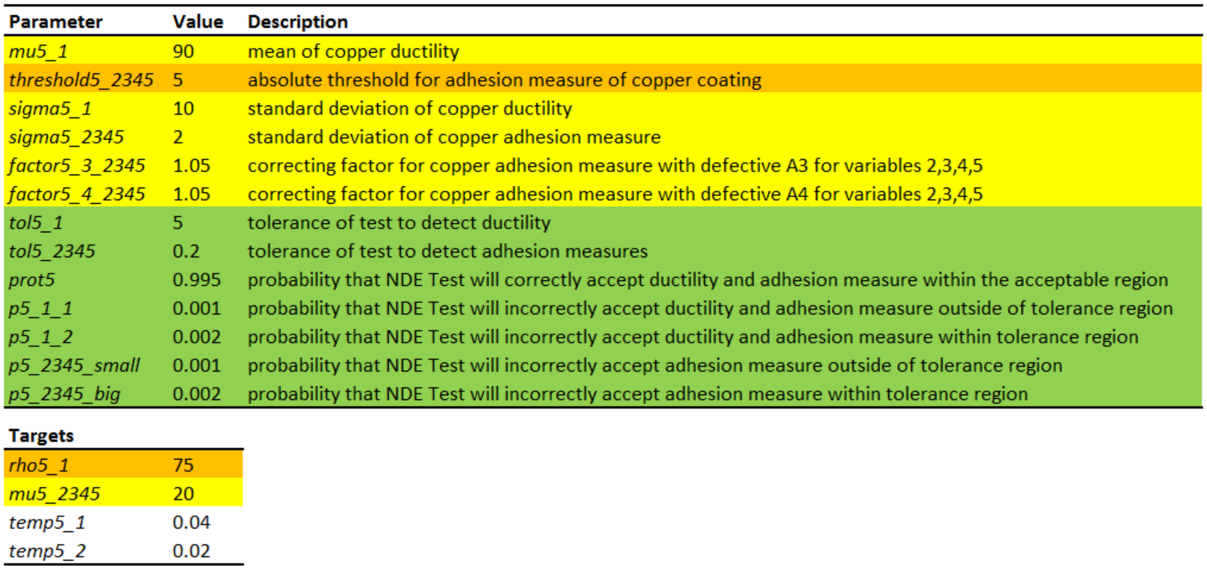
Table 8: Parameters for State 3 (yellow – V; orange – A; green – R; white – unused)



Parameter	Value	Description
threshold4_12	1	absolute threshold for weld depths
threshold4_3	5	absolute threshold for weld brittleness
sigma4_12	0.3	standard deviation around target
sigma4_3	1	standard deviation around target
factor4_1_12	1.05	correcting factor for weld depths with defective A1
factor4_1_3	1.05	correcting factor for weld brittleness with defective A1
factor4_2_12	1.05	correcting factor for weld depths with defective A2
factor4_2_3	1.05	correcting factor for weld brittleness with defective A2
factor4_3_12	1.05	correcting factor for weld depths with defective A3
factor4_3_3	1.05	correcting factor for weld brittleness with defective A3
tol4_12	0.1	tolerance of test to detect weld depths
tol4_3	0.2	tolerance of test to detect weld brittleness
prot4	0.995	probability that NDE Test will correctly accept state 4 variables within the acceptable region
p4_12_small	0.001	probability that NDE Test will incorrectly accept weld depths outside the tolerance regions
p4_12_big	0.002	probability that NDE Test will incorrectly accept weld depths within the tolerance regions
p4_3_small	0.001	probability that NDE Test will incorrectly accept weld brittleness 3 outside the tolerance region
p4_3_big	0.002	probability that NDE Test will incorrectly accept weld brittleness within the tolerance region

Targets	
mu4_12	10
mu4_3	30
temp4_1	0.1
temp4_2	0.02

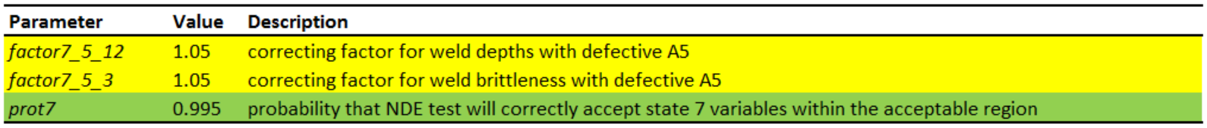
Table 9: Parameters for State 4 (yellow – V; orange – A; green – R; white – unused)



Parameter	Value	Description
mu5_1	90	mean of copper ductility
threshold5_2345	5	absolute threshold for adhesion measure of copper coating
sigma5_1	10	standard deviation of copper ductility
sigma5_2345	2	standard deviation of copper adhesion measure
factor5_3_2345	1.05	correcting factor for copper adhesion measure with defective A3 for variables 2,3,4,5
factor5_4_2345	1.05	correcting factor for copper adhesion measure with defective A4 for variables 2,3,4,5
tol5_1	5	tolerance of test to detect ductility
tol5_2345	0.2	tolerance of test to detect adhesion measures
prot5	0.995	probability that NDE Test will correctly accept ductility and adhesion measure within the acceptable region
p5_1_1	0.001	probability that NDE Test will incorrectly accept ductility and adhesion measure outside of tolerance region
p5_1_2	0.002	probability that NDE Test will incorrectly accept ductility and adhesion measure within tolerance region
p5_2345_small	0.001	probability that NDE Test will incorrectly accept adhesion measure outside of tolerance region
p5_2345_big	0.002	probability that NDE Test will incorrectly accept adhesion measure within tolerance region

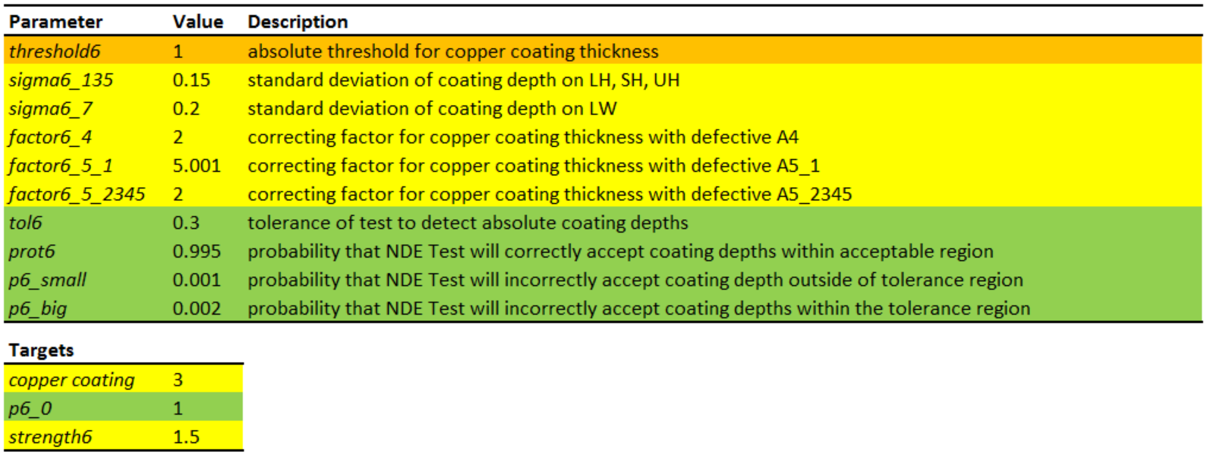
Targets	
rho5_1	75
mu5_2345	20
temp5_1	0.04
temp5_2	0.02

Table 10: Parameters for State 5 (yellow – V; orange – A; green – R; white – unused)



Parameter	Value	Description
factor7_5_12	1.05	correcting factor for weld depths with defective A5
factor7_5_3	1.05	correcting factor for weld brittleness with defective A5
prot7	0.995	probability that NDE test will correctly accept state 7 variables within the acceptable region

Table 11: Parameters for State 7 (yellow – V; orange – A; green – R; white – unused)



Parameter	Value	Description
threshold6	1	absolute threshold for copper coating thickness
sigma6_135	0.15	standard deviation of coating depth on LH, SH, UH
sigma6_7	0.2	standard deviation of coating depth on LW
factor6_4	2	correcting factor for copper coating thickness with defective A4
factor6_5_1	5.001	correcting factor for copper coating thickness with defective A5_1
factor6_5_2345	2	correcting factor for copper coating thickness with defective A5_2345
tol6	0.3	tolerance of test to detect absolute coating depths
prot6	0.995	probability that NDE Test will correctly accept coating depths within acceptable region
p6_small	0.001	probability that NDE Test will incorrectly accept coating depth outside of tolerance region
p6_big	0.002	probability that NDE Test will incorrectly accept coating depths within the tolerance region

Targets	
copper coating	3
p6_0	1
strength6	1.5

Table 12: Parameters for State 6 (yellow – V; orange – A; green – R; white – unused)

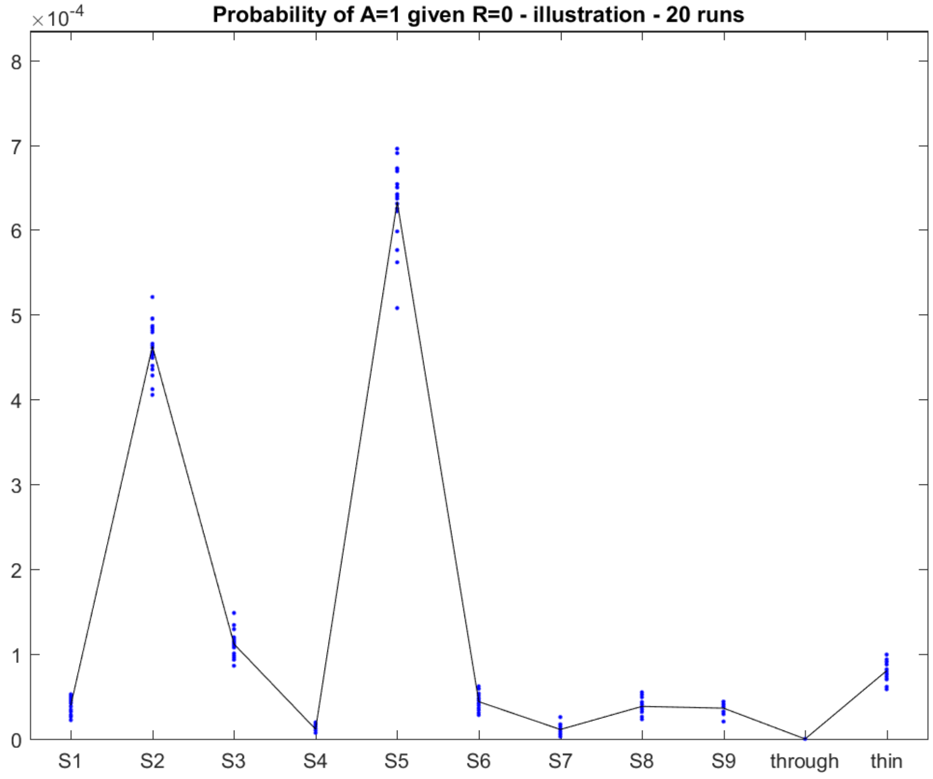
Simulation Results

20 replicates of 500,000 containers have been simulated. The results are shown in Figures 7 and 8. Interesting features include:

- At each of the states 1 to 9, there is a non-zero probability that a defective UFC will have been passed along to the next state.
- The probabilities differ from simulation run to simulation run, but they tend to cluster around specific values, which supports the likelihood that the model is stable for a given parameter set.
- States S_2 and S_5, are substantially more likely to be erroneously accepted by the process, for the given parameter set.
- In none of the simulation were through-wall defects present, although a number of thin-wall defects went undetected.
- At each stage, the probability of a damaged UFC container being sent to the next stage is never more than 7.5×10^{-4}, which seems encouraging.

In hindsight, these results are not entirely surprising, since the probability of capturing a defective UFC are highly correlated with the magnitudes of the various tests' tolerance and the accompanying probabilities in the tolerance regions, as well as with the number of sub-states where something could go wrong (from a detection standpoint).

The graphs in Figure 8 also highlight an important property of the model: the cumulative number of rejected UFCs ($R = 1$) naturally increases at every stage. Since we only care about those containers that eventually will find their way to the repository ($R = 0$), we are looking for high ratios between the first column and second column of each histogram. However, if the combined heights of the last two columns becomes too important, this could be a sign that the probabilities that are used to reject UFCs (defective or not) may be too stringent.



State	Mean	SD	Min	Q1	Median	Q3	Max
1	4.0E-05	9.1E-06	2.2E-05	3.4E-05	4.2E-05	4.7E-05	5.3E-05
2	4.6E-04	2.9E-05	4.1E-04	4.5E-04	4.6E-04	4.8E-04	5.2E-04
3	1.1E-04	1.5E-05	8.6E-05	1.0E-04	1.1E-04	1.2E-04	1.5E-04
4	1.1E-05	3.5E-06	7.3E-06	9.1E-06	1.1E-05	1.3E-05	2.0E-05
5	6.3E-04	4.4E-05	5.1E-04	6.2E-04	6.4E-04	6.6E-04	7.0E-04
6	4.4E-05	9.6E-06	2.8E-05	3.9E-05	4.2E-05	5.1E-05	6.2E-05
7	1.1E-05	5.3E-06	2.9E-06	7.9E-06	1.0E-05	1.4E-05	2.6E-05
8	3.8E-05	8.0E-06	2.3E-05	3.2E-05	3.8E-05	4.4E-05	5.5E-05
9	3.6E-05	6.8E-06	2.0E-05	3.2E-05	3.8E-05	4.1E-05	4.4E-05
Through	0	0	0	0	0	0	0
Thin	8.1E-05	1.1E-05	5.9E-05	7.3E-05	7.9E-05	9.1E-05	9.9E-05

Figure 7: Simulation results of the illustration example, for 20 replicates: the conditional probabilities $P(A_j = 1|R_j = 0)$ and their descriptive statistics are given for each state.

Of course, this is the result of a single run of 20 simulations, **with a single (and arbitrarily selected) parameter set**. Are these results robust? How likely are they to survive a switch to a different parameter set? We attempt to answer some of these questions in the following section. In the meantime, let us urge caution: without a set of reasonable parameter values, a significant amount of parameter space exploration is required before general conclusions can be reached.

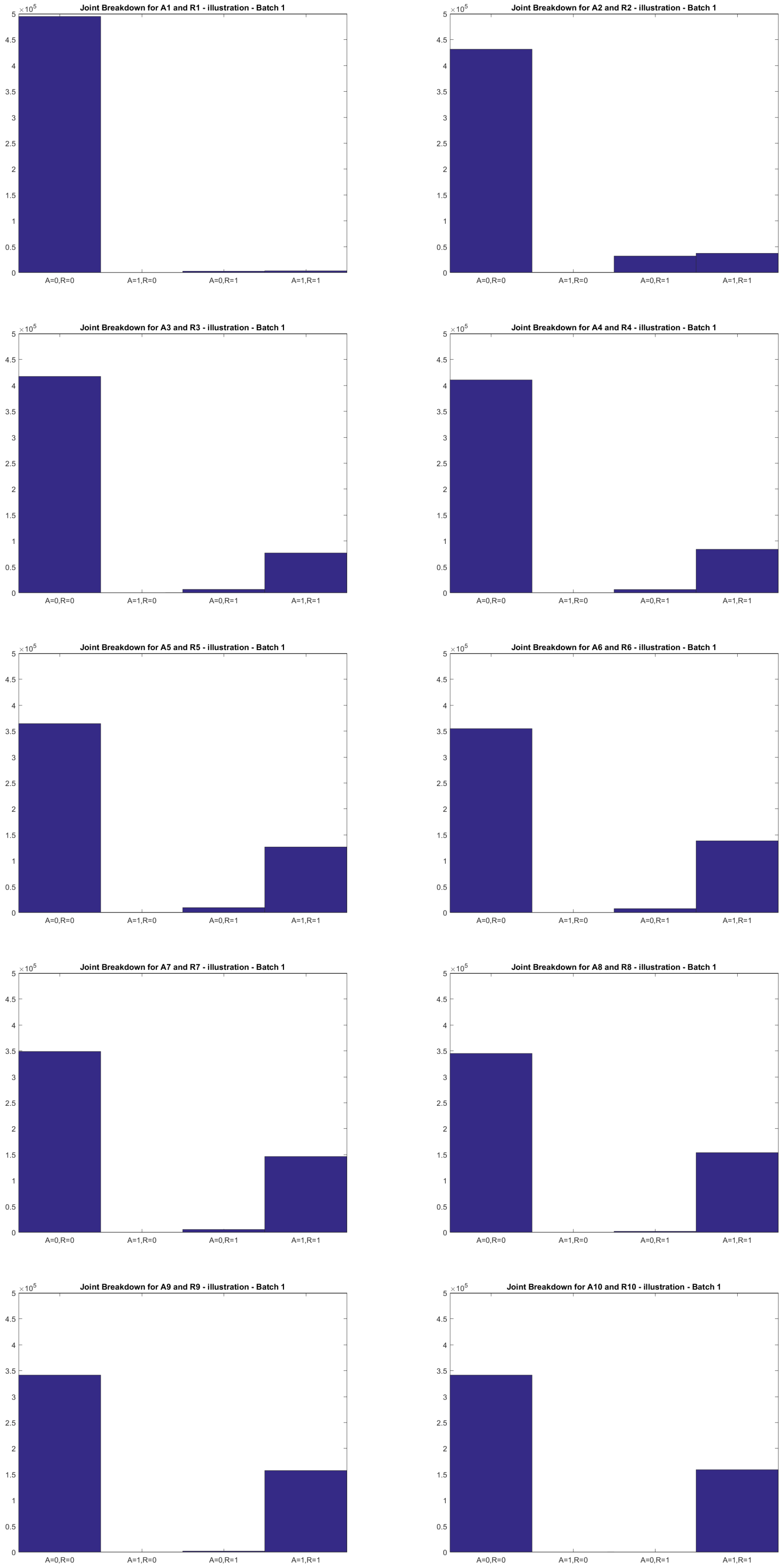
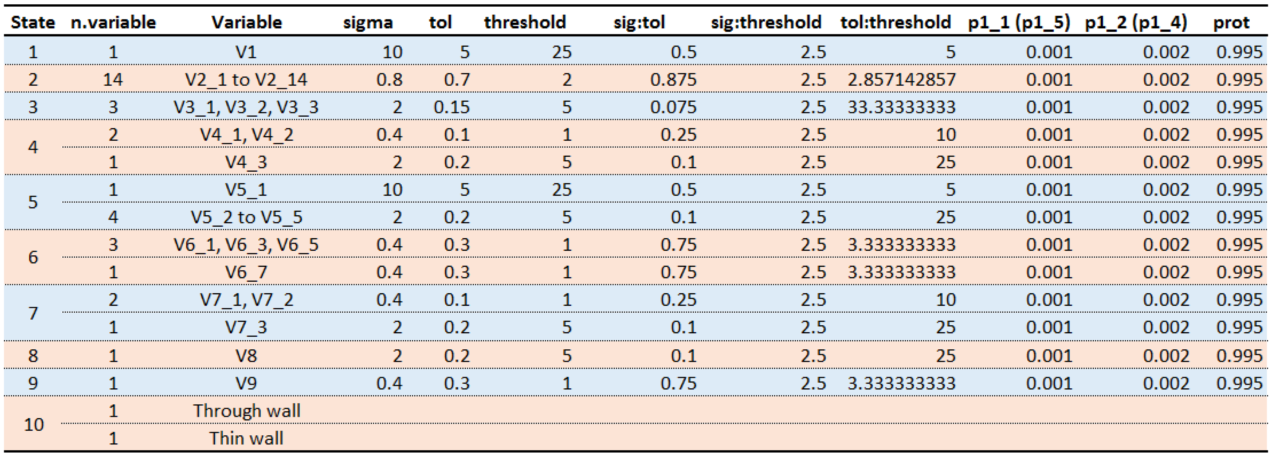


Figure 8: Simulation results of the illustration example, for the first of the 20 replicates: from left to right (within a graph), relative frequencies $P(A_j = 0, R_j = 0)$, $P(A_j = 1, R_j = 0)$, $P(A_j = 0, R_j = 1)$, $P(A_j = 1, R_j = 1)$ for all states.



State	n.variable	Variable	sigma	tol	threshold	sig:tol	sig:threshold	tol:threshold	p1_1 (p1_5)	p1_2 (p1_4)	prot
1	1	V1	10	5	25	0.5	2.5	5	0.001	0.002	0.995
2	14	V2_1 to V2_14	0.8	0.7	2	0.875	2.5	2.857142857	0.001	0.002	0.995
3	3	V3_1, V3_2, V3_3	2	0.15	5	0.075	2.5	33.33333333	0.001	0.002	0.995
4	2	V4_1, V4_2	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
	1	V4_3	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
5	1	V5_1	10	5	25	0.5	2.5	5	0.001	0.002	0.995
	4	V5_2 to V5_5	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
6	3	V6_1, V6_3, V6_5	0.4	0.3	1	0.75	2.5	3.333333333	0.001	0.002	0.995
	1	V6_7	0.4	0.3	1	0.75	2.5	3.333333333	0.001	0.002	0.995
7	2	V7_1, V7_2	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
	1	V7_3	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
8	1	V8	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
9	1	V9	0.4	0.3	1	0.75	2.5	3.333333333	0.001	0.002	0.995
10	1	Through wall									
	1	Thin wall									

Table 13: Parameter set for Scenario 1

3.4 Simulation Results for Eight Scenarios

We now present the results of 8 different simulation scenarios. As before, the emphasis should be taken away from the final probabilities as absolute numbers: rather, we aim to show how varying the parameters affects the final probabilities.

Scenario 1 (Baseline)

The parameter set for Scenario 1 is shown in Table 13; simulation results can be found in Figure 9.

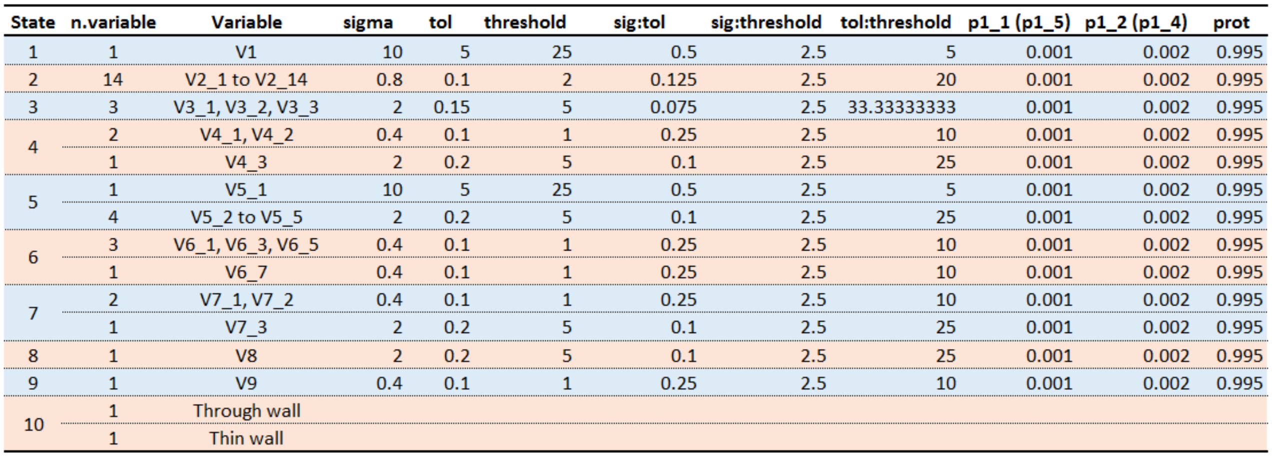
Parameter Set Description:

- σ-to-threshold ratio is set to 2:5 for all states.
- For states 2, 6, and 9, the tolerance-to-threshold ratios vary from 2.9 to 3.3; for the rest of the states, these ratios vary between 5 and 25.
- $p_{i,1}$, $p_{i,2}$, and prot are set to 0.001, 0.002, and 0.995 for all states.
- The factors influencing mean or standard deviation when the parent states are defective are all set to 1.05.
- The tolerance varies from state to state.

This parameter set should give, on average, a value of $P(A_1 = 1|R_1 = 0) = 4.25 \times 10^{-5}$.

Expected Results:

- Since the ratio of σ-to-threshold is held constant at 2:5 throughout the process, with the average $P(A_1 = 1|R_1 = 0)$ of 4.25×10^{-5}, we expect that probability of undetected through-wall defect to be small for this scenario.
- Since the ratio of σ-to-threshold is held constant, we also expect the conditional probability $P(A_i = 1|R_i = 0)$ at each state to be heavily dependant of the number of variables introduced at each state.



State	n.variable	Variable	sigma	tol	threshold	sig:tol	sig:threshold	tol:threshold	p1_1 (p1_5)	p1_2 (p1_4)	prot
1	1	V1	10	5	25	0.5	2.5	5	0.001	0.002	0.995
2	14	V2_1 to V2_14	0.8	0.1	2	0.125	2.5	20	0.001	0.002	0.995
3	3	V3_1, V3_2, V3_3	2	0.15	5	0.075	2.5	33.33333333	0.001	0.002	0.995
4	2	V4_1, V4_2	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
	1	V4_3	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
5	1	V5_1	10	5	25	0.5	2.5	5	0.001	0.002	0.995
	4	V5_2 to V5_5	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
6	3	V6_1, V6_3, V6_5	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
	1	V6_7	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
7	2	V7_1, V7_2	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
	1	V7_3	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
8	1	V8	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
9	1	V9	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
10	1	Through wall									
	1	Thin wall									

Table 14: Parameter set for Scenario 2

Results:

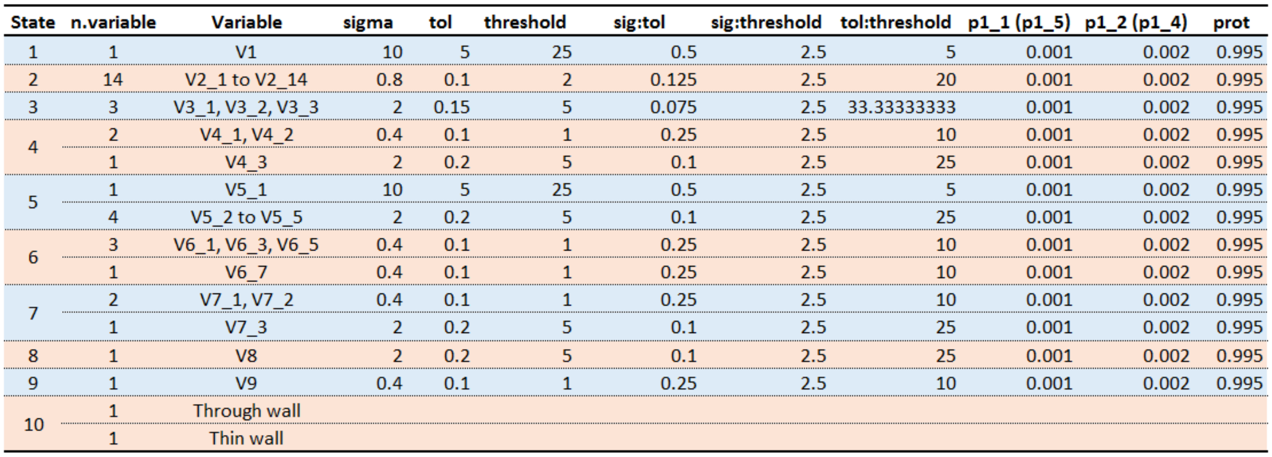
- Given the parameter sets specified above, the shape of $P(A_i = 1|R_i = 0)$ in Figure 9 seems adequate at all states. States 1, 3, 4, 5, 7, and 8 have relatively small probabilities of being mistakenly accepted, and this can be explained by the fact that each of these states has between one to five components, and tolerance-to-threshold ratios are very high.
- On the other hand, States 2, 6, and 9 have large spikes. State 2 has the largest spike, which is explained by it consisting of 14 sub-states. State 6 has a lesser, but still noticeable, spike compared to the rest, which may be due to the low tolerance-to-threshold ratio. It should also be noted that as State 9 uses the same parameters as State 6 with fewer sub-states, it should also show a spike, but with a lesser intensity.
- A direct consequence of having large spikes in states 6 and 9 is that we observe large values for $P(A_{\text{thin}} = 1|R_{\text{thin}} = 0)$ value for the thin-wall. Finally, we also observe small but not negligible values of $P(A_{\text{through}} = 1|R_{\text{through}} = 0)$ for through-wall defects.

Scenario 2

The parameter set for Scenario 2 is shown in Table 14; simulation results can be found in Figure 10 and a comparison with Scenario 1 can be seen in Figure 17.

Parameter Set Description:

- The new parameter set is based on the baseline setting.
- Tolerance-to-threshold ratio for States 2 and 6 are increased to similar levels given in other states. (i.e., At States 2 and 6, the measurement error become smaller compared to baseline scenario)
- $p_{i,1}$, $p_{i,2}$, and prot are set to 0.001, 0.002, and 0.995 for all states.
- The factors influencing mean or standard deviation in the case of defective batch, are all set to 1.05.



State	n.variable	Variable	sigma	tol	threshold	sig:tol	sig:threshold	tol:threshold	p1_1 (p1_5)	p1_2 (p1_4)	prot
1	1	V1	10	5	25	0.5	2.5	5	0.001	0.002	0.995
2	14	V2_1 to V2_14	0.8	0.1	2	0.125	2.5	20	0.001	0.002	0.995
3	3	V3_1, V3_2, V3_3	2	0.15	5	0.075	2.5	33.33333333	0.001	0.002	0.995
4	2	V4_1, V4_2	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
	1	V4_3	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
5	1	V5_1	10	5	25	0.5	2.5	5	0.001	0.002	0.995
	4	V5_2 to V5_5	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
6	3	V6_1, V6_3, V6_5	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
	1	V6_7	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
7	2	V7_1, V7_2	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
	1	V7_3	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
8	1	V8	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
9	1	V9	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
10	1	Through wall									
	1	Thin wall									

Table 15: Parameter set for Scenario 3 (not shown, smaller values for strength_2 and strength_6.

Expected Results:

- Since we are only changing the tolerance levels at States 2 and 6, States 1, 3, 4, 5, 7, and 8 should remain at the similar level compared to Scenario 1.
- Since the tolerance levels are increased in States 2 and 6, $P(A=1|R=0)$ for States 2, 6, 9, thin-wall and through-wall should be reduced.

Results:

- Compared to the Scenario 1, the change in tolerance-to-threshold ratio shows a minor reduction in $P(A=1|R=0)$ at States 2 and 6. However, as States 2, 6, and 9 still show much higher spikes compared to States 1, 3, 4, 5, 7, and 8, we believe that there are parameters that are unique to States 2 and 6 that are causing such high spikes.

Scenario 3

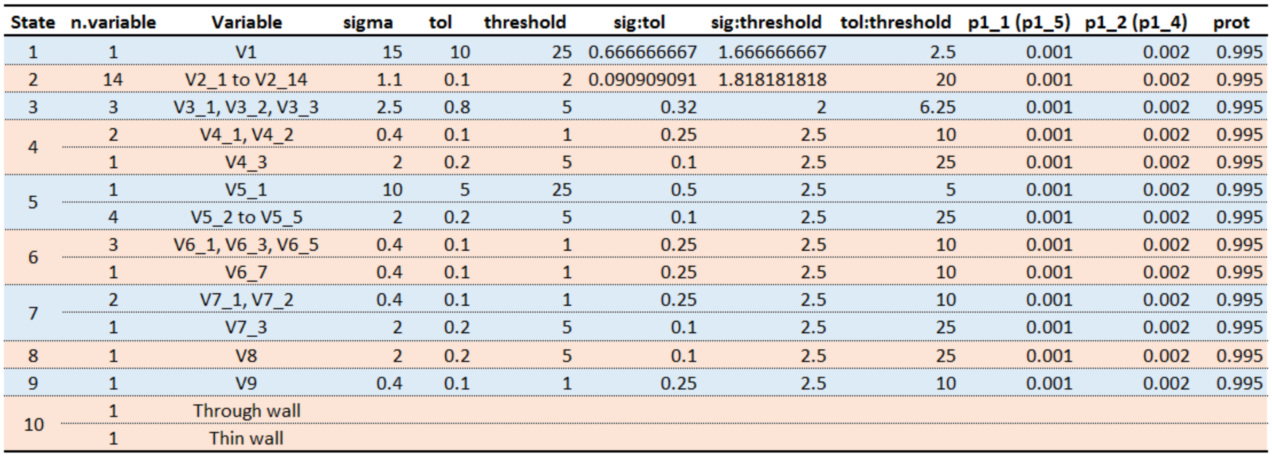
The parameter set for Scenario 3 is shown in Table 15; simulation results can be found in Figure 11 and a comparison with Scenario 2 can be seen in Figure 18.

Parameter Set Description:

- In this scenario, we will investigate the effect of parameters strength_2 and strength_6, which represent the magnitude of the effect of the folded normal distribution in States 2 and 6.
- In Scenarios 1 and 2, strength_2 and strength_6 were set to 1, and 1.5, respectively. Both of these values are reduced to 0.2. These will become the default values for the next 6 scenarios.

Expected Results:

- Since strength_2 and strength_6 affect the magnitude of shift in means, we expect that the reduction in these terms will affect $P(A_1=1|R_1=0)$ at States 2 and 6.



State	n.variable	Variable	sigma	tol	threshold	sig:tol	sig:threshold	tol:threshold	p1_1 (p1_5)	p1_2 (p1_4)	prot
1	1	V1	15	10	25	0.666666667	1.666666667	2.5	0.001	0.002	0.995
2	14	V2_1 to V2_14	1.1	0.1	2	0.090909091	1.818181818	20	0.001	0.002	0.995
3	3	V3_1, V3_2, V3_3	2.5	0.8	5	0.32	2	6.25	0.001	0.002	0.995
4	2	V4_1, V4_2	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
	1	V4_3	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
5	1	V5_1	10	5	25	0.5	2.5	5	0.001	0.002	0.995
	4	V5_2 to V5_5	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
6	3	V6_1, V6_3, V6_5	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
	1	V6_7	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
7	2	V7_1, V7_2	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
	1	V7_3	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
8	1	V8	2	0.2	5	0.1	2.5	25	0.001	0.002	0.995
9	1	V9	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
10	1	Through wall									
	1	Thin wall									

Table 16: Parameter set for Scenario 4

Results:

- As shown in Figure 18, there are clear reductions in $P(A_1 = 1|R_1 = 0)$ at States 2 and 6.
- Also, with given parameter sets, the probability of through-wall is zero for all runs.
- At the same time, the probability of thin-wall is greatly decreased.

Scenario 4

The parameter set for Scenario 4 is shown in Table 16; simulation results can be found in Figure 12 and a comparison with Scenario 3 can be seen in Figure 19.

Parameter Set Description:

- The following scenario is a modification to the parameter sets provided in Scenario 3.
- σ-to-threshold ratios are reduced in States 1, 2, and 3. The ratios are now between 1.67 to 2.
- We are interested in determining whether failure at earlier stages affect the probability of through-wall.

Expected Results:

- We expect that $P(A = 1|R = 0)$ will be inflated at States 1, 2, and 3.

Results:

- Figure 19, clearly indicate inflation of $P(A = 1|R = 0)$ at Stages 1, 2, and 3.
- However, there is no visible impact on latter stages.
- Furthermore, with given parameter sets, the probability of through-wall is zero for all runs.

State	n.variable	Variable	sigma	tol	threshold	sig:tol	sig:threshold	tol:threshold	p1_1 (p1_5)	p1_2 (p1_4)	prot
1	1	V1	15	10	25	0.666666667	1.666666667	2.5	0.001	0.002	0.995
2	14	V2_1 to V2_14	1.1	0.1	2	0.090909091	1.818181818	20	0.001	0.002	0.995
3	3	V3_1, V3_2, V3_3	2.5	0.8	5	0.32	2	6.25	0.001	0.002	0.995
4	2	V4_1, V4_2	0.4	0.1	1	0.25	2.5	10	0.01	0.02	0.995
	1	V4_3	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
5	1	V5_1	10	5	25	0.5	2.5	5	0.01	0.02	0.995
	4	V5_2 to V5_5	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
6	3	V6_1, V6_3, V6_5	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
	1	V6_7	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
7	2	V7_1, V7_2	0.4	0.1	1	0.25	2.5	10	0.01	0.02	0.995
	1	V7_3	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
8	1	V8	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
9	1	V9	0.4	0.1	1	0.25	2.5	10	0.001	0.002	0.995
10	1	Through wall									
	1	Thin wall									

Table 17: Parameter set for Scenario 5

Scenario 5

The parameter set for Scenario 5 is shown in Table 17; simulation results can be found in Figure 13 and a comparison with Scenario 4 can be seen in Figure 20.

Parameter Set Description:

- The following scenario is a modification to the parameter sets provided in Scenario 4.
- In previous scenarios, $p_{i,1}$, and $p_{i,2}$ were set to 0.001, and 0.002, respectively at all states. They are inflated to 0.01 and 0.02.
- In this scenario, two main goals are to determine the effect of inflated $p_{i,1}$, and $p_{i,2}$, as well as their impact on subsequent states.

Expected Results:

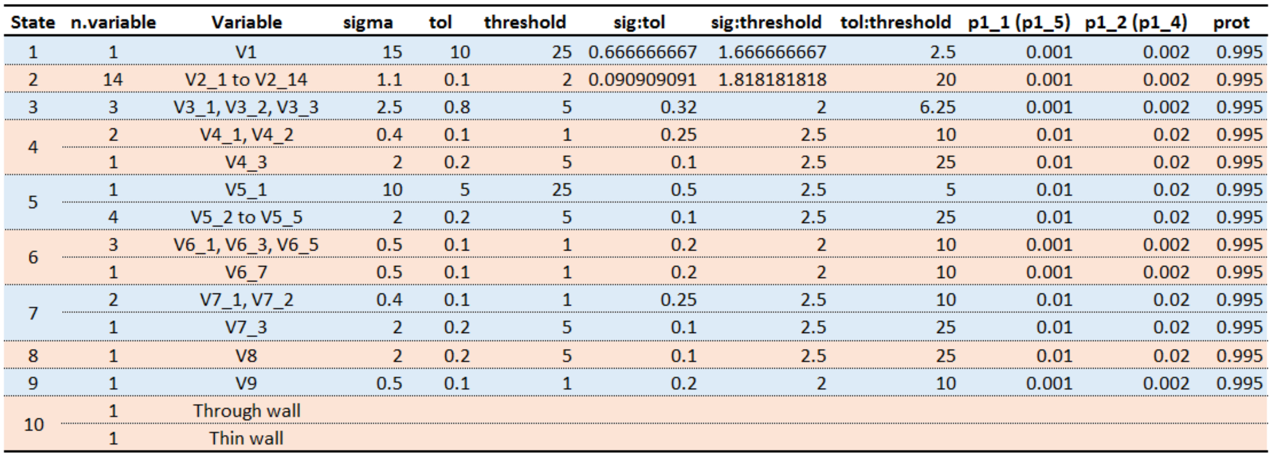
- $P(A_1 = 1|R_1 = 0)$ at States 4 and 5are expected to inflate.
- Since States 7 and 8 share the parameters with States 4 and 5, these states are likely affected as well.

Results:

- Due to inflation in $p_{i,1}$, and $p_{i,2}$, States 4 and 5 show greater $P(A = 1|R = 0)$.
- While $P(A = 1|R = 0)$ are at a similar level in States 4 and 5, these probabilities are impacted at different magnitudes between States 7 and 8. This is likely due to the fact that State 7 has three components, while State 8 has only one component.
- Even though State 9 is dependent on State 7, no significant impact is observed at State 9.

Scenario 6

The parameter set for Scenario 6 is shown in Table 18; simulation results can be found in Figure 14 and a comparison with Scenario 5 can be seen in Figure 21.



State	n.variable	Variable	sigma	tol	threshold	sig:tol	sig:threshold	tol:threshold	p1_1 (p1_5)	p1_2 (p1_4)	prot
1	1	V1	15	10	25	0.666666667	1.666666667	2.5	0.001	0.002	0.995
2	14	V2_1 to V2_14	1.1	0.1	2	0.090909091	1.818181818	20	0.001	0.002	0.995
3	3	V3_1, V3_2, V3_3	2.5	0.8	5	0.32	2	6.25	0.001	0.002	0.995
4	2	V4_1, V4_2	0.4	0.1	1	0.25	2.5	10	0.01	0.02	0.995
	1	V4_3	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
5	1	V5_1	10	5	25	0.5	2.5	5	0.01	0.02	0.995
	4	V5_2 to V5_5	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
6	3	V6_1, V6_3, V6_5	0.5	0.1	1	0.2	2	10	0.001	0.002	0.995
	1	V6_7	0.5	0.1	1	0.2	2	10	0.001	0.002	0.995
7	2	V7_1, V7_2	0.4	0.1	1	0.25	2.5	10	0.01	0.02	0.995
	1	V7_3	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
8	1	V8	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
9	1	V9	0.5	0.1	1	0.2	2	10	0.001	0.002	0.995
10	1	Through wall									
	1	Thin wall									

Table 18: Parameter set for Scenario 6

Parameter Set Description:

- Here, parameters in States 6 and 9 are introduced. Parameters at other states are held constant.
- σ-to-threshold ratio is reduced from 2.5 to 2 in States 6 and 9.
- As State 10 is built on States 6 and 9, our main interest lies in determining the effect on thin-wall, as well as through-wall.

Expected Results:

- $P(A=1|R=0)$ at States 6 and 9 should be inflated.
- The likelihood of thin-wall and through-wall should also be inflated.

Results:

- As expected, $P(A=1|R=0)$ at States 6 and 9 are increased significantly.
- While the likelihood of thin-wall has increased, no case of through-wall is reported in all runs.

Scenario 7

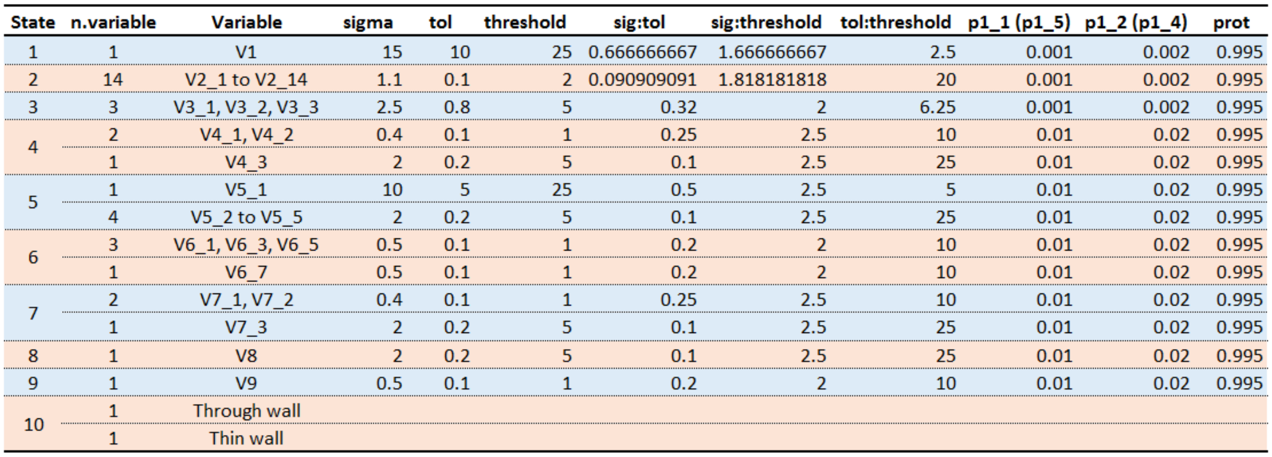
The parameter set for Scenario 7 is shown in Table 19; simulation results can be found in Figure 15 and a comparison with Scenario 6 can be seen in Figure 22.

Parameter Set Description:

- In addition to the changes implemented in Scenario 6, $p_{i,1}$, and $p_{i,2}$ are changed to 0.01, and 0.02 in States 6 and 9.

Expected Results:

- In a similar way to Scenario 6, $P(A_1=1|R_1=0)$ are expected to increase in States 6 and 9.



State	n.variable	Variable	sigma	tol	threshold	sig:tol	sig:threshold	tol:threshold	p1_1 (p1_5)	p1_2 (p1_4)	prot
1	1	V1	15	10	25	0.666666667	1.666666667	2.5	0.001	0.002	0.995
2	14	V2_1 to V2_14	1.1	0.1	2	0.090909091	1.818181818	20	0.001	0.002	0.995
3	3	V3_1, V3_2, V3_3	2.5	0.8	5	0.32	2	6.25	0.001	0.002	0.995
4	2	V4_1, V4_2	0.4	0.1	1	0.25	2.5	10	0.01	0.02	0.995
	1	V4_3	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
5	1	V5_1	10	5	25	0.5	2.5	5	0.01	0.02	0.995
	4	V5_2 to V5_5	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
6	3	V6_1, V6_3, V6_5	0.5	0.1	1	0.2	2	10	0.01	0.02	0.995
	1	V6_7	0.5	0.1	1	0.2	2	10	0.01	0.02	0.995
7	2	V7_1, V7_2	0.4	0.1	1	0.25	2.5	10	0.01	0.02	0.995
	1	V7_3	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
8	1	V8	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
9	1	V9	0.5	0.1	1	0.2	2	10	0.01	0.02	0.995
10	1	Through wall									
	1	Thin wall									

Table 19: Parameter set for Scenario 7

- The probabilities of thin-wall and through-wall are positively affected.

Results:

- States 6 and 9 have further increased $P(A_1 = 1|R_1 = 0)$.
- While the likelihood of thin-wall become extremely large, the event of through-wall is not reported in any runs.

Scenario 8

The parameter set for Scenario 8 is shown in Table 20; simulation results can be found in Figure 16 and a comparison with Scenario 7 can be seen in Figure 23.

Parameter Set Description:

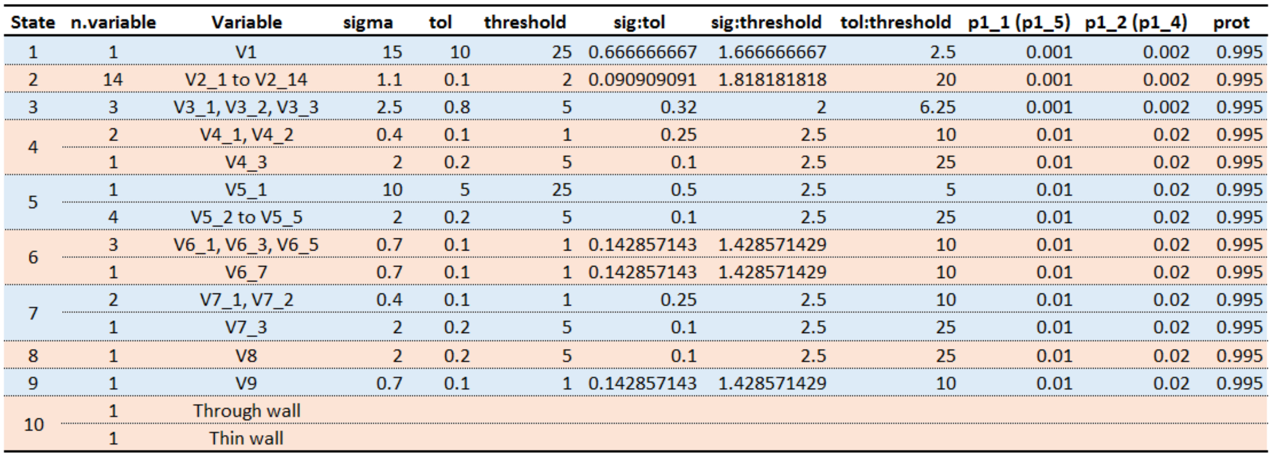
- In the last scenario, σ-to-threshold ratio in States 6 and 9 are further reduced to 1.42.

Expected Results:

- Inflation in $P(A_1 = 1|R_1 = 0)$ at States 6 and 9 is expected.
- Possible increase in the likelihood of thin-wall and through-wall.

Results:

- Again, $P(A_1 = 1|R_1 = 0)$ at States 6 and 9 are increased.
- While it is small, the probability of through-wall is positive in all twenty runs. The average likelihood is now 1.14×10^{-4}.



State	n.variable	Variable	sigma	tol	threshold	sig:tol	sig:threshold	tol:threshold	p1_1 (p1_5)	p1_2 (p1_4)	prot
1	1	V1	15	10	25	0.666666667	1.666666667	2.5	0.001	0.002	0.995
2	14	V2_1 to V2_14	1.1	0.1	2	0.090909091	1.818181818	20	0.001	0.002	0.995
3	3	V3_1, V3_2, V3_3	2.5	0.8	5	0.32	2	6.25	0.001	0.002	0.995
4	2	V4_1, V4_2	0.4	0.1	1	0.25	2.5	10	0.01	0.02	0.995
	1	V4_3	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
5	1	V5_1	10	5	25	0.5	2.5	5	0.01	0.02	0.995
	4	V5_2 to V5_5	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
6	3	V6_1, V6_3, V6_5	0.7	0.1	1	0.142857143	1.428571429	10	0.01	0.02	0.995
	1	V6_7	0.7	0.1	1	0.142857143	1.428571429	10	0.01	0.02	0.995
7	2	V7_1, V7_2	0.4	0.1	1	0.25	2.5	10	0.01	0.02	0.995
	1	V7_3	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
8	1	V8	2	0.2	5	0.1	2.5	25	0.01	0.02	0.995
9	1	V9	0.7	0.1	1	0.142857143	1.428571429	10	0.01	0.02	0.995
10	1	Through wall									
	1	Thin wall									

Table 20: Parameter set for Scenario 8

Lookup Tables

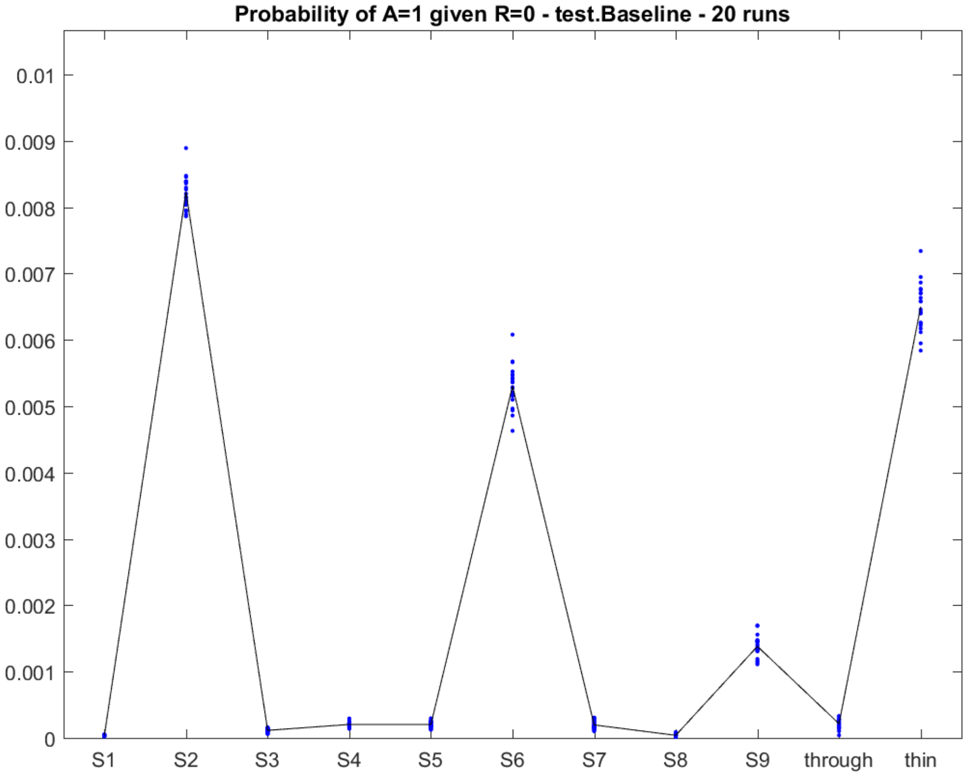
The given lookup tables serve as guidelines to determine the expected conditional probability of a damaged UFC misreported as undamaged (i.e., $P(A=1|R=0)$). The values in the table are generated based on normal distributions with one-sided thresholds (such as is the case with V_1 in State 1). Other variables are also generated based on normal distributions or on order statistics based on normal distributions and folded normal distributions.

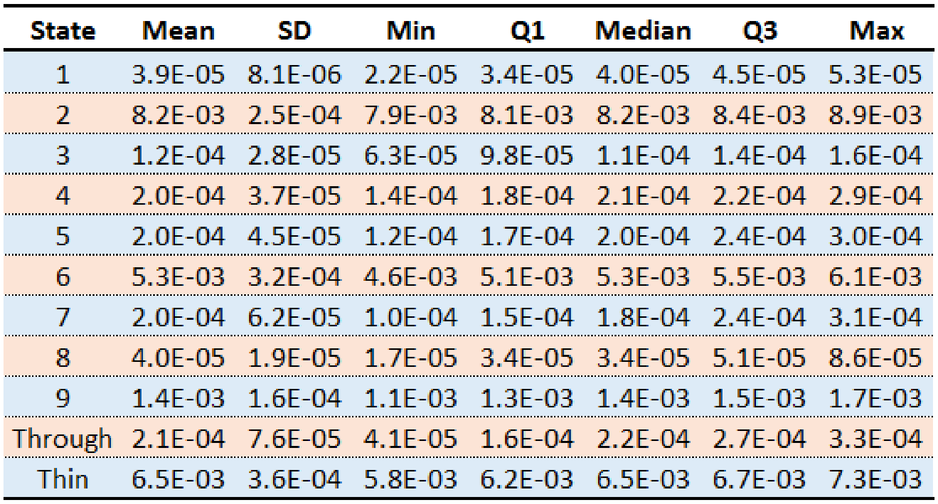
Therefore, while these tables do not provide the exact expected probability $P(A=1|R=0)$ for each state, they provide a rough estimate of expected probability for each component at each state.

At the same time, comparisons within these tables provide an insight as to the effect that the parameters σ, tolerance, threshold, $p_1 = p_{\text{small}}$, and $p_2 = p_{\text{big}}$ have on $P(A=1|R=0)$. Consider, for instance, the third table of Table 21, where it is assumed that $p_1 = 0.001$, $p_2 = 0.002$, prot $= 0.99$, and tol $= 5$. The first row of that table shows that when σ is held constant at 1 (and the tolerance is held constant at 5), an increase in threshold values results in rapid reduction in $P(A=1|R=0)$. Similarly, a focus on the first column shows that an increase in sigma leads to inflated values of $P(A=1|R=0)$. The other tables can be used in a similar fashion.

References

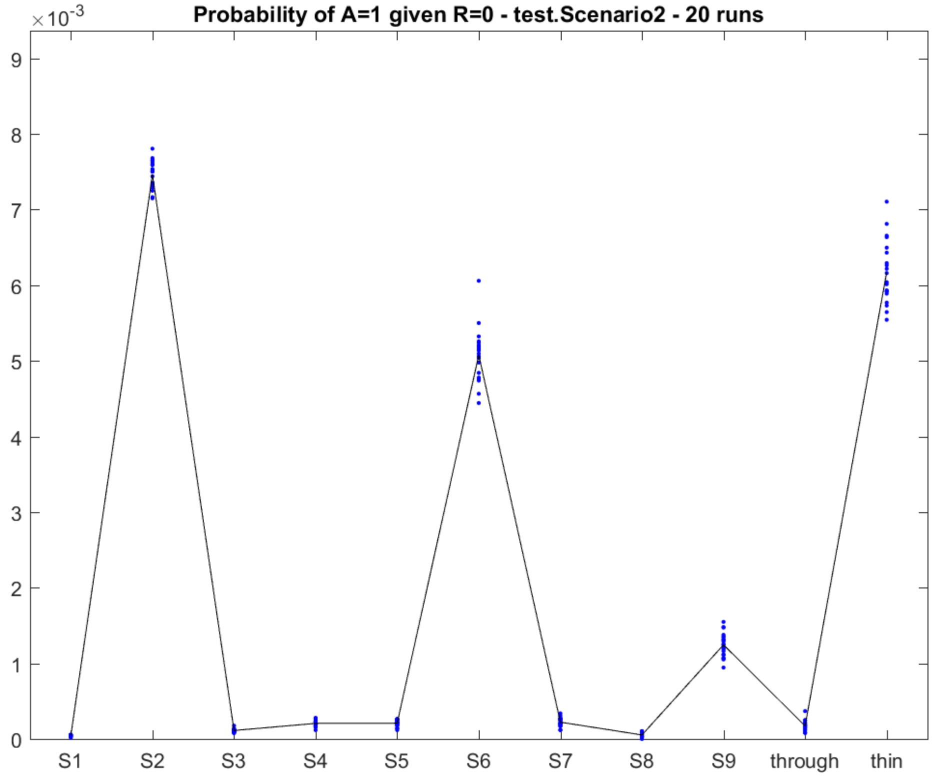
- Boyle, C., Overview of the NWMO and the Mark II Used Fuel Container, presentation deck from the NWMO.

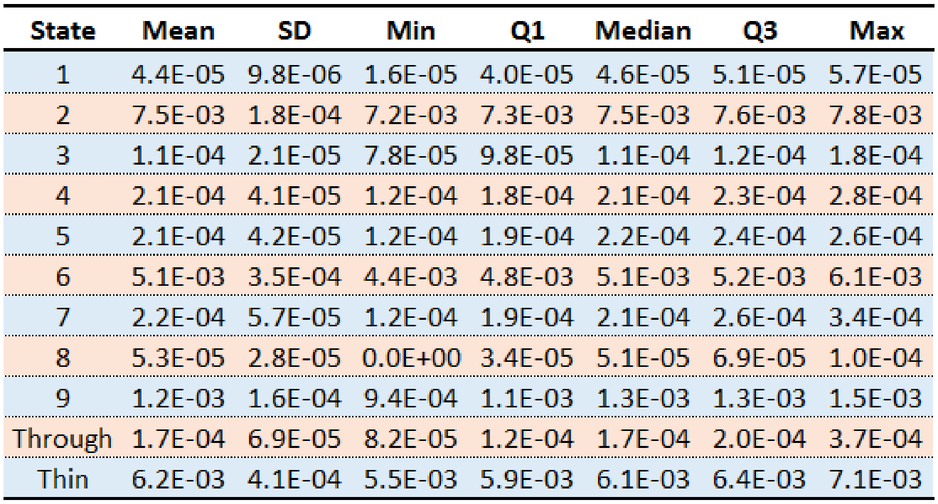




State	Mean	SD	Min	Q1	Median	Q3	Max
1	3.9E-05	8.1E-06	2.2E-05	3.4E-05	4.0E-05	4.5E-05	5.3E-05
2	8.2E-03	2.5E-04	7.9E-03	8.1E-03	8.2E-03	8.4E-03	8.9E-03
3	1.2E-04	2.8E-05	6.3E-05	9.8E-05	1.1E-04	1.4E-04	1.6E-04
4	2.0E-04	3.7E-05	1.4E-04	1.8E-04	2.1E-04	2.2E-04	2.9E-04
5	2.0E-04	4.5E-05	1.2E-04	1.7E-04	2.0E-04	2.4E-04	3.0E-04
6	5.3E-03	3.2E-04	4.6E-03	5.1E-03	5.3E-03	5.5E-03	6.1E-03
7	2.0E-04	6.2E-05	1.0E-04	1.5E-04	1.8E-04	2.4E-04	3.1E-04
8	4.0E-05	1.9E-05	1.7E-05	3.4E-05	3.4E-05	5.1E-05	8.6E-05
9	1.4E-03	1.6E-04	1.1E-03	1.3E-03	1.4E-03	1.5E-03	1.7E-03
Through	2.1E-04	7.6E-05	4.1E-05	1.6E-04	2.2E-04	2.7E-04	3.3E-04
Thin	6.5E-03	3.6E-04	5.8E-03	6.2E-03	6.5E-03	6.7E-03	7.3E-03

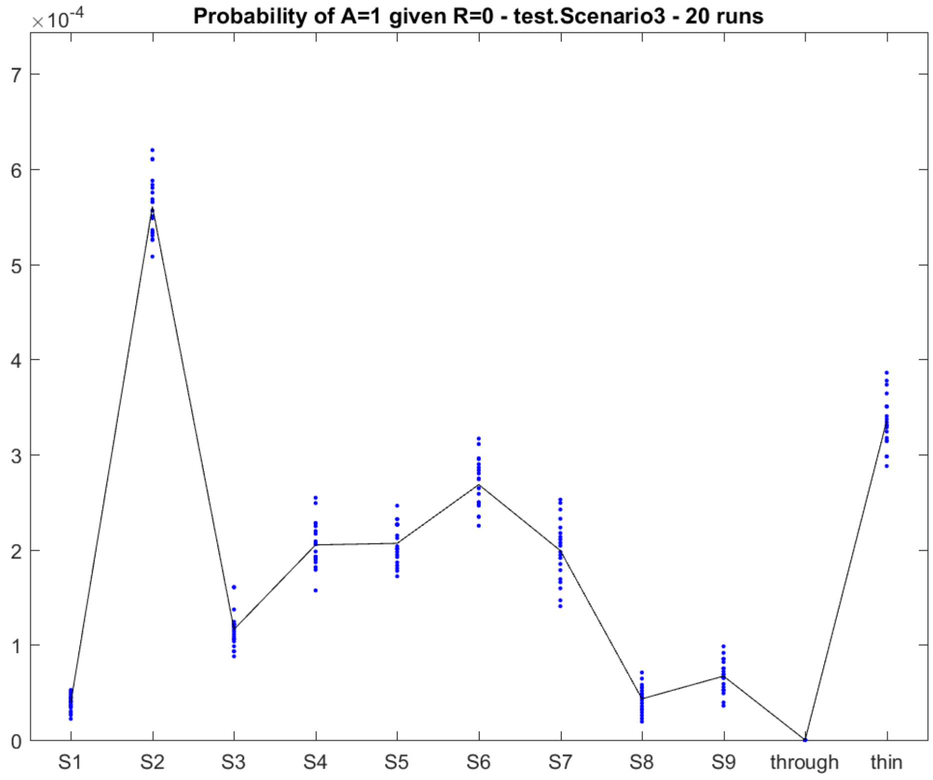
Figure 9: Simulation results for Scenario 1: conditional probabilities $P(A_j = 1|R_j = 0)$ for each state and descriptive statistics.





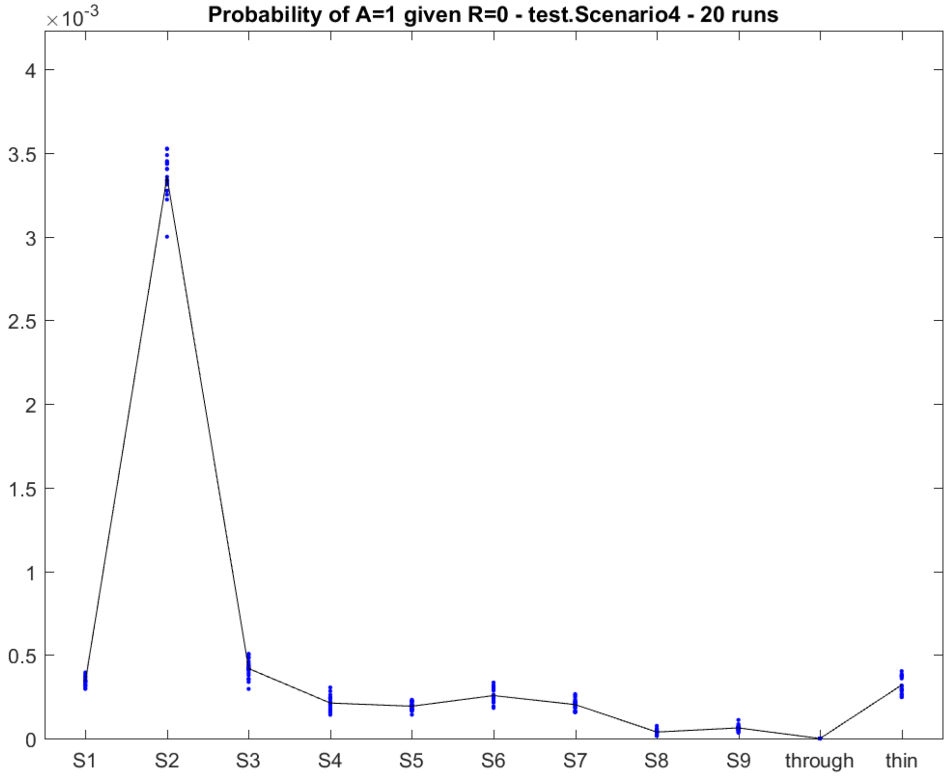
State	Mean	SD	Min	Q1	Median	Q3	Max
1	4.4E-05	9.8E-06	1.6E-05	4.0E-05	4.6E-05	5.1E-05	5.7E-05
2	7.5E-03	1.8E-04	7.2E-03	7.3E-03	7.5E-03	7.6E-03	7.8E-03
3	1.1E-04	2.1E-05	7.8E-05	9.8E-05	1.1E-04	1.2E-04	1.8E-04
4	2.1E-04	4.1E-05	1.2E-04	1.8E-04	2.1E-04	2.3E-04	2.8E-04
5	2.1E-04	4.2E-05	1.2E-04	1.9E-04	2.2E-04	2.4E-04	2.6E-04
6	5.1E-03	3.5E-04	4.4E-03	4.8E-03	5.1E-03	5.2E-03	6.1E-03
7	2.2E-04	5.7E-05	1.2E-04	1.9E-04	2.1E-04	2.6E-04	3.4E-04
8	5.3E-05	2.8E-05	0.0E+00	3.4E-05	5.1E-05	6.9E-05	1.0E-04
9	1.2E-03	1.6E-04	9.4E-04	1.1E-03	1.3E-03	1.3E-03	1.5E-03
Through	1.7E-04	6.9E-05	8.2E-05	1.2E-04	1.7E-04	2.0E-04	3.7E-04
Thin	6.2E-03	4.1E-04	5.5E-03	5.9E-03	6.1E-03	6.4E-03	7.1E-03

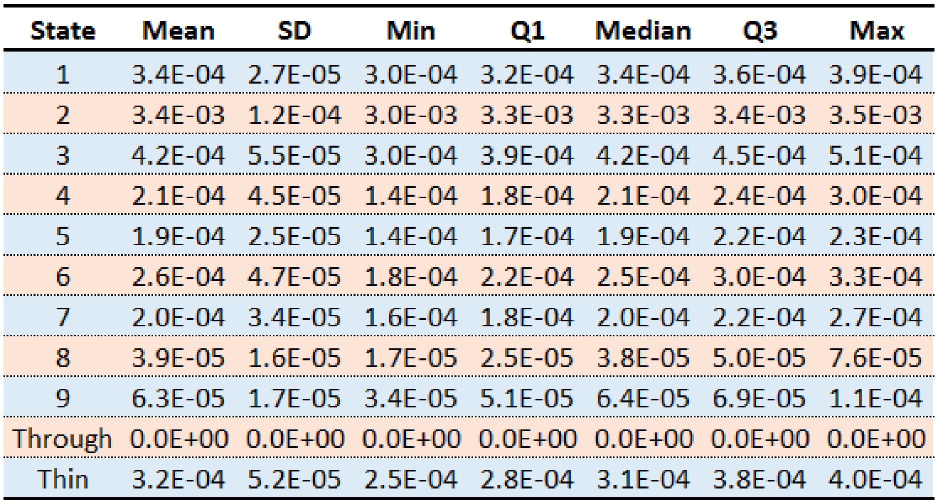
Figure 10: Simulation results for Scenario 2: conditional probabilities $P(A_j = 1|R_j = 0)$ for each state and descriptive statistics.



State	Mean	SD	Min	Q1	Median	Q3	Max
1	3.9E-05	8.1E-06	2.2E-05	3.4E-05	4.0E-05	4.5E-05	5.3E-05
2	5.6E-04	3.2E-05	5.1E-04	5.3E-04	5.6E-04	5.8E-04	6.2E-04
3	1.2E-04	1.9E-05	8.8E-05	1.1E-04	1.2E-04	1.2E-04	1.6E-04
4	2.1E-04	2.4E-05	1.6E-04	1.9E-04	2.0E-04	2.2E-04	2.5E-04
5	2.1E-04	2.1E-05	1.7E-04	1.9E-04	2.0E-04	2.3E-04	2.5E-04
6	2.7E-04	2.6E-05	2.3E-04	2.5E-04	2.7E-04	2.9E-04	3.2E-04
7	2.0E-04	3.3E-05	1.4E-04	1.8E-04	2.0E-04	2.2E-04	2.5E-04
8	4.3E-05	1.4E-05	1.9E-05	3.2E-05	4.5E-05	5.2E-05	7.1E-05
9	6.7E-05	1.7E-05	3.6E-05	5.5E-05	6.7E-05	7.7E-05	9.8E-05
Through	0	0	0	0	0	0	0
Thin	3.4E-04	2.7E-05	2.9E-04	3.2E-04	3.3E-04	3.5E-04	3.9E-04

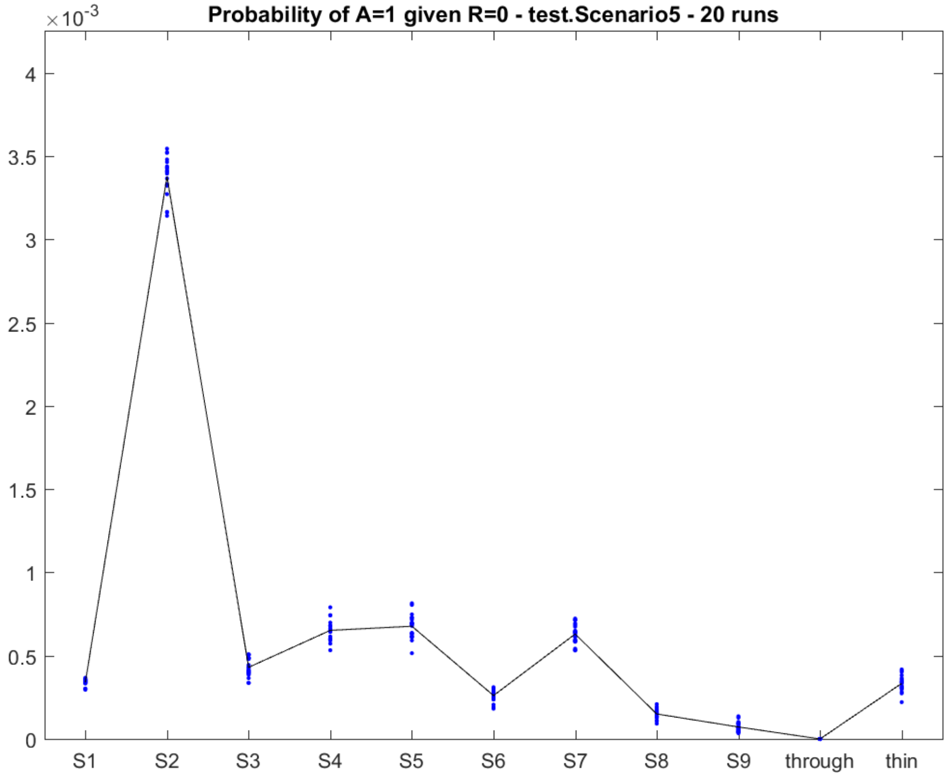
Figure 11: Simulation results for Scenario 3: conditional probabilities $P(A_j = 1|R_j = 0)$ for each state and descriptive statistics.

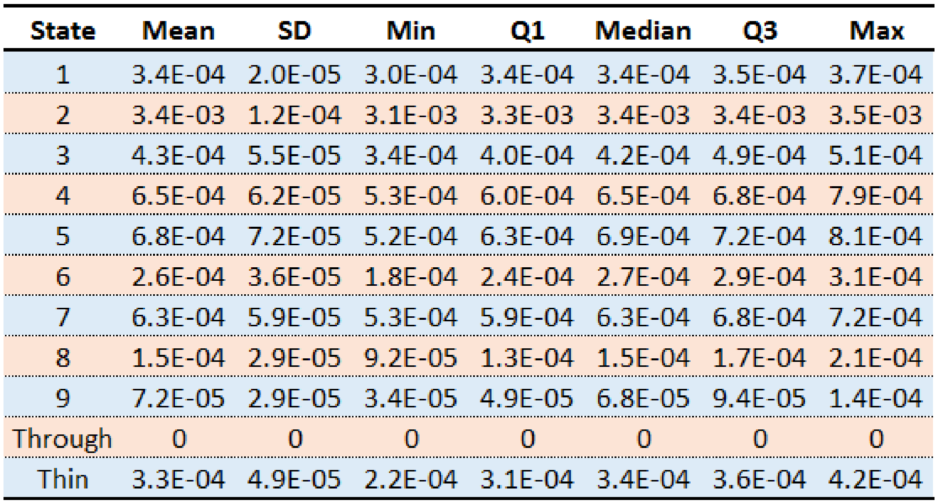




State	Mean	SD	Min	Q1	Median	Q3	Max
1	3.4E-04	2.7E-05	3.0E-04	3.2E-04	3.4E-04	3.6E-04	3.9E-04
2	3.4E-03	1.2E-04	3.0E-03	3.3E-03	3.3E-03	3.4E-03	3.5E-03
3	4.2E-04	5.5E-05	3.0E-04	3.9E-04	4.2E-04	4.5E-04	5.1E-04
4	2.1E-04	4.5E-05	1.4E-04	1.8E-04	2.1E-04	2.4E-04	3.0E-04
5	1.9E-04	2.5E-05	1.4E-04	1.7E-04	1.9E-04	2.2E-04	2.3E-04
6	2.6E-04	4.7E-05	1.8E-04	2.2E-04	2.5E-04	3.0E-04	3.3E-04
7	2.0E-04	3.4E-05	1.6E-04	1.8E-04	2.0E-04	2.2E-04	2.7E-04
8	3.9E-05	1.6E-05	1.7E-05	2.5E-05	3.8E-05	5.0E-05	7.6E-05
9	6.3E-05	1.7E-05	3.4E-05	5.1E-05	6.4E-05	6.9E-05	1.1E-04
Through	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
Thin	3.2E-04	5.2E-05	2.5E-04	2.8E-04	3.1E-04	3.8E-04	4.0E-04

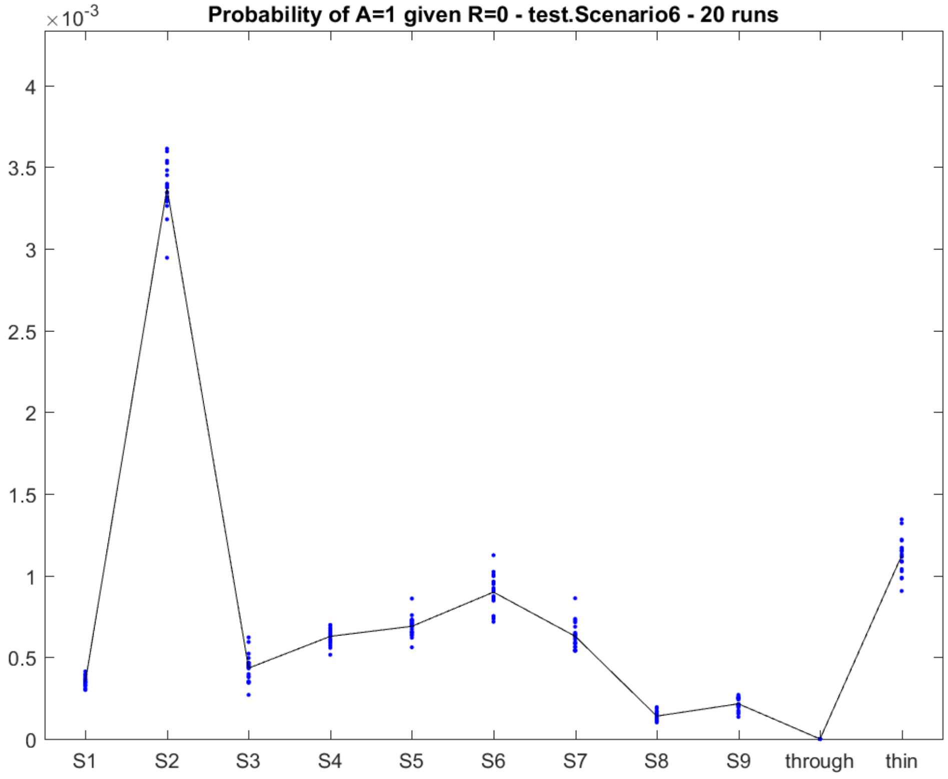
Figure 12: Simulation results for Scenario 4: conditional probabilities $P(A_j = 1|R_j = 0)$ for each state and descriptive statistics.

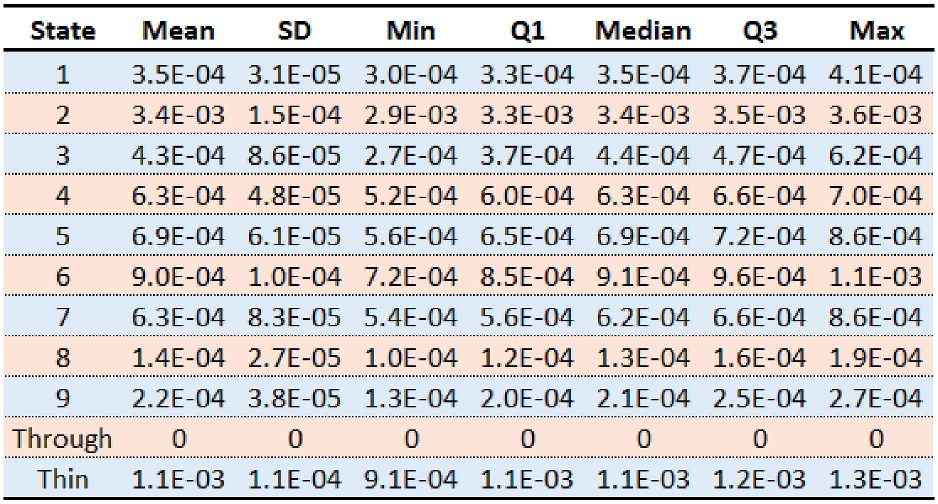




State	Mean	SD	Min	Q1	Median	Q3	Max
1	3.4E-04	2.0E-05	3.0E-04	3.4E-04	3.4E-04	3.5E-04	3.7E-04
2	3.4E-03	1.2E-04	3.1E-03	3.3E-03	3.4E-03	3.4E-03	3.5E-03
3	4.3E-04	5.5E-05	3.4E-04	4.0E-04	4.2E-04	4.9E-04	5.1E-04
4	6.5E-04	6.2E-05	5.3E-04	6.0E-04	6.5E-04	6.8E-04	7.9E-04
5	6.8E-04	7.2E-05	5.2E-04	6.3E-04	6.9E-04	7.2E-04	8.1E-04
6	2.6E-04	3.6E-05	1.8E-04	2.4E-04	2.7E-04	2.9E-04	3.1E-04
7	6.3E-04	5.9E-05	5.3E-04	5.9E-04	6.3E-04	6.8E-04	7.2E-04
8	1.5E-04	2.9E-05	9.2E-05	1.3E-04	1.5E-04	1.7E-04	2.1E-04
9	7.2E-05	2.9E-05	3.4E-05	4.9E-05	6.8E-05	9.4E-05	1.4E-04
Through	0	0	0	0	0	0	0
Thin	3.3E-04	4.9E-05	2.2E-04	3.1E-04	3.4E-04	3.6E-04	4.2E-04

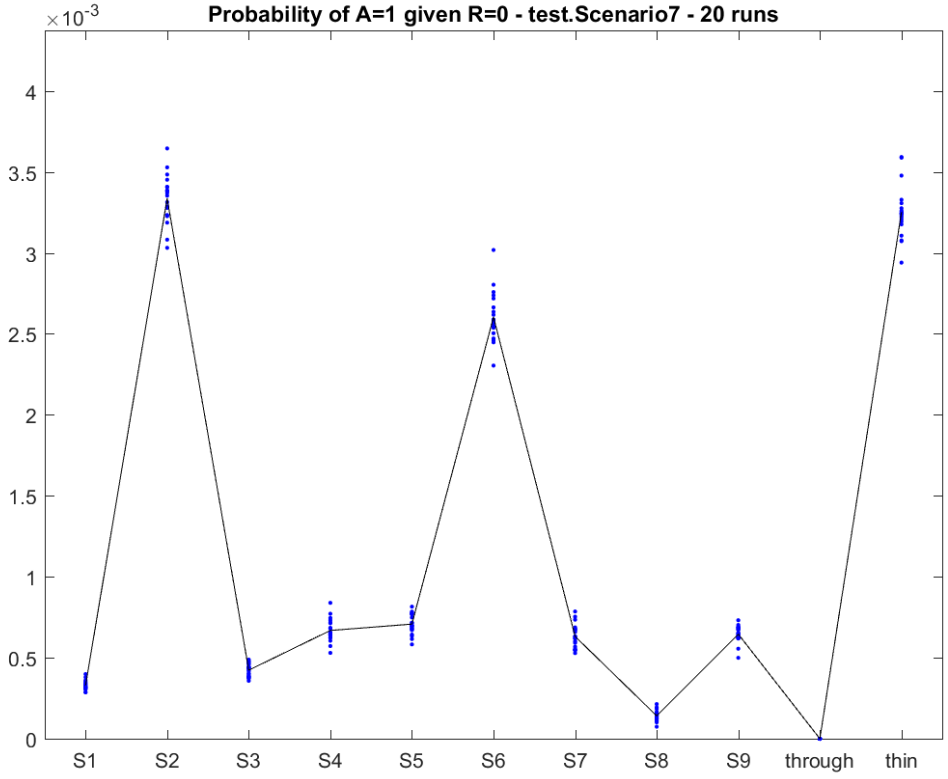
Figure 13: Simulation results for Scenario 5: conditional probabilities $P(A_j = 1|R_j = 0)$ for each state and descriptive statistics.

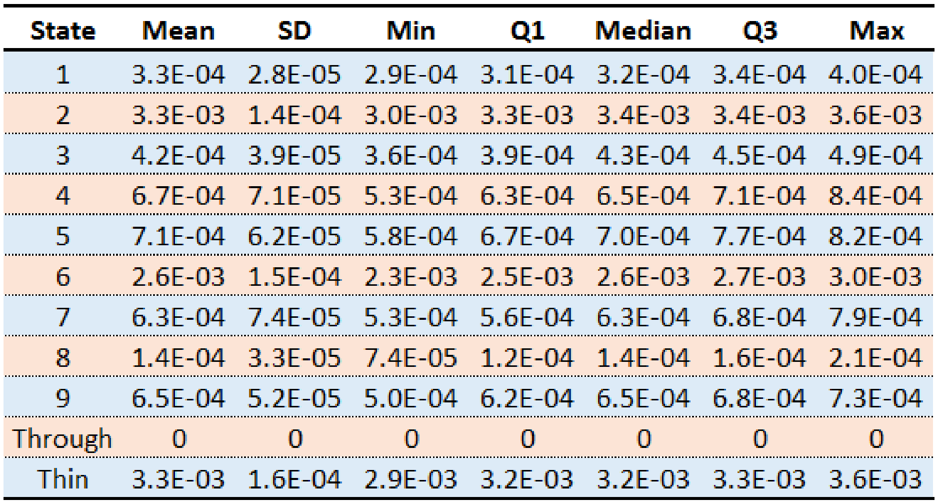




State	Mean	SD	Min	Q1	Median	Q3	Max
1	3.5E-04	3.1E-05	3.0E-04	3.3E-04	3.5E-04	3.7E-04	4.1E-04
2	3.4E-03	1.5E-04	2.9E-03	3.3E-03	3.4E-03	3.5E-03	3.6E-03
3	4.3E-04	8.6E-05	2.7E-04	3.7E-04	4.4E-04	4.7E-04	6.2E-04
4	6.3E-04	4.8E-05	5.2E-04	6.0E-04	6.3E-04	6.6E-04	7.0E-04
5	6.9E-04	6.1E-05	5.6E-04	6.5E-04	6.9E-04	7.2E-04	8.6E-04
6	9.0E-04	1.0E-04	7.2E-04	8.5E-04	9.1E-04	9.6E-04	1.1E-03
7	6.3E-04	8.3E-05	5.4E-04	5.6E-04	6.2E-04	6.6E-04	8.6E-04
8	1.4E-04	2.7E-05	1.0E-04	1.2E-04	1.3E-04	1.6E-04	1.9E-04
9	2.2E-04	3.8E-05	1.3E-04	2.0E-04	2.1E-04	2.5E-04	2.7E-04
Through	0	0	0	0	0	0	0
Thin	1.1E-03	1.1E-04	9.1E-04	1.1E-03	1.1E-03	1.2E-03	1.3E-03

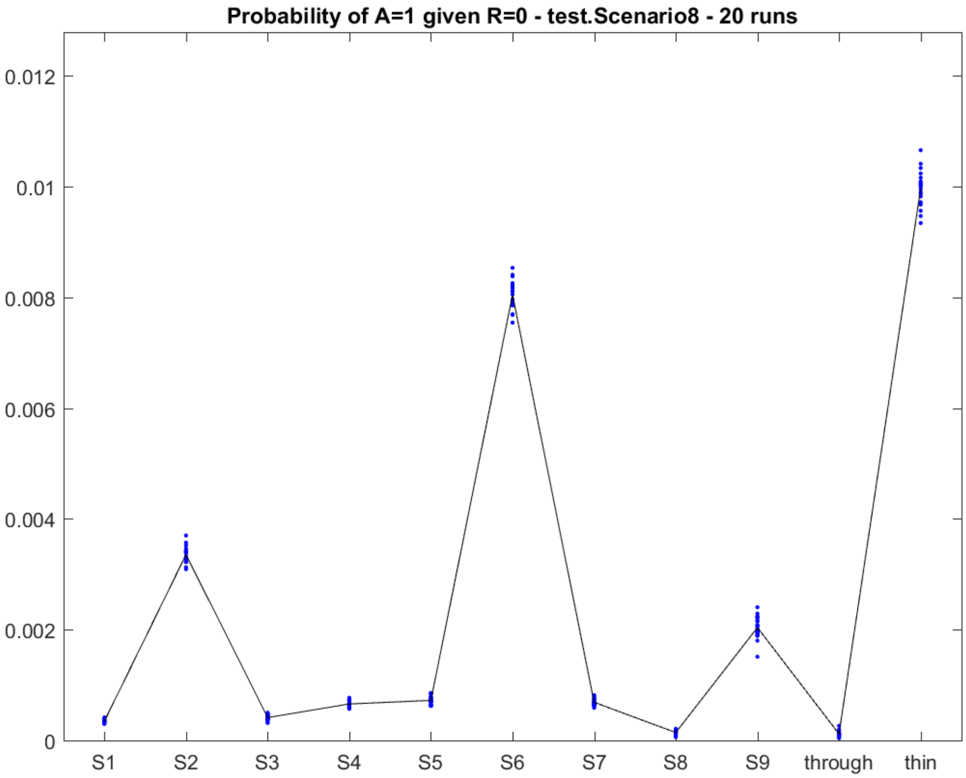
Figure 14: Simulation results for Scenario 6: conditional probabilities $P(A_j = 1|R_j = 0)$ for each state and descriptive statistics.





State	Mean	SD	Min	Q1	Median	Q3	Max
1	3.3E-04	2.8E-05	2.9E-04	3.1E-04	3.2E-04	3.4E-04	4.0E-04
2	3.3E-03	1.4E-04	3.0E-03	3.3E-03	3.4E-03	3.4E-03	3.6E-03
3	4.2E-04	3.9E-05	3.6E-04	3.9E-04	4.3E-04	4.5E-04	4.9E-04
4	6.7E-04	7.1E-05	5.3E-04	6.3E-04	6.5E-04	7.1E-04	8.4E-04
5	7.1E-04	6.2E-05	5.8E-04	6.7E-04	7.0E-04	7.7E-04	8.2E-04
6	2.6E-03	1.5E-04	2.3E-03	2.5E-03	2.6E-03	2.7E-03	3.0E-03
7	6.3E-04	7.4E-05	5.3E-04	5.6E-04	6.3E-04	6.8E-04	7.9E-04
8	1.4E-04	3.3E-05	7.4E-05	1.2E-04	1.4E-04	1.6E-04	2.1E-04
9	6.5E-04	5.2E-05	5.0E-04	6.2E-04	6.5E-04	6.8E-04	7.3E-04
Through	0	0	0	0	0	0	0
Thin	3.3E-03	1.6E-04	2.9E-03	3.2E-03	3.2E-03	3.3E-03	3.6E-03

Figure 15: Simulation results for Scenario 7: conditional probabilities $P(A_j = 1 | R_j = 0)$ for each state and descriptive statistics.



State	Mean	SD	Min	Q1	Median	Q3	Max
1	3.5E-04	2.7E-05	3.0E-04	3.3E-04	3.5E-04	3.6E-04	4.2E-04
2	3.4E-03	1.5E-04	3.1E-03	3.2E-03	3.4E-03	3.4E-03	3.7E-03
3	4.1E-04	5.0E-05	3.2E-04	3.8E-04	4.1E-04	4.5E-04	5.0E-04
4	6.6E-04	6.2E-05	5.7E-04	6.1E-04	6.6E-04	7.2E-04	7.7E-04
5	7.2E-04	7.3E-05	6.2E-04	6.8E-04	7.1E-04	7.7E-04	8.6E-04
6	8.0E-03	2.6E-04	7.5E-03	7.9E-03	8.1E-03	8.2E-03	8.5E-03
7	6.9E-04	6.0E-05	5.9E-04	6.5E-04	6.9E-04	7.2E-04	8.2E-04
8	1.4E-04	3.9E-05	6.2E-05	1.2E-04	1.5E-04	1.7E-04	2.1E-04
9	2.0E-03	2.0E-04	1.5E-03	1.9E-03	2.0E-03	2.2E-03	2.4E-03
Through	1.2E-04	5.0E-05	4.2E-05	8.3E-05	1.1E-04	1.3E-04	2.6E-04
Thin	1.0E-02	3.2E-04	9.3E-03	9.8E-03	1.0E-02	1.0E-02	1.1E-02

Figure 16: Simulation results for Scenario 8: conditional probabilities $P(A_j = 1|R_j = 0)$ for each state and descriptive statistics.

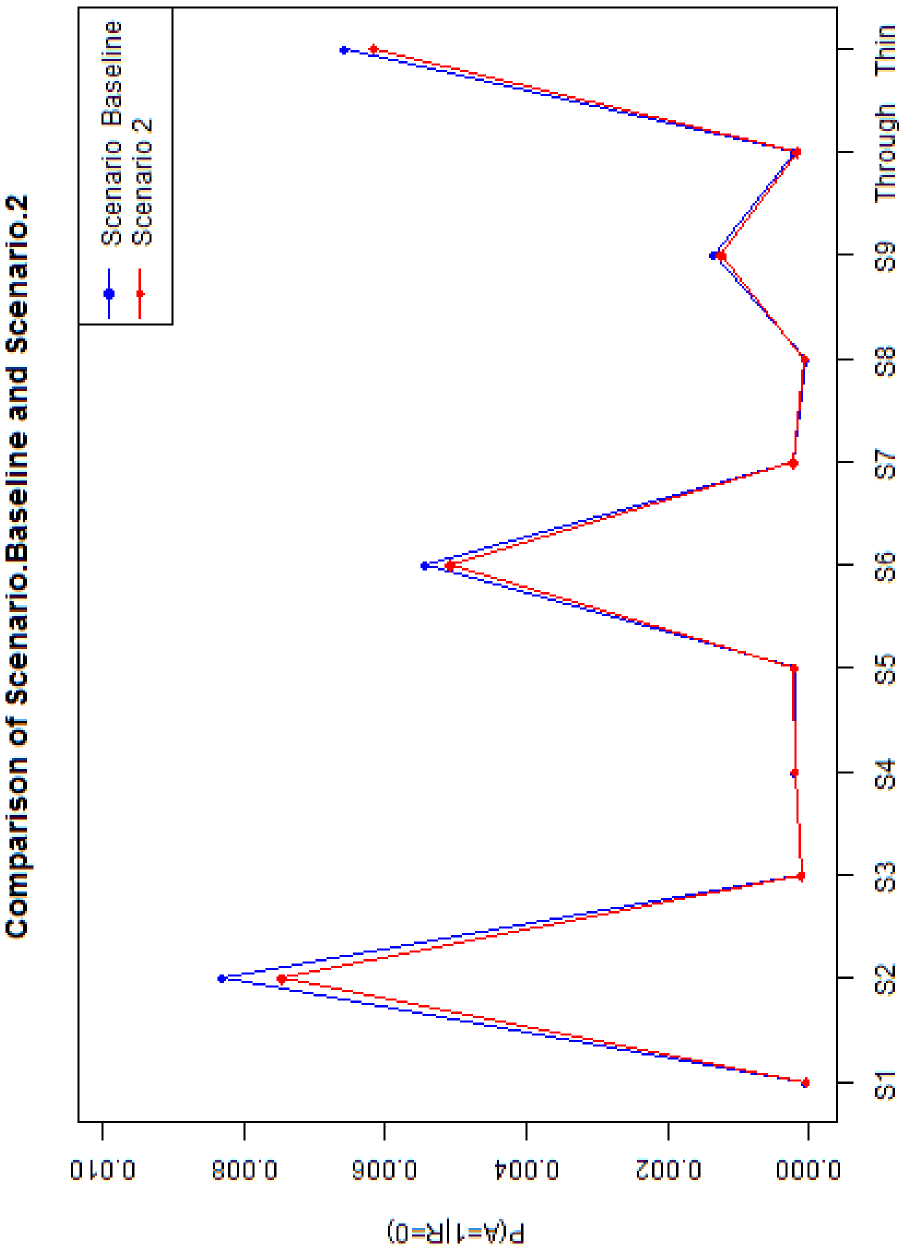


Figure 17: Comparison of simulation results between Scenarios 1 and 2.

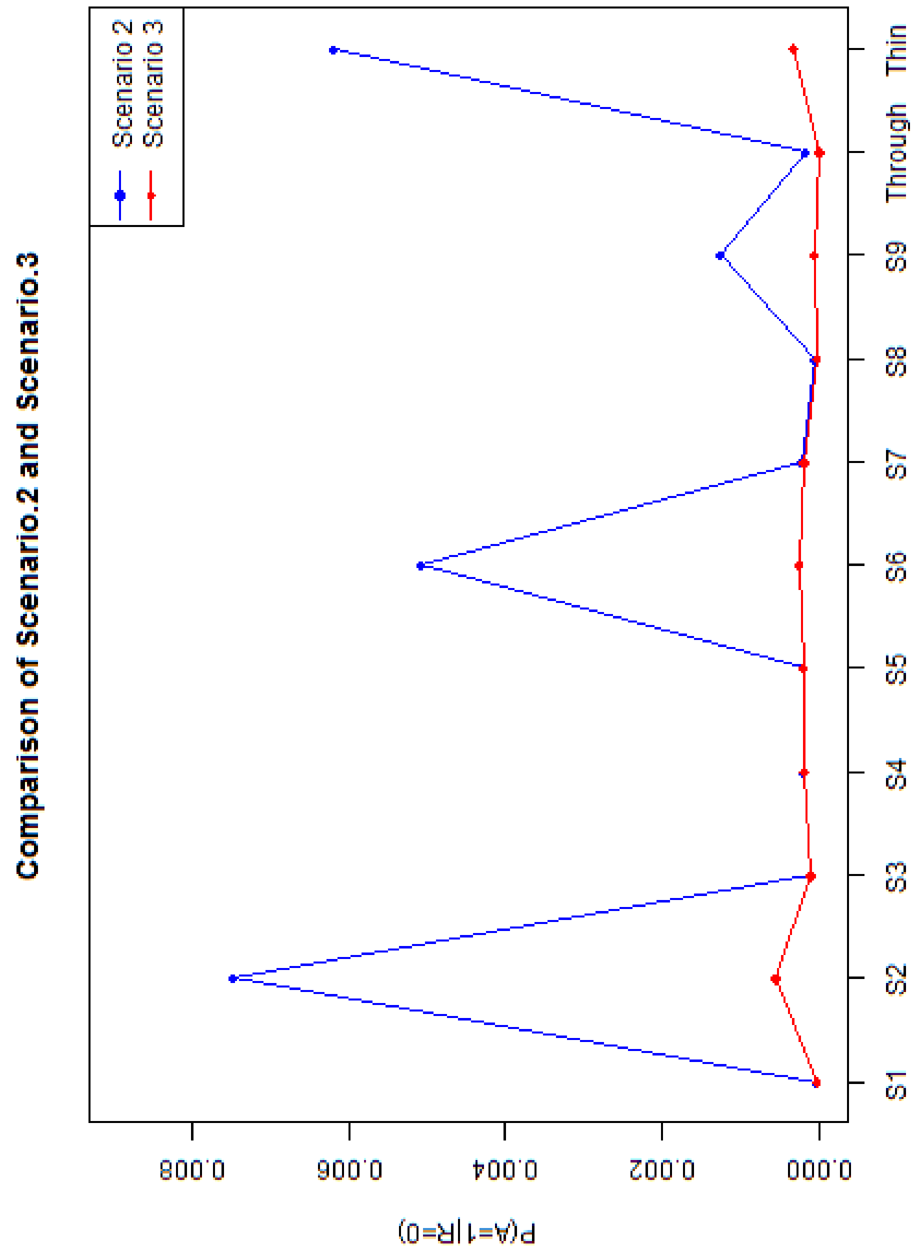


Figure 18: Comparison of simulation results between Scenarios 2 and 3.

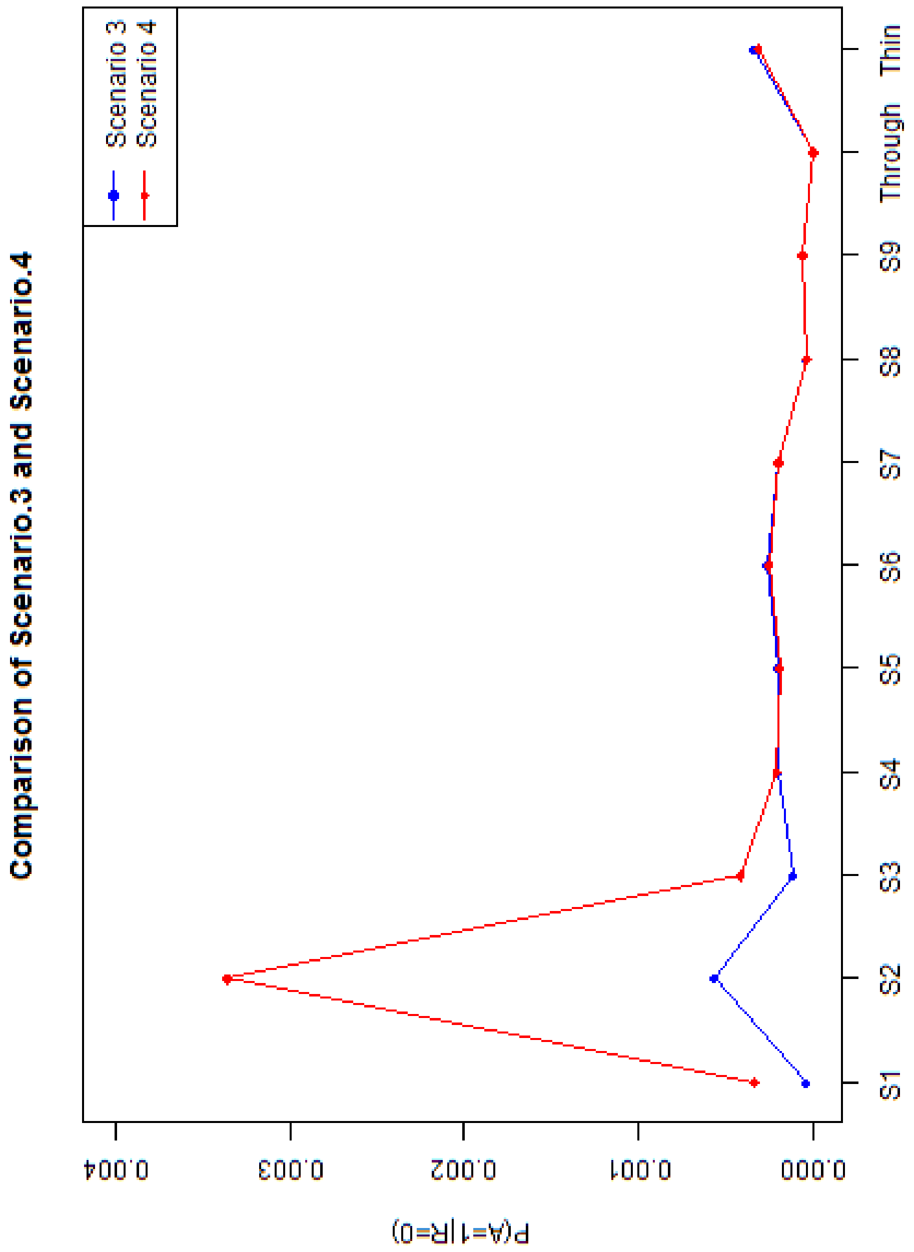


Figure 19: Comparison of simulation results between Scenarios 3 and 4.

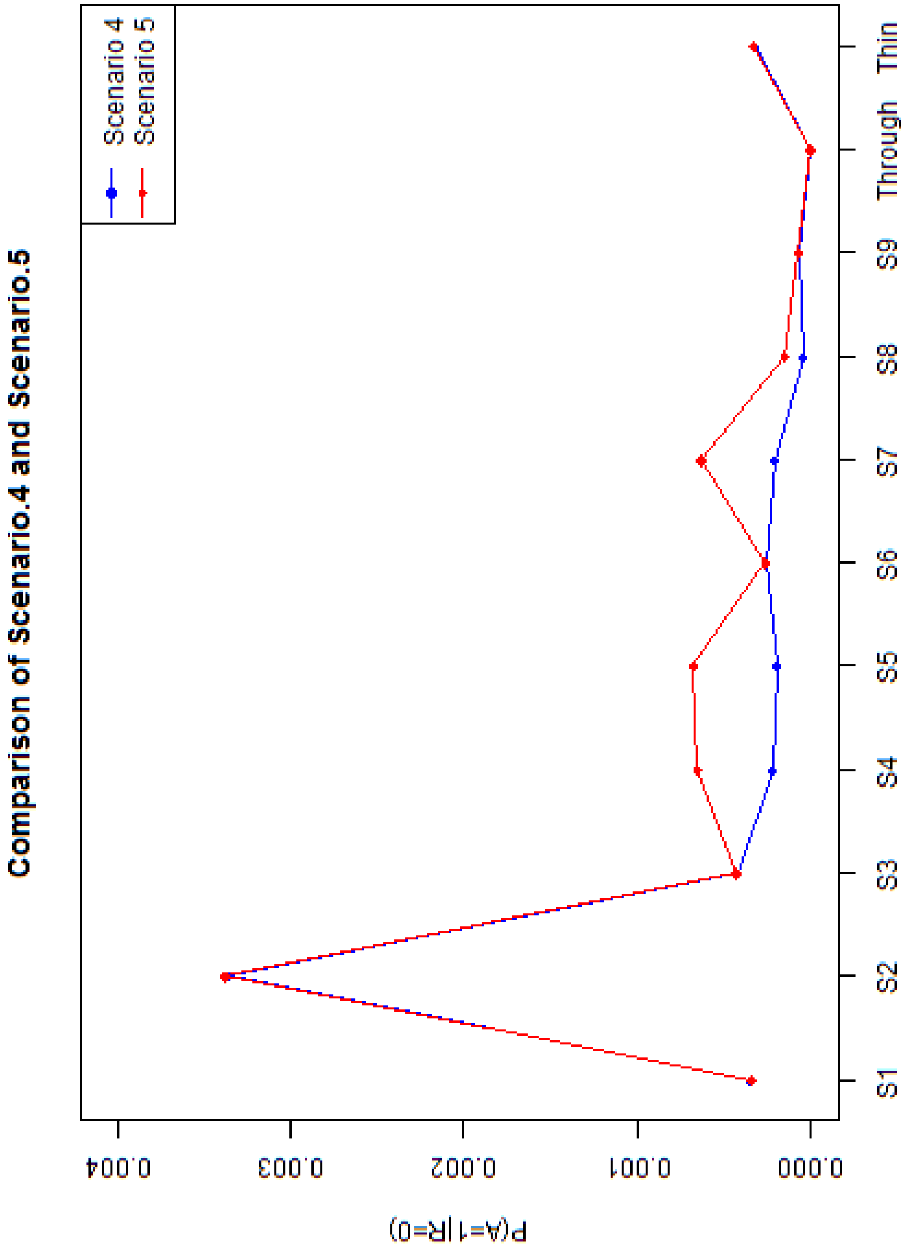


Figure 20: Comparison of simulation results between Scenarios 4 and 5.

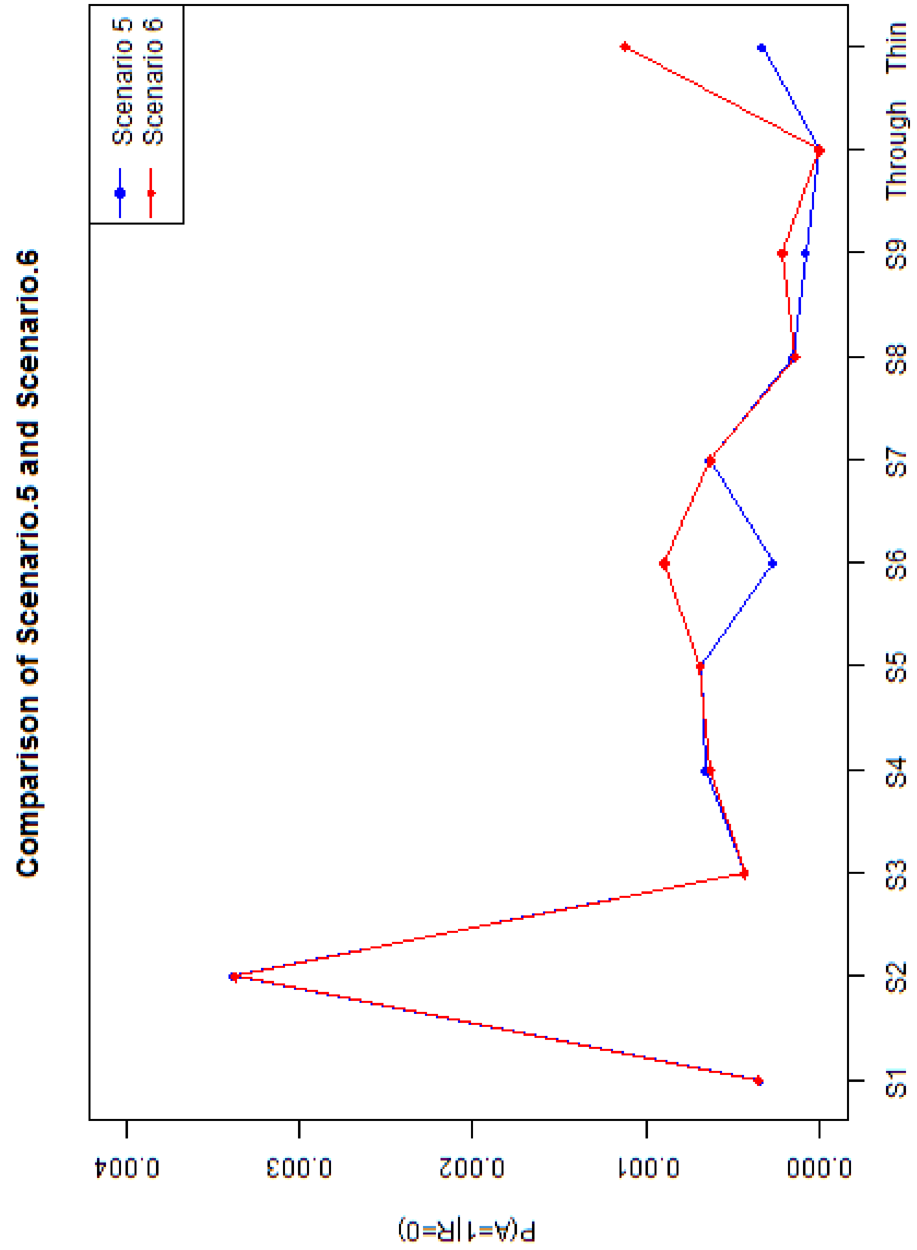


Figure 21: Comparison of simulation results between Scenarios 5 and 6.

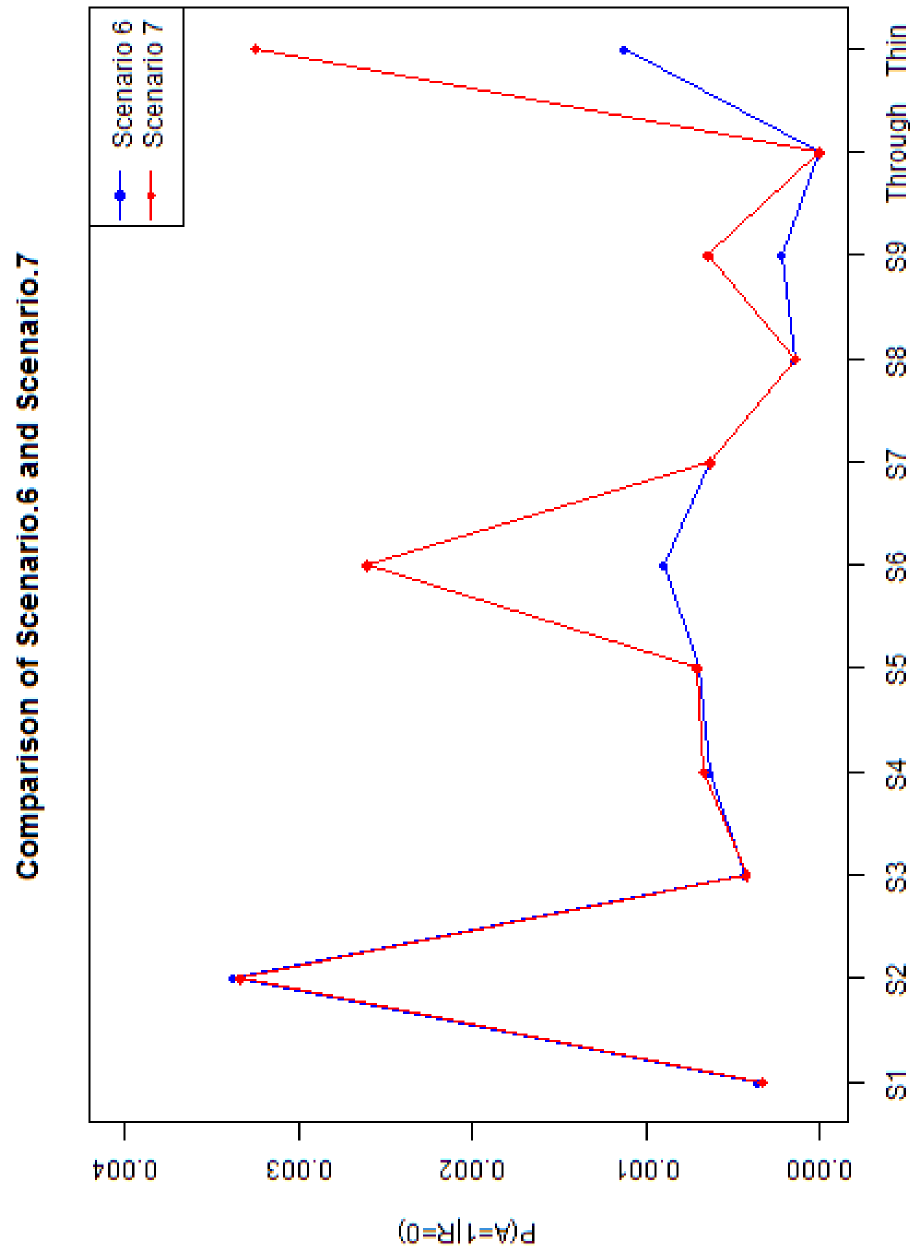


Figure 22: Comparison of simulation results between Scenarios 6 and 7.

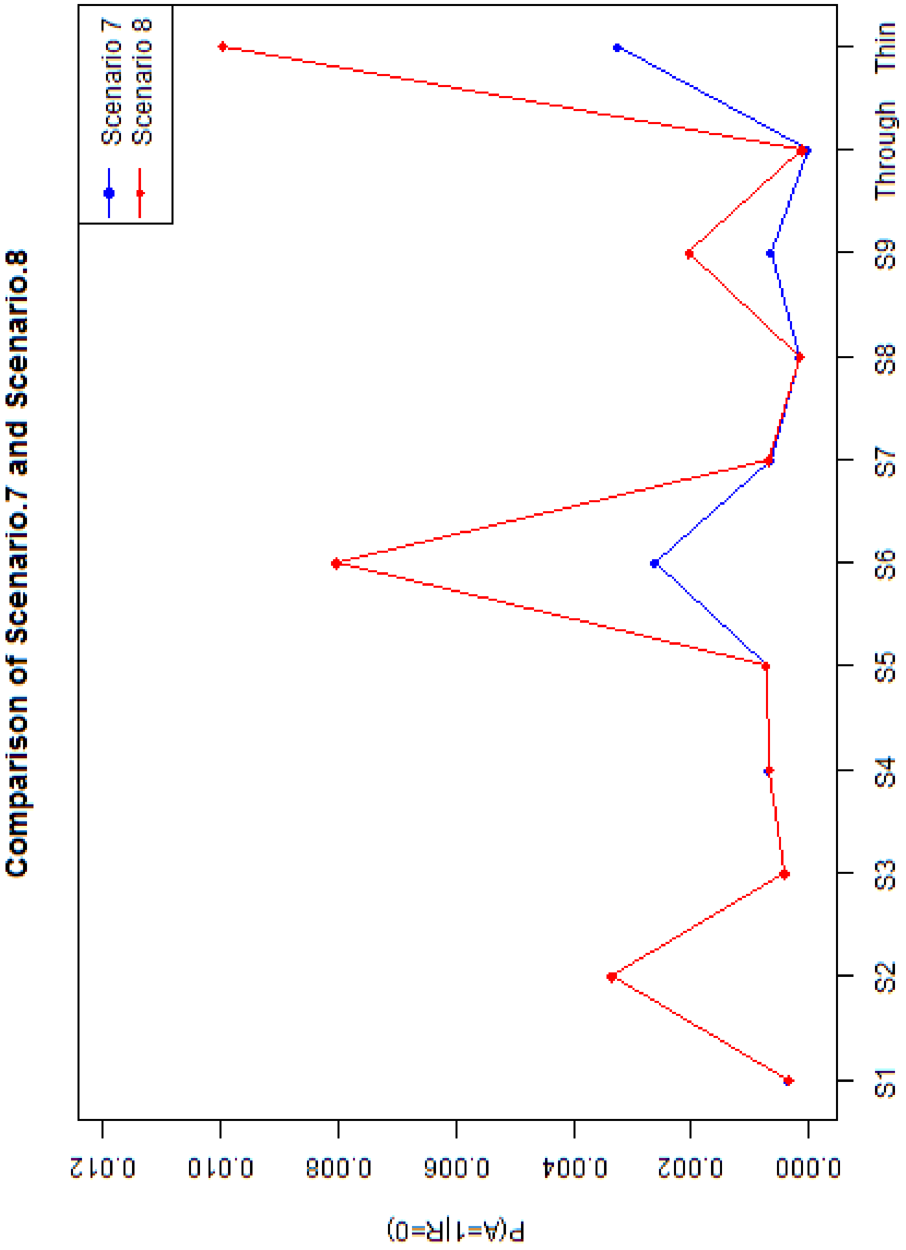


Figure 23: Comparison of simulation results between Scenarios 7 and 8.

sigma=5	threshold=1	threshold=2	threshold=3	threshold=4	threshold=5	threshold=6	threshold=7	threshold=8	threshold=9	threshold=10
tol=1	0.008128	0.00590837	0.0042627	0.0030422	0.00214057	0.00148007	0.00100247	0.00066312	0.00042722	0.00026741
tol=2	0.00824742	0.00600244	0.00433537	0.00309716	0.00218118	0.00150932	0.00102295	0.00067704	0.00043639	0.000273245
tol=3	0.00835336	0.00608264	0.00439491	0.00314043	0.00221189	0.00153058	0.00103726	0.00068639	0.0004423	0.000276862
tol=4	0.00844367	0.00614832	0.00444177	0.00317315	0.00223422	0.00154542	0.00104687	0.00069242	0.00044596	0.000279016
tol=5	0.00851764	0.00620003	0.00447722	0.00319694	0.00224982	0.00155539	0.00105306	0.00069616	0.00044815	0.000280249
tol=6	0.00857587	0.00623915	0.00450298	0.00321356	0.00226028	0.00156182	0.0010569	0.00069838	0.0004494	0.000280926
tol=7	0.00861991	0.00626758	0.00452098	0.00322471	0.00226703	0.0015658	0.00105919	0.00069965	0.00045008	0.000281285
tol=8	0.00865193	0.00628743	0.00453306	0.0032319	0.00227122	0.00156817	0.00106049	0.00070035	0.00045045	0.000281466
tol=9	0.00867429	0.00630076	0.00454085	0.00323636	0.00227371	0.00156953	0.00106121	0.00070072	0.00045063	0.000281555
tol=10	0.0086893	0.00630936	0.00454568	0.00323902	0.00227514	0.00157028	0.00106159	0.00070091	0.00045072	0.000281597

threshold=5	tol=1	tol=2	tol=3	tol=4	tol=5	tol=6	tol=7	tol=8	tol=9	tol=10
sigma=1	3.47E-09	3.47E-09	3.47E-09	3.47E-09	3.47E-09	3.47E-09	3.47E-09	3.47E-09	3.47E-09	3.47E-09
sigma=2	7.42E-05	7.54E-05	7.56E-05	7.56E-05	7.56E-05	7.56E-05	7.56E-05	7.56E-05	7.56E-05	7.56E-05
sigma=3	0.0005831	0.00059667	0.00060295	0.00060555	0.00060652	0.00060684	0.00060693	0.00060696	0.00060697	0.000606967
sigma=4	0.00135296	0.00138279	0.00140209	0.00141382	0.00142053	0.00142413	0.00142595	0.00142681	0.00142719	0.001427356
sigma=5	0.00214057	0.00218118	0.00221189	0.00223422	0.00224982	0.00226028	0.00226703	0.00227122	0.00227371	0.002275136
sigma=6	0.00286229	0.00290839	0.00294635	0.00297677	0.00300046	0.00301842	0.00303167	0.00304116	0.00304778	0.003052276
sigma=7	0.00350075	0.00354897	0.00359078	0.0036263	0.00365586	0.00367998	0.00369925	0.00371434	0.00372592	0.003734627
sigma=8	0.00405976	0.00410819	0.0041516	0.00418992	0.00422321	0.00425169	0.00427568	0.00429557	0.00431181	0.004324858
sigma=9	0.00454882	0.00459642	0.00464008	0.00467963	0.00471503	0.00474631	0.00477363	0.00479719	0.00481725	0.004834135
sigma=10	0.00497806	0.00502429	0.0050674	0.00510719	0.00514355	0.00517646	0.00520593	0.00523208	0.00525504	0.005275003

tol=5	threshold=1	threshold=2	threshold=3	threshold=4	threshold=5	threshold=6	threshold=7	threshold=8	threshold=9	threshold=10
sigma=1	0.00227673	0.00028163	1.64E-05	3.83E-07	3.47E-09	1.19E-11	1.55E-14	7.53E-18	1.37E-21	9.22E-26
sigma=2	0.00536866	0.00227646	0.00086553	0.00028163	7.56E-05	1.64E-05	2.82E-06	3.83E-07	4.11E-08	3.47E-09
sigma=3	0.00700444	0.00405781	0.0022722	0.00121157	0.00060652	0.0002815	0.00011991	4.65E-05	1.64E-05	5.19E-06
sigma=4	0.00793585	0.00531328	0.00350431	0.00226227	0.00142053	0.00086237	0.00050333	0.00028104	0.0001495	7.55E-05
sigma=5	0.00851764	0.00620003	0.00447722	0.00319694	0.00224982	0.00155539	0.00105306	0.00069616	0.00044815	0.000280249
sigma=6	0.00891158	0.00684972	0.00524008	0.00398218	0.00300046	0.00223724	0.0016477	0.00119644	0.00085506	0.000600454
sigma=7	0.0091954	0.00734392	0.00584744	0.0046362	0.00365586	0.00286368	0.00222557	0.00171407	0.00130671	0.000984951
sigma=8	0.00940967	0.007732	0.00634029	0.00518414	0.00422321	0.00342494	0.00276282	0.00221511	0.00176373	0.001393563
sigma=9	0.0095773	0.00804477	0.00674747	0.00564781	0.00471503	0.00392377	0.00325305	0.00268532	0.00220585	0.001802125
sigma=10	0.00971213	0.00830225	0.00708925	0.00604434	0.00514355	0.00436678	0.0036971	0.0031202	0.00262388	0.002197683

Table 21: Lookup tables – $p_1 = 0.001$, $p_2 = 0.002$, prot $= 0.99$

sigma=5	threshold=1	threshold=2	threshold=3	threshold=4	threshold=5	threshold=6	threshold=7	threshold=8	threshold=9	threshold=10
tol=1	0.01566569	0.01150683	0.00838486	0.00604149	0.00429008	0.00299255	0.00204409	0.00136315	0.00088508	0.000558161
tol=2	0.0168406	0.0124362	0.00910514	0.00658754	0.00469426	0.00328404	0.00224848	0.0015022	0.00097668	0.00061648
tol=3	0.01788072	0.0132272	0.00969446	0.007017	0.0049998	0.00349582	0.00239119	0.0015955	0.00103574	0.000652621
tol=4	0.01876579	0.0138743	0.01015792	0.00734164	0.00522178	0.0036437	0.00248696	0.00165567	0.00107235	0.000674143
tol=5	0.01948971	0.01438313	0.01050823	0.00757749	0.00537678	0.00374293	0.00254872	0.00169296	0.00109415	0.000686459
tol=6	0.02005888	0.01476771	0.01076272	0.00774217	0.00548079	0.00380693	0.00258699	0.00171517	0.00110662	0.000693232
tol=7	0.02048901	0.01504708	0.01094041	0.00785267	0.00554787	0.00384658	0.00260979	0.00172787	0.00111348	0.00069681
tol=8	0.02080144	0.01524213	0.01105964	0.00792393	0.00558943	0.0038702	0.00262283	0.00173486	0.0011171	0.000698627
tol=9	0.02101956	0.01537301	0.01113652	0.00796809	0.00561418	0.00388371	0.00263	0.00173855	0.00111894	0.000699514
tol=10	0.02116591	0.0154574	0.01118417	0.00799439	0.00562835	0.00389114	0.00263379	0.00174043	0.00111984	0.00069993

threshold=5	tol=1	tol=2	tol=3	tol=4	tol=5	tol=6	tol=7	tol=8	tol=9	tol=10
sigma=1	8.62E-09	8.63E-09	8.63E-09	8.63E-09	8.63E-09	8.63E-09	8.63E-09	8.63E-09	8.63E-09	8.63E-09
sigma=2	0.00017447	0.00018571	0.00018773	0.00018802	0.00018805	0.00018805	0.00018805	0.00018805	0.00018805	0.00018805
sigma=3	0.0012702	0.00140568	0.00146835	0.00149432	0.00150397	0.00150717	0.00150813	0.00150838	0.00150844	0.001508455
sigma=4	0.00280098	0.0030983	0.0032906	0.0034075	0.00347429	0.00351016	0.00352825	0.00353683	0.00354066	0.003542258
sigma=5	0.00429008	0.00469426	0.0049998	0.00522178	0.00537678	0.00548079	0.00554787	0.00558943	0.00561418	0.005628348
sigma=6	0.0056144	0.00607263	0.00644974	0.00675166	0.0069868	0.00716495	0.00729625	0.00739038	0.00745602	0.007500552
sigma=7	0.00676454	0.00724339	0.00765822	0.00801038	0.00830336	0.00854221	0.00873302	0.00888239	0.00899698	0.009083113
sigma=8	0.00775955	0.00824004	0.00867043	0.00904999	0.00937958	0.00966138	0.00989861	0.01009524	0.01025571	0.010384648
sigma=9	0.00862296	0.00909487	0.00952734	0.00991886	0.01026899	0.01057829	0.01084818	0.01108084	0.01127894	0.011445562
sigma=10	0.00937635	0.0098344	0.01026112	0.01065473	0.01101422	0.0113393	0.01163037	0.0118884	0.01211489	0.012311734

tol=5	threshold=1	threshold=2	threshold=3	threshold=4	threshold=5	threshold=6	threshold=7	threshold=8	threshold=9	threshold=10
sigma=1	0.00564421	0.00070025	4.07E-05	9.53E-07	8.63E-09	2.97E-11	3.85E-14	1.87E-17	3.40E-21	2.29E-25
sigma=2	0.01323436	0.00564148	0.00214996	0.00070022	0.00018805	4.07E-05	7.00E-06	9.53E-07	1.02E-07	8.63E-09
sigma=3	0.01698188	0.00993647	0.0055992	0.00299724	0.00150397	0.000699	0.00029797	0.00011565	4.07E-05	1.29E-05
sigma=4	0.0187034	0.01268896	0.00845448	0.00550053	0.00347429	0.0021185	0.00124054	0.00069436	0.00037003	0.00018716
sigma=5	0.01948971	0.01438313	0.01050823	0.00757749	0.00537678	0.00374293	0.00254872	0.00169296	0.00109415	0.000686459
sigma=6	0.01985916	0.01546356	0.01196732	0.00918855	0.0069868	0.00525182	0.00389557	0.0028465	0.00204556	0.001443437
sigma=7	0.02003579	0.01619045	0.01303116	0.01043475	0.00830336	0.00655838	0.00513582	0.00398292	0.00305556	0.002316409
sigma=8	0.02011863	0.01670528	0.01383337	0.01141523	0.00937958	0.00766801	0.0062322	0.00503178	0.00403263	0.003205658
sigma=9	0.02015382	0.01708642	0.01445782	0.01220324	0.01026899	0.0086103	0.0071896	0.0059751	0.00493969	0.004060065
sigma=10	0.02016404	0.01737911	0.01495741	0.01284963	0.01101422	0.00941606	0.00802526	0.00681625	0.00576701	0.004858478

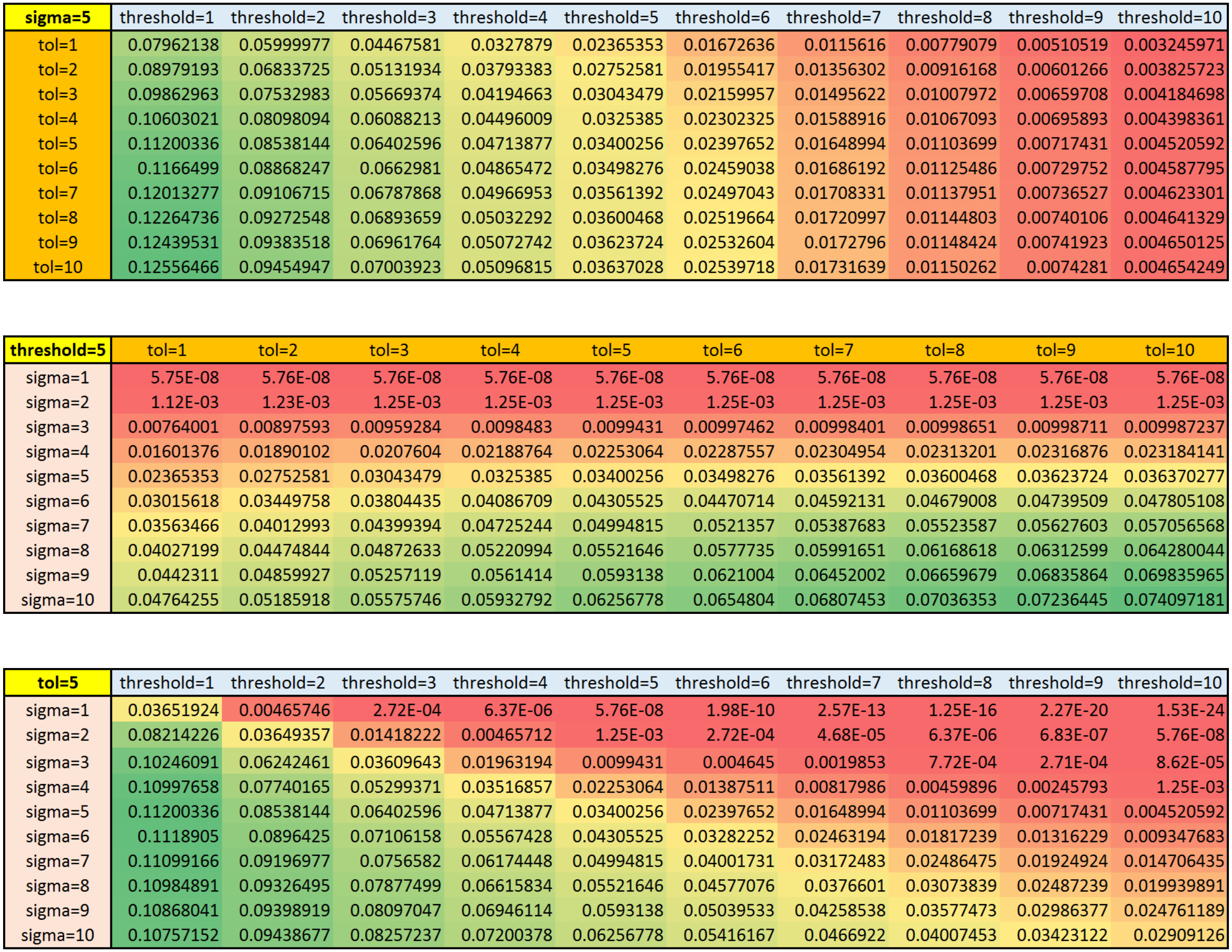
Table 22: Lookup tables – $p_1 = 0.01$, $p_2 = 0.02$, prot $= 0.99$

sigma=5	threshold=1	threshold=2	threshold=3	threshold=4	threshold=5	threshold=6	threshold=7	threshold=8	threshold=9	threshold=10
tol=1	0.008128	0.00590837	0.0042627	0.0030422	0.00214057	0.00148007	0.00100247	0.00066312	0.00042722	0.00026741
tol=2	0.00824742	0.00600244	0.00433537	0.00309716	0.00218118	0.00150932	0.00102295	0.00067704	0.00043639	0.000273245
tol=3	0.00835336	0.00608264	0.00439491	0.00314043	0.00221189	0.00153058	0.00103726	0.00068639	0.0004423	0.000276862
tol=4	0.00844367	0.00614832	0.00444177	0.00317315	0.00223422	0.00154542	0.00104687	0.00069242	0.00044596	0.000279016
tol=5	0.00851764	0.00620003	0.00447722	0.00319694	0.00224982	0.00155539	0.00105306	0.00069616	0.00044815	0.000280249
tol=6	0.00857587	0.00623915	0.00450298	0.00321356	0.00226028	0.00156182	0.0010569	0.00069838	0.0004494	0.000280926
tol=7	0.00861991	0.00626758	0.00452098	0.00322471	0.00226703	0.0015658	0.00105919	0.00069965	0.00045008	0.000281285
tol=8	0.00865193	0.00628743	0.00453306	0.0032319	0.00227122	0.00156817	0.00106049	0.00070035	0.00045045	0.000281466
tol=9	0.00867429	0.00630076	0.00454085	0.00323636	0.00227371	0.00156953	0.00106121	0.00070072	0.00045063	0.000281555
tol=10	0.0086893	0.00630936	0.00454568	0.00323902	0.00227514	0.00157028	0.00106159	0.00070091	0.00045072	0.000281597

threshold=5	tol=1	tol=2	tol=3	tol=4	tol=5	tol=6	tol=7	tol=8	tol=9	tol=10
sigma=1	3.47E-09	3.47E-09	3.47E-09	3.47E-09	3.47E-09	3.47E-09	3.47E-09	3.47E-09	3.47E-09	3.47E-09
sigma=2	7.42E-05	7.54E-05	7.56E-05	7.56E-05	7.56E-05	7.56E-05	7.56E-05	7.56E-05	7.56E-05	7.56E-05
sigma=3	0.0005831	0.00059667	0.00060295	0.00060555	0.00060652	0.00060684	0.00060693	0.00060696	0.00060697	0.000606967
sigma=4	0.00135296	0.00138279	0.00140209	0.00141382	0.00142053	0.00142413	0.00142595	0.00142681	0.00142719	0.001427356
sigma=5	0.00214057	0.00218118	0.00221189	0.00223422	0.00224982	0.00226028	0.00226703	0.00227122	0.00227371	0.002275136
sigma=6	0.00286229	0.00290839	0.00294635	0.00297677	0.00300046	0.00301842	0.00303167	0.00304116	0.00304778	0.003052276
sigma=7	0.00350075	0.00354897	0.00359078	0.0036263	0.00365586	0.00367998	0.00369925	0.00371434	0.00372592	0.003734627
sigma=8	0.00405976	0.00410819	0.0041516	0.00418992	0.00422321	0.00425169	0.00427568	0.00429557	0.00431181	0.004324858
sigma=9	0.00454882	0.00459642	0.00464008	0.00467963	0.00471503	0.00474631	0.00477363	0.00479719	0.00481725	0.004834135
sigma=10	0.00497806	0.00502429	0.0050674	0.00510719	0.00514355	0.00517646	0.00520593	0.00523208	0.00525504	0.005275003

tol=5	threshold=1	threshold=2	threshold=3	threshold=4	threshold=5	threshold=6	threshold=7	threshold=8	threshold=9	threshold=10
sigma=1	0.00227673	0.00028163	1.64E-05	3.83E-07	3.47E-09	1.19E-11	1.55E-14	7.53E-18	1.37E-21	9.22E-26
sigma=2	0.00536866	0.00227646	0.00086553	0.00028163	7.56E-05	1.64E-05	2.82E-06	3.83E-07	4.11E-08	3.47E-09
sigma=3	0.00700444	0.00405781	0.0022722	0.00121157	0.00060652	0.0002815	0.00011991	4.65E-05	1.64E-05	5.19E-06
sigma=4	0.00793585	0.00531328	0.00350431	0.00226227	0.00142053	0.00086237	0.00050333	0.00028104	0.0001495	7.55E-05
sigma=5	0.00851764	0.00620003	0.00447722	0.00319694	0.00224982	0.00155539	0.00105306	0.00069616	0.00044815	0.000280249
sigma=6	0.00891158	0.00684972	0.00524008	0.00398218	0.00300046	0.00223724	0.0016477	0.00119644	0.00085506	0.000600454
sigma=7	0.0091954	0.00734392	0.00584744	0.0046362	0.00365586	0.00286368	0.00222557	0.00171407	0.00130671	0.000984951
sigma=8	0.00940967	0.007732	0.00634029	0.00518414	0.00422321	0.00342494	0.00276282	0.00221511	0.00176373	0.001393563
sigma=9	0.0095773	0.00804477	0.00674747	0.00564781	0.00471503	0.00392377	0.00325305	0.00268532	0.00220585	0.001802125
sigma=10	0.00971213	0.00830225	0.00708925	0.00604434	0.00514355	0.00436678	0.0036971	0.0031202	0.00262388	0.002197683

Table 23: Lookup tables – $p_1 = 0.1$, $p_2 = 0.2$, prot $= 0.99$



sigma=5	threshold=1	threshold=2	threshold=3	threshold=4	threshold=5	threshold=6	threshold=7	threshold=8	threshold=9	threshold=10
tol=1	0.07962138	0.05999977	0.04467581	0.0327879	0.02365353	0.01672636	0.0115616	0.00779079	0.00510519	0.003245971
tol=2	0.08979193	0.06833725	0.05131934	0.03793383	0.02752581	0.01955417	0.01356302	0.00916168	0.00601266	0.003825723
tol=3	0.09862963	0.07532983	0.05669374	0.04194663	0.03043479	0.02159957	0.01495622	0.01007972	0.00659708	0.004184698
tol=4	0.10603021	0.08098094	0.06088213	0.04496009	0.0325385	0.02302325	0.01588916	0.01067093	0.00695893	0.004398361
tol=5	0.11200336	0.08538144	0.06402596	0.04713877	0.03400256	0.02397652	0.01648994	0.01103699	0.00717431	0.004520592
tol=6	0.1166499	0.08868247	0.0662981	0.04865472	0.03498276	0.02459038	0.01686192	0.01125486	0.00729752	0.004587795
tol=7	0.12013277	0.09106715	0.06787868	0.04966953	0.03561392	0.02497043	0.01708331	0.01137951	0.00736527	0.004623301
tol=8	0.12264736	0.09272548	0.06893659	0.05032292	0.03600468	0.02519664	0.01720997	0.01144803	0.00740106	0.004641329
tol=9	0.12439531	0.09383518	0.06961764	0.05072742	0.03623724	0.02532604	0.0172796	0.01148424	0.00741923	0.004650125
tol=10	0.12556466	0.09454947	0.07003923	0.05096815	0.03637028	0.02539718	0.01731639	0.01150262	0.0074281	0.004654249

threshold=5	tol=1	tol=2	tol=3	tol=4	tol=5	tol=6	tol=7	tol=8	tol=9	tol=10
sigma=1	5.75E-08	5.76E-08	5.76E-08	5.76E-08	5.76E-08	5.76E-08	5.76E-08	5.76E-08	5.76E-08	5.76E-08
sigma=2	1.12E-03	1.23E-03	1.25E-03	1.25E-03	1.25E-03	1.25E-03	1.25E-03	1.25E-03	1.25E-03	1.25E-03
sigma=3	0.00764001	0.00897593	0.00959284	0.0098483	0.0099431	0.00997462	0.00998401	0.00998651	0.00998711	0.009987237
sigma=4	0.01601376	0.01890102	0.0207604	0.02188764	0.02253064	0.02287557	0.02304954	0.02313201	0.02316876	0.023184141
sigma=5	0.02365353	0.02752581	0.03043479	0.0325385	0.03400256	0.03498276	0.03561392	0.03600468	0.03623724	0.036370277
sigma=6	0.03015618	0.03449758	0.03804435	0.04086709	0.04305525	0.04470714	0.04592131	0.04679008	0.04739509	0.047805108
sigma=7	0.03563466	0.04012993	0.04399394	0.04725244	0.04994815	0.0521357	0.05387683	0.05523587	0.05627603	0.057056568
sigma=8	0.04027199	0.04474844	0.04872633	0.05220994	0.05521646	0.0577735	0.05991651	0.06168618	0.06312599	0.064280044
sigma=9	0.0442311	0.04859927	0.05257119	0.0561414	0.0593138	0.0621004	0.06452002	0.06659679	0.06835864	0.069835965
sigma=10	0.04764255	0.05185918	0.05575746	0.05932792	0.06256778	0.0654804	0.06807453	0.07036353	0.07236445	0.074097181

tol=5	threshold=1	threshold=2	threshold=3	threshold=4	threshold=5	threshold=6	threshold=7	threshold=8	threshold=9	threshold=10
sigma=1	0.03651924	0.00465746	2.72E-04	6.37E-06	5.76E-08	1.98E-10	2.57E-13	1.25E-16	2.27E-20	1.53E-24
sigma=2	0.08214226	0.03649357	0.01418222	0.00465712	1.25E-03	2.72E-04	4.68E-05	6.37E-06	6.83E-07	5.76E-08
sigma=3	0.10246091	0.06242461	0.03609643	0.01963194	0.0099431	0.004645	0.0019853	7.72E-04	2.71E-04	8.62E-05
sigma=4	0.10997658	0.07740165	0.05299371	0.03516857	0.02253064	0.01387511	0.00817986	0.00459896	0.00245793	1.25E-03
sigma=5	0.11200336	0.08538144	0.06402596	0.04713877	0.03400256	0.02397652	0.01648994	0.01103699	0.00717431	0.004520592
sigma=6	0.1118905	0.0896425	0.07106158	0.05567428	0.04305525	0.03282252	0.02463194	0.01817239	0.01316229	0.009347683
sigma=7	0.11099166	0.09196977	0.0756582	0.06174448	0.04994815	0.04001731	0.03172483	0.02486475	0.01924924	0.014706435
sigma=8	0.10984891	0.09326495	0.07877499	0.06615834	0.05521646	0.04577076	0.0376601	0.03073839	0.02487239	0.019939891
sigma=9	0.10868041	0.09398919	0.08097047	0.06946114	0.0593138	0.05039533	0.04258538	0.03577473	0.02986377	0.024761189
sigma=10	0.10757152	0.09438677	0.08257237	0.07200378	0.06256778	0.05416167	0.0466922	0.04007453	0.03423122	0.02909126

Table 24: Lookup tables – $p_1 = 0.1$, $p_2 = 0.2$, prot $= 0.999$

4 Prototype Modeling of Selected Repository Interactions

A causal network, linking together system states and events, based on a sequence of necessary and sufficient causes, acted as a high level backbone for the model of selected components of the engineered barrier system. To determine the focus of the prototype project, a number of possible subsets of the overall causal network (causal chains) were presented to system experts, who then provided feedback and suggestions about their structure.

Based on this feedback, two main causal chains were chosen for the prototype project- a corrosion chain and a UFC pressure chain. It is worth noting here that the level of detail (and associated assumptions) implemented in this model, was in part set based on the goal of meeting the proof of concept objective of the prototype phase within an appropriate amount of time. However, the model framework has been constructed such that it can easily allow for both the addition of greater levels of detail, in terms of object properties and relationships represented, and the abstraction of detail where deemed appropriate.

To generate the specific details of these chosen causal chains, the relevant end state of the system – exposure of the container contents to the environment – was first defined, and then a series of necessary and sufficient conditions were constructed that could lead to this end result, with each of the identified conditions themselves being connected to other necessary or sufficient conditions, consisting of other system states (see Figure 27).

The structure developed in the conceptual model was then implemented. The primary output of the simulation model was length of time before which the contents of the UFC were exposed to the environment under a given set of starting conditions. Analysis of the simulation models involved an exploration of the model behavior using statistical analysis across parameter sets. Parameter sets were chosen to maximize the exploration of key parts of the parameter space, and specific scenarios of interest.

4.1 Causal Chain Events, States, Processes and Objects

The resulting system model was constructed from four main elements: objects (and their properties), processes, states and events. For the purposes of the prototype model, most system processes (e.g. corrosion processes, glacier pressure loading, placement room environment evolution) were modeled in a relatively simple manner. The emphasis here was in having processes that provided inputs to other parts of the model within appropriate ranges. In future phases of model construction, these abstract process components could be replaced with outputs from existing detailed component models.

As previously noted, two major causal pathways were identified as potentially leading to the exposure of the contents of the UFC (see Figure 27): exposure as a result of chemical alteration of the UFC and exposure as a result of mechanical damage to the UFC. Two specific possible instances of these pathways were chosen to be modeled during the prototype phase- corrosion of the steel core of the UFC from the outside in, as an instance of the chemical path to exposure, and a punch through of the surface of the UFC, as influenced by the presence or absence of glaciation above the repository, as an instance of the mechanical path.

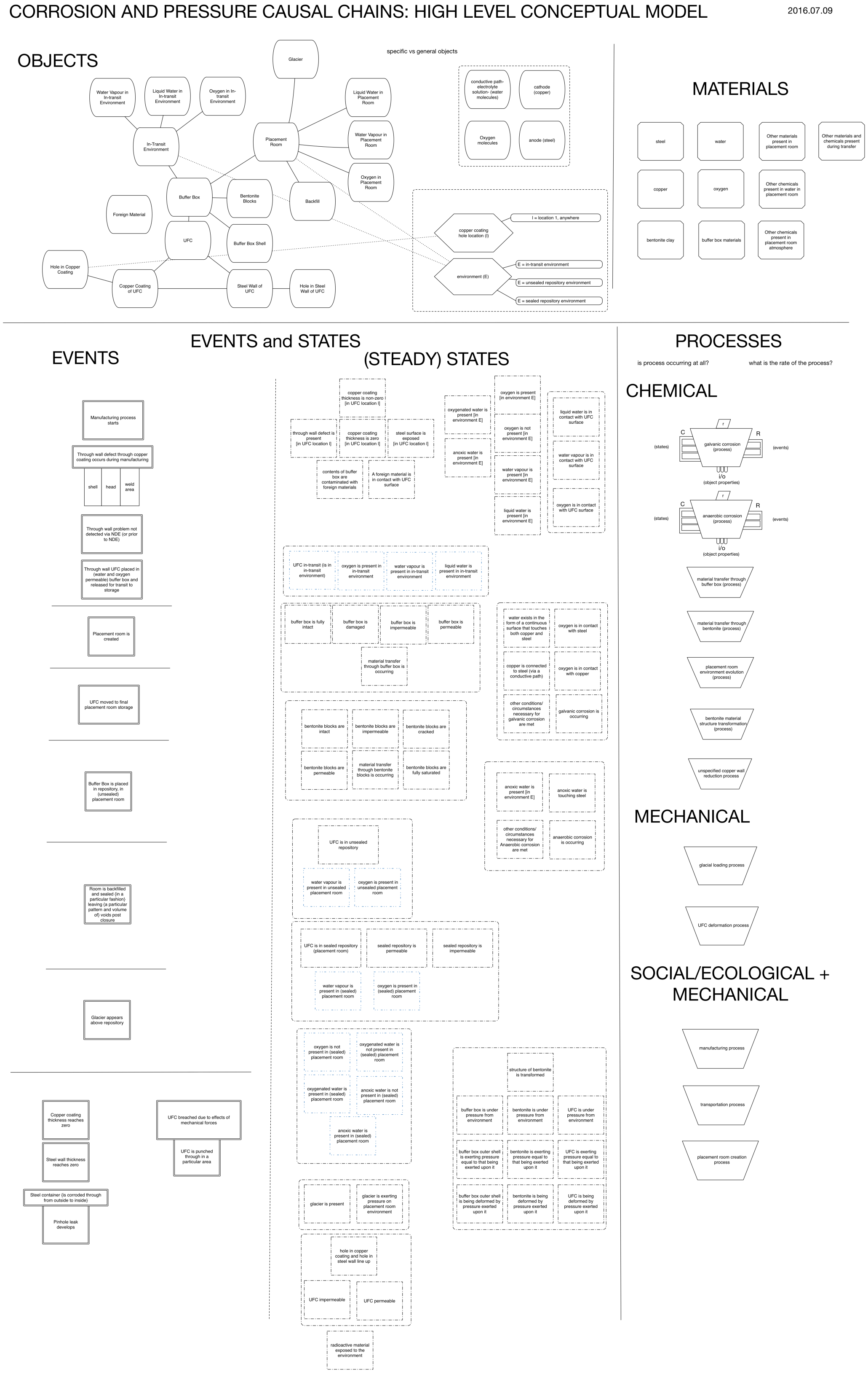


Figure 24: A high level schematic of objects, processes, events and states involved in the two chosen causal chains (see accompanying file for larger figure)

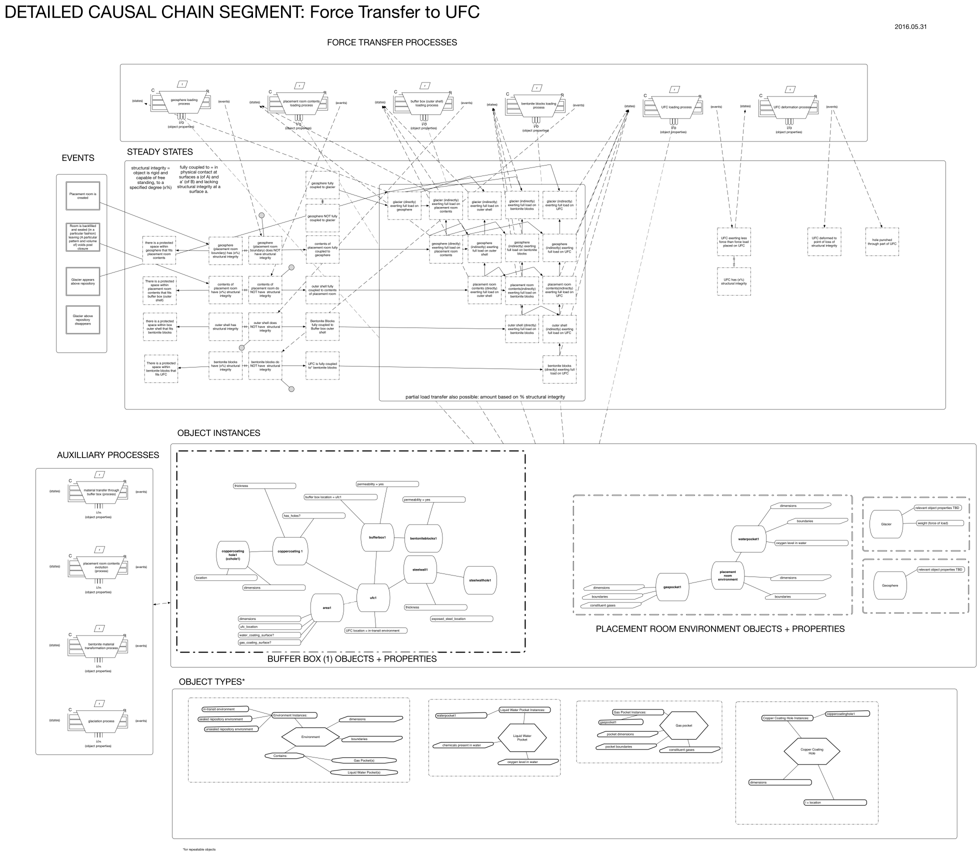


Figure 25: Detailed schematic of the connections and logical relationships for the UFC pressure chain (see accompanying file for larger figure)

Because the single end state (contents exposure) branched off into two main pathways (corrosion and UFC pressure) the causal network was constructed in two separate parts, or segements, one for each of these main pathways (see Tables 25, 26 and 27 for a list of model events and states associated with each chain). The presence of possible interactions between the two chains were then taken into account by constructing shared objects and shared processes that jointly influenced, and were influenced by, the events and states in the chains (see Table 28 for a list of system objects and processes).

The behaviour of the system was advanced in defined intervals, or time steps. At any given time step, particular states – representing a particular set of object property values in the system – could 'fire' with a certain probability, but only if the state's necessary and/or sufficient conditions were also firing at that time step. System processes – system actions or behaviours carried out during a given time step – might also be started by the truth value of particular states, and could in turn determine the truth value of particular states, which could influence model behaviour at the next time step. Processes might also interact with and be influenced by objects in the model. If all of the necessary and sufficient conditions defined in the network were met at a given time step, the final state in the model– contents exposure– would also fire with a certain probability, indicating that this final event was occurring at that time step. Note that the system behaviour was tracked for 1 000 000 years, in increments (time steps) of either 1 or 10 years.

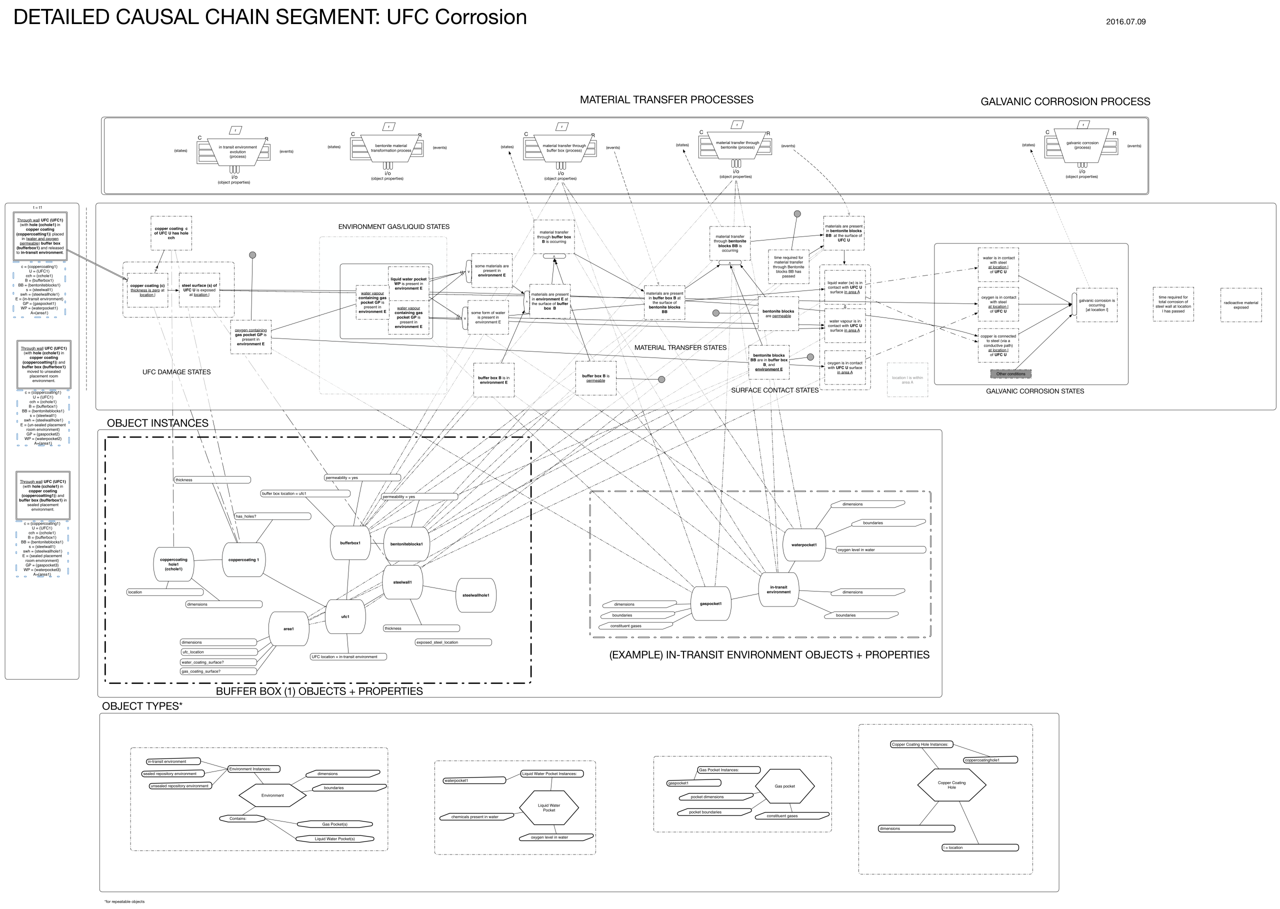


Figure 26: Detailed schematic of the connections and logical relationships for the corrosion chain (see accompanying file for larger figure)

4.2 Modeling Assumptions and Parameters

As must occur when constructing models, some assumptions were made in terms of what to include or exclude from the model and how to represent various aspects of the model. Parameters were chosen based on NWMO documentation, relevant literature and discussions with SMEs.

4.2.1 Assumptions and Limitations

The model currently makes a number of assumptions about the system, many of which relate to either the presence or absence of interactions between particular system components, or the relationship between system properties. Because of the structure of the model, incorporating these interactions or augmenting the nature of these relationships would be relatively straight forward. It is generally recommended that as many interactions as possible be incorporated into the model, to allow for emergent causal effects. For the purposes of the prototype, however, to keep this phase of the project tractable, the following assumptions were made:

- It is assumed that the bentonite blocks are partially saturated at the start of the simulation (when the UFC is placed in the buffer box). As a result it is assumed for most scenarios

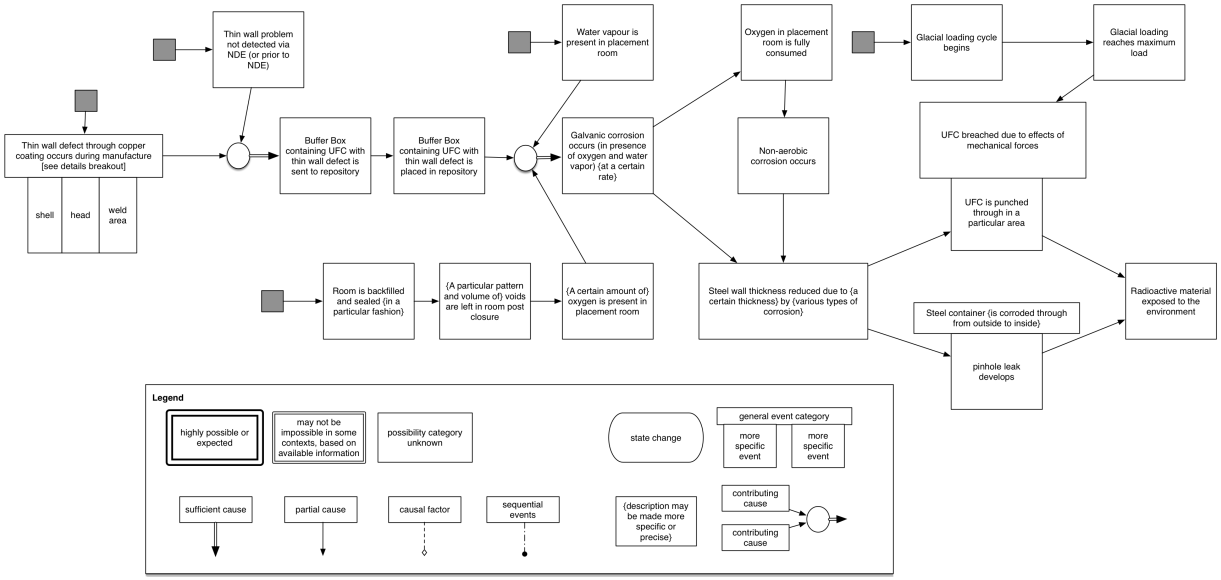
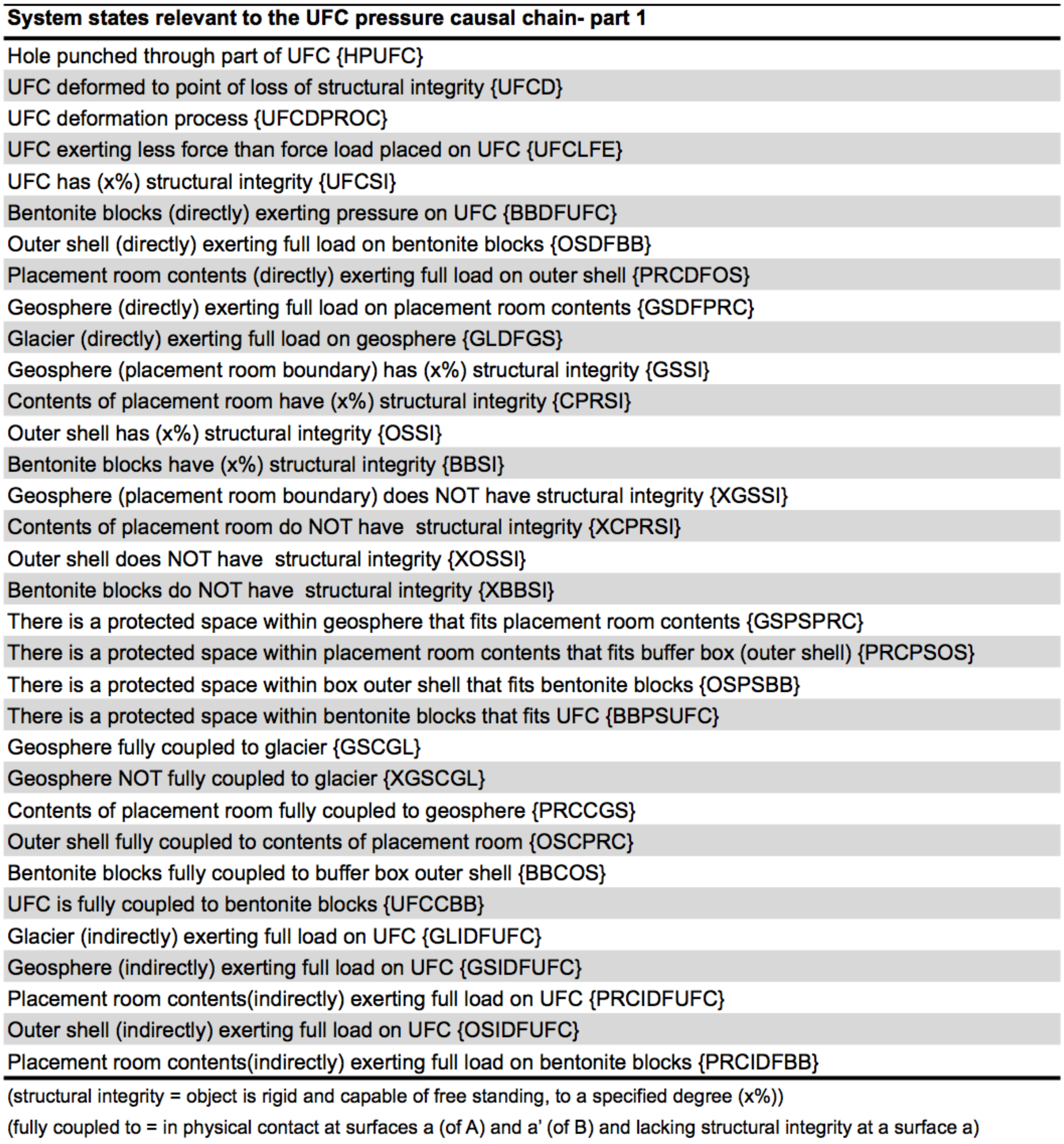


Figure 27: Initial representation of prototype causal chains, based on discussions with SMEs (see accompanying file for larger figure)

(unless otherwise specified) that water and oxygen are present at the beginning of the simulation.

- It is currently assumed that the rate of the galvanic corrosion reaction is not influenced by the amount of oxygen present at the surface of the UFC- rather, oxygen presence is currently a binary variable- either it is present or it isn't. This then determines the type of corrosion but doesn't influence the rate of that particular type of corrosion.
- It is currently assumed that the relationship between the load strength of the UFC and the thickness of the UFC is simply proportional. Exploring more complex and precise relationships between these two variables is left for future work.
- It is also currently assumed that the relationship between the level of (relative) humidity present at the surface of the UFC and the rate of galvanic corrosion is simply proportional. Again, exploring more complex and precise relationships is left for future work.
- It is currently assumed that the rate of anaerobic corrosion is not affected by the level of humidity present at the surface of the UFC.
- Hydrostatic pressure, and effects of hydrostatic pressure, are not directly included in the current version of the model, although they are incorporated indirectly, to some extent, in the pressure profile.
- Temperature and effects of temperature (e.g. on chemical process rates) are not explicitely modeled.
- It is assumed that there is no connection between pressure in the system (as exerted on the UFC) and rates of chemical reactions at the surface of the UFC.

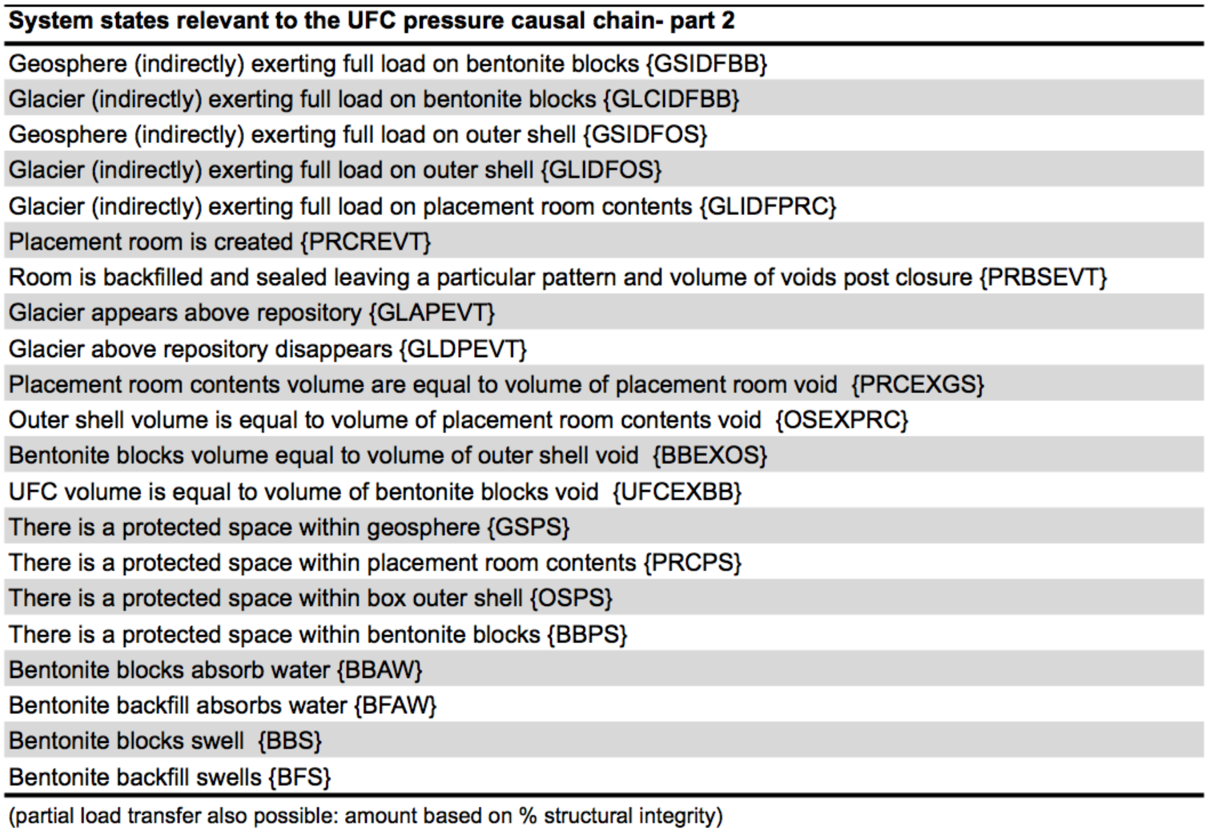


System states relevant to the UFC pressure causal chain- part 1
Hole punched through part of UFC {HPUFC}
UFC deformed to point of loss of structural integrity {UFCD}
UFC deformation process {UFCDPROC}
UFC exerting less force than force load placed on UFC {UFCLFE}
UFC has (x%) structural integrity {UFCSI}
Bentonite blocks (directly) exerting pressure on UFC {BBDFUFC}
Outer shell (directly) exerting full load on bentonite blocks {OSDFBB}
Placement room contents (directly) exerting full load on outer shell {PRCDFOS}
Geosphere (directly) exerting full load on placement room contents {GSDFPRC}
Glacier (directly) exerting full load on geosphere {GLDFGS}
Geosphere (placement room boundary) has (x%) structural integrity {GSSI}
Contents of placement room have (x%) structural integrity {CPRSI}
Outer shell has (x%) structural integrity {OSSI}
Bentonite blocks have (x%) structural integrity {BBSI}
Geosphere (placement room boundary) does NOT have structural integrity {XGSSI}
Contents of placement room do NOT have structural integrity {XCPRSI}
Outer shell does NOT have structural integrity {XOSSI}
Bentonite blocks do NOT have structural integrity {XBBSI}
There is a protected space within geosphere that fits placement room contents {GSPSPRC}
There is a protected space within placement room contents that fits buffer box (outer shell) {PRCPSOS}
There is a protected space within box outer shell that fits bentonite blocks {OSPSBB}
There is a protected space within bentonite blocks that fits UFC {BBPSUFC}
Geosphere fully coupled to glacier {GSCGL}
Geosphere NOT fully coupled to glacier {XGSCGL}
Contents of placement room fully coupled to geosphere {PRCCGS}
Outer shell fully coupled to contents of placement room {OSCPRC}
Bentonite blocks fully coupled to buffer box outer shell {BBCOS}
UFC is fully coupled to bentonite blocks {UFCCBB}
Glacier (indirectly) exerting full load on UFC {GLIDFUFC}
Geosphere (indirectly) exerting full load on UFC {GSIDFUFC}
Placement room contents(indirectly) exerting full load on UFC {PRCIDFUFC}
Outer shell (indirectly) exerting full load on UFC {OSIDFUFC}
Placement room contents(indirectly) exerting full load on bentonite blocks {PRCIDFBB}

(structural integrity = object is rigid and capable of free standing, to a specified degree (x%))

(fully coupled to = in physical contact at surfaces a (of A) and a' (of B) and lacking structural integrity at a surface a)

Table 25: UFC pressure chain states and events – Part 1



System states relevant to the UFC pressure causal chain- part 2
Geosphere (indirectly) exerting full load on bentonite blocks {GSIDFBB}
Glacier (indirectly) exerting full load on bentonite blocks {GLCIDFBB}
Geosphere (indirectly) exerting full load on outer shell {GSIDFOS}
Glacier (indirectly) exerting full load on outer shell {GLIDFOS}
Glacier (indirectly) exerting full load on placement room contents {GLIDFPRC}
Placement room is created {PRCREVT}
Room is backfilled and sealed leaving a particular pattern and volume of voids post closure {PRBSEVT}
Glacier appears above repository {GLAPEVT}
Glacier above repository disappears {GLDPEVT}
Placement room contents volume are equal to volume of placement room void {PRCEXGS}
Outer shell volume is equal to volume of placement room contents void {OSEXPRC}
Bentonite blocks volume equal to volume of outer shell void {BBEXOS}
UFC volume is equal to volume of bentonite blocks void {UFCEXBB}
There is a protected space within geosphere {GSPS}
There is a protected space within placement room contents {PRCPS}
There is a protected space within box outer shell {OSPS}
There is a protected space within bentonite blocks {BBPS}
Bentonite blocks absorb water {BBAW}
Bentonite backfill absorbs water {BFAW}
Bentonite blocks swell {BBS}
Bentonite backfill swells {BFS}

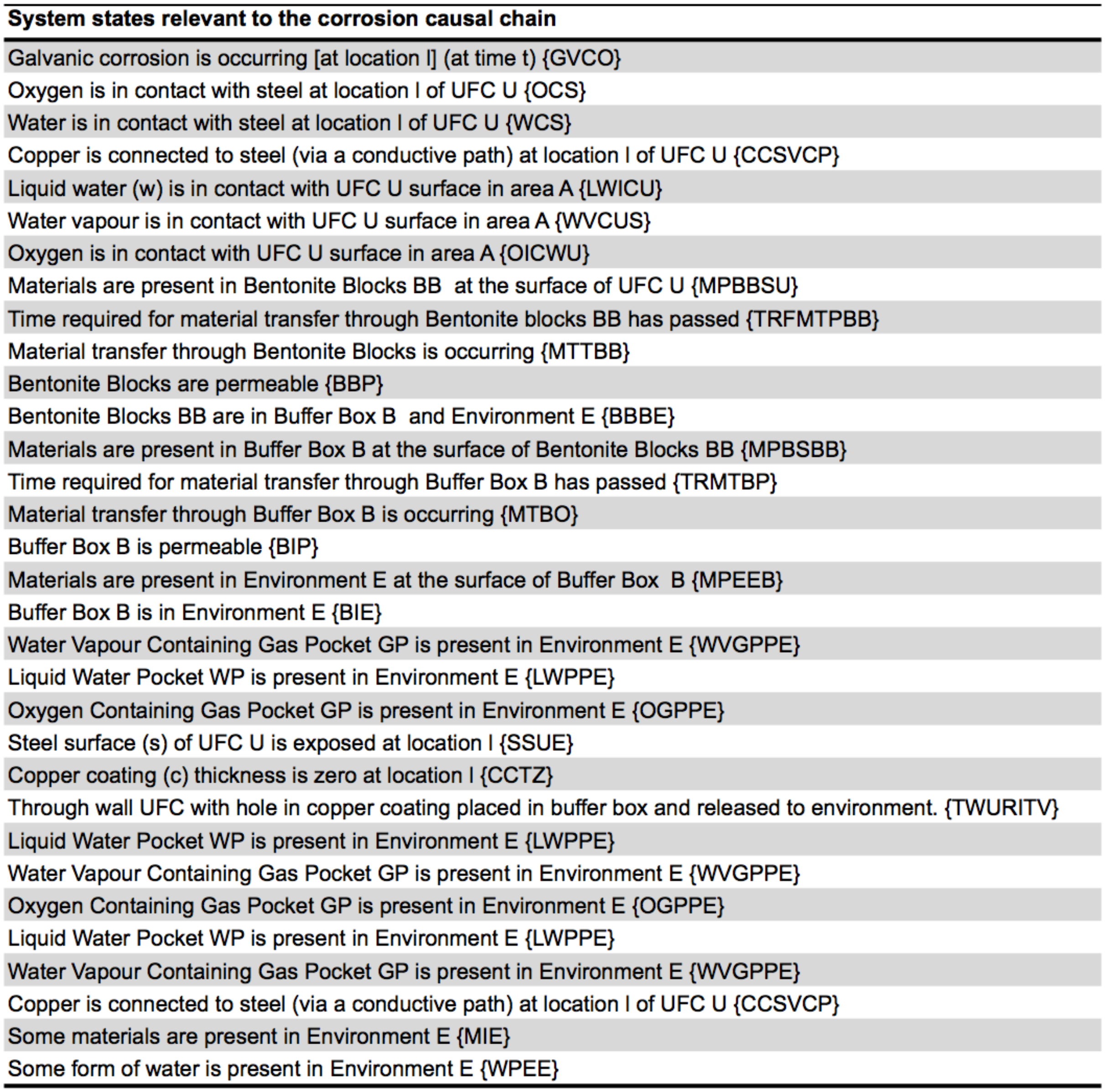
(partial load transfer also possible: amount based on % structural integrity)

Table 26: UFC pressure chain states and events – Part 2

4.2.2 Parameters

The model has two main types of parameters: Probability parameters are values between 0 and 1 that correspond to the probability of states firing in the model. System parameters (e.g. thickness of the steel wall of the UFC, maximum rate of corrosion) are set, when possible, based on available known values for particular system components. In cases where these values (or their range or distribution) are not known, a possible range for the parameter value is chosen based on available literature, and then specific values are selected based on varying the order of magnitude of the parameter value within this range. See Table 29 for a list of key parameter values. In general these parameters can be seen as representing a range of values that include the expected value for a system property, the highest anticipated value for that property at any point in time during the evolution of the system, and, possibly, also the highest physically possible value for that parameter.

Using these range of values as a basis, parameter sets– combinations of values assigned to the model parameters– were chosen to explore specific scenarios of interest. See Tables 30, 31 and 32 for a list of parameter values associated with each scenario. To generate results, the model was run in either a deterministic or stochastic mode. In the deterministic mode, model behaviours at each time step were driven solely by logical-mathematical relationships. In the probabilistic mode the deterministic model was expanded to include uncertainty in the system behaviour, as represented by both probabilties of occurrence of states and probability distributions of values of different aspects of the system.



System states relevant to the corrosion causal chain
Galvanic corrosion is occurring [at location l] (at time t) {GVCO}
Oxygen is in contact with steel at location l of UFC U {OCS}
Water is in contact with steel at location l of UFC U {WCS}
Copper is connected to steel (via a conductive path) at location l of UFC U {CCSVCP}
Liquid water (w) is in contact with UFC U surface in area A {LWICU}
Water vapour is in contact with UFC U surface in area A {WVCUS}
Oxygen is in contact with UFC U surface in area A {OICWU}
Materials are present in Bentonite Blocks BB at the surface of UFC U {MPBBSU}
Time required for material transfer through Bentonite blocks BB has passed {TRFMTPBB}
Material transfer through Bentonite Blocks is occurring {MTTBB}
Bentonite Blocks are permeable {BBP}
Bentonite Blocks BB are in Buffer Box B and Environment E {BBBE}
Materials are present in Buffer Box B at the surface of Bentonite Blocks BB {MPBSBB}
Time required for material transfer through Buffer Box B has passed {TRMTBP}
Material transfer through Buffer Box B is occurring {MTBO}
Buffer Box B is permeable {BIP}
Materials are present in Environment E at the surface of Buffer Box B {MPEEB}
Buffer Box B is in Environment E {BIE}
Water Vapour Containing Gas Pocket GP is present in Environment E {WVGPPE}
Liquid Water Pocket WP is present in Environment E {LWPPE}
Oxygen Containing Gas Pocket GP is present in Environment E {OGPPE}
Steel surface (s) of UFC U is exposed at location l {SSUE}
Copper coating (c) thickness is zero at location l {CCTZ}
Through wall UFC with hole in copper coating placed in buffer box and released to environment. {TWURITV}
Liquid Water Pocket WP is present in Environment E {LWPPE}
Water Vapour Containing Gas Pocket GP is present in Environment E {WVGPPE}
Oxygen Containing Gas Pocket GP is present in Environment E {OGPPE}
Liquid Water Pocket WP is present in Environment E {LWPPE}
Water Vapour Containing Gas Pocket GP is present in Environment E {WVGPPE}
Copper is connected to steel (via a conductive path) at location l of UFC U {CCSVCP}
Some materials are present in Environment E {MIE}
Some form of water is present in Environment E {WPEE}

Table 27: Corrosion states

4.3 Analysis Approach

4.3.1 Deterministic Mode Scenarios

In the deterministic mode, varying the initial parameters could change the behavior and final outcome, of the model, but the initial conditions set fully determined the behavior of the model. This is an overly simplistic representation of the system, as it does not allow for any degree of stochasticity or a representation of levels of uncertainty in the behaviour of the system. However, this mode is useful in two ways: First, the deterministic mode allows for a relatively straightforward exploration of component interactions and system behaviours. As a result, it more clearly

	System Processes
Primary	System pressure exertion process
	Galvanic corrosion process
	Anaerobic corrosion process
Secondary*	Material transfer through buffer box outer shell (process)
	Material transfer through bentonite (process)
	Placement room environment evolution (process)
	Bentonite material transformation process

	System Objects
	UFC
	Bentonite Blocks
	Bentonite Outer Shell (removed)
	Contents of Placement Room (Backfill)
	Placement Room Water Pocket
	Placement Room Oxygen Pocket

*initially implemented but then simplified or omitted based on conversations with SMEs

Table 28: Key system objects and processes

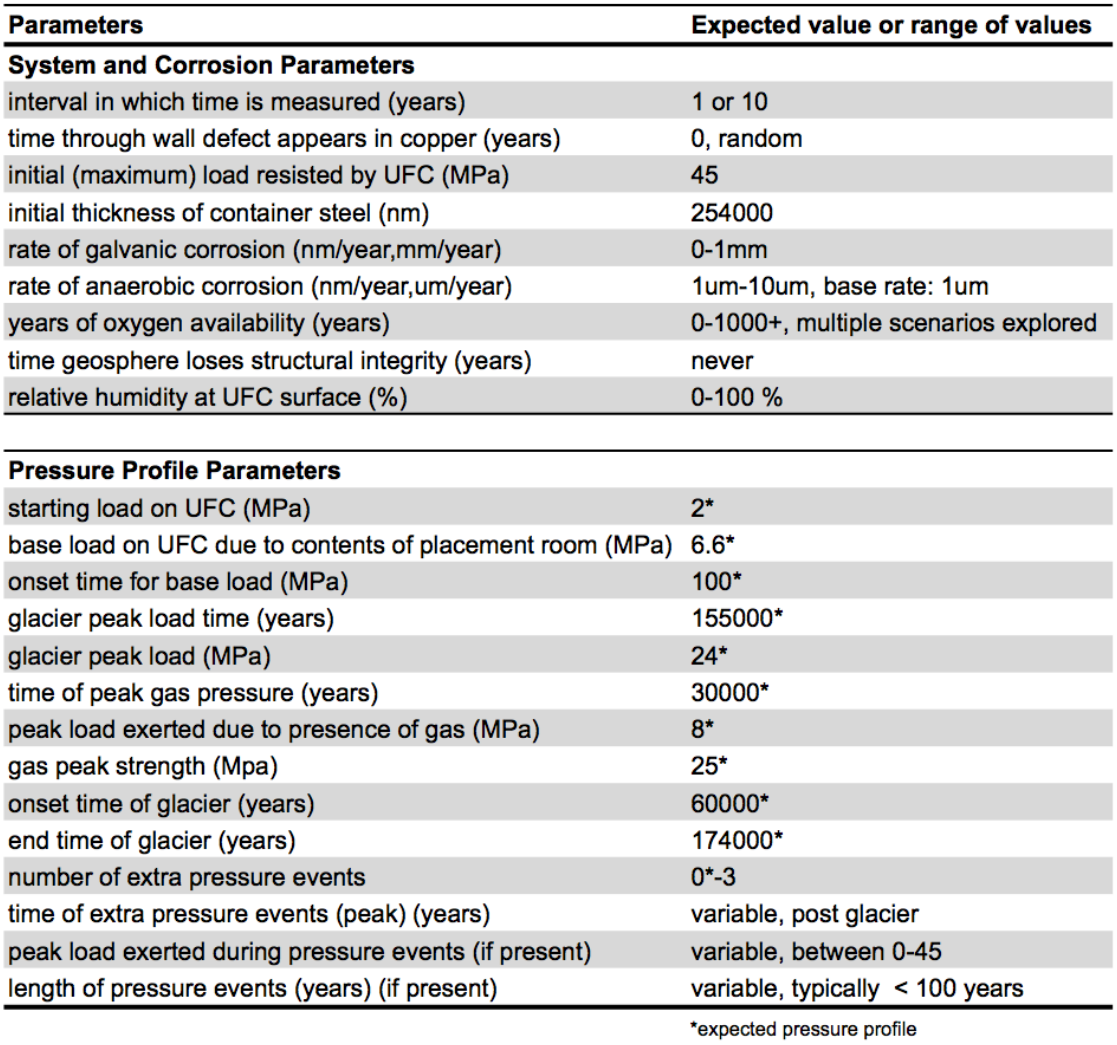
highlights emergent interaction effects (if any) between components. Second, it can act as an explicit reflection of the way system behaviours may be conceptualized when people hypothesize about and attempt to understand causal behaviours within the system.

Within this deterministic context, it was also fairly easy to generate unanticipated but still possible scenarios, some of which led to the end state of container contents exposure and some of which did not, as this process only involved finding parameter values that were both within the range of the physically possible and that, given the known structure of the system, would then logically lead to the relevant end state. In this context, the deterministic scenarios were intended as a useful preliminary to the introduction of uncertainty into the model, as they can demonstrate some of the underlying causality at play in the results which are produced as a result of the more complex model behaviours that result from probability being introduced into the system.

4.3.2 Stochastic Mode Scenarios

Probablistic models often involve predictions at the population level- i.e. how many out of a certain number of containers will have the following property? Within the population, what is the range and distribution of values that can be expected? However, in the case of the barrier system model, this interpretation is less useful, as there is only intended to be one barrier system. Thus, interpreting the results of the model as 'x% of all barrier systems will have this property', or 'x% of barrier systems will have a corrosion rate within this range of values', does not necessarily provide us with an estimate of the probability that the actual barrier system will have a particular property of interest, or behave in a particular manner.

An alternate way to interpret a probabilistic model is to take what is referred to as a possible worlds approach (Kripke, 1963). In this case, we would first consider a set of possible worlds, each of which represent a possible description of what will occur (e.g. in some possible worlds, this container will corrode at a steady rate of 100 um/year. In other possible words, this container

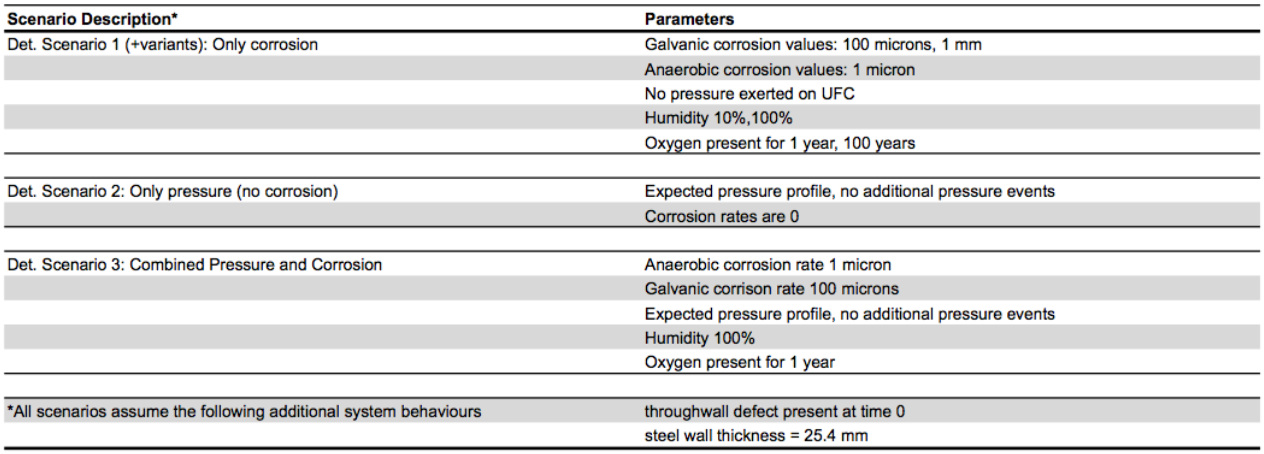


Parameters	**Expected value or range of values**
System and Corrosion Parameters	
interval in which time is measured (years)	1 or 10
time through wall defect appears in copper (years)	0, random
initial (maximum) load resisted by UFC (MPa)	45
initial thickness of container steel (nm)	254000
rate of galvanic corrosion (nm/year,mm/year)	0-1mm
rate of anaerobic corrosion (nm/year,um/year)	1um-10um, base rate: 1um
years of oxygen availability (years)	0-1000+, multiple scenarios explored
time geosphere loses structural integrity (years)	never
relative humidity at UFC surface (%)	0-100 %
Pressure Profile Parameters	
starting load on UFC (MPa)	2*
base load on UFC due to contents of placement room (MPa)	6.6*
onset time for base load (MPa)	100*
glacier peak load time (years)	155000*
glacier peak load (MPa)	24*
time of peak gas pressure (years)	30000*
peak load exerted due to presence of gas (MPa)	8*
gas peak strength (Mpa)	25*
onset time of glacier (years)	60000*
end time of glacier (years)	174000*
number of extra pressure events	0*-3
time of extra pressure events (peak) (years)	variable, post glacier
peak load exerted during pressure events (if present)	variable, between 0-45
length of pressure events (years) (if present)	variable, typically < 100 years

*expected pressure profile

Table 29: Key system parameters

will corrode at a steady rate of 150 um/year, in other possible worlds, the rate of the corrosion will fluctuate in some manner between these two values). We can use this possible world interpretation when we are thinking about both the role of stochastic elements in the model, and also the end result of the model. Under this interpretation, we could say that probabilities in a model represents our level of certainty, or uncertainty, that the actual system will be in one of a particular subset of possible worlds. So, for example, if we say that we have fairly high uncertainty about the precise end point of oxygen presence, but fairly low uncertainty regarding whether or not there will be oxygen after 1000 years, then this essentially says that we don't have much certainty regarding which set of possible worlds the actual world will be in with respect to the precise time at which oxygen will be consumed, but we have high certainty about the possible world set in terms of possible worlds where oxygen is or is not present at 1000 years. This can then be represented using probabilities- e.g. if we say that we are highly confident, but still not 100% confident that there will be no oxygen present at any time after 1000 years, then this can be represented as there being a very low but non-zero probability that oxygen will be present after 1000 years.



Scenario Description*	**Parameters**
Det. Scenario 1 (+variants): Only corrosion	Galvanic corrosion values: 100 microns, 1 mm
	Anaerobic corrosion values: 1 micron
	No pressure exerted on UFC
	Humidity 10%,100%
	Oxygen present for 1 year, 100 years
Det. Scenario 2: Only pressure (no corrosion)	Expected pressure profile, no additional pressure events
	Corrosion rates are 0
Det. Scenario 3: Combined Pressure and Corrosion	Anaerobic corrosion rate 1 micron
	Galvanic corrison rate 100 microns
	Expected pressure profile, no additional pressure events
	Humidity 100%
	Oxygen present for 1 year
*All scenarios assume the following additional system behaviours	throughwall defect present at time 0
	steel wall thickness = 25.4 mm

Table 30: Deterministic Scenarios

Within the context of the simulation methodology, these probabilities are then effectively translated into a specific possible world with each run of the model. The end result of multiple model runs is a set of possible worlds that reflect the probabilities that have been set in the model, which themselves reflect the level of certainty about which possible world we can expect to be the actual possible world. Thus the result of the simulation can be broadly interpreted as: based on the model results (and given the model structure, assumptions and levels of certainty associated with particular components of the model) we have the follow (high or low) level of certainty that the actual world will be in this set of possible worlds.

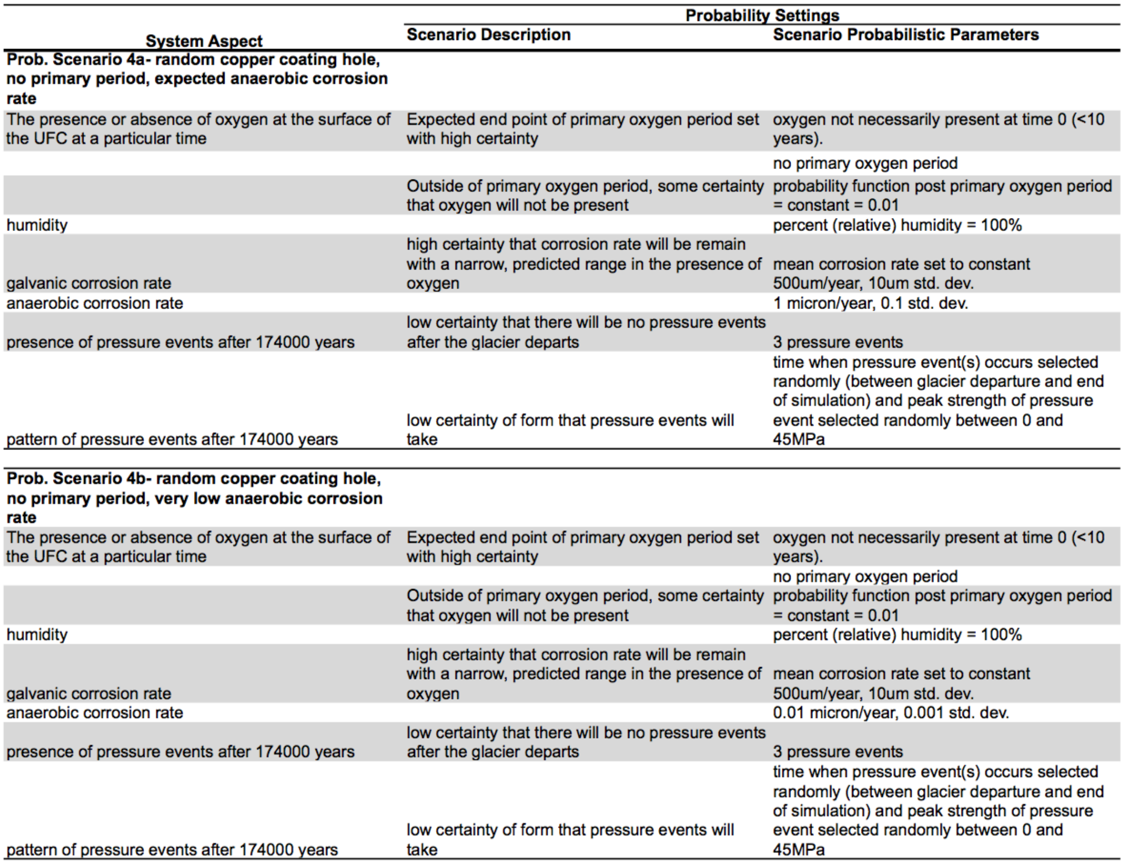
Inserting and altering probabilities in the model in this way allows for an exploration of the risk involved in creation of the system, relative to current levels of certainty about the system, combined with a counterfactual exploration of what the consequences may be if assumptions about the anticipated behaviour of the model are either themselves incorrect, or attributed an excessively high level of certainty.

Thus, for the engineered barrier system, in the stochastic mode probability represents a number of aspects of both the system itself and available knowledge of the system, including:

- a level of uncertainty with respect to the whether a particular event will or will not happen (either at all, or under particular circumstances)
- a level of uncertainty with respect to the value or range of a system object property
- a level of certainty regarding the presence of necessary and sufficient conditions for a particular event
- the presence, at a particular time, of non-explicit sufficient conditions for an event
- a correlation relationship between two aspects of the model

	Probability Settings	
System Aspect	Scenario Description	Scenario Probabilistic Parameters
Prob. Scenario 1- high certainty that system will behave as anticipated		
The presence or absence of oxygen at the surface of the UFC at a particular time	Expected end point of primary oxygen period set with high certainty	primary oxygen end time mean = 100 years, 10 years std. dev.
	Within primary oxygen period, probability of presence of oxygen at a given time step is highly probable, representing high certainty that oxygen will be present at this time	probability function for primary oxygen period = constant = 0.9
	Outside of primary oxygen period, high certainty that oxygen will not be present	probability function post primary oxygen period = constant = 0.2
humidity		humidity = 100%
galvanic corrosion rate	high certainty that corrosion rate will be remain with a narrow, predicted range in the presence of oxygen	mean corrosion rate set to constant 100um/year, 10um std. dev.
anaerobic corrosion rate		1um/year, 0.1um std. dev.
presence of pressure events after 174000 years	high certainty that there will be no pressure events after the glacier departs	0 probability of post glacier pressure events
Prob. Scenario 2- low certainty that system will behave as anticipated peri and post end of the primary oxygen period		
The presence or absence of oxygen at the surface of the UFC at a particular time	Expected end point of primary oxygen period set with low certainty	primary oxygen end time 1000 years, 100 std. dev.
	Within primary oxygen period, probability of presence of oxygen at a given time step is highly probable, representing high certainty that oxygen will be present at this time	probability function for primary oxygen period = constant = 0.9
	Outside of primary oxygen period, low certainty that oxygen will not be present	probability function post primary oxygen period = constant = 0.7
humidity		humidity = 10%
galvanic corrosion rate	high certainty that corrosion rate will be remain with a narrow, predicted range in the presence of oxygen	mean corrosion rate set to constant 500um/year, 10um std. dev.
anaerobic corrosion rate		1um/year, 0.1 um std. dev.
presence of pressure events after 174000 years		0 post glacier pressure events
presence of pressure events after 174000 years	high certainty that there will be no pressure events after the glacier departs	0 probability of post glacier pressure events
Prob. Scenario 3a- no primary oxygen period		
The presence or absence of oxygen at the surface of the UFC at a particular time	Expected end point of primary oxygen period set with high certainty	oxygen not necessarily present at time 0 (<10 years).
		no primary oxygen period
	Outside of primary oxygen period, some certainty that oxygen will not be present	probability function post primary oxygen period = constant = 0.1
humidity		percent (relative) humidity = 100%
galvanic corrosion rate	high certainty that corrosion rate will be remain with a narrow, predicted range in the presence of oxygen	mean corrosion rate set to constant 500um/year, 10 um, std. dev.
anaerobic corrosion rate		1um/year, 0.1 um std. dev.
presence of pressure events after 174000 years	low certainty that there will be no pressure events after the glacier departs	3 pressure events
pattern of pressure events after 174000 years	low certainty of form that pressure events will take	time when pressure event(s) occurs selected randomly (between glacier departure and end of simulation) and peak strength of pressure event selected randomly between 0 and 45MPa
Prob. Scenario 3b- no primary oxygen period, low anaerobic corrosion rate		
The presence or absence of oxygen at the surface of the UFC at a particular time	Expected end point of primary oxygen period set with high certainty	oxygen not necessarily present at time 0 (<10 years). Aerobic decomposition begins immediately with probability 1
	Within primary oxygen period, probability of presence of oxygen at a given time step is highly probable, representing high certainty that oxygen will be present at this time	probability function for primary oxygen period = constant = 1
	Outside of primary oxygen period, low certainty that oxygen will not be present	probability function post primary oxygen period = constant = 0.1
humidity		percent (relative) humidity = 100%
galvanic corrosion rate	high certainty that corrosion rate will be remain with a narrow, predicted range in the presence of oxygen	mean corrosion rate set to constant 500um/year, 10um std. dev.
anaerobic corrosion rate		0.10um/year, 0.1 um std. dev.
presence of pressure events after 174000 years	low certainty that there will be no pressure events after the glacier departs	3 pressure events
pattern of pressure events after 174000 years	low certainty of form that pressure events will take	time when pressure event(s) occurs selected randomly (between glacier departure and end of simulation) and peak strength of pressure event selected randomly between 0 and 45MPa

Table 31: Probabilistic scenarios – Part 1



System Aspect	Probability Settings	
	Scenario Description	Scenario Probabilistic Parameters
Prob. Scenario 4a- random copper coating hole, no primary period, expected anaerobic corrosion rate		
The presence or absence of oxygen at the surface of the UFC at a particular time	Expected end point of primary oxygen period set with high certainty	oxygen not necessarily present at time 0 (<10 years).
		no primary oxygen period
	Outside of primary oxygen period, some certainty that oxygen will not be present	probability function post primary oxygen period = constant = 0.01
humidity		percent (relative) humidity = 100%
galvanic corrosion rate	high certainty that corrosion rate will be remain with a narrow, predicted range in the presence of oxygen	mean corrosion rate set to constant 500um/year, 10um std. dev.
anaerobic corrosion rate		1 micron/year, 0.1 std. dev.
presence of pressure events after 174000 years	low certainty that there will be no pressure events after the glacier departs	3 pressure events
pattern of pressure events after 174000 years	low certainty of form that pressure events will take	time when pressure event(s) occurs selected randomly (between glacier departure and end of simulation) and peak strength of pressure event selected randomly between 0 and 45MPa
Prob. Scenario 4b- random copper coating hole, no primary period, very low anaerobic corrosion rate		
The presence or absence of oxygen at the surface of the UFC at a particular time	Expected end point of primary oxygen period set with high certainty	oxygen not necessarily present at time 0 (<10 years).
		no primary oxygen period
	Outside of primary oxygen period, some certainty that oxygen will not be present	probability function post primary oxygen period = constant = 0.01
humidity		percent (relative) humidity = 100%
galvanic corrosion rate	high certainty that corrosion rate will be remain with a narrow, predicted range in the presence of oxygen	mean corrosion rate set to constant 500um/year, 10um std. dev.
anaerobic corrosion rate		0.01 micron/year, 0.001 std. dev.
presence of pressure events after 174000 years	low certainty that there will be no pressure events after the glacier departs	3 pressure events
pattern of pressure events after 174000 years	low certainty of form that pressure events will take	time when pressure event(s) occurs selected randomly (between glacier departure and end of simulation) and peak strength of pressure event selected randomly between 0 and 45MPa

Table 32: Probabilistic scenarios – Part 2

4.4 Results

4.4.1 Deterministic Mode Scenarios

Within the deterministic context, both expected and unanticipated but possible scenarios were explored. In the case of the unanticipated scenarios, system properties took on values within recognized physically possible ranges, but at times, or over durations, or with magnitudes, other than what is anticipated.

4.4.1.1 Deterministic Scenario 1: Corrosion Alone As can be seen in Figures 28 through 31, in the absence of pressure exerted on the UFC by other components of the barrier system, in scenarios where the rates of corrosion and amount of oxygen are set within expected bounds, the container relatively slowly corrodes in the presence of a through wall defect in the copper coating. So long as the mean rate of corrosion is above 25.4 nanometers/year, the container will always corrode through within the 1,000,000 year time-span, and the container contents will be exposed to the environment. The specific time at which the contents are exposed is determined in part by how long oxygen is present in the system and in part by the humidity at the surface of the UFC, as shown in Figures 28, 29, 30 and 31.

4.4.1.2 Deterministic Scenario 2: Pressure Alone As can be seen in Figure 32, in the absence of corrosion pressure alone is not expected to cause the system to fail, even if the glacier exerts the largest amount of pressure anticipated by the Long-Term Stability Analysis of APM Mark II Conceptual Design in Sedimentary and Crystalline Rock Settings, and even if unexpected pressure events (assumed to be under 45 MPa) occur post glacier, because there is nothing to decrease the load strength of the container in this situation (as currently modeled).

4.4.1.3 Deterministic Scenario 3: Corrosion and Pressure Combined As can be seen in Figure 33, when pressure and corrosion are combined in the system, the container gradually weakens over time due to corrosion, and eventually the pressure within the system causes the container contents to become exposed via a breach of the UFC due to load exerted on the UFC, even if the load exerted on the UFC is relatively low.

4.4.1.4 Summary of Deterministic Results These deterministic scenarios collectively illustrate that, in both anticipated and unanticipated scenarios, the container contents do become exposed to the environment. This is the case when corrosion is acting alone as well as when combining the two causal chains. However, although such deterministic results can usefully lay bare the underlying behaviours of the system, they do not allow for predictions of the probabilities of particular events. It should also be noted here that, as the system is currently represented (for the prototype phase), the pressure and corrosion chains are not coupled in both directions: although system properties affected by corrosion (e.g. steel wall thickness) influence some pressure related properties (e.g. load strength of UFC), pressure related properties do not in return influence corrosion related properties. As a result, overall system behaviour is relatively non-complex, and fairly predictable in a deterministic context.

4.4.2 Probabilistic Mode Scenarios

The probabilistic scenarios considered involve uncertainty surrounding a number of model elements:

- The presence or absence of oxygen at the surface of the UFC at a particular time
- The level of humidity at the surface of the UFC at a particular time
- the corrosion rate at a particular time
- the presence of pressure events after 174,000 years
- the pattern of pressure events after 174,000 years

The level of certainty, and thus, probability related values, were varied for each of these aspects of the model (see Table 31). In addition to this, two more scenarios were considered in an exploratory context– for both of these scenarios, the through wall defect was not assumed to be present immediately post manufacturing. Rather, in these scenarios the hole in the copper coating could appear at any time post enclosure, with equal probability.

4.4.2.1 Probabilistic Scenario 1: High Certainty for Quick Absence of Oxygen, Variability of Corrosion Rate, Absence of Additional Pressure Events In this scenario, the certainty (and thus probability) that oxygen would be present when expected, as well as absent when expected,

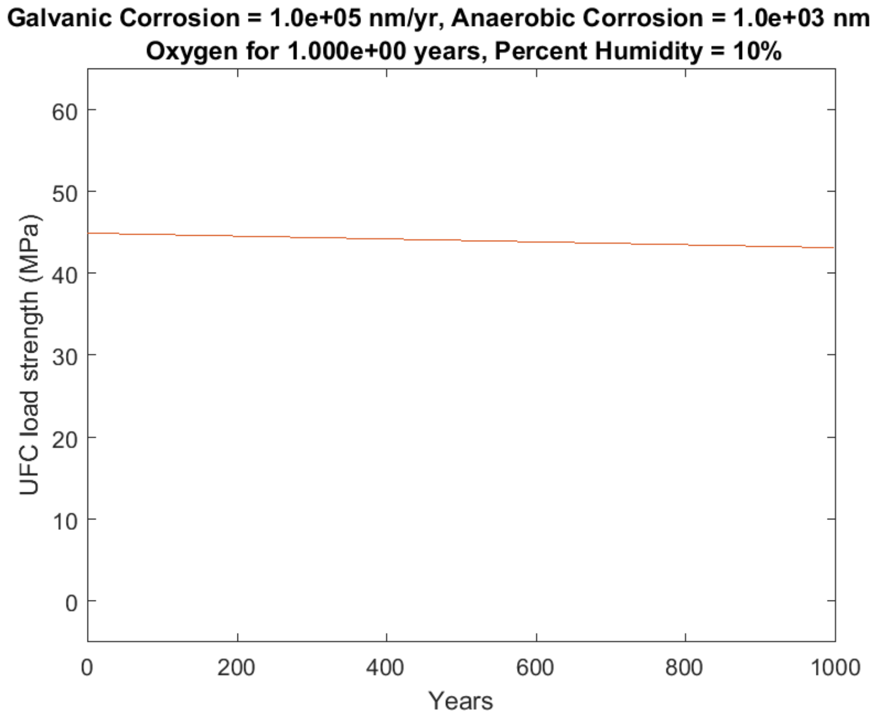


Figure 28: Scenario 1: Effects of corrosion alone on the load strength of the container – short galvanic period, low humidity. Under these conditions, the galvanic corrosion effect is fairly negligible.

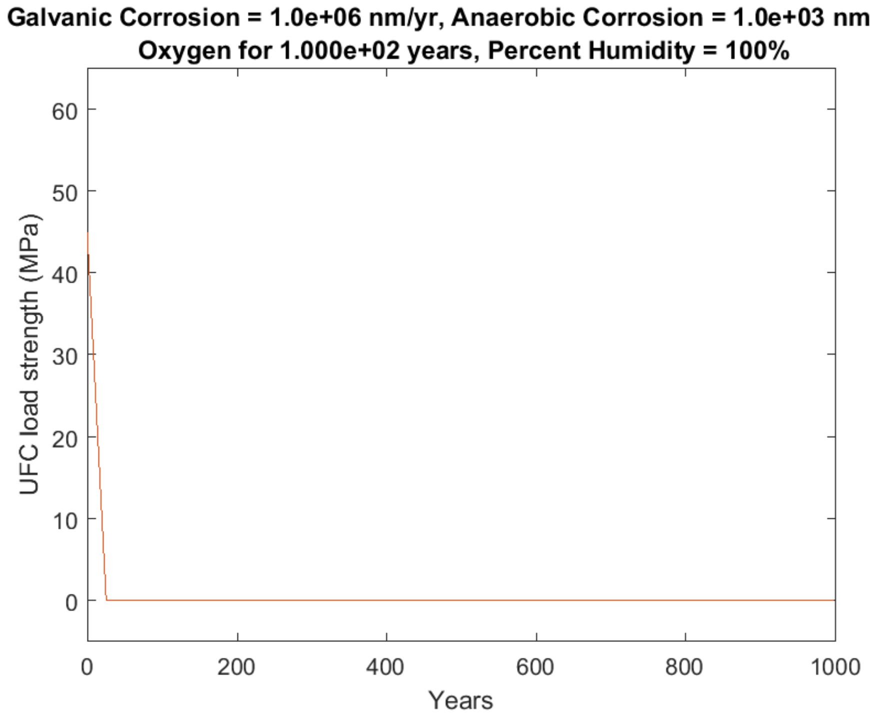


Figure 29: Deterministic Scenario 1b: Lengthening the galvanic period past the expected length results in a relatively quick UFC contents exposure time, particularly if humidity is high.

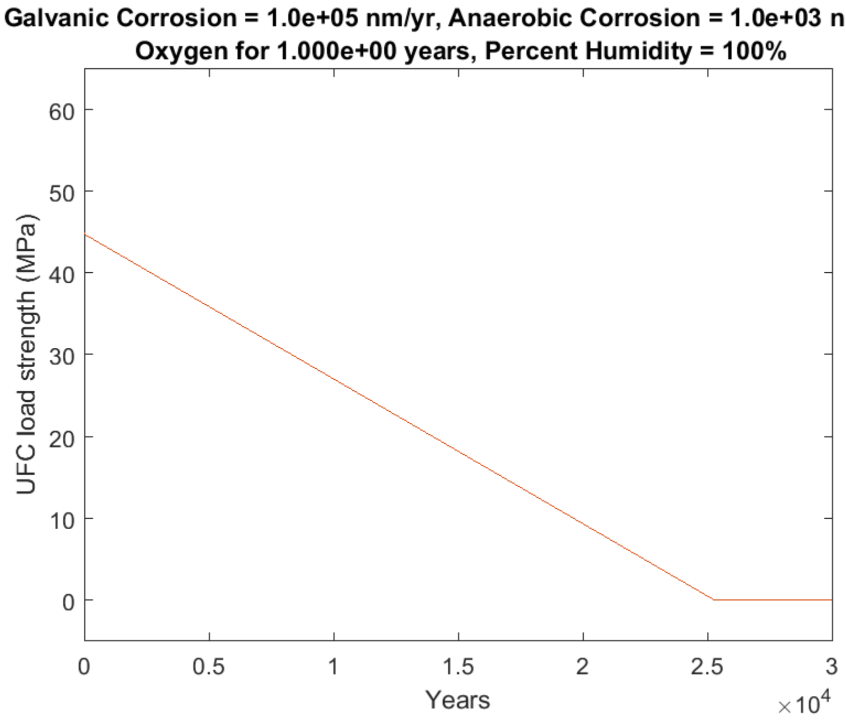


Figure 30: Deterministic Scenario 1c: If the primary oxygen period is short, galvanic corrosion has minimal effect, but anaerobic corrosion eventually leads to contents exposure

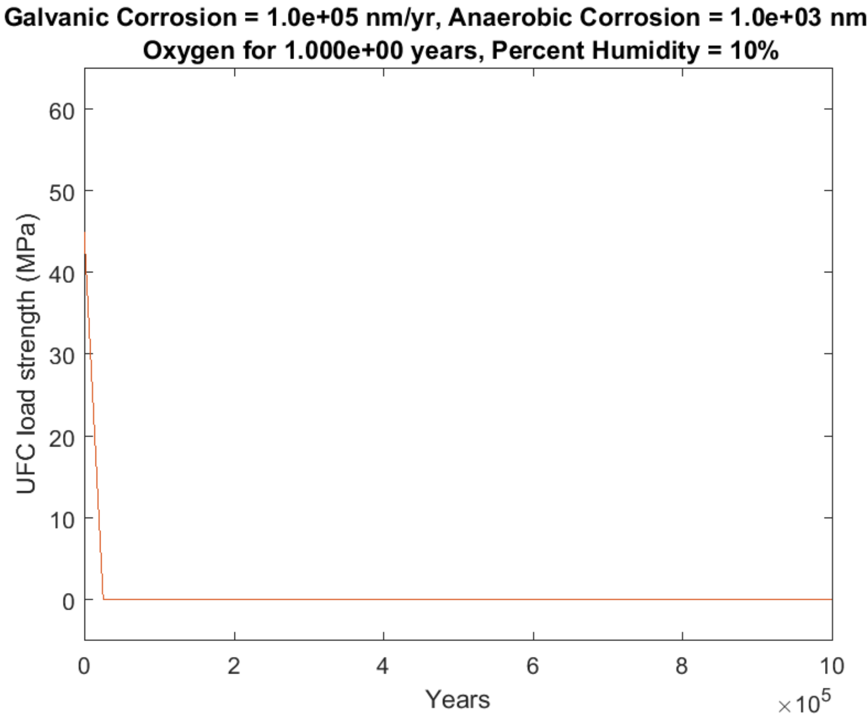


Figure 31: Deterministic Scenario 1d: Showing time to contents exposure relative to the full time period being considered provides a better sense of the rate of anaerobic corrosion.

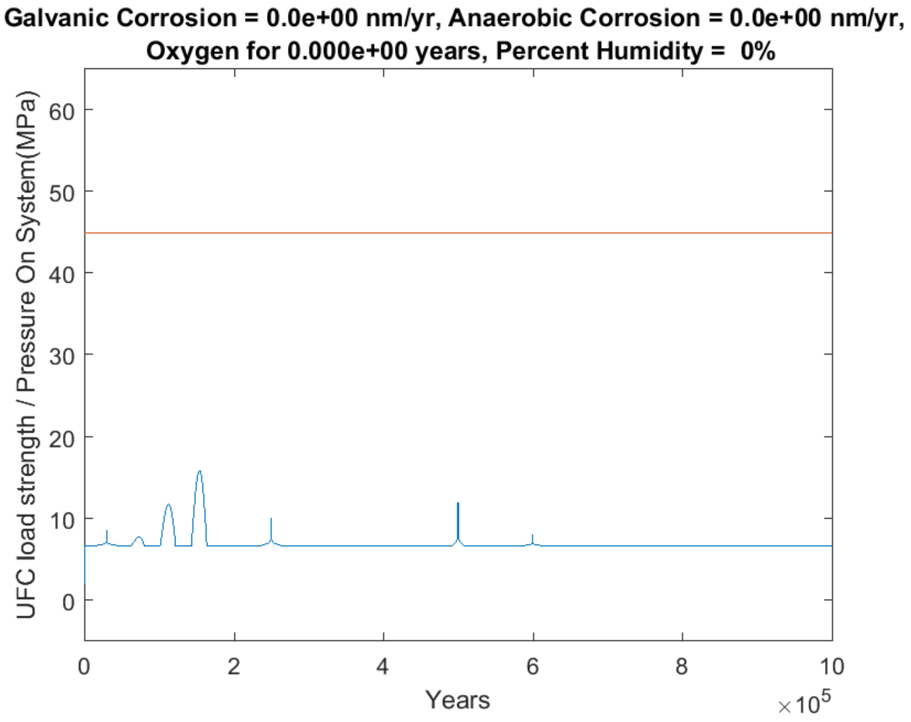


Figure 32: Deterministic Scenario 2: Container behaviour under system pressure but in the absence of corrosion, including three unexpected post glacier pressure events. As expected, container contents are never exposed under these conditions.

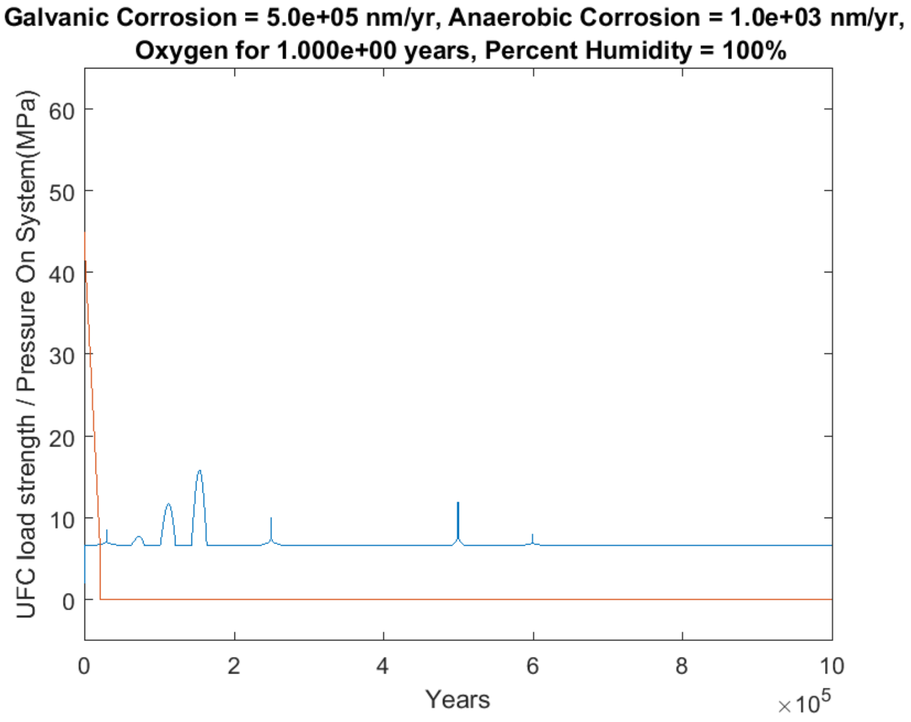


Figure 33: Deterministic Scenario 3: Container behaviour under both system pressure and corrosion, including three unexpected pressure events, with one year of galvanic corrosion.

was fairly high (the mean length of time of the preliminary oxygen period was set at 100 years to allow for some variability in the length of this period), the variability of the corrosion rates were minimal, and there were no unexpected pressure events. Figure 34 shows a typical run of the simulation. Figure 35 shows the frequency of times when exposure occurred. The resulting cumulative probability distribution function, providing probability that contents would be exposed by the time a particular point in time was reached, can be seen in Figure 36.

4.4.2.2 Probabilistic Scenario 2: Low Certainty for Oxygen Behaviour, Variability of Corrosion Rate, Absence of Additional Pressure Events In this scenario, the certainty that oxygen would be present when expected, and absent when expected was low. As a result, variability of the end point of the first oxygen period was high, and there was a relatively high probability at time steps after this period that oxygen might reappear in the system. The variability of the corrosion rates were also set to be relatively high. Figure 37 shows a typical run of the simulation. Figure 38 shows the frequency of times when exposure occurred. The resulting cumulative probability distribution function, providing probability that contents would be exposed by the time a particular point in time was reached, can be seen in Figure 39.

4.4.2.3 Probabilistic Scenarios 3a and 3b: No Primary Oxygen Period Oxygen is expected to leave the barrier system very rapidly. Thus, as can be seen in the deterministic scenarios, despite the high rate of galvanic corrosion, the main corrosion factor in the model is expected to be anaerobic. Because the current model was generally set to proceed in 10 year increments, for computational reasons, two anaerobic scenarios were investigated in order to effectively encompass the possibility of rapid reduction of oxygen in the system (e.g. < 1 year). However in these scenarios, the model was set such that oxygen could still reappear in the system, at any given time, with a specified probability (see Table 31). Two scenarios were explored, one with an expected anaerobic corrosion rate, and one with a very low anaerobic corrosion rate.

Figure 40 and 43 show typical runs of the anaerobic only simulations for each scenario. The resulting histograms and cumulative probability distribution functions, providing probability that contents will be exposed by a particular point in time, can be seen in Figures 41, 42, 44 and 42.

4.4.2.4 Probabilistic Scenarios 4a and 4b: Hole in Copper Over Time, No Primary Oxygen Period The observed behaviour of the system when a through-wall defect in the coating was immediately present in the UFC– in particular the noted effects of oxygen presence and corrosion rate on the (typically rapid) exposure time of the UFC contents– motivated a further, preliminary investigation of what impact the appearance of a hole in the copper coating at other times post enclosure might have on the behaviour of the system. To that end, two additional scenarios were considered (see Table 32). The results showed a relatively evenly spaced time to failure for the expected anaerobic rate (see Figures 46, 47 and 48). However, when the anaerobic rate was reduced, an interaction effect with pressure became evident, and the presence of the glacier became a determining event in the exposure of the contents of the UFC to the environment (see Figures 49, 50 and 51).

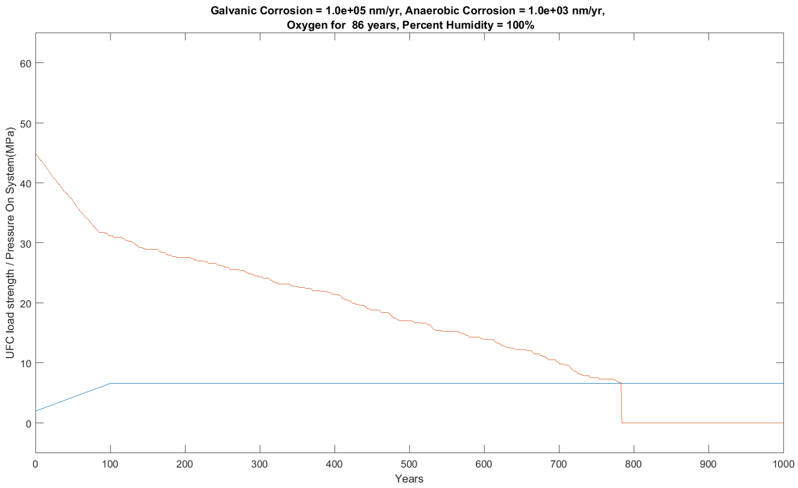


Figure 34: Probabilistic Scenario 1: A typical simulation run showing time to exposure under expected conditions.

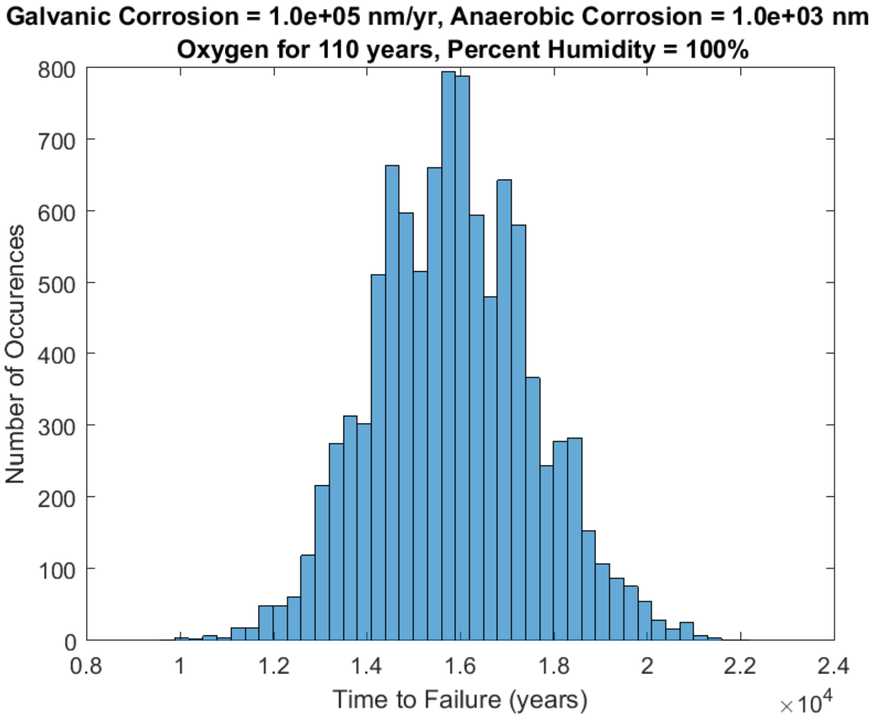


Figure 35: Probabilistic Scenario 1: Histogram of time to exposure of UFC contents, under expected conditions, in the presence of a through wall defect.

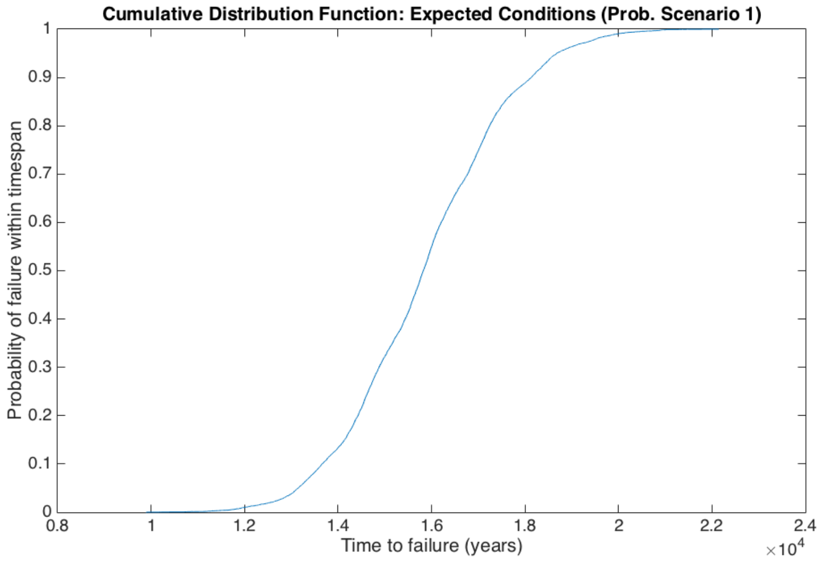


Figure 36: Probabilistic Scenario 1: Probability of content exposure either at or before a particular time (cumulative distribution function) under expected system conditions, in the presence of a through wall defect.

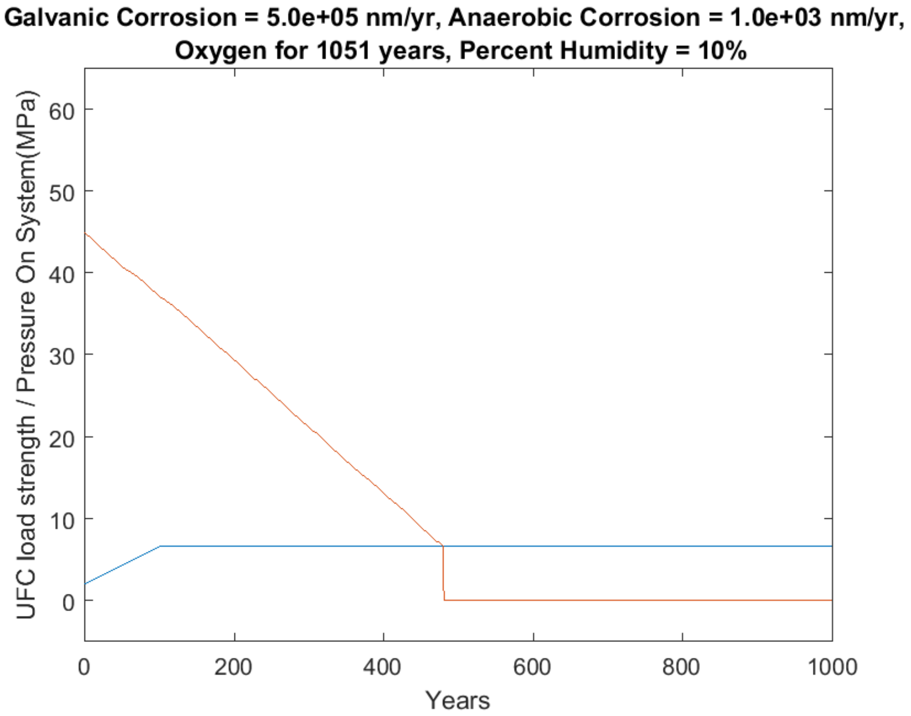


Figure 37: Probabilistic Scenario 2: An illustrative simulation run, with some uncertainty in system behaviour.

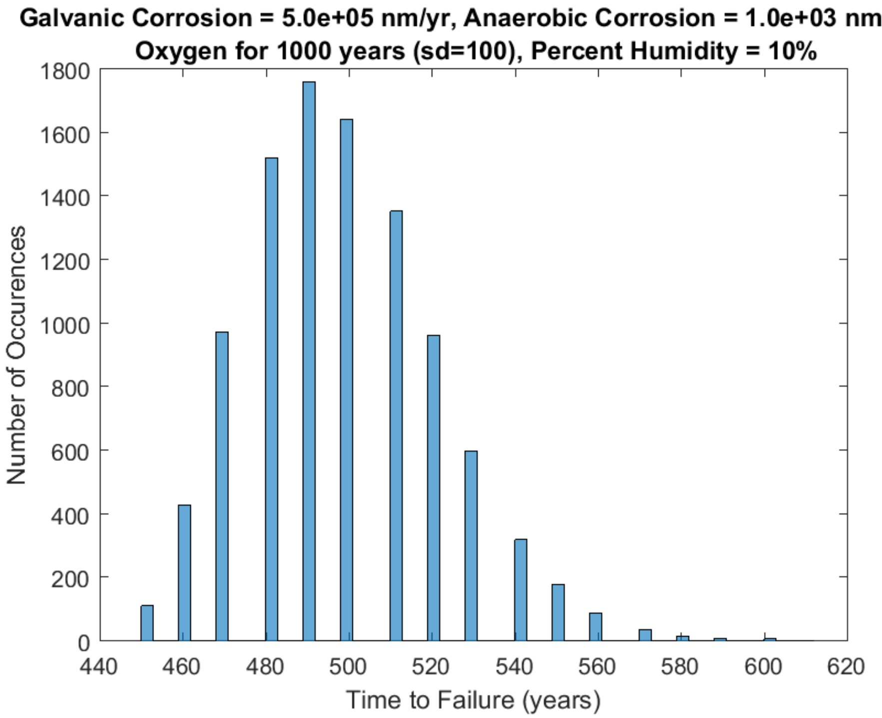


Figure 38: Probabilistic Scenario 2: Histogram of time to exposure of UFC contents, given uncertainty about behaviour of the aspects of the system (gaps in the histogram are due to the choice of 10 year time intervals, which are more visible when dealing with short time periods. Results are expected to be equivalent for 1 year time intervals.

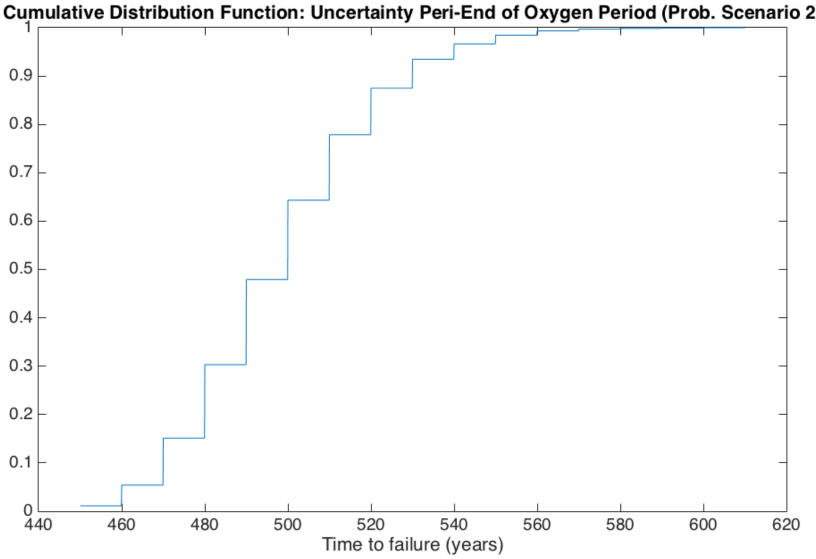


Figure 39: Probabilistic Scenario 2: Probability of content exposure either at or before a particular time (cumulative distribution function) given some uncertainty about system behaviour.

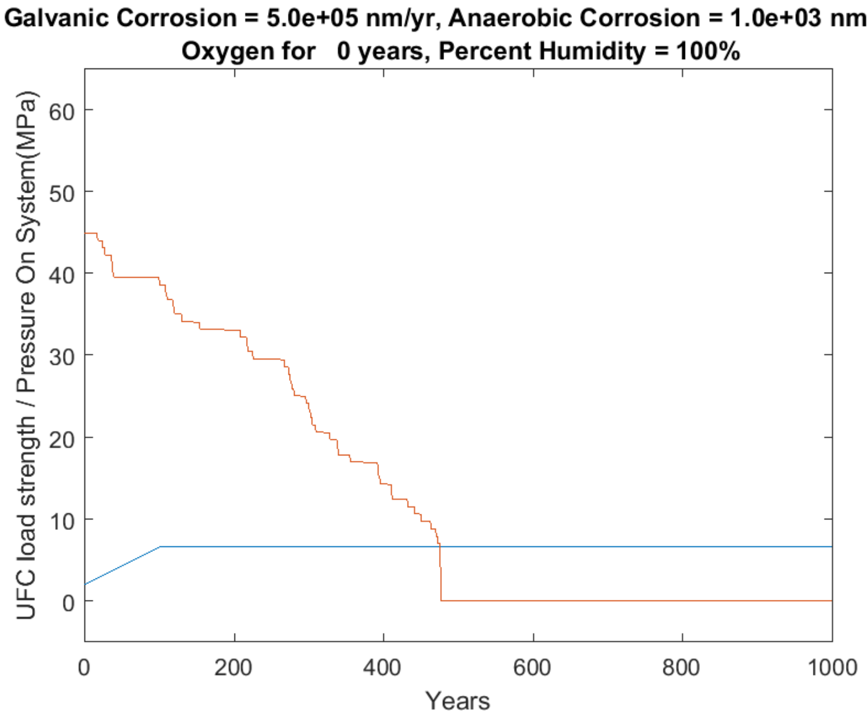


Figure 40: Probabilistic Scenario 3a: A single simulation run showing time to exposure, with no primary oxygen period, but some probability of oxygen appearing at each time step.

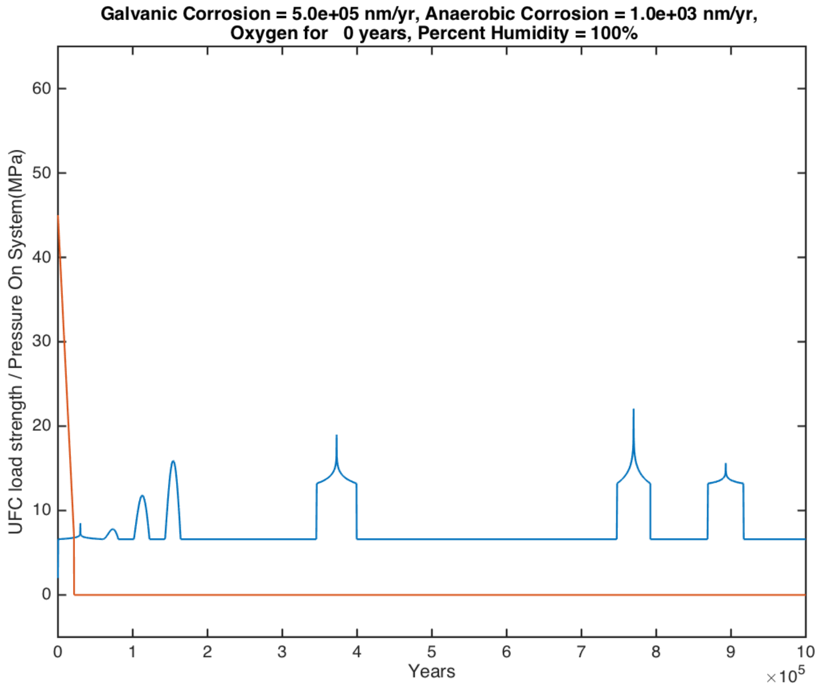


Figure 41: Probabilistic Scenario 3a: Histogram of time to exposure of UFC contents, , with no primary oxygen period, but some probability of oxygen appearing at each time. step.

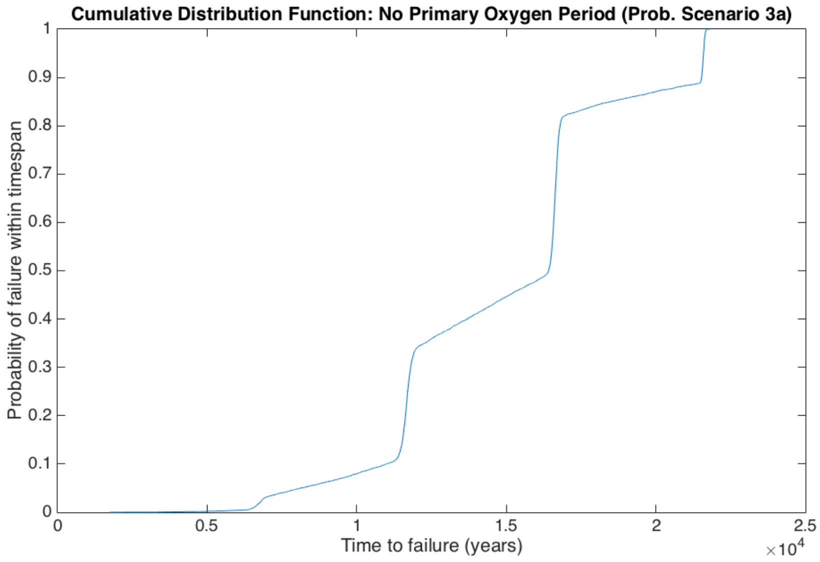


Figure 42: Probabilistic Scenario 3a: Probability of content exposure either at or before a particular time (cumulative distribution function), with no primary oxygen period, but some probability of oxygen appearing at each time. step.

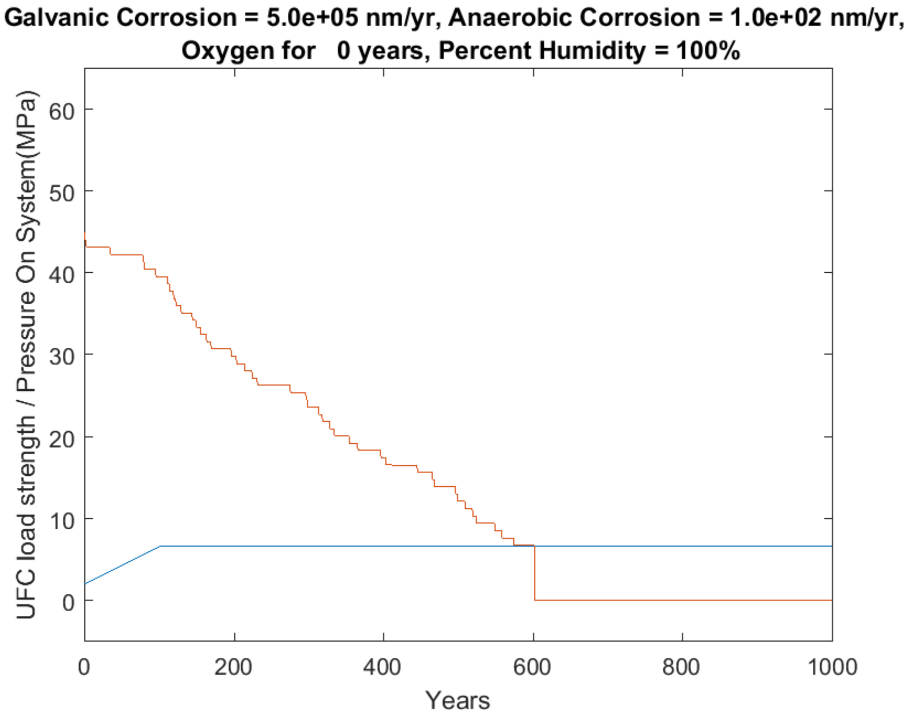


Figure 43: Scenario 3b: a single simulation run showing time to exposure, no primary oxygen period, low anaerobic corrosion rate rate

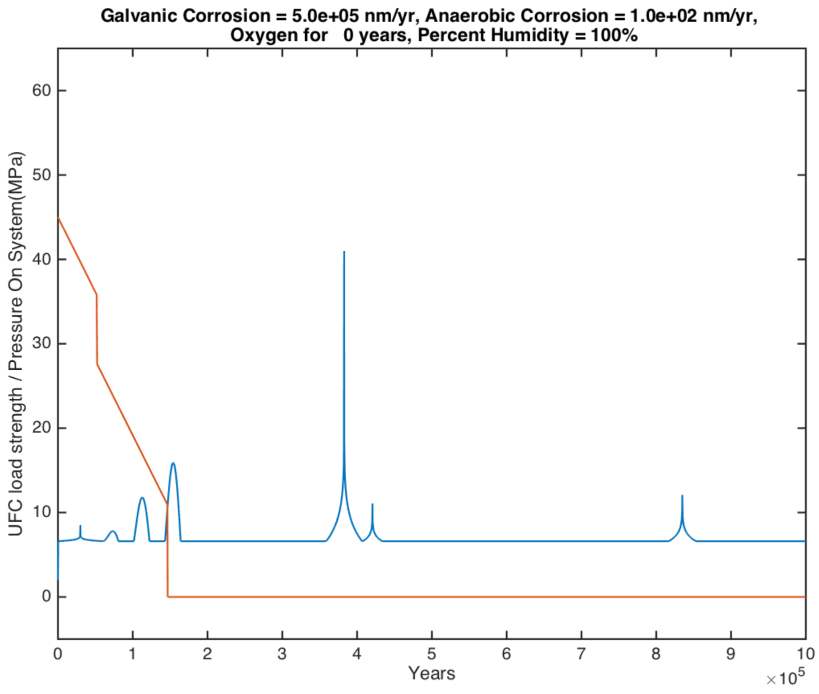


Figure 44: Probabilistic Scenario 3b: Histogram of time to exposure of UFC contents, no primary oxygen period, low anaerobic corrosion rate.

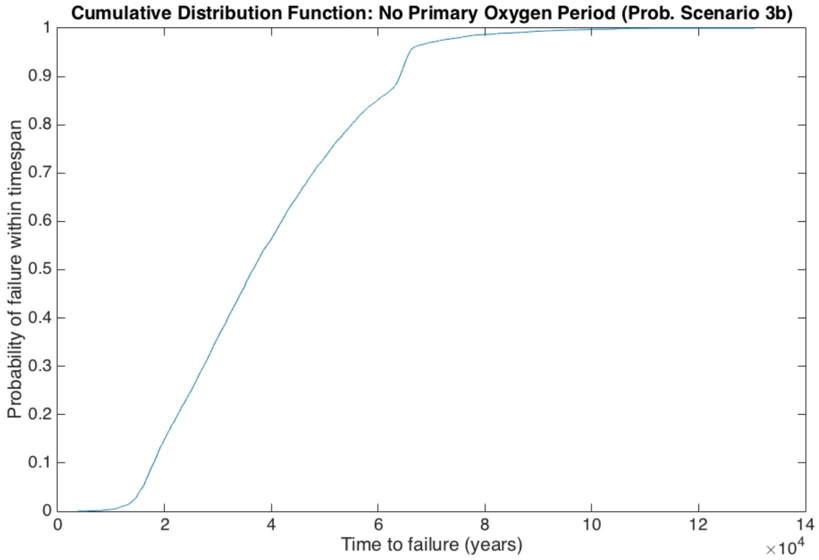


Figure 45: Probabilistic Scenario 3b: Probability of content exposure either at or before a particular time (cumulative distribution function) no primary oxygen period, low anaerobic corrosion rate.

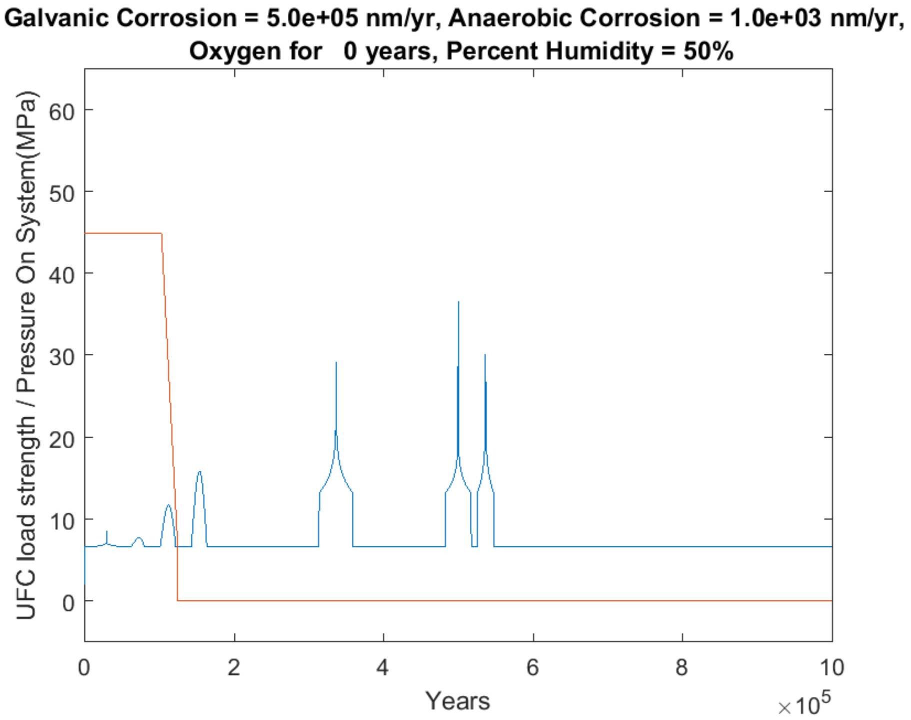


Figure 46: Probabilistic Scenario 4a: A single simulation run showing post enclosure appearance of a hole in the copper coating, no primary oxygen period, expected anaerobic rate of corrosion

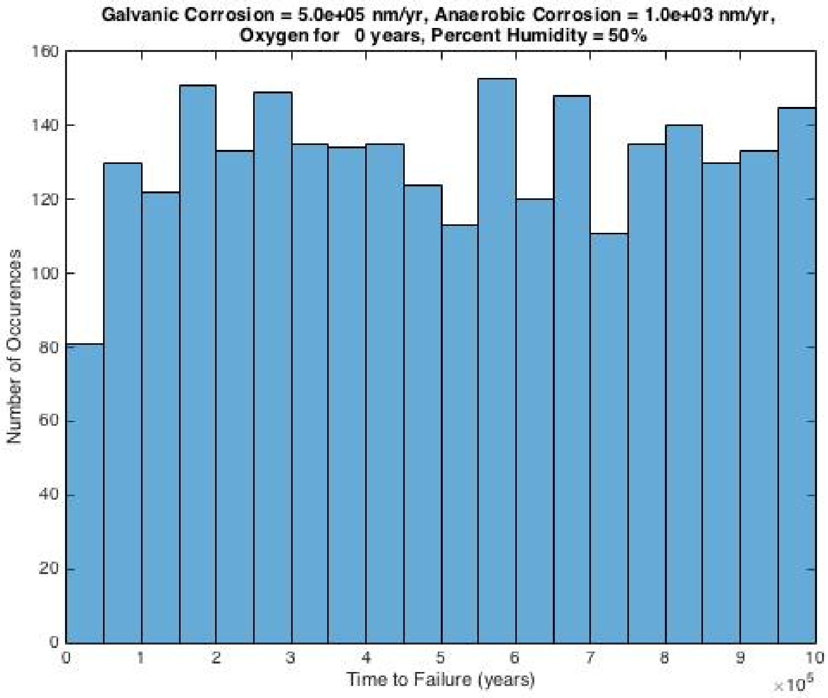


Figure 47: Probabilistic Scenario 4a: A histogram of time to exposure when a hole can appear in the copper coating post closure, expected anaerobic corrosion.

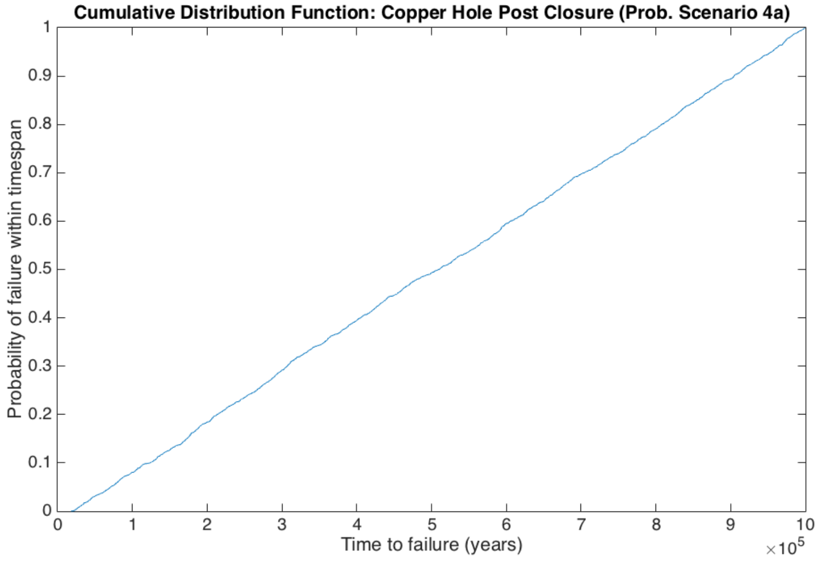


Figure 48: Probabilistic Scenario 4a: Probability of content exposure either at or before a particular time (cumulative distribution function) given appearance of a hole in the copper coating at some point post closure, expected anaerobic corrosion.

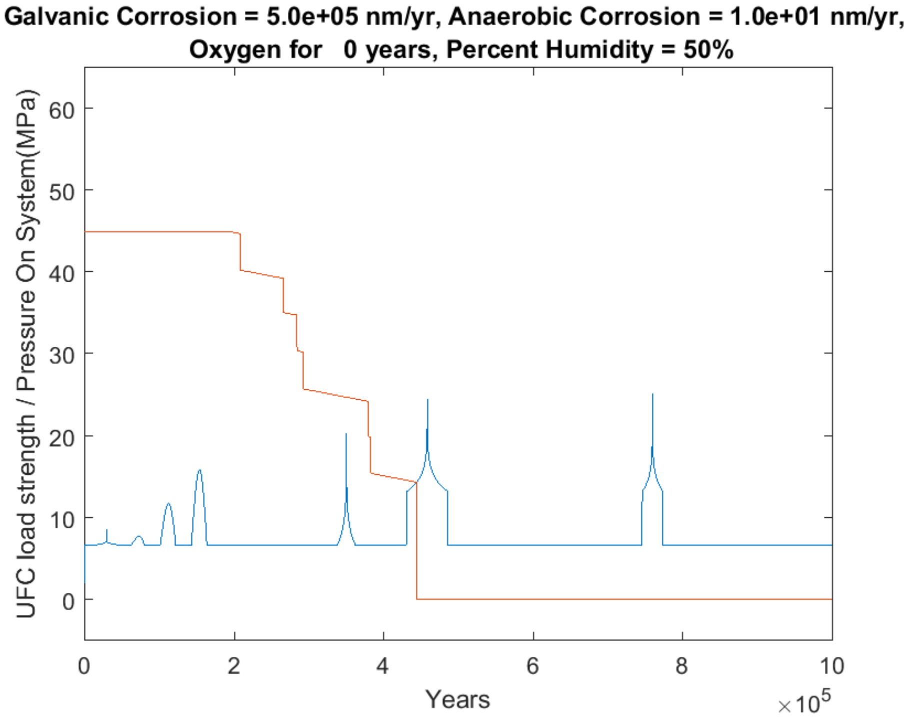


Figure 49: Probabilistic Scenario 4b: A single simulation run showing post enclosure appearance of a hole in the copper coating, no primary oxygen period, low anaerobic rate of corrosion

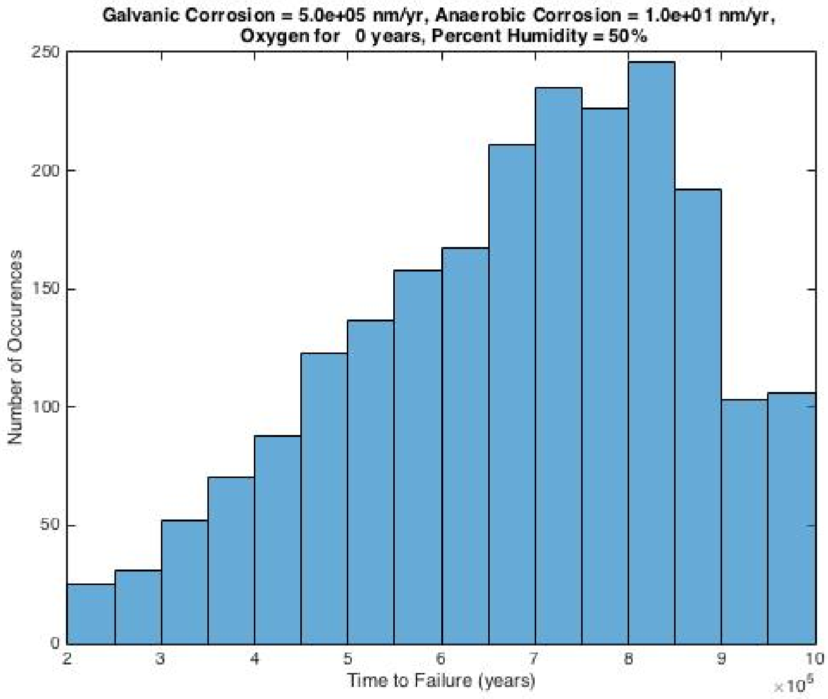


Figure 50: Probabilistic Scenario 4b: A histogram of time to exposure when a hole can appear in the copper coating post closure, low anaerobic corrosion.

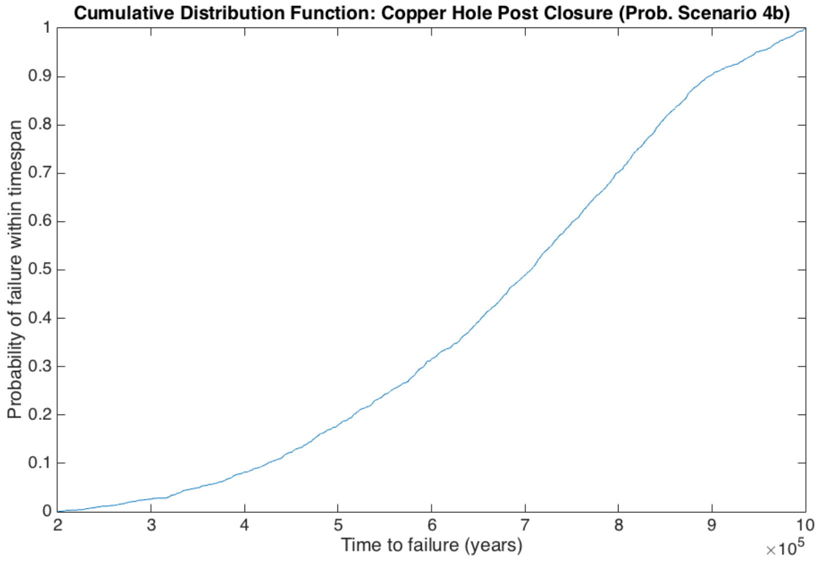


Figure 51: Probabilistic Scenario 4b: Probability of content exposure either at or before a particular time (cumulative distribution function) given appearance of a hole in the copper coating at some point post closure, low anaerobic corrosion.

4.5 Discussion

Key points arising from the construction of the prototype causal chain model:

- The prototype phase allowed for the development of several key methodologies required for the prediction of the behaviour of the engineered barrier system, including strategies for a methodical analysis of available information, consultation with key subject matter experts and incorporation of their knowledge into the end model, and conversion of the conceptual model into an implemented model that was constructed with an appropriate level of detail.

- Given that the prototype model only encompassed a small number of the components and aspects of the engineered barrier system, the results presented here should not be considered indicative of actual system behaviours. As well, further discussions with subject matter experts about appropriate model parameter values will need to be carried out prior to incorporation of this model into a more comprehensive system model.

- If this model were indicative of system behaviour, the results would suggest that the presence of a through wall defect in the copper coating results in a high probability of container content exposure in a relatively short period of time (typically $<$ 50 000 years).

- It is also clear that, for the causal chains chosen, rate of corrosion was an overriding factor in the behaviour of the system as a whole. Although not presented at this time, it is worth noting that an initial exploration of system behaviour with very low corrosion rates yielded notably different interaction patterns between pressure and corrosion parameters (e.g. unanticipated pressure events post glaciation played a much larger role in whether or not contents were exposed).

- There was relatively little mutual interaction between the two causal chains chosen for the prototype: although corrosion was affected by pressure, as modeled, pressure in the system did not significantly effect corrosion. Nonetheless, a detailed exploration and conceptual analysis of the system prior to modeling allowed for an exploration of potential interactions between components. System behavior was explored in the presence and absence of these components to confirm the appropriate level of abstraction for causal chain processes, states and objects. This level of detail was left latent within the model, such that in the event that new object interactions or process information was obtained, these interactions could be easily represented.

- One benefit of presenting the behaviour of the model first deterministically and then probabilistically is that it makes both the model interactions and the role of uncertainty in the model more visible. This may be useful in meeting the stated goal of being able to clearly communicate model behaviours and probabilities to stakeholders.

- A key aspect of the developed methodology was the ability to incorporate level of certainty of knowledge into the model, and explore the potential consequences of this on predictability of the behaviour of the system. A focus of future phases should be an exploration of the implications of levels of certainty about aspects of the system, based on input from subject matter experts.

- Combining the cumulative distribution function for the chosen scenarios has the potential to provide a perspective on the overall probability that contents of the container will be exposed by a given point in time. However, to accurately provide a combined cumulative distribution function, more information is required with respect to cumulative distributions for failure in the absence of holes in the copper coating. Possible next steps for this will be discussed further in recommendations.

References

- Kripke, S. (1963). Semantical Considerations on Modal Logic. Acta Philosophica Fennica 16, pp. 83-94

5 Recommendations

A primary purpose of models is to act as cognitive tools that support efforts to understand and anticipate the range of potential behaviours of a given system of interest. In relation to this, the process of constructing a whole-system level model of the engineered barrier system will accomplish two separate but important tasks: First, it will allow system experts to make tangible, explicit and concrete their existing (and possibly contrasting) hypotheses about potential system behaviours. As is the case with the FMECA process, this will effectively enable subject matter expert perspectives to be captured in such a way that they can be discussed and compared more directly and explicitly. Turning knowledge and information into working models in this way allows for a concrete exploration of the implications of different hypotheses about how the system may behave, as well as the consequences of being more or less accurate in this understanding.

Second, construction of such a model will allow the NWMO to explore the possibility space of behaviours of the engineered barrier system in a methodical and quantitative manner. In particular, the proposed method will allow for the consideration of how the likelihood of certain aspects of system behaviour occurring can influence, along multiple pathways, the likelihood of occurrence of chosen states of interest (e.g. exposure of the contents of the container).

Given this, we recommend that the NWMO continue to expand its current suite of models by constructing a series of ‘light’ (partial) causal chain models, which can then be selectively combined to understand interactions between selected aspects of the system. This selective combining of models may not immediately lead to the creation of a single system level model. However, we recommend that these models be constructed using the overarching framework presented in the prototype phase so that they can, in principle, be combined into more encompassing models as this becomes desirable and appropriate.

As well, based on the results of this prototype project, in constructing these ‘light’ system models, we recommend that the NWMO focus on initially incorporating as many interactions between system objects as possible, rather than making up front assumptions about which interactions can be implicitly captured in a small number of aggregate system parameters. Level of detail may then be removed from the model once it is shown that there are no emergent interactions between different system components.

At the same time, we suggest that the NWMO begin to aggregate and structure two existing resources relating to system behaviour, in preparation for inclusion and integration into the higher level whole-system model backbone: existing simulations, in order to determine their potential relationships to the causal network backbone, and system documentation, from which information can be extracted in a structured manner in order to uncover potentially unanticipated interactions between system components.

One potential end product of such a series of models would be a combined distribution function for the probability that the contents of the container would be exposed across a given time span, taking into account a wide variety of model behaviour scenarios. However, in order to generate such a probability failure curve, we require cumulative distribution functions for each of the exclusive scenarios as well as a probability of occurrence for each of them.

For instance, consider the exclusive list of options indexed by

$S_{i,j}$: UFC placed in the repository with i undetected through-wall defect(s) and j undetected thin-wall defects.

If we further assume that, under some profile under investigation, each of those items has a probability failure curve given by $p_{i,j}(t)$, and a probability $q_{i,j}$ of occurring in the first place, then the combined failure curve for the ensemble of options is simply

$$\sum_{i,j} q_{i,j} p_{i,j}(t).$$

Substantially more work needs to be done before this failure probability curve can be approximated in a useful manner.

Finally, the NWMO can improve its control over the UFC manufacturing process with a better understanding of the role (and impact) played by various combinations of failure probabilities and system parameters at each stage. While the current manufacturing model provides some insight into this issue, the day will be carried by experimental tests and results at the various stages of the process. We strongly encourage the NWMO to design such tests and collect data that can be used by stochastic manufacturing process models (see accompanying Excel spreadsheet for details). New variables may need to be introduced, the model structure may need to be modified (in particular with respect to the effect that a defective parent state may have on a child variable), and some parameter values may need to be changed.

Note that, under the current model, the target values (i.e., the means of the distributions) are of less importance than the various ratios between the threshold, variance, and tolerance, as well as the probabilities of incorrectly accepting a UFC when the variable lies within the acceptable, tolerance and “bad” regions. Since, however, future model iterations could incorporate some modifications to this approach, determining the target values of each variable could still prove to be a valuable exercise.