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Towards Systematically Deriving Defence Mechanisms from Functional Requirements of Cyber-Physical Systems

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ABSTRACT

The threats faced by cyber-physical systems (CPSs) in critical infrastructure have motivated the development of different attack detection mechanisms, such as those that monitor for violations of *invariants*, i.e. properties that always hold in normal operation. Given the complexity of CPSs, several existing approaches focus on deriving invariants automatically from data logs, but these can miss possible system behaviours if they are not represented in that data. Furthermore, resolving any design flaws identified in this process is costly, as the CPS is already built. In this position paper, we propose a systematic method for deriving invariants *before* a CPS is built by analysing its *functional requirements*. Our method, inspired by the *axiomatic design* methodology for systems, iteratively analyses dependencies in the design to construct equations and process graphs that model the invariant relationships between CPS components. As a preliminary study, we applied it to the design of a water treatment plant testbed, implementing checkers for two invariants by using decision trees, and finding that they could detect some examples of attacks on the testbed with high accuracy and without false positives. Finally, we explore how developing our method further could lead to more robust CPSs and reduced costs by identifying design weaknesses before systems are implemented.

CCS CONCEPTS

• **Computer systems organization** → **Embedded and cyber-physical systems**; • **Security and privacy** → *Intrusion detection systems*; • **General and reference** → *Design*.

KEYWORDS

Cyber-physical systems; systematic design framework; anomaly detection; axiomatic design; supervised machine learning

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1 INTRODUCTION

Cyber-physical systems (CPSs), in which software components and physical processes are tightly integrated, are prevalent in the automation of critical infrastructure, e.g. as the industrial control systems of power grids and water purification plants. The potentially serious consequences of such systems being compromised [29, 31, 37] has motivated the development of different countermeasures for attack detection and prevention, including techniques based on anomaly detection [3, 7, 10, 13, 18, 20, 25, 28, 30, 32, 34, 36, 38, 43, 45, 46], fingerprinting [8, 9, 22, 26, 35, 49], and fuzzing [16, 17, 48].

Another popular approach is to monitor *invariants* of a CPS [23], i.e. properties that *always* hold under normal operating conditions, and the violation of which might suggest the presence of an attacker in the system. Invariants are typically relations over the sensor readings and actuator states of a system, a simple example being that “if the tank level is above x , then pump p should be ON”. Given the complexity of CPSs in general, several approaches (e.g. [14, 15, 21]) aim to derive such invariants automatically from sources of data, for instance, the time series of sensor readings and actuator states logged by a supervisory control and data acquisition system (SCADA). There is a risk, however, that viable system behaviours are missed if they are not represented in that data (e.g. rarely occurring), and addressing any design flaws identified is costly as the CPS is already built. Invariants can be derived manually by system engineers [4–6, 12, 19], but if done so in an ad hoc manner, may also lead to properties being missed.

In this position paper, we propose a systematic method to support the derivation of invariants *before* a CPS is built by analysing its *functional requirements*. Our goal is to further integrate security concerns in the design stage, ensuring that invariants can be traced from requirements through to implemented defence mechanisms, and to potentially save costs by identifying weak points before the design is executed. Our approach, inspired by *axiomatic design* [47]—a design science methodology for systems—iteratively analyses dependencies in the CPS to construct equations and process graphs that model the required invariant relationships between sensors and actuators. Checkers for these invariants can then be implemented

using techniques such as decision trees, and when deployed with the built CPS, can monitor its data for any violations of the properties.

To evaluate the viability of our proposals, we applied our method to the design of Secure Water Treatment (SWaT) [2, 40], a scaled-down version of a real-world water purification plant. SWaT is a complex multi-stage CPS involving physical and chemical processes such as ultrafiltration, de-chlorination, and reverse osmosis. We used our method to decompose eight high-level functional requirements into 44 concrete ones, tracing dependencies down to specific sensors and actuators. We illustrate how this information can be used to construct invariants, represented either as equations or process graphs. Finally, as a preliminary study, we implemented checkers for two of the invariants by training supervised machine learning (ML) models (i.e. decision trees) on equation inputs/outputs, finding that they could detect relevant attacks in both a dataset *and* on the real testbed with high levels of accuracy and without false positives.

Summary of Contributions. We propose a method for systematically deriving invariants from the functional requirements of a CPS. Through a preliminary study on a real-world critical infrastructure testbed, we demonstrate the feasibility of constructing effective invariant-based checkers for CPSs that can be traced all the way back to the system’s requirements. Furthermore, our study demonstrates the potential of a cross-disciplinary approach that utilises methodologies from design science (i.e. axiomatic design) to structure and analyse the dependencies present in critical infrastructure.

This work extends the initial ideas of Palleti et al. [44], who explored how axiomatic design could help analyse the requirements of a water distribution network. We go further by applying it to a water purification plant and deriving invariant-based checkers that can be used for its defence.

Organisation. The rest of the paper is organised as follows. Section 2 briefly describes the SWaT architecture, as well as the axiomatic design theory our method is inspired by. Next, our systematic design framework is presented in Section 3. Section 4 discusses the effectiveness of our invariant checkers in a preliminary study. Finally, Section 5 concludes this paper.

2 BACKGROUND

In this section, we present an overview of the water purification plant that forms the case study of this position paper. Following this, we discuss the axiomatic design theory that our proposed approach is based on.

2.1 SWaT Testbed

The Secure Water Treatment (SWaT) testbed [2, 40] is a scaled-down version of a modern water purification plant, intended for supporting research into cyber-security solutions for critical infrastructure. SWaT is able to produce up to five gallons of safe drinking water per minute across six distinct co-operating stages (Figure 1) involving chemical processes like ultrafiltration, de-chlorination, and reverse osmosis. Each stage is controlled by a Programmable Logic Controller (PLC), which communicates with sensors and actuators through a field-bus network, and with each other through a

24-port Ethernet switch. A SCADA workstation connects a human-machine interface to all of the PLCs, facilitating monitoring and control of the plant by human operators. The physical state of SWaT, as observed by the sensors, is recorded by a historian server at pre-specified intervals. A SWaT dataset is available, consisting of all the data recorded by this server over a period of several days, including a few during which the testbed was subjected to attacks [1, 24].

An overview of the six sub-processes of SWaT is given in Figure 1. A number of the testbed’s 68 sensors and actuators are depicted, with sensors including Flow Indicator Transmitters (FITs), Analyzer Indicator Transmitters (AITs), and Level Indicator Transmitters (LITs). Actuators include Motorised Valves (MVs) for controlling the inflow of water into tanks, and Pumps (Ps) for pumping it out.

Stage One. At the bottom of raw water tank T-101, a motorised valve (MV-101) is opened to allow raw water to flow in. An electromagnetic flow transmitter (FIT-101) reads the flow rate of this water, and sends it to the PLC. Pump P-101 transfers water from T-101 to the ultrafiltration feed water tank T-301 in stage three, passing through the chemical dosing of stage two. The operation of P-101 is interlocked to the level indicator transmitter (LIT-301) in tank T-301.

Stage Two. Chemical dosing is applied in this stage. The chemical properties of the incoming raw water are measured using analyser indicator transmitters AIT-201, AIT-202, and AIT-203. This information is used by the PLC to control pumps P-201, P-202, and P-203, adjusting the dosing and thus the water’s chemical properties before it enters stage three.

Stage Three. Ultrafiltration (UF) is performed in this stage. Raw water, after being dosed with chemicals in stage two, is fed into an UF unit. The operation of P-301 is interlocked with the level indicator transmitter LIT-401 for the reverse osmosis (RO) feed water tank (T-401) in stage four. Thus, P-301 is stopped when the water level in T-401 is high, and P-301 is turned on and MV-302 opened when the water level in tank T-401 reaches the low marker. Flow meter FIT-301 measures the incoming flow rate to the UF unit. The differential pressure indicator transmitter (DPIT) continuously monitors the difference in inlet pressure and outlet pressure. If the UF membranes are clogged, the DPIT triggers an alarm and a backwash sequence begins in stage six. AIT-301, AIT-302, and AIT-303 measure and transmit (to the PLC) various chemical parameters of the water entering the UF feed water tank T-301.

Stage Four. De-chlorination is performed in this stage: any free chlorine in the water coming out of the UF unit is removed using a combination of an ultraviolet de-chlorinator and sodium bisulphate. P-401 is started when T-401 reaches the high marker, moving water through the de-chlorinator unit. The hardness analyser (AIT-401) monitors and indicates the level of hardness to avoid scaling within the RO system.

Stage Five. Reverse osmosis (RO) is applied in stage five. The RO system is designed to provide bulk reduction of inorganic impurities. The RO permeate stream is channeled to the RO permeate tank (T-601) when MV-501 is opened. Before reaching the tank, the RO permeate conductivity analyser (AIT-504) analyses water conductivity, and if above the threshold, water is diverted to a reject tank T-602 by opening valve MV-503. The rejected water is used to clean the UF membranes in the backwash process. RO permeate pump P-601 recycles water from T-601 back to T-101.

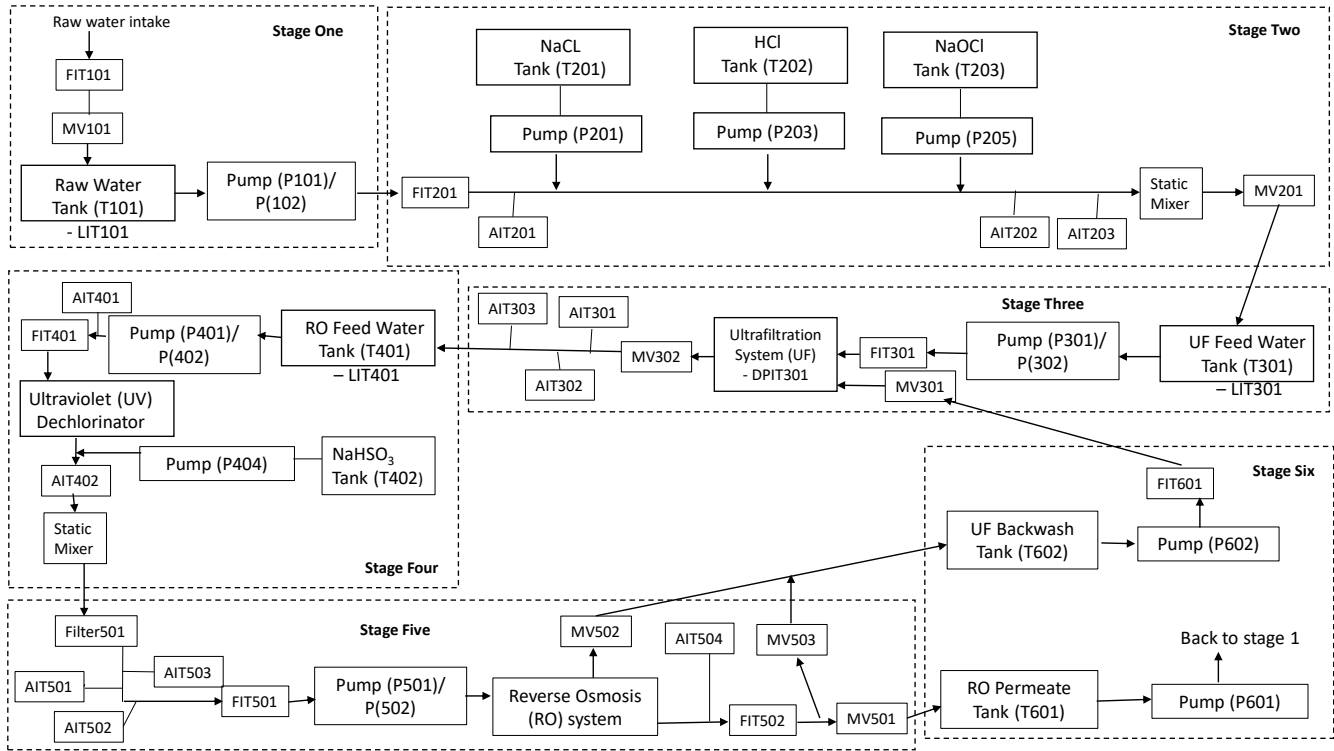


Figure 1: The sub-processes of SWaT

Stage Six. Finally, stage six consists of a backwash process. UF membranes need cleaning to remove solid particles. This cleaning is achieved through the backwash process, which is programmed to start every 30 minutes. It is also started when the pressure drop across the membrane goes above a pre-set threshold. The rejected RO water from tank T-602 is moved through the UF unit by starting pump P-602.

2.2 Axiomatic Design Theory

Axiomatic design is a systems design methodology, developed by Nam Pyo Suh [47], that uses matrix methods to systematically analyse the transformation of customer needs into functional requirements, design parameters, and process variables. The objective of the theory is to create a scientific base for the design process by building upon a suite of fundamental theories from logic and rationale thinking. Researchers have applied this theory in areas such as manufacturing [41, 50] and software development [33, 42].

In axiomatic design, functional requirements (FRs) express *what* we want to achieve, i.e. the specific behaviours we want from the design. Design parameters (DPs) are elements of the physical design that are chosen to *realise* the FRs. Finally, process variables (PVs) are elements of the process design controlling the DPs (e.g. continuous or discrete values characterising the process). Matrix methods are used by the designer to map FRs to DPs in the physical domain. For example, suppose that the top-level of a design involved two FRs

and two DPs. These can then be related using the following matrix:

$$\begin{bmatrix} FR_1 \\ FR_2 \end{bmatrix} = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} \begin{bmatrix} DP_1 \\ DP_2 \end{bmatrix}$$

The square matrix is a binary (or Boolean) matrix, indicating the coupling between FRs and DPs. After identifying the couplings at a high level (e.g. where one DP might represent *all* pumps), the designer would decompose the FRs and DPs further (e.g. with one DP representing exactly *one* of the pumps) until achieving a fine-grained set of dependencies in the design. The decomposed matrices can then be subjected to analyses to assess and mitigate the effects of coupling.

In our work (Section 3), axiomatic design is *not* used to design a CPS from the ground-up, but rather, its principles are applied to an existing design to support the derivation of invariants based on the dependencies it implies, and to help assess where weak points might exist (e.g. due to certain couplings). In SWaT, DPs will correspond to components such as tank level sensors and motorised valves, each of which can function within specific values of PVs. This paves the way for a simple and high-level of analysis to establish the relations between DPs that represent normal CPS behaviour. These relations are then taken as our invariants.

3 DESIGN FRAMEWORK

Our proposed systematic design approach consists of three parts: an axiomatic design analysis, the construction of mathematical equations over DPs, and the construction of process graphs, i.e. directed

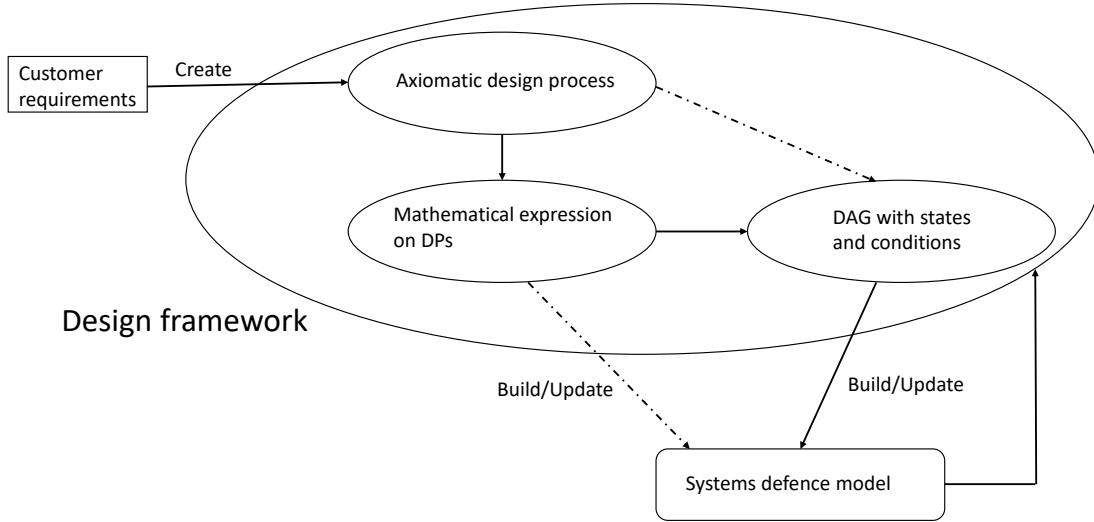


Figure 2: Overview of our proposed method

acyclic graphs (DAGs) over physical states and conditions. These equations and DAGs characterise invariant relationships between the DPs, and their input/output relations are fed into supervised ML algorithms to learn classifiers that can be used to detect attacks. Figure 2 summarises the relationship between these steps.

The workflow begins by transforming the customer’s needs (e.g. build a six-stage water treatment plant) into a list of high-level FRs (e.g. track water level of tanks) with some associated high-level DPs (e.g. sensing mechanisms) and PVs (e.g. value ranges). These are systematically and iteratively decomposed into fine-grained FRs, with particular sensors/actuators as DPs, as guided by the axiomatic design theory. At this stage, the dependencies between particular DPs are transformed into *invariants*, i.e. mathematical equations over the DP states (e.g. “if DP₁ is on and DP₂ is low then the system is anomalous”). The design engineers determine which combination of DP states are normal/anomalous, optionally using DAGs with states and conditions to guide their reasoning about paths through the system. Supervised ML algorithms are then trained on the input/output relations of these equations or paths, resulting in classifiers that detect when sensor and actuator data is violating the underlying invariants.

The classifiers, and the invariants underlying them, embody key characteristics of the design as identified by the engineer through a systematic method. We envisage that this has the potential to complement defence mechanisms based on black-box approaches (e.g. [15]), where invariant relationships are based only on observable data after the system has been implemented, and which might not reflect all invariants implied by the design. Furthermore, as our invariants are constructed at the design stage, it may be possible to involve them in early simulations of the processes, and to iteratively modify the system design before it is implemented (Figure 2) if any weak points are identified.

$$\begin{pmatrix} FR1 \\ FR2 \\ FR3 \\ FR4 \\ FR5 \\ FR6 \\ FR7 \\ FR8 \end{pmatrix} = \begin{pmatrix} X & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & X & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & X & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & X & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & X & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & X & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & X & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & X \end{pmatrix} \begin{pmatrix} DP1 \\ DP2 \\ DP3 \\ DP4 \\ DP5 \\ DP6 \\ DP7 \\ DP8 \end{pmatrix} \quad (1)$$

$$\begin{pmatrix} FR1 \\ FR2 \\ FR3 \\ FR4 \\ FR5 \\ FR6 \\ FR7 \\ FR8 \end{pmatrix} = \begin{pmatrix} X & y & y & y & 0 & y & y & 0 \\ y & X & y & 0 & 0 & 0 & y & 0 \\ y & y & X & 0 & 0 & 0 & y & 0 \\ y & 0 & 0 & X & y & 0 & 0 & 0 \\ 0 & 0 & 0 & y & X & 0 & 0 & y \\ y & 0 & 0 & 0 & 0 & X & y & 0 \\ y & y & y & 0 & 0 & y & X & 0 \\ 0 & 0 & 0 & 0 & y & 0 & 0 & X \end{pmatrix} \begin{pmatrix} DP1 \\ DP2 \\ DP3 \\ DP4 \\ DP5 \\ DP6 \\ DP7 \\ DP8 \end{pmatrix} \quad (2)$$

For the rest of this paper, we use the SWaT water purification testbed as a worked example to show how the steps of our approach are applied, and how invariant-based classifiers can be derived.

3.1 Axiomatic Design Process

Based on the requirements of SWaT, a top-level decomposition and design are given in Table 1. By the axiomatic design principles, this first level should be a functionally *uncoupled* design guaranteeing that each DP satisfies exactly one FR. This is reflected by the matrix of Equation (1), a diagonal matrix in which each FR is related only to its given DP from Table 1.

Next, the engineer analyses the DPs against the FRs and updates the corresponding Boolean value of the matrix if there is an *information state coupling* between them. This type of coupling differs

Table 1: Top-level decomposition of SWaT

No	Functional Requirements (FRs)	Design Parameters (DPs)	Process Variables (PVs)
1	FR1: Feed water to water tanks/systems	DP1: DOL/VSD Pumps	Features - Switch (On/Off) and Speed
2	FR2: Track level of water in tanks	DP2: Sensing mechanisms	Value range
3	FR3: Track flow rate of water	DP3: EMF sensors	Value range
4	FR4: Monitor chemical properties of water	DP4: Chemical properties sensors	Value range
5	FR5: Feed chemicals to water	DP5: Dosing Pumps	Switch (On/Off)
6	FR6: Track water pressure	DP6: Pressure sensors	Value range
7	FR7: Direct flow of water	DP7: Motorised valves	Switch (On/Off)
8	FR8: Track level of chemicals in tanks	DP8: Level switch	Value range

Table 2: Second-level decomposition of FRs and DPs

No	Functional Requirements (FRs)	Design Parameters (DPs)	Process Variables (PVs)
1	FR1.1: Pump raw water from stage one to UF feed tank in stage three	DP1.1: P-101,P-102	On/Off
2	FR1.2: Pump water from stage three to RO feed tank in stage four	DP1.2: P-301,P-302	On/Off
3	FR1.3: Pump water from stage four through de-chlorination system	DP1.3: P-401,P-402	On/Off
4	FR1.4: Pump (VSD) water from stage five to tanks in stage six	DP1.4: P-501,P-502	On/Off
5	FR1.5: Pump water from RO permeate tank to raw water tank in stage one	DP1.5: P-601	On/Off
6	FR1.6: Pump water for UF backwash system	DP1.6: P-602	On/Off
7	FR1.7: Pump water for RO/UF cleaning	DP1.7: P-603	On/Off
8	FR2.1: Determine water level in raw water tank of stage one	DP2.1: LIT-101	$0 < \alpha < \max_a$
9	FR2.2: Determine water level in UF feed tank of stage three	DP2.2: LIT-301	$0 < \alpha < \max_b$
10	FR2.3: Determine water level in RO feed tank of stage four	DP2.3: LIT-401	$0 < \alpha < \max_c$
11	FR2.4: Determine water level in RO permeate tank of stage six	DP2.4: LS-601	$Low_d < \alpha < High_d$
12	FR2.5: Determine water level in UF backwash tank of stage six	DP2.5: LS-602	$Low_e < \alpha < High_e$
13	FR2.6: Determine water level in CIP tank of stage six	DP2.6: LS-603	$Low_f < \alpha < High_f$
14	FR3.1: Measure raw water flow rate in stage one	DP3.1: FIT-101	$Low_g < \alpha < High_g$
15	FR3.2: Measure water flow rate in stage two	DP3.2: FIT-201	$Low_h < \alpha < High_h$
16	FR3.3: Measure water flow rate in stage three	DP3.3: FIT-301	$Low_i < \alpha < High_i$
17	FR3.4: Measure water flow rate in stage four	DP3.4: FIT-401	$Low_j < \alpha < High_j$
18	FR3.5: Measure water flow rate in stage five	DP3.5: FIT-501,FIT-502,FIT-503,FIT-504	$Low_k < \alpha < High_k$
19	FR3.6: Measure water flow rate in stage six	DP3.6: FIT-601	$Low_l < \alpha < High_l$
20	FR4.1: Calculate chemical properties of water	DP4.1: AIT-201,AIT-202,AIT-203,AIT-301,AIT-302,AIT-303 AIT-401,AIT-402,AIT-501,AIT-502,AIT-503,AIT-504	$Low_m < \alpha < High_m$
21	FR5.1: Pump chemicals to water	DP5.1: P-201,P-202,P-203,P-204,P-205,P-206,P-207,P-208, P-403,P-404	On/Off
22	FR6.1: Measure UF filter differential pressure	DP6.1: DPIT-301	$0 < \alpha < \max_n$
23	FR6.2: Measure RO membrane inlet pressure	DP6.2: PIT-501	$0 < \alpha < \max_o$
24	FR6.3: Measure RO membrane pressure	DP6.3: PIT-502	$0 < \alpha < \max_p$
25	FR6.4: Measure RO reject pressure	DP6.4: PIT-503	$0 < \alpha < \max_q$
26	FR7.1: Control water flow direction	DP7.1: MV-101,MV-201,MV-301,MV-302,MV-303,MV-304, MV-501,MV-502,MV-503,MV-504	On/Off
27	FR8.1: Determine NaCl level in NaCl tank of stage two	DP8.1: LS-201	$Low_r < \alpha < \max_r$
28	FR8.2: Determine HCl level in HCl tank of stage two	DP8.2: LS-202	$Low_s < \alpha < \max_s$
29	FR8.3: Determine NaOCl level in NaOCl tank of stage two	DP8.3: LS-203	$Low_t < \alpha < \max_t$
30	FR8.4: Determine NaHSO3 level in NaHSO3 tank of stage four	DP8.4: LS-401	$Low_u < \alpha < \max_u$

from the physical coupling used in the conventional axiomatic design theory because it considers state information. Inserting this information state coupling into Equation (1) results in Equation (2), where y (or X on the diagonal) indicates some dependencies, and a zero (0) denotes the absence of them. Note that these dependencies are represented symmetrically: for example, if DP7 is (information state) coupled with FR2, then FR7 is coupled with DP2.

Equation (2) shows that DP7 is depended on by FR1, FR2, and FR7: for example, a motorised valve (DP7) is opened to feed water into a tank when the level is low (FR2) and the pump is on (FR1), i.e. the state of some valve depends on the state of some tank and pump. Note however that Equation (2) presents design information that is very high-level and broadly defined. For instance, FR3—“track

flow rate of water”—relates to *multiple* different locations and flow sensors in SWaT. Another example is FR1—“feed water to water tanks/systems”—when in reality there are multiple water pumps in six different stages of SWaT. In order to derive meaningful invariants that relate concrete components of the CPS, our method requires that the top-level design of Equation (2) is iteratively decomposed until there is only a *point-to-point mapping* between each FR and DP. For illustration purposes, such a mapping is shown in the third-level decomposition of Table 6 at the end of the paper.

For simplicity, rather than use a point-to-point mapping, we decompose the eight FRs of Equation (2) into the 30 FRs of the second-level decomposition in Table 2. This is much more concrete than the top-level decomposition as it factors in particular sensors

Table 3: Linking second-level decomposition of FRs to dependent DPs

No	Functional Requirements (FRs)	Design Parameters (DPs)
1	FR1.1: Pump raw water from stage one to UF feed tank in stage three	DP1.1: P-101, P-102 DP1.1.1: P-101 Other DPs: DP2.1(LIT-101), DP2.2(LIT-301), DP7.1(MV-201) DP1.1.2: P-102 Other DPs: DP2.1(LIT-101), DP2.2(LIT-301), DP7.1(MV-201)
2	FR1.2: Pump water from stage three to RO feed tank in stage four	DP1.2: P-301, P-302 DP1.2.1: P-301 Other DPs: DP2.2(LIT-301), DP2.3(LIT-401), DP7.1(MV-302) DP1.2.2: P-302 Other DPs: DP2.2(LIT-301), DP2.3(LIT-401), DP7.1(MV-302)
3	FR1.3: Pump water from stage four through de-chlorination system	DP1.3: P-401, P-402 DP1.3.1: P-401 Other DPs: DP1.4(P-501,P-502), DP2.3(LIT-401) DP1.3.2: P-402 Other DPs: DP1.4(P-501,P-502), DP2.3(LIT-401)
4	FR1.4: Pump (VSD) water from stage five to tanks in stage six	DP1.4: P-501, P-502 DP1.4.1: P-501 Other DPs: DP1.3(P-401,P-402), DP7.1(MV-501) DP1.4.2: P-502 Other DPs: DP1.3(P-401,P-402), DP7.1(MV-501)
5	FR1.5: Pump water from RO permeate tank to raw water tank in stage one	DP1.5: P-601 Other DPs: DP2.1(LIT-101), DP2.4(LS-601)
6	FR1.6: Pump water for UF backwash system	DP1.6: P-602 Other DPs: DP2.5(LS-602), DP7.1(MV-301)
7	FR1.7: Pump water for RO/UF cleaning	DP1.7: P-603 Other DPs: DP2.6(LS-603)
8	FR2.1: Determine water level in raw water tank of stage one	DP2.1: LIT-101 Other DPs: DP1.1(P-101,P-102), DP1.5(P-601), DP2.4(LS-601), DP7.1(MV-101)
9	FR2.2: Determine water level in UF feed tank of stage three	DP2.2: LIT-301 Other DPs: DP1.1(P-101,P-102), DP1.2(P-301,P-302), DP7.1(MV-201)
10	FR2.3: Determine water level in RO feed tank of stage four	DP2.3: LIT-401 Other DPs: DP1.2(P-301,P-302), DP1.3(P-401,P-402), DP7.1(MV-302)
11	FR2.4: Determine water level in RO permeate tank of stage six	DP2.4: LS-601 Other DPs: DP1.5(P-601), DP2.1(LIT-101)
12	FR2.5: Determine water level in UF backwash tank of stage six	DP2.5: LS-602 Other DPs: DP1.6(P-602), DP7.1(MV-301)
13	FR2.6: Determine water level in CIP tank of stage six	DP2.6: LS-603 Other DPs: DP1.7(P-603), DP7.1(MV-301)
14	FR3.1: Measure raw water flow rate in stage one	DP3.1: FIT-101 Other DPs: DP2.1(LIT-101), DP7.1(MV-101)
15	FR3.2: Measure water flow rate in stage two	DP3.2: FIT-201 Other DPs: DP1.1(P-101,P-102), DP2.2(LIT-301), DP7.1(MV-201)
16	FR3.3: Measure water flow rate in stage three	DP3.3: FIT-301 Other DPs: DP1.2(P-301,P-302), DP2.3(LIT-401), DP7.1(MV-302)
17	FR3.4: Measure water flow rate in stage four	DP3.4: FIT-401 Other DPs: DP1.3(P-401,P-402), DP2.3(LIT-401)
18	FR3.5: Measure water flow rate in stage five	DP3.5: FIT-501,FIT-502,FIT-503,FIT-504 DP3.5.1: FIT-501 Other DPs: DP1.3(P-401,P-402) DP3.5.2: FIT-502 Other DPs: DP1.4(P-501,P-502) DP3.5.3: FIT-503 Other DPs: DP1.4(P-501,P-502) DP3.5.4: FIT-504 Other DPs: DP1.3(P-401,P-402)
19	FR3.6: Measure water flow rate in stage six	DP3.6: FIT-601 Other DPs: DP1.6(P-602), DP2.5(LS-602), DP7.1(MV-301)
20	FR4.1: Calculate chemical properties of water	DP4.1: AIT-201,AIT-202,AIT-203,AIT-301,AIT-302,AIT-303, AIT-401,AIT-402,AIT-501,AIT-502,AIT-503,AIT-504 DP4.1.1: AIT-201 Other DPs: DP1.1.1(P-101), DP1.1.2(P-102) DP4.1.2: AIT-202 Other DPs: DP1.1.1(P-101), DP1.1.2(P-102) DP4.1.3: AIT-203 Other DPs: DP1.1.1(P-101), DP1.1.2(P-102) DP4.1.4: AIT-301 Other DPs: DP1.2.1(P-301), DP1.2.2(P-302) DP4.1.5: AIT-302 Other DPs: DP1.2.1(P-301), DP1.2.2(P-302) DP4.1.6: AIT-303 Other DPs: DP1.2.1(P-301), DP1.2.2(P-302) DP4.1.7: AIT-401 Other DPs: DP1.3.1(P-401), DP1.3.2(P-402) DP4.1.8: AIT-402 Other DPs: DP1.3.1(P-401), DP1.3.2(P-402) DP4.1.9: AIT-501 Other DPs: DP1.3.1(P-401), DP1.3.2(P-402) DP4.1.10: AIT-502 Other DPs: DP1.3.1(P-401), DP1.3.2(P-402) DP4.1.11: AIT-503 Other DPs: DP1.3.1(P-401), DP1.3.2(P-402) DP4.1.11: AIT-504 Other DPs: DP1.4.1(P-501), DP1.4.2(P-502)
21	FR5.1: Pump chemicals to water	DP5.1: P-201,P-202,P-203,P-204,P-205,P-206,P-207,P-208,P-403,P-404 DP5.1.1: P-201 Other DPs: DP4.1.1(AIT-201), DP7.1.2(MV-201) DP5.1.2: P-202 Other DPs: DP4.1.1(AIT-201), DP7.1.2(MV-201) DP5.1.3: P-203 Other DPs: DP4.1.2(AIT-202), DP7.1.2(MV-201) DP5.1.4: P-204 Other DPs: DP4.1.2(AIT-202), DP7.1.2(MV-201) DP5.1.5: P-205 Other DPs: DP4.1.3(AIT-203), DP7.1.2(MV-201) DP5.1.6: P-206 Other DPs: DP4.1.3(AIT-203), DP7.1.2(MV-201) DP5.1.7: P-207 Other DPs: DP4.1.5(AIT-302) DP5.1.8: P-208 Other DPs: DP4.1.5(AIT-302) DP5.1.9: P-403 Other DPs: DP4.1.8(AIT-402) DP5.1.10: P-404 Other DPs: DP4.1.8(AIT-402)
22	FR6.1: Measure UF filter differential pressure	DP6.1: DPIT-301 Other DPs: DP1.2.1(P-301), DP1.2.2(P-302), DP7.1(MV-302)
23	FR6.2: Measure RO membrane inlet pressure	DP6.2: PIT-501 Other DPs: DP1.4.1(P-501), DP1.4.2(P-502)
24	FR6.3: Measure RO membrane pressure	DP6.3: PIT-502 Other DPs: DP1.4.1(P-501), DP1.4.2(P-502), DP7.1.7(MV-501), DP7.1.9(MV-503)
25	FR6.4: Measure RO reject pressure	DP6.4: PIT-503 Other DPs: DP1.4.1(P-501), DP1.4.2(P-502), DP7.1.8(MV-502), DP7.1.10(MV-504)

Figure 3(a) shows a subsystem in stage one of SWaT and the interconnection of some dependent devices identified from the axiomatic design analysis (row 26 of Table 4), along with the physical tank (T-101) and PLC that controls the components. Figures 3(b) and

4 then visualise how the state of one DP (MV-101) changes according to the other (LIT-101), for both the normal and the (inverted) anomalous cases. In both graphs, we consider the cases when the tank level is below one of its low thresholds (Low or LowLow), or

Table 4: Linking second-level decomposition of FRs to dependent DPs (continued)

No	Functional Requirements (FRs)	Design Parameters (DPs)
26	FR7.1: Control water flow direction	DP7.1: MV-101, MV-201, MV-301, MV-302, MV-303, MV-304, MV-501, MV-502, MV-503, MV-504 DP7.1.1: MV-101 Other DPs: DP2.1(LIT-101) DP7.1.2: MV-201 Other DPs: DP1.1.1(P-101), DP1.1.2(P-102), DP2.2(LIT-301) DP7.1.3: MV-301 Other DPs: DP1.6(P-602), DP2.5(LS-602), DP2.6(LS-603) DP7.1.4: MV-302 Other DPs: DP1.2.1(P-301), DP1.2.2(P-302), DP2.3(LIT-401) DP7.1.5: MV-303 Other DPs: DP1.2.1(P-301), DP1.2.2(P-302) DP7.1.6: MV-304 Other DPs: DP1.2.1(P-301), DP1.2.2(P-302) DP7.1.7: MV-501 Other DPs: DP1.4.1(P-501), DP1.4.2(P-502) DP7.1.8: MV-502 Other DPs: DP1.4.1(P-501), DP1.4.2(P-502) DP7.1.9: MV-503 Other DPs: DP1.4.1(P-501), DP1.4.2(P-502) DP7.1.10: MV-504 Other DPs: DP1.4.1(P-501), DP1.4.2(P-502)
27	FR8.1: Determine NaCl level in NaCl tank of stage two	DP8.1: LS-201 Other DPs: DP5.1.1(P-201), DP5.1.2(P-202)
28	FR8.2: Determine HCl level in HCl tank of stage two	DP8.2: LS-202 Other DPs: DP5.1.3(P-203), DP5.1.4(P-204)
29	FR8.3: Determine NaOCl level in NaOCl tank of stage two	DP8.3: LS-203 Other DPs: DP5.1.5(P-205), DP5.1.6(P-206), DP5.1.7(P-207), DP5.1.8(P-208)
30	FR8.4: Determine NaHSO3 level in NaHSO3 tank of stage four	DP8.4: LS-401 Other DPs: DP5.1.9(P-403), DP5.1.10(P-404)

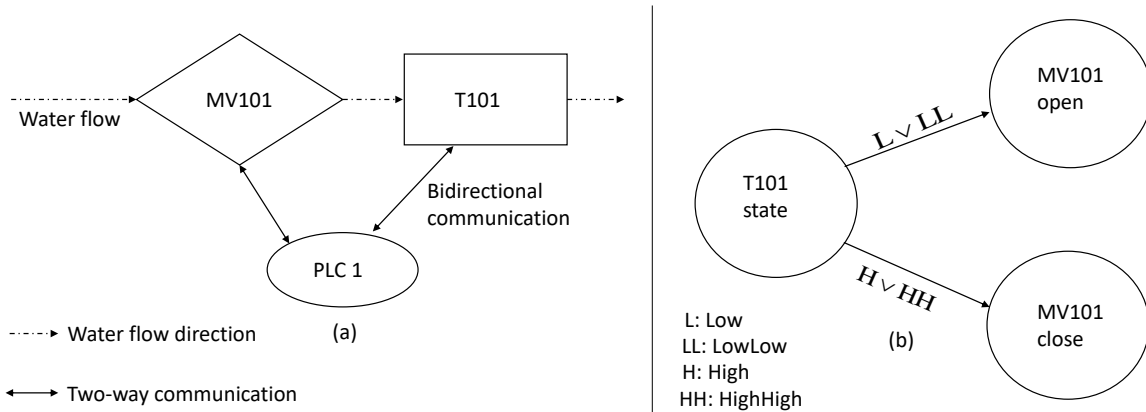


Figure 3: (a) Subsystem in stage one of SWaT; (b) A process graph in stage one of SWaT for normal cases

Table 5: Mathematical state expressions and assessments

State Expression (Input)	Assessment (Output)
!MV-101 and !LIT-101	Anomaly
!MV-101 and LIT-101	No anomaly
MV-101 and !LIT-101	No anomaly
MV-101 and LIT-101	Anomaly

above one of its high thresholds (High or HighHigh). MV-101 can be either open or closed, and the graphs reflect the states it should switch to according to different level thresholds of the tank. The idea is that the designer traverses through the different paths in the normal case of Figures 3(b), and then concludes that all other possible paths are abnormal cases, thus deriving Figure 4. For example, if the tank level is low (L or LL), then the correct behaviour is for the valve to open and allow water to flow in; remaining closed (risking an underflow scenario) is thus anomalous.

These paths in Figures 3(b) and 4 provide direct and indirect information for deciding the outcome of an attack, and the identified anomaly cases should be investigated further to prevent successful attacks. This information is useful because it gives the designer the possibility to employ different types of defence mechanisms at certain locations based on cost and impact analysis. The graphs provide visual representations of paths which may be easier to communicate and analyse in comparison to mathematical expressions. A deeper analysis of Figures 3(b) and 4 by the designer may lead to the discovery of a successful concrete attack such as spoofing of data. For example: if LIT-101 for T-101 is spoofed to be at H instead of L, then P-101 starts pumping water out of T-101. In a short time, T-101 is going to be emptied. A prolonged period of pumping water from an empty tank can damage the pumps. A solution to prevent such an attack is to use data encryption for network communication between devices. As this weakness is determined at the design phase of the system, the cost of protecting against such an attack is likely to be less than if the attack had been discovered after the implementation of hardware and software.

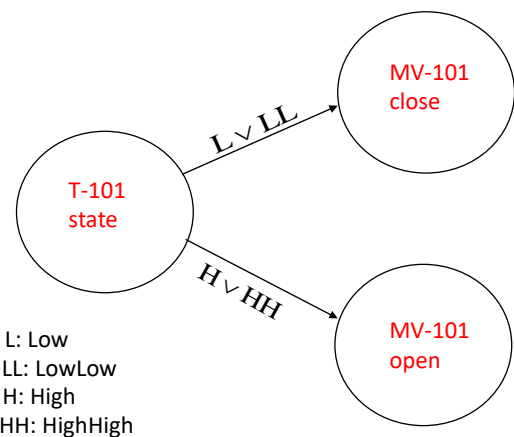


Figure 4: A process graph depicting anomalous cases

4 PRELIMINARY EVALUATION

In this section, we present a preliminary study in which we assess how effective our invariants are for implementing *attack detection mechanisms* in SWaT. First, we derive two invariants from our design framework: one concerning sensors and actuators in stage one only, and another concerning sensors and actuators across three stages (1–3). Next, we train supervised machine learning algorithms (e.g. decision trees, naïve Bayes) on the inputs/outputs of the equations and process graphs associated with the invariants. The training results in *classifiers* that can judge actual sensor/actuator data as ‘normal’ or ‘anomalous’ with respect to the invariant relationships they were trained on. Finally, we deploy these classifiers on both the SWaT dataset [1] as well as the actual testbed to assess how effective they are at detecting some relevant attacks.

Experiment and Results. The first invariant (#1) we derived concerns the relationship between MV-101 and LIT-101. This dependency was identified from our design analysis, in particular, from DP7.1.1, row 26 of Table 4. The completed mathematical equations and their corresponding process graphs are given in Table 5, Figure 3(b), and Figure 4. As this dependency involved only two components, it was feasible to completely classify all Boolean combinations of their discretised values as normal or anomalous. This might not be the case for larger sets of dependencies, which is why supervised learning algorithms may be required in general.

The second invariant (#2) concerns the relationship between LIT-301, MV-201, P-101, and P-102. These dependencies were also identified from our design analysis, in particular, from DP7.1.2, row 26 of Table 4. Mathematical equations and process graphs were constructed for these components in an analogous way to the first invariant.

We trained both supervised decision tree and naïve Bayes learning algorithms on the inputs/outputs of the mathematical equations and process graphs of these invariants. We applied the classifiers

to the SWaT dataset [1] and found that *no false positives* were reported, i.e. at no point did ‘normal’ data in the labelled dataset get misclassified as ‘anomalous’. Likewise, when implemented for the actual testbed, we found that the classifiers did not report any false positives throughout our experiments. We investigated the effectiveness of the classifiers against relevant attacks in both the SWaT dataset as well as on the testbed itself. We found that our decision tree classifiers achieved 100% accuracy in the prediction of normal/anomalous labels throughout these attacks, and that our naïve Bayes classifiers achieved 100% and 93.75% accuracy for the two invariants respectively. The two attack tests we considered for the SWaT testbed (of potentially many more) are discussed below.

While we are motivated by the results, we are actively working on building a larger set of invariants/classifiers to be sure that the results do generalise, and are keen to compare the effectiveness of our invariants against those derived using other approaches, e.g. those that used only data and not the system design at all.

Attack Test #1. The following attack scenario was successfully detected using the SWaT testbed.

Components to attack: Motorised valve MV-101, and level indicator transmitter LIT-101 (both in stage one).

Objective: Damage or reduce the reliability of MV-101.

Launch state: At time t , the water level of LIT-101 is above 800mm.

Attack: At time $t++$, an attacker begins *manually* turning MV-101 on and off several times.

Results: Successfully detected. The attack violated the classifier of invariant #1 for MV-101, LIT-101.

SWaT’s defences could be strengthened against this attack by overriding attempts to manually turn on MV-101 if the water level reported by LIT-101 is above its high (H) or critically high (HH) thresholds. This would block the attack, although would rely on the assumption that the value of LIT-101 is correct can be trusted (additional invariants and classifiers concerning LIT-101 could help to mitigate this threat).

Attack Test #2. This second attack test case was also successfully executed and detected using the SWaT testbed.

Components to attack: Pumps P-101, P-102, and motorised valve MV-201.

Objective: Damage or reduce the reliability of P-101, P-102, and MV-201.

Launch state: At time t , the water level reported by LIT-301 is above 1000mm.

Attack: At time $t++$, an attacker manually turns on MV-201. Next, the attacker manually starts pump P-102. Finally, the attacker manually starts pump P-101.

Results: Successfully detected. The attack violated the classifier of invariant #2 for LIT-301, MV-201, P-101, P-102.

SWaT’s defences could be strengthened by overriding attempts to turn on MV-201 if the water level reported by LIT-301 is above its high (H) or critically high (HH) thresholds. This would prevent the attack from happening, but again, would require additional mechanisms or improvements to the design to ensure that the value of LIT-301 can be trusted.

5 CONCLUSION

In this position paper, we proposed a method for systematically deriving invariants from the functional requirements of a CPS, in order to: (1) integrate security concerns at the design stage; (2) ensure that invariants can be traced from requirements through to implemented defence mechanisms; (3) identify all invariants implicit in the design, not just those represented in datasets; and (4) potentially save costs by identifying weak points before the CPS is built. Inspired by the axiomatic design methodology for systems, our method iteratively analyses dependencies in a given CPS to construct equations and process graphs that represent invariant relations between sensor readings and actuator states. We demonstrated the potential use of this approach in a preliminary study on the SWaT water treatment testbed, implementing checkers for two invariants using decision trees, and finding that they detected relevant attacks without false positives.

Our method provides a step-by-step approach from requirements to the implementation of invariant checkers, and does not require any complex mathematical modelling or dataset-based training. This may help to ensure that detected attacks or system malfunctions can be *explained*, not just in terms of the equations or process graph that they violated, but also in terms of the functional requirements that they were derived from, providing systems engineers with a rich amount of context.

In ongoing work, we plan to extend our preliminary study for SWaT by implementing more invariant-based checkers from our requirements analysis, and evaluating them against a wider array of attacks. We also plan to compare the effectiveness of our invariants against those derived by other approaches (both automated and manual ones) in order to better understand the added security benefits of analysing the CPS design directly. Finally, we plan to assess the generalisability of our approach by applying it to other industrial control systems (e.g. the WADI water distribution plant), and potentially to CPSs from other domains, such as building management or healthcare systems.

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Table 6: Third-level decomposition of FRs and DPs

No	Functional Requirements (FRs)	Design Parameters (DPs)	Process Variables (PVs)
1	FR1.1.1: Feed raw water from stage one to UF feed tank in stage three using pump P-101	DP1.1.1: P-101	On/Off
2	FR1.1.2: Feed raw water from stage one to UF feed tank in stage three using pump P-102	DP1.1.2: P-102	On/Off
3	FR1.2.1: Feed water from stage three to RO feed tank in stage four using pump P-301	DP1.2.1: P-301	On/Off
4	FR1.2.2: Feed water from stage three to RO feed tank in stage four using pump P-302	DP1.2.2: P-302	On/Off
5	FR1.3.1: Pump water from stage four through de-chlorination system using pump P-401	DP1.3.1: P-401	On/Off
6	FR1.3.2: Pump water from stage four through de-chlorination system using pump P-402	DP1.3.2: P-402	On/Off
7	FR1.4.1: Pump (VSD) water from stage five to tanks in stage six using pump P-501	DP1.4.1: P-501	On/Off
8	FR1.4.2: Pump (VSD) water from stage five to tanks in stage six using pump P-502	DP1.4.2: P-502	On/Off
9	FR3.5.1: Compute RO membrane inlet flow meter in stage five	DP3.5.1: FIT-501	$0 \leq \alpha \leq \max_{k1}$
10	FR3.5.2: Compute RO permeate flow meter in stage five	DP3.5.2: FIT-502	$0 \leq \alpha \leq \max_{k2}$
11	FR3.5.3: Compute RO reject flow meter in stage five	DP3.5.3: FIT-503	$0 \leq \alpha \leq \max_{k3}$
12	FR3.5.4: Compute RO re-circulation flow meter in stage five	DP3.5.4: FIT-504	$0 \leq \alpha \leq \max_{k4}$
13	FR4.1.1: Calculate chemical dosing conductivity of water in stage two	DP4.1.1: AIT-201	$0 \leq \alpha \leq \max_{m1}$
14	FR4.1.2: Calculate chemical dosing pH of water in stage two	DP4.1.2: AIT-202	$0 \leq \alpha \leq \max_{m2}$
15	FR4.1.3: Calculate chemical dosing ORP of water in stage two	DP4.1.3: AIT-203	$0 \leq \alpha \leq \max_{m3}$
16	FR4.1.4: Calculate UF permeate pH of water in stage three	DP4.1.4: AIT-301	$0 \leq \alpha \leq \max_{m4}$
17	FR4.1.5: Calculate UF permeate ORP of water in stage three	DP4.1.5: AIT-302	$0 \leq \alpha \leq \max_{m5}$
18	FR4.1.6: Calculate UF permeate conductivity of water in stage three	DP4.1.6: AIT-303	$0 \leq \alpha \leq \max_{m6}$
19	FR4.1.7: Calculate RO feed hardness of water in stage four	DP4.1.7: AIT-401	$0 \leq \alpha \leq \max_{m7}$
20	FR4.1.8: Calculate RO ORP of water in stage four	DP4.1.8: AIT-402	$0 \leq \alpha \leq \max_{m8}$
21	FR4.1.9: Calculate RO feed pH of water in stage five	DP4.1.9: AIT-501	$0 \leq \alpha \leq \max_{m9}$
22	FR4.1.10: Calculate RO feed ORP of water in stage five	DP4.1.10: AIT-502	$0 \leq \alpha \leq \max_{m10}$
23	FR4.1.11: Calculate RO feed conductivity of water in stage five	DP4.1.11: AIT-503	$0 \leq \alpha \leq \max_{m11}$
24	FR4.1.12: Calculate RO permeate conductivity of water in stage five	DP4.1.12: AIT-504	$0 \leq \alpha \leq \max_{m12}$
25	FR5.1.1: Feed NaCl dosing in stage two using pump P-201	DP5.1.1: P-201	On/Off
26	FR5.1.2: Feed NaCl dosing in stage two using pump P-202	DP5.1.2: P-202	On/Off
27	FR5.1.3: Feed HCl dosing in stage two using pump P-203	DP5.1.3: P-203	On/Off
28	FR5.1.4: Feed HCl dosing in stage two using pump P-204	DP5.1.4: P-204	On/Off
29	FR5.1.5: Feed NaOCl dosing in stage two using pump P-205 (FAC)	DP5.1.5: P-205	On/Off
30	FR5.1.6: Feed NaOCl dosing in stage two using pump P-206 (FAC)	DP5.1.6: P-206	On/Off
31	FR5.1.7: Feed NaOCl dosing to stage three UF cleaning using pump P-207 (UF)	DP5.1.7: P-207	On/Off
32	FR5.1.8: Feed NaOCl dosing to stage three UF cleaning using pump P-208 (UF)	DP5.1.8: P-208	On/Off
33	FR5.1.9: Feed NaHSO3 dosing in stage four using pump P-403	DP5.1.9: P-403	On/Off
34	FR5.1.10: Feed NaHSO3 dosing in stage four using pump P-404	DP5.1.10: P-404	On/Off
35	FR7.1.1: Direct raw water inlet in stage one	DP7.1.1: MV-101	On/Off
36	FR7.1.2: Direct water flow in stage two	DP7.1.2: MV-201	On/Off
37	FR7.1.3: Direct UF backwash in stage three	DP7.1.3: MV-301	On/Off
38	FR7.1.4: Direct UF feed water in stage three	DP7.1.4: MV-302	On/Off
39	FR7.1.5: Direct UF backwash drain in stage three	DP7.1.5: MV-303	On/Off
40	FR7.1.6: Direct UF drain in stage three	DP7.1.6: MV-304	On/Off
41	FR7.1.7: Direct RO permeate in stage five	DP7.1.7: MV-501	On/Off
42	FR7.1.8: Direct RO backwash in stage five	DP7.1.8: MV-502	On/Off
43	FR7.1.9: Direct RO permeate reject in stage five	DP7.1.9: MV-503	On/Off
44	FR7.1.10: Direct RO reject in stage five	DP7.1.10: MV-504	On/Off