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# ElChemo: A Cross-Domain Interoperability in a Chemical Plant

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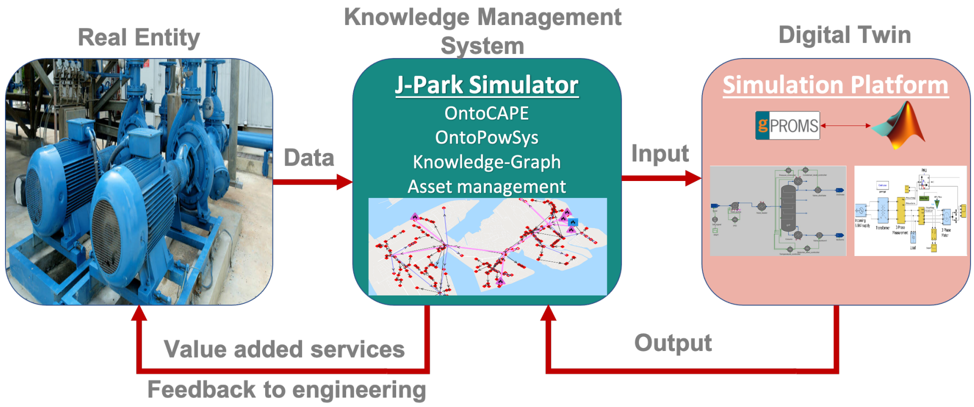
## Abstract

In this paper we propose a novel framework capable of establishing machine-to-machine (M2M) interactions between chemical and electrical systems in the industry. The semantic framework termed as ElChemo addresses the challenges in M2M interaction of entities from different silos, such as differences in the domains' behaviour, the heterogeneities arising from different vocabularies and software. The OntoTwin ontology has been developed based on OntoPowSys and OntoEIP ontologies, which are parts of an intelligent platform called the "J-Park Simulator (JPS)". The ElChemo framework uses Description Logic (DL) and SPIN reasoning techniques to establish the interaction between the chemical and electrical systems in a plant. As use-case we study a depropaniser section of a chemical plant and its corresponding electrical system as a use case scenario to demonstrate the interoperability between the two silos within the ElChemo framework. The results indicate that the proposed approach can achieve significant economic benefits.




### Highlights

- OntoTwin ontology for cross-domain coupling of chemical and electrical domains in a chemical plant.
- Implement ElChemo framework as a component of J-Park Simulator.
- Ensure product quality and power quality in ElChemo framework by using the SPARQL Inference Notation (SPIN).
- Discuss the potential of integrating ElChemo framework into agent composition framework.

# Contents

# 1 Introduction

Advanced industrial production systems, such as petrochemical, manufacturing, and many other industries, consist of complex interconnected processes. The breakdown of critical equipment such as pumps, motors, compressors, and generators can, therefore lead to the loss of equipment and result in the shut down of the whole production process [41]. Thus, improving equipment and production systems safety, reliability, availability, and reducing maintenance and production costs have become a major focus for an industrial plant [20, 34]. A better understanding of machine-to-machine (M2M) interactions is an important step towards achieving these goals [21, 23]. Industry 4.0 [24, 40], also known as the Fourth Industrial Revolution, has led to several advancements in M2M interaction that allows for increased automation and seamless exchange of information between heterogeneous silos in industrial manufacturing processes [42]. To ultimately realise the potential of Industry 4.0, the manufacturers need to provide end-to-end integration of various assets in a factory, such as vertical integration through connected and smart manufacturing and horizontal integration through connected discrete operational systems [9, 33].

Semantic Web [4] technologies have been used to improve the collaboration between tools in different domains [35]. We propose the Semantic Web technologies as a good candidate to be used in building frameworks that helps tools to collaborate and share information seamlessly across multiple domains. One such example is the J-Park Simulator (JPS) project where tools from various domains interact in an Eco-Industrial Park (EIP) to make informed decisions for solving cross-domain problems [14]. To reduce the semantic interoperability gap between tools and to make data more reliable and available, several solutions have been proposed. One such effort to detect fault diagnoses was established by linking process, electrical and logical connectivity derived from smart P&IDs [15] which are stored in the eXtensible Markup Language (XML) format [38]. Graph databases [5] are used to store data generated by computer-aided engineering tools. A set of rules is used for querying connections between process, electrical and logical connectives [38]. However, this platform does not utilise any ontology [25] approach to establish semantic interoperability between these entities. An effort similar to the work presented in this paper is the decision support platform for a process plant floor [47]. It uses the SatisFactory ontology. This ontology defines a model for pilot plants for chemical processes. Furthermore, the platform allows users to observe the plant's status and the plant's downtime estimation. Tools such as SCADA [7] access the knowledge-based platform through middleware to visualise the plant [47]. Although the platform is a significant step forward in using the ontology approach to monitor a pilot plant, there are some areas that can be improved. For example, the platform does not guarantee the consistency of data stored in the knowledge base. In addition, the SatisFactory ontology does not support features in a model's main component, such as bottoms, distillate, and mole fraction that are important for chemical plants.

The closest effort to the work presented in this paper is the ontology-based framework [31] that aims to present process supervision in a chemical plant. The chemical data used in this project are stored in a heavyweight ontology. The ontology is implemented by using OWL2 language [17] and it is expressed by using *SROIQ* [19] Description Logics (DLs) syntax [31]. The ontology has only implemented terms from the chemical domain, grouped into three modules: equipment, control, and supervision. The forward-chaining reasoning algorithm is employed to support process supervision and the characterisation of hazards in chemical plants. While the project uses semantic web standards for querying and reasoning, it does not support semantic interoperability between tools in various domains such as chemical and electrical domains. Although the Semantic Web Rule Language (SWRL) [18] is used to implement rules in this knowledge base, it is not expressive enough to implement very intricate rules for plant supervision as listed in Section 5.2. The OntoSafe ontology [32] introduces knowledge that represents the state and condition of a plant. It extends OntoCAPE [28] with new aspects that establish the connection between changes in the process information. The ontology is a part of a multi-agent based distributed intelligent system ENCORE [32] for process supervision. However, the ENCORE does not support reasoning, such as DL consistency in process supervision, to ensure data quality. The semantic interoperability is not supported between different domains.

This paper addresses the aforementioned research challenges and its major objectives are:

- To describe OntoTwin ontology for cross-domain clustering in a chemical plant.
- To outline the implementation details of the ElChemo framework mainly designed for semantic interoperability between tools in the chemical and electrical domains and ensure the plant's smooth and reliable operation as a component of the JPS.
- To integrate DL based inference engine to detect inconsistency and the SPARQL Inferencing Notation (SPIN) [22] inference engine to detect constraint violations, for monitoring and suggesting optimal operating decisions.
- To discuss the potential of integrating the ElChemo framework into agent composition framework.

The paper starts with an introduction of the JPS, an intelligent semantic web-based platform. The subsequent section describes the OntoTwin ontology that was developed for knowledge modelling in a cross-domain environment. The model descriptions for the chemical and corresponding electrical systems are then illustrated along with a sample calculation for transformer sizing. The paper then describes the implementation of the ElChemo framework. This is followed by an overview of a potential extension of the ElChemo framework by using an agent composition approach. The results obtained from the proposed framework are described in the subsequent section. The final section provides the conclusion and future work scope for further improvements.

# 2 The World Avatar - A Dynamic Knowledge Graph

Large scale heterogeneous systems such as industrial symbioses constitute components such as power generators, storage tanks, and buildings, which are from diverse domains. An efficient and optimum operation of such an integrated complex environment would require cooperation and knowledge from several domains. However, the communication friction arising from the semantic and syntactic heterogeneities across domains hinders such an integration. The World Avatar concept intends to capture the idea of representing every aspect of the real world in a digital "mirror" world. This is essentially an extension of the Digital Twin notion, where, taking an example from Industry 4.0, a device or a unit operation in an industrial process has a corresponding virtual representation. Within The World Avatar project we have been developing the J-Park Simulator (JPS).

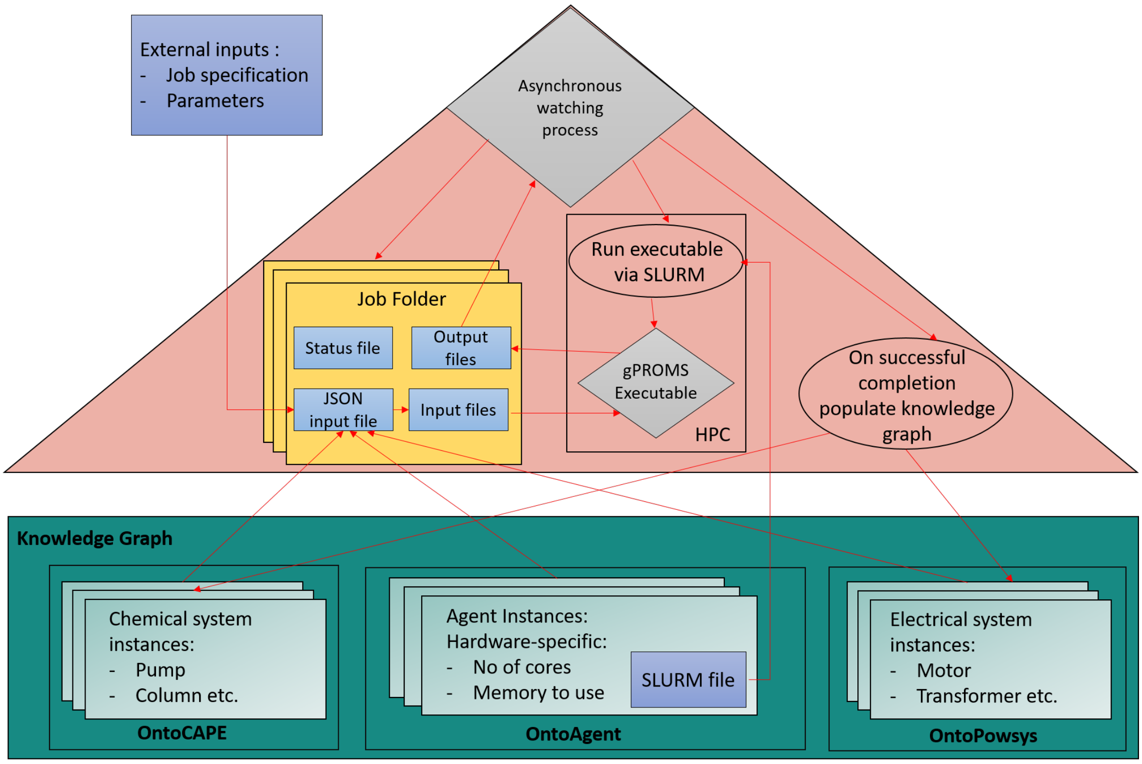



**Figure 1:** *Elements of the gPROMS agent (red triangle) and how they interact with the knowledge graph (green box). An asynchronous watcher (grey diamond) manages running the gPROMS executable (grey diamond) with all associated input and output files (blue boxes). This agent follows the generic template described in [29].*

The JPS serves as a common platform for establishing cross-domain correlations and interoperability in a modern industrial production environment. One of the primary objectives of the JPS is to create a cyber-physical system wherein every entity of the production process has its digital twin [45]. These digital twins will be capable of emulating the actual behaviour of the physical entity. They can be used to improve the product quality of the industrial processes. The JPS includes a Knowledge Management System (KMS) [44], which is capable of storing and analysing information from various domains that include chemical, electrical, and logistical [27]. It also has a semantic web-based agent framework whose tasks can vary from querying of the knowledge graph to executing complex mathematical models [10].

# 3 OntoTwin: A Cross-Domain Ontology

The OntoTwin, a cross-domain ontology, is used to define both chemical and electrical system models shown in Figure 2 and Figure 3. In this section, we will use DL syntax to express the ontology. The ontology has been developed using the OWL2 DL language. Table 1 lists a part of the OntoTwin knowledge base which comprises 50 concept names, 23 role names, and 70 axioms. The listed axioms are used for checking constraint violations and DL consistency of the chemical and electrical systems. It is derived from two interconnected ontologies i.e. OntoEIP [14] and OntoPowSys [11].

The depropaniser section performs a separation process called distilling, which is a type of unit operation (see axioms 1 and 2). The process streams coming in and out of the depropaniser section have a process state and an operational mode i.e., continuous in nature (see axioms 3 and 4). Axiom 16 shows that a pump is a machine present in the chemical system and is realised in the electrical system as an electrical motor (axioms 36, 39 and 40) by using the role inclusion axioms $56-59$. Axioms $13-16$ and 20 express that the feed pump is used to maintain the outlet pressure in the chemical system. The process stream is then fed to the distillation column, which realises separation (see axiom 5). The distillation column has thermodynamic temperature and pressure as input variables, as expressed in axioms $17-19$ and $21-23$. It has two output streams named bottoms and distillate. Both have product quality expressed as mole fraction of the major component in the stream. Formally, axioms 7, 9, 11, 12, 24, 25, and 26 define the connectivity between outlet process streams. At this point, the SPIN [22] inference engine is responsible for ensuring the plant operation provides the required quality of the product. To achieve it, the SPIN inference engine uses constraint violations shown in Figure 7, the implementation of which is explained in detail in Section 5.2.

The power transformer is used to step down the incoming voltage level expressed in axioms $36-38$. The class *ConstantProperty* is used to describe the rated parameters for all equipment present in the electrical system. These values are used to compare with the real-time values, due to any change in a process stream. At this stage, the SPIN inference engine is used to check the various Power Quality (PQ) parameters such as frequency deviation or voltage fluctuation of the incoming supply by using implemented constraint violations on top of *ConstantProperty*, *ScalarQuantity* and *PhysicalQuantity* concept names expressed in axioms $27-35$ [6].

**Table 1:** *Selected concept inclusion axioms and individual assertions in the OntoTwin knowledge base.*

| S.No | DLs concept inclusion axioms and individual assertions |
|---|---|
| 1 | Separation $\sqsubseteq$ UnitOperation |
| 2 | Distilling $\sqsubseteq$ Separation |
| 3 | ProcessStream $\equiv$ ProcessState $\sqcap$ $\forall$ hasOperationMode.ModeOfOperation |

Continued on next page

Table 1 – continued from previous page

| S.No | DLs concept inclusion axioms and individual assertions |
|---|---|
| 4 | ModeOfOperation(Continuous) |
| 5 | Distillation $\sqsubseteq$ Separation |
| 6 | Distillation $\sqsubseteq \forall$ hasInputAtNumberedTray.ProcessState |
| 7 | Distillation $\sqsubseteq$ ($\leq$ 1 hasTopProduct.$\top$) $\sqcap$ ($\geq$ 1 hasTopProduct.$\top$) |
| 8 | Distillation $\sqsubseteq$ ($\leq$ 1 hasDistillateToFeedRatio.$\top$) $\sqcap$ ($\geq$ 1 hasDistillateToFeedRatio.$\top$) |
| 9 | Distillation $\sqsubseteq$ ($\leq$ 1 hasBottomProduct.$\top$) $\sqcap$ ($\geq$ 1 hasBottomProduct.$\top$) |
| 10 | Separation $\sqsubseteq \geq$ 2 hasOutput.$\top$ |
| 11 | Bottoms $\sqsubseteq$ ProcessStream |
| 12 | Distillate $\sqsubseteq$ ProcessStream |
| 13 | ScalarValue $\sqsubseteq$ QuantitativeValue |
| 14 | Pump $\sqsubseteq \exists$ hasOutletPressure.OutletPressure |
| 15 | Pump $\sqsubseteq \exists$ hasPumpHead.QuantitativeValue |
| 16 | Pump $\sqsubseteq$ Machine |
| 17 | Temperature $\sqsubseteq \forall$ hasDimension.PhysicalDimension |
| 18 | PhysicalDimension(thermodynamic_temperature) |
| 19 | Temperature $\sqsubseteq$ ThermodynamicStateProperty |
| 20 | OutletPressure $\sqsubseteq$ Pressure |
| 21 | Pressure $\sqsubseteq \forall$ hasDimension.Mechanics |
| 22 | Mechanics(pressure) |
| 23 | Pressure $\sqsubseteq$ ThermodynamicStateProperty |
| 24 | MoleFraction $\sqsubseteq \forall$ hasDimension.DerivedDimension |
| 25 | DerivedDimension(mole_fraction) |
| 26 | MoleFraction $\sqsubseteq$ PhaseComponentFraction |
| 27 | RatedPower $\sqsubseteq$ ConstantProperty |
| 28 | RatedVoltage $\sqsubseteq$ ConstantProperty |

Continued on next page

Table 1 – continued from previous page

| S.No | DLs concept inclusion axioms and individual assertions |
|---|---|
| 29 | RatedCurrent $\sqsubseteq$ ConstantProperty |
| 30 | RatedFrequency $\sqsubseteq$ ConstantProperty |
| 31 | ActivePower $\sqsubseteq$ ScalarQuantity |
| 32 | AbsorbedActivePower $\sqsubseteq$ ActivePower |
| 33 | Voltage $\sqsubseteq$ PhysicalQuantity |
| 34 | Current $\sqsubseteq$ PhysicalQuantity |
| 35 | Frequency $\sqsubseteq$ ScalarQuantity |
| 36 | ElectricalEquipment $\sqsubseteq$ CompositeSystem |
| 37 | PowerConverter $\sqsubseteq$ ElectricalEquipment |
| 38 | PowerTransformer $\sqsubseteq$ PowerConverter |
| 39 | PowerLoad $\sqsubseteq$ ElectricalEquipment |
| 40 | ElectricalMotor $\sqsubseteq$ PowerLoad |
| 41 | Bottoms $\sqcap$ Distillate $\sqsubseteq \bot$ |
| 42 | TimeInstant $\sqsubseteq$ TemporalEntity |
| 43 | PrefixedDerivedUnit $\sqsubseteq$ SI_DerivedUnit |
| 44 | SI_DerivedUnit $\sqsubseteq$ SI_Unit |
| 45 | SI_Unit $\sqsubseteq$ UnitOfMeasure |
| 46 | hasProperty $\sqsubseteq$ inter-objectRelation |
| 47 | hasProperty $\equiv$ isPropertyOf$^{-}$ |
| 48 | $\top \sqsubseteq \leqslant 1$ hasProperty$^{-}$ |
| 49 | $\exists$ hasProperty.$\top \sqsubseteq$ System |
| 50 | $\top \sqsubseteq \forall$ hasProperty.Property |
| 51 | hasValue $\sqsubseteq$ inter-objectRelation |
| 52 | hasValue $\equiv$ isValueOf$^{-}$ |
| 53 | $\top \sqsubseteq \leqslant 1$ hasValue$^{-}$ |
| 54 | $\exists$ hasValue.$\top \sqsubseteq$ Property |
| 55 | $\top \sqsubseteq \forall$ hasValue.Value |
| 56 | hasPart $\sqsubseteq$ inter-objectRelation |

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Table 1 – continued from previous page

| S.No | DLs concept inclusion axioms and individual assertions |
|---|---|
| 57 | hasPart $\equiv$ isPartOf$^{-}$ |
| 58 | $\exists$ hasPart. $\top \sqsubseteq$ Object |
| 59 | $\top \sqsubseteq \forall$ hasPart.Object |
| 60 | hasUnitOfMeasure $\sqsubseteq$ object-featureRelation |
| 61 | $\exists$ hasUnitOfMeasure.$\top \sqsubseteq$ QuantitativeValue |
| 62 | $\top \sqsubseteq \forall$ hasUnitOfMeasure.UnitOfMeasure |
| 63 | hasActivePowerAbsorbed $\sqsubseteq$ hasProperty |
| 64 | $\top \sqsubseteq \forall$ hasActivePowerAbsorbed.AbsorbedActivePower |
| 65 | hasFrequency $\sqsubseteq$ hasProperty |
| 66 | $\top \sqsubseteq \forall$ hasFrequency.Frequency |
| 67 | $\top \sqsubseteq \forall$ hasTime.TemporalEntity |
| 68 | hasRatedFrequency $\sqsubseteq$ hasProperty |
| 69 | hasOutletPressure $\sqsubseteq$ hasProperty |
| 70 | isConnectedTo $\sqsubseteq$ inter-objectRelation |

# 4 Model Description

This section first introduces the chemical process modelling of a depropaniser section within a typical natural gas processing plant. Next, the corresponding electrical system model is presented wherein a sample calculation of a transformer design capacity is discussed. Finally, the proposed integrated modelling approach is presented wherein a relationship between the chemical process model and the corresponding electrical model is established.

## 4.1 Chemical Process System

The chemical process system modelled in this paper considers the depropaniser section of a natural gas processing plant. The system was developed as a dynamic model in gPROMS [2, 43] as shown in Figure 2.

The feed conditions to the depropaniser section are provided in Table 5 of the Appendix. The chemical system involves the following equipment:

- Feed pump: It energises the feed stream to the required pressure. It is equipped with a variable frequency drive to ensure constant outlet pressure. Each pump is

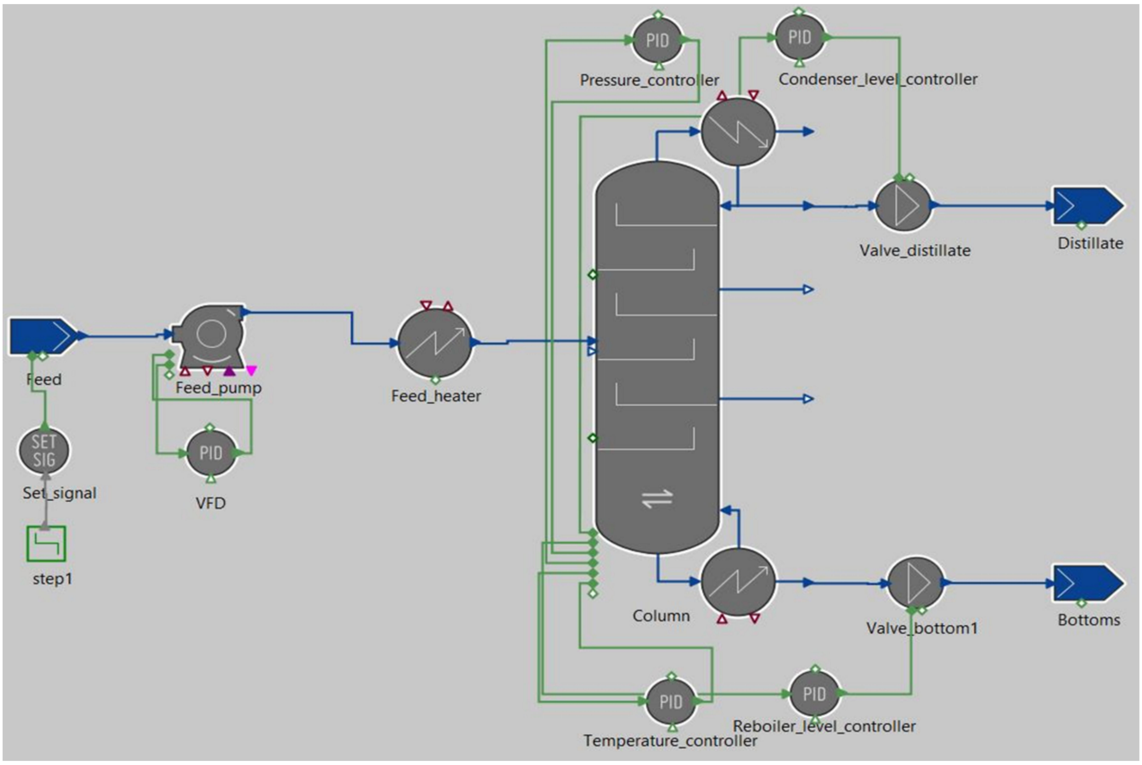


**Figure 2:** *An gPROMS [2] dynamic model of a separation unit in a chemical plant.*

equipped with an electrical motor that drives its shaft, and it is necessary to model it in the electrical system. To have a more realistic model, a suitable commercial pump with known characteristics is chosen. The design properties of the pump are provided in Table 6 of the Appendix.

- Feed pre-heater: The energised stream from the feed pump enters the feed pre-heater and is heated to a temperature of 330 $K$.
- Distillation column: The feed from the pre-heater is then sent to the distillation column for the separation of propane from isobutane. We have used a tray-type column, and the properties are listed in Table 7 in the Appendix.

Section A.1 in the Appendix provides the details of other equipment in the flowsheet.

## 4.2 Electrical System

Figure 3 shows the corresponding electrical system model representation of the chemical process system. The electrical model comprises a 6.6 $kV$ three-phase AC voltage source used to supply power to the transformer's load. The incoming 6.6 $kV$ voltage is stepped down to 400 $V$ using a three-phase two winding step down transformer (refer to Table 9). A constant resistive load rated 5 $kW$ is assumed to represent other plant loads such as lighting. An electrical motor rated 200 $kW$ that drives the feed pump in the chemical

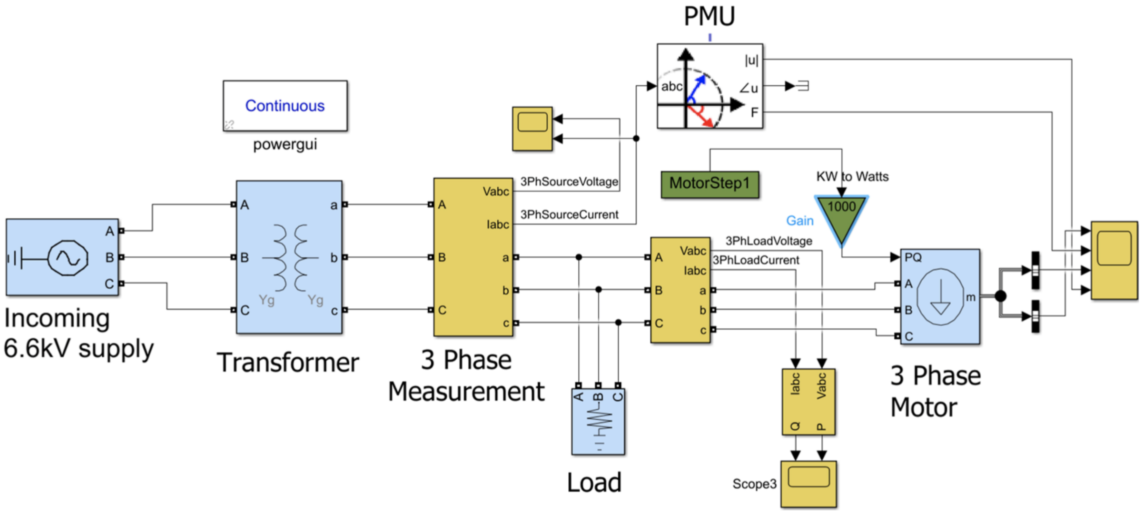


**Figure 3:** *A dynamic electrical system model of the corresponding chemical system developed using MATLAB/Simulink [26].*

system is connected to the transformer. The motor is modelled as a dynamic load, and its characteristics are listed in Table 10. The active power demand profile for the motor generated from the chemical process model is fed to the dynamic load. The electrical model is used to study the effects of process disturbance on the PQ at the Point of Common Coupling (PCC) [37]. PCC refers to a point in the transmission and distribution network, electrically nearest to a connected person's installation, at which other customers' loads are or may be connected.

### 4.2.1 Transformer Design Capacity Calculation

A transformer is an electrical equipment that transfers electrical power from one circuit magnetically to another without changing frequency. It helps to either step up or step down the voltage in an electrical system. The rated power capacity of a transformer in an electrical system depends on the load connected to it. In the proposed electrical system, a constant resistive load rated 5 $kW$ and a dynamic motor load rated 200 $kW$ is connected to the transformer. The total active power demand from the transformer is the sum of the active power consumed by the resistive load and the dynamic motor load. The total rated value adds up to be 205 $kW$. Note that the reactive power for each chemical process load is assumed to be half of its kW demand. Since the constant load is resistive, it operates at a unity power factor, i.e., it does not require any reactive power. The total reactive power demand from the transformer is the reactive power consumed by the motor, i.e., 100 $kVAR$. The total power (apparent power) required in an electrical system is expressed as the complex summation of the active and reactive power. The real part is the active power, and the imaginary being the reactive power.

The apparent power rating (S) for the transformer is given as:

$$S = (P + jQ) \tag{1}$$

*i.e.* ,

$$S = (205 + j100)kVA \tag{2}$$

where $S$ is the apparent power, $P$ is the active power, and $Q$ is the reactive power. The absolute value of $S$ is 228 $kVA$. This is the actual loading on the transformer. According to the standard design practices, a design margin of 10 % is incorporated. In order to cater for a future increase in demand, an additional buffer of 20 % is also considered while sizing the transformer. The transformer's final power rating based on these calculations turns out to be 300 $kVA$. In general, a transformer of a higher rating (around 500 $kVA$) will be chosen to ensure smooth operation. In this paper, we have chosen a transformer rating of 300 $kVA$ to study the impact of PQ disturbances arising from the chemical system. Note that for a distribution transformer, the power factor of 0.9 is assumed. The deviation in frequency at the Low Voltage (LV) side of the transformer is measured using a Phasor Measurement Unit (PMU).

### 4.3 Proposed Integrated Modelling Approach

The main idea behind integrating the chemical and electrical models is to identify the electrical footprint of the equipment present in the chemical plant in terms of the power consumed ($kW$). The power ($kW$) consumption is considered as the specified load profile for monitoring the real-time PQ disturbances in the corresponding electrical system model. The electrical power consumed by the chemical process load is directly obtained as one of the chemical process model's output parameters and stored in the JPS knowledge graph. This output is then fed as an input to the electrical model to detect the real-time PQ disturbances in the network. The next section elucidates the implementation of the decision support framework for the integrated modelling approach.

## 5 ElChemo Framework: Design and Implementation

This section outlines the design and implementation of the ElChemo semantic web-based framework that is a component of the JPS. It establishes cross-domain semantic interoperability between modelling tools in chemical and electrical engineering. It also extends the JPS knowledge graph with the data from both the chemical process model and its corresponding electrical system. The proposed approach utilises semantic web technologies, queries, and automated reasoning to efficiently make an autonomous operational decision and design optimisation in a chemical plant [3]. The main objective of the work done in [12] is to integrate data from the chemical process and electrical subsystems to perform plant-wide diagnoses. The data generated from these tools are exported to a graph database. However, that infrastructure lacked a reasoning engine to guarantee the quality of process flow data and semantic interoperability between computer-aided engineering tools. In addition, it did not offer users the option to monitor the PQ performance of an electrical system. The ElChemo aims to address the inadequacy of the work mentioned in the previous section as follows:

- To employ OntoTwin cross-domain ontology. The ontology supports semantic query, reasoning, and semantic interoperability between chemical process simulation tools and the tools used for mathematical simulations of the hybrid power system.

- To use the consistency reasoning technique in DL to ensure the consistency of data used in chemical processes and mathematical simulation tools.
- To employ the SPIN [22] to
  - detect constraint violations of the distillate and bottoms product quality;
  - detect changes in process flow rate for the distillate column;
  - detect frequency deviations and voltage fluctuations in the electrical system due to the corresponding change in process flow rate.
- To improve semantic interoperability between different tools in the chemical plant as a component of the JPS.

## 5.1 Implementation of the ElChemo Framework

This section describes the implementation details of the ElChemo framework by using the Unified Modeling Language (UML) [39]. Figure 4 and Figure 5 depict the UML use case and sequence diagram of the ElChemo framework. The design process parameters for the chemical system are read from text files and are then populated in the JPS knowledge graph. JPS agent architecture ensures logical consistency of the knowledge graph by running HermiT reasoner [30] whenever there is a change in the knowledge graph. The coordination agent is responsible for initiating the simulation of the depropaniser section of the process plant and the corresponding electrical system of the processing plant.

The coordination agent first initiates the simulation of the chemical processing plant by calling the gPROMS agent. The gPROMS agent performs the SPARQL query to retrieve the data from the knowledge graph. This data is used to initialise the gPROMS model. The model is executed on a High Performance Computing (HPC) system using the SLURM job scheduler. Figure 6 provides an overview of the gPROMS agent execution. The gPROMS agent continuously monitors for any request for model executions. Once the agent receives a request, a job ID is assigned and the data required to execute the model are retrieved through SPARQL queries. The retrieved data is then processed to match the format required by the gPROMS software. These files along with the executable are then transferred from the host computer to the HPC using SSH File Transfer Protocol (SFTP). The SLURM job scheduler submits the job to be executed on the HPC. The agent continuously monitors the job status and waits for job completion. As soon as the job is completed, the generated output files are transferred back to the host computer. Information about the output file including the location, date of creation and the agent that created it are annotated in JPS metadata repository so that it can be accessed by other agents. The annotated output file is then analysed using the SPIN [22] inference engine to check for logical consistency and constraint violation as shown in Figure 4 and Figure 5. The ElChemo framework will terminate when any constraint violation is detected. For example, the SPIN engine will detect a constraint violation if the distillate mole fraction

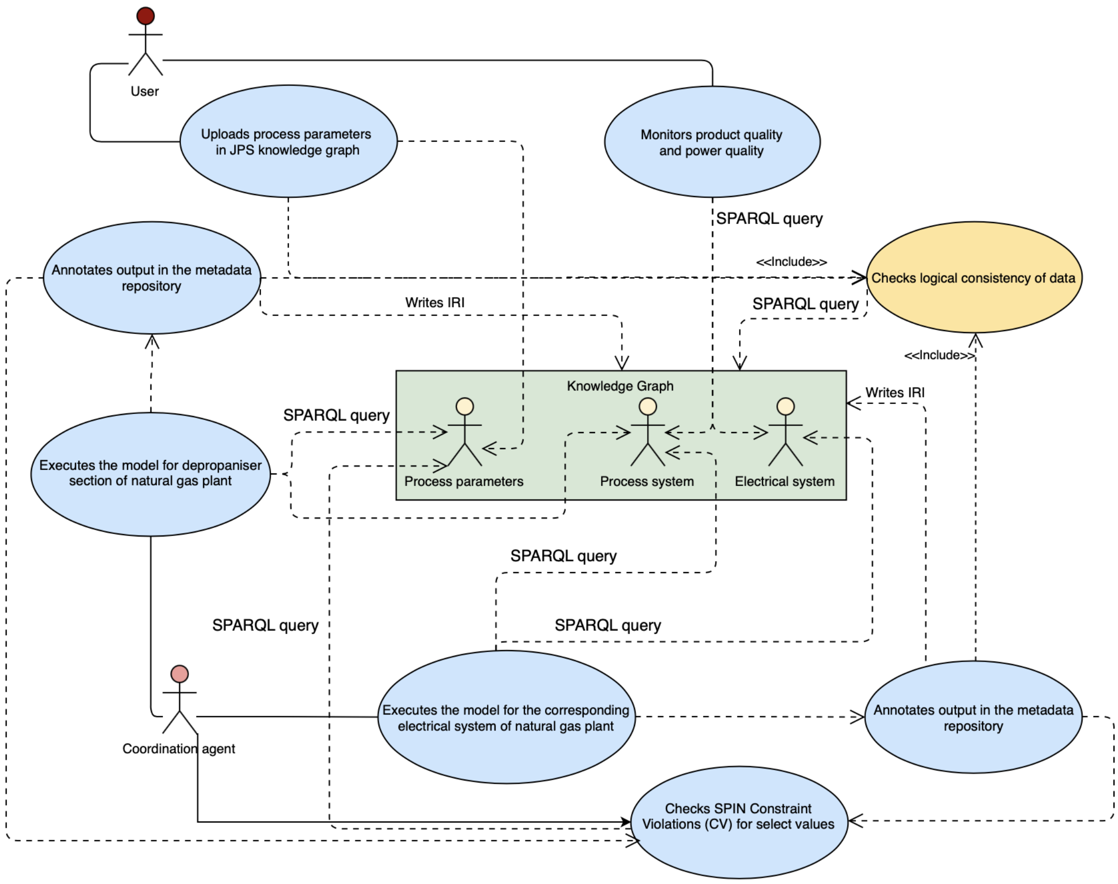


**Figure 4:** *The use case of ElChemo framework. The yellow shaded action represents a part of the JPS framework that is used to maintain the consistency of the knowledge graph. The green shaded portion represents the knowledge graph and the blue shaded actions represent the ElChemo framework. The solid lines represent actions triggered by the agents and the dotted lines represent actions within the agents.*

of propane and/or bottoms mole fraction of isobutane is less than 0.973. It has to be noted that, at present the SPIN constraint validation is applied only on select data points (minimum and maximum values) from the output for improving agent run times. After the successful execution of the gPROMS agent, and no constraint violation detection by the SPIN agent, the coordination agent initiates the Matlab agent. It sends the metadata IRI and the electrical system IRI to the Matlab agent. The execution of the corresponding electrical system performed in a similar way as the chemical system. Users can monitor and check the product quality and PQ when the systems are subjected to any change in the operating condition.

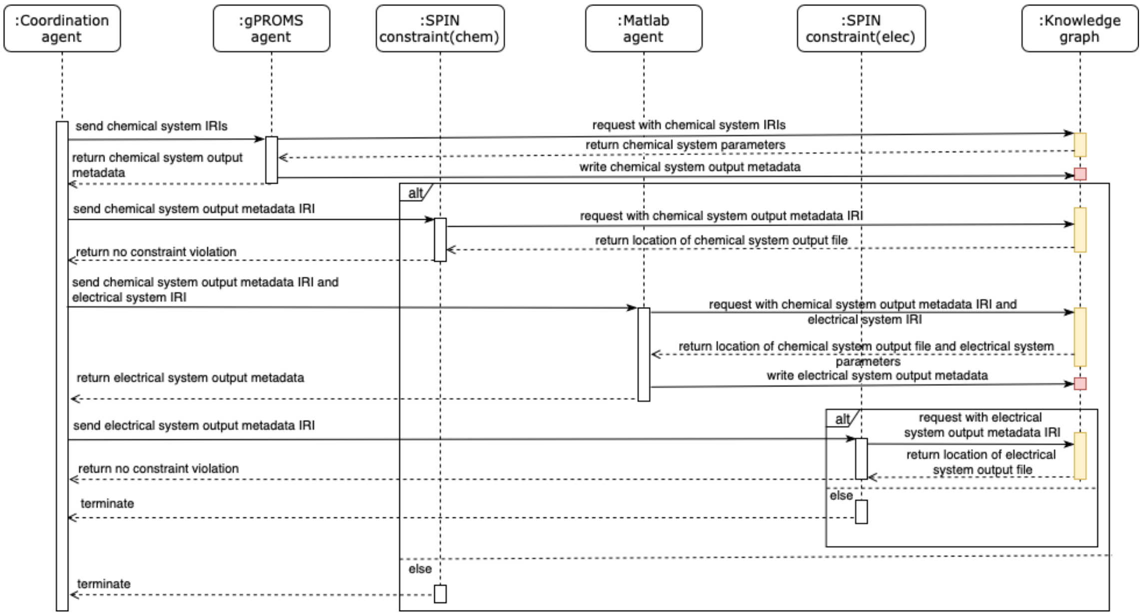


**Figure 5:** *UML sequence diagram of ElChemo framework depicting the interaction between the different agents and the knowledge graph. Actions where the agent retrieves data from the knowledge graph are shaded in yellow and those where the agent populates the knowledge graph are shaded in magenta.*

## 5.2 Implementation of Constraints Violation in the ElChemo Framework

This section provides a formal description of constraints that ensures the stable operation of the plant. The inference engines use these constraints to detect any deviation for the product quality and PQ from acceptable limits due to any change in the plant's operation. We divide these constraints into two groups. The first group is for monitoring the chemical process, whereas the second group is for monitoring the power network. All constraints are expressed using a restricted first-order language adapted from [8]. The dictionary of the language consists of a countable set of functional and relational symbols, logical connectivity ($\wedge$ and $\vee$), universal quantifier ($\forall$), and existential quantifier ($\exists$), constants that are real numbers, variables, and parenthesis.

$$(\forall x, z, v, w)(\exists_1 nvb)(Bottoms(x) \wedge hasProperty(x, z) \wedge MoleFraction(z) \wedge representsOccurenceOf(z, w) \wedge hasValue(z, v) \wedge numericalValue(v, nvb) \wedge (nvb \geq 0.973)) \quad (3)$$

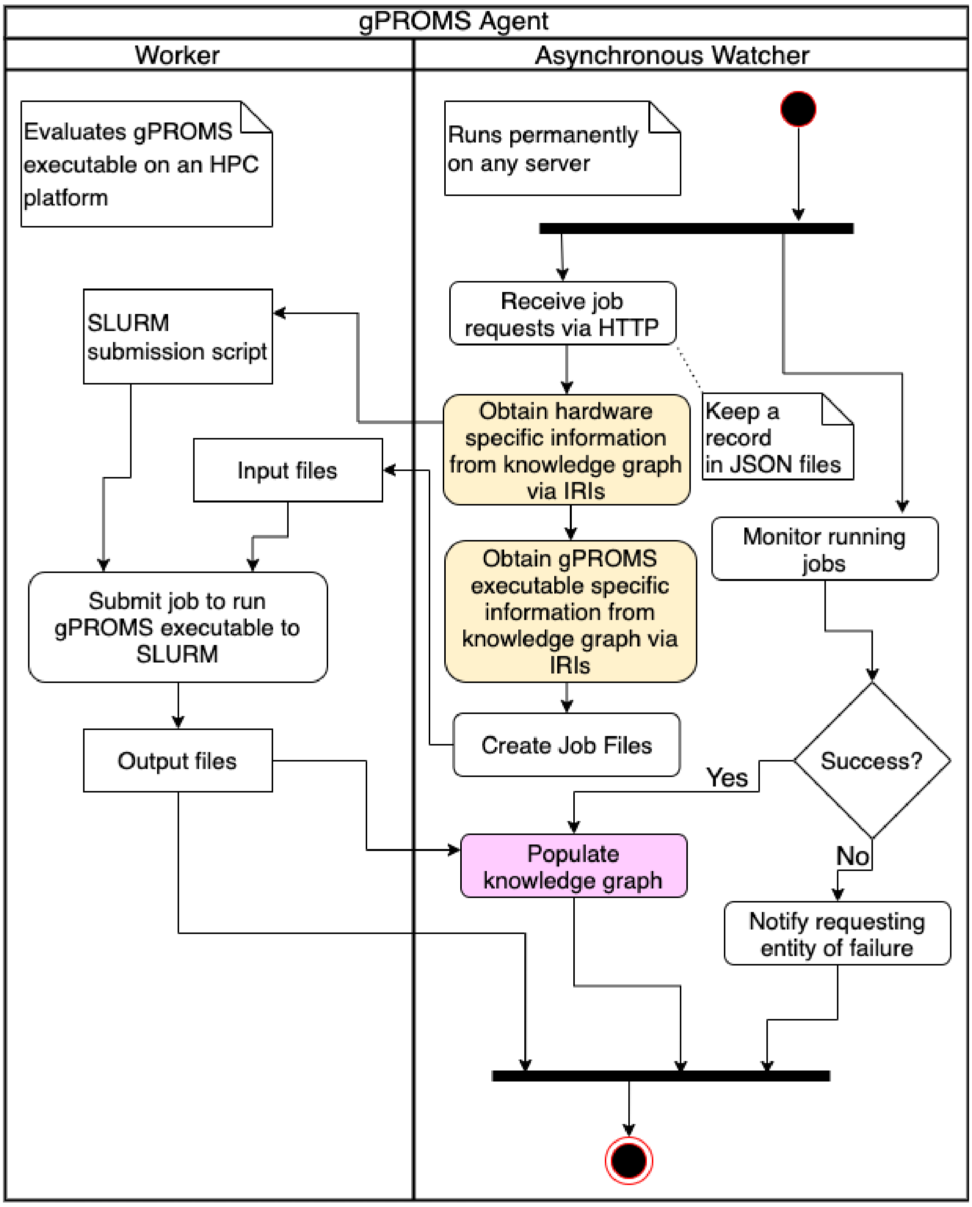


**Figure 6:** *UML activity diagram of the gPROMS agent that enables the execution of gPROMS simulation asynchronously on an HPC platform upon HTTP requests. The yellow shaded actions represent the data retrieval operation of the agent from the knowledge graph, whereas the magenta shaded action represents the knowledge graph populating operation of the agent.*

$$(\forall x, z, v, w)(\exists_1 nvd)(Distillate(x) \land hasProperty(x,z)$$
$$\land MoleFraction(z) \land representsOccurenceOf(z,w) \land hasValue(z,v)$$
$$\land numericalValue(v,nvd) \land (nvd \geq 0.973)) \tag{4}$$

$$(\forall x, w, p, q, r, z)(\exists_1 s, t)((Bottoms(x) \vee Distillate(x)) \wedge hasProperty(x, r) \wedge MoleFraction(r) \wedge hasValue(r, p) \wedge numericalValue(p, s) \wedge hasProperty(x, z) \wedge MoleFraction(z) \wedge hasValue(z, q) \wedge numericalValue(q, t) \wedge (s + t = 1.00)) \quad (5)$$

The rules (3, 4, 5) represent the formal expressions for the violation of the mole fraction of the products. The rule 3 states that there is a unique value for a mole fraction of isobutane in all bottoms that contain isobutane, and the value of the mole fraction must not be less than 0.973. The rule 4 is a modification of rule 3 wherein it is applied to distillate. The rule 5 states that the sum of the mole fraction of all the components for a process stream (either bottoms or distillate) must be equal to 1.

A

```
# Bottoms mole fraction for Isobutane is smaller than 0.973.
CONSTRUCT {
    _: b0 a spin:ConstraintViolation .
    _:b0 spin:violationRoot ?this .
    _:b0 rdfs:label "Bottoms mole fraction for Isobutane is smaller than 0.973" .
}
WHERE {
    ?s network_system:leaves ?this .
    ?s a :Bottoms .
    ?s system:hasProperty ?mf1 .
    ?mf1 a phase_system:MoleFraction .
    ?mfl phase_system:representsOccurenceOf :Isobutane .
    ?mf1 system:hasValue ?v_mf1 .
    ?v_mf1 system:numericalValue ?mf1_num_value .
    FILTER (?mf1_num_value < 0.973) .
}
```

B

```
# Distillate mole fraction for Propane is smaller than 0.973.
CONSTRUCT {
    _:b0 a spin:ConstraintViolation .
    _:b0 spin:violationRoot ?this .
    _:b0 rdfs:label " Distillate mole fraction for Propane is smaller than 0.973" .
}
WHERE {
    ?s network_system:leaves ?this .
    ?s a :Distillate .
    ?s system:hasProperty ?mf2 .
    ?mf2 a phase_system:MoleFraction .
    ?mf2 phase_system:representsOccurenceOf :Propane .
    ?mf2 system:hasValue ?v_mf2 .
    ?v_mf2 system:numericalValue ?mf2_num_value .
    FILTER (?mf2_num_value < 0.973) .
}
```

C

```
# Validates whether sum of all mole fraction of some process stream is not equal to 1.
CONSTRUCT {
    _:b0 a spin:ConstraintViolation .
    _:b0 spin:violationRoot ?this .
    _:b0 rdfs:label "Sum of all numerical values for mole fraction of Distilling is not equal to one" .
}
WHERE {
    ?s network_system:leaves ?this .
    ?s a ?type .
    ?s system:hasProperty ?mf1 .
    ?mf1 a phase_system:MoleFraction .
    ?mf1 system:hasValue ?v_mf1 .
    ?v_mf1 system:numericalValue ?mf1_num_value .
    ?s system:hasProperty ?mf2 .
    ?mf2 a phase_system:MoleFraction .
    ?mf2 system:hasValue ?v_mf2 .
    ?v_mf2 system:numericalValue ?mf2_num_value .
    BIND ((?mf1_num_value + ?mf2_num_value) AS ?total) .
    FILTER ((?total > 1.01) || (?total < 0.99)) .
    FILTER ((?mf1) != (?mf2)) .
    FILTER (?type != owl:NameIndividual) .
}
```

**Figure 7:** *Implementation of constraint violation to check the distillate mole fraction of propane and bottoms mole fraction of isobutane by using the SPIN [22].*

Figure 7 (A, B, C) depicts the implementation of rules (3, 4, 5) in SPIN [22] respectively. The concerned knowledge graph is validated by using SPIN inference engine via implemented rules. For rule 5, there is a relative tolerance of one percent because of minor variations during model validation. It means that any sum of the mole fractions outside the range of 0.99 to 1.01 is not acceptable as shown in Figure 7 (C). Rules A and B shown in Figure 7 differ only in type of process stream and chemical species used in checking constraint violation. Consequently, these two rules can be implemented by using *spin:Template* [22] and having the type of process stream as an input parameter. These two constraints (A and B) thus become the instances of this template. This is a flexible way to implement a number of rules into a single spin template [22].

# 6 ElChemo Framework: Agent Composition Approach

This section examines how the current ElChemo framework presented above can be integrated into the agent composition framework discussed in [46]. The paper describes how the automatic agent discovery and composition can generate cross-domain applications. The agent composition framework is based upon the adaptation of the Minimal Service Model (MSM) ontology [36] into a light-weight agent ontology called OntoAgent [13]. The purpose of implementing an agent composition framework is to fulfill tasks that require the consecutive execution of more than one agent, without any hard-coded coordination. An agent composition framework creates plans for agent coordination in an automated and dynamic fashion, thus increasing the efficiency and flexibility of coordinating agents. The agents operate on the JPS knowledge graph and collaborate with each other. The agents are envisioned to be capable of automatically and autonomously integrate and standardise knowledge from different domains. The formal definition of an ElChemo agent composition framework is presented below:

**Definition 1.** *Formal ElChemo agent composition framework is a tuple $\omega = (A, F, O, M, B, T)$ where A is a countable set of agents, F is a countable set of agent function, O is a countable set of agent operations, M is a countable set of agent memory, B is a countable set of agent behaviours, and T is a countable set of agent transitions. All of these sets are disjoint.*

Based on Definition (1), the proposed ElChemo agent composition framework consists of five agents $A = \{a_1, a_2, \ldots, a_5\}$. Agent $a_1$ runs operation $o_1$ named as *data read from knowledge graph* to create agent memory $m \in M$ which is a part of the JPS knowledge graph. Formally, we write this as tuple $a_1(o_1, m)$. In a practical scenario, the data should have behaviour $b_1 \in B$ as a *real-time data* from sensors installed in the plant. The modified tuple $a_1$ is expressed as $a_1(o_1, m, b_1)$. The agent architecture in JPS ensures logical consistency of the knowledge graph by running consistency checks whenever the knowledge graph is updated. Once the memory $m$ is deemed to be logically consistent, then it is sent to agent $a_2$ named as *gPROMS agent wrapper*. The agent $a_2$ has functionality $f_1$ which performs the dynamic simulation of the chemical system. It is expressed as $a_1(o_1, m) \xrightarrow{t_1} a_2(f_1, m)$, where $t_1$ is transition between agents $a_1$ and $a_2$, whereas memory $m$ is updated memory with the data that are the outputs of performing function $f_1$. After completing function $f_1$, the knowledge graph is updated and agent $a_3$ performs operation $o_2$ named as *constraint violation* on data stored in memory $m$. Formally, we express this as $a_1(o_1, m) \xrightarrow{t_2} a_3(o_2, m)$. If the agent $a_3$ does not detect any constraint violation, then agent $a_1$ *reads* the updated data from the memory. These data are used in execution of agent $a_4$ named as *Matlab agent wrapper* that performs function $f_2$ on memory $m$. The function $f_2$ performs the dynamic simulation of the corresponding electrical system due to any change in the chemical system. This step is formally expressed as $a_1(o_1,m) \xrightarrow{t_3} a_4(f_2,m)$. Finally, the framework runs the agent $a_5(o_3,m)$ that checks the memory $m$ for constraint violations for data generated by the execution of agent $a_4$.

The formal agent composition approach proposed in this section fits the developed agent composition framework in [46]. Our formal agent description includes a set of agents described in the semantic agent composition framework by using OntoAgent ontology. The formal agent composition framework defines agent compositions by using agent transitions. The semantic agent composition framework described in [46] lacks a reasoning technique that can be implemented in an agent composition framework. The formal approach specified in this section proposes a framework that will be able to automatically compose the agents and detect violation of any rule implemented for the agent composition framework.

# 7 Results and Discussion

Section 7 is divided into two subsections to illustrate the two-factor advantage as a consequence of cross-domain clustering of chemical and electrical systems described in Section 4. Section 7.1 demonstrates two case studies based on ElChemo framework. It utilises several semantic web technologies, including the SPIN constraint violations, to establish the interactions between the models from chemical and electrical domains. These are then utilised to choose the optimum operating decision that ensures a resilient and reliable operation of the system in the event of a change in the feed flow rate of the chemical plant's depropaniser section. The reliability of the chemical system in this context has been defined as its ability to maintain the product quality within the desired product specification, thereby reducing off-spec production. The PQ disturbances are detected and monitored for the electrical system to ensure minimum downtime of the network due to the increase in feed flow rate, resulting in the smooth operation of the depropaniser section. Section 7.2 showcases the optimum equipment sizing based upon the operational decision derived in Section 7.1, leading to cost-savings.

## 7.1 Operational Optimisation

The increase in the demand for the final product leads to the change in the feed flow rate of the depropaniser section from 52 $kg/s$ to 62 $kg/s$ in the minimum possible time while ensuring stable operation of the system and maintaining the product quality within the specified limits. The case studies introduce the changes that occur as single step change or multiple-step changes over a duration of time. In both case studies, the responses from the chemical and electrical systems are studied.

#### 7.1.1 Case 1

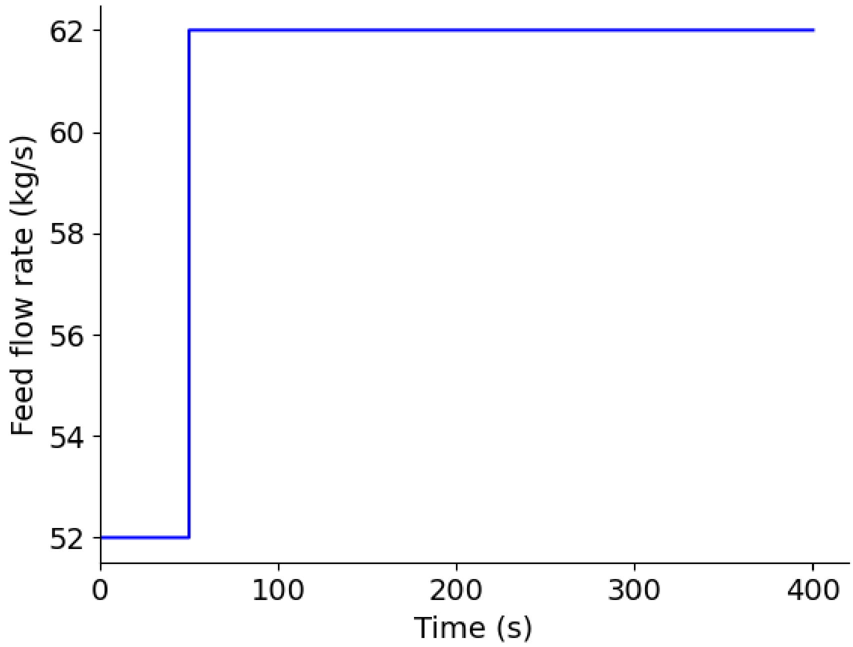


**Figure 8:** *Feed flow rate curve for case 1.*

In the first case, the feed flow rate change is introduced as a single step change of magnitude $10kg/s$ at time $t = 50s$ as shown in Figure 8. This is achieved by the sudden opening of the feed control valve. Table 2 represents a section of the Abox assertions that depicts maintaining the desired pump's outlet pressure to meet the specified product demand at a particular instant of time. Axiom 1 in the Table 2 instantiates the pump $P-001$. Axioms 2 to 8 represents how the outlet pressure is stored in the JPS knowledge graph. The next three axioms showcase how the corresponding instant of time is linked to the outlet pressure value. The last two axioms describe how an individual, such as $P-001$ (axiom 1 of Table 2) defined in a chemical domain, is related to an electrical motor $EM-001$ defined in the electrical domain.

**Table 2:** *Abox assertions for pump outlet pressure to maintain in feed flow rate.*

| S.No | Individual assertions |
|---|---|
| 1 | Pump(P-001) |
| 2 | OutletPressure(OP-P-001) |
| 3 | hasOutletPressure(P-001, OP-P-001) |
| 4 | ScalarValue(V-OP-P-001) |

Continued on next page

Table 2 – continued from previous page

| S.No | Individual assertions |
|---|---|
| 5 | hasValue(OP-P-001, V-OP-P-001) |
| 6 | numericalValue(V-OP-P-001, 52) |
| 7 | PrefixedDerivedUnit(kg/s) |
| 8 | hasUnitOfMeasure(V-OP-P-001, kg/s) |
| 9 | TimeInstant(T-V-OP-P-001) |
| 10 | hasTime(V-OP-P-001, T-V-OP-P-001) |
| 11 | second(T-V-OP-P-001, 49.90) |
| 12 | ElectricalMotor(EM-001) |
| 13 | hasPart(P-001, EM-001) |

As the flow rate increases, the pump motor draws more power to meet the required outlet pressure, as shown in Figure 9. This power is stored in the JPS knowledge graph and expressed as Abox assertions given in Table 3 at a given instant of time. Tbox concept inclusion axioms for all Abox assertions is given in Table 1.

**Table 3:** *Abox assertions for pump motor power response to change in feed flow rate.*

| S.No | Individual assertions |
|---|---|
| 1 | ElectricalMotor(EM-001) |
| 2 | AbsorbedActivePower(APA-EM-001) |
| 3 | hasActivePowerAbsorbed(EM-001, APA-EM-001) |
| 4 | ScalarValue(V-APA-EM-001) |
| 5 | hasValue(APA-EM-001, V-APA-EM-001) |
| 6 | numericalValue(V-APA-EM-001, 126842.70) |
| 7 | PrefixedDerivedUnit(kW) |
| 8 | hasUnitOfMeasure(V-APA-EM-001, kW) |
| 9 | TimeInstant(T-V-APA-EM-001) |
| 10 | hasTime(V-APA-EM-001, T-V-APA-EM-001) |
| 11 | second(T-V-APA-EM-001, 49.90) |
| 12 | PowerTransformer(PTr-001) |

Continued on next page

Table 3 – continued from previous page

| S.No | Individual assertions |
|---|---|
| 13 | isConnectedTo(EM-001, PTr-001) |

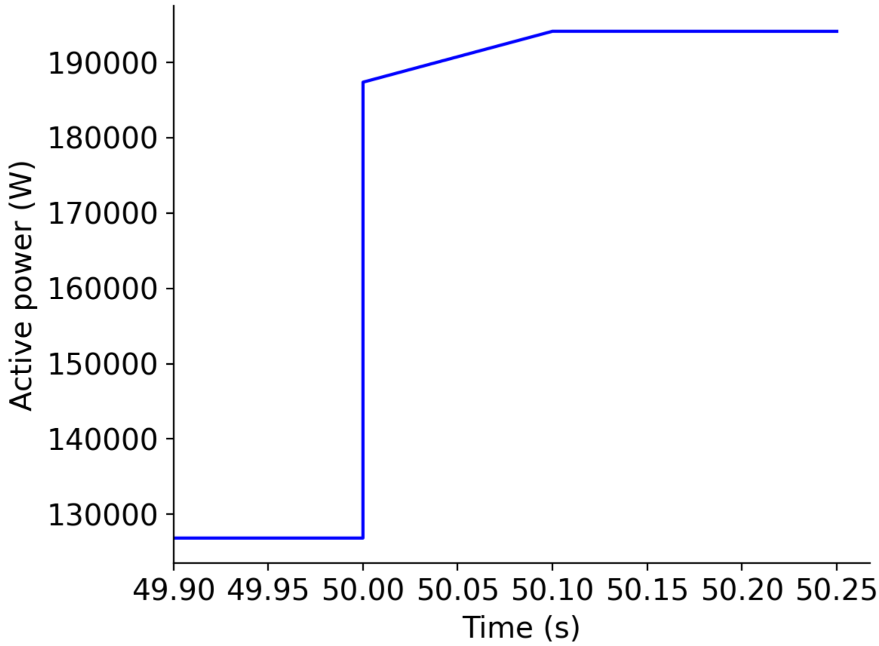


**Figure 9:** *Motor power response to change in feed flow rate for case* 1.

The first assertion in the Table 3 defines the electrical motor $EM-001$ as an instance of $ElectricalMotor$ class of the OntoTwin ontology. The second to eighth assertions establish the relationships between the electrical motor and the power consumed by it. The next three assertions describe the corresponding instant of time. The last two assertions establish the relationship that the electrical motor $EM-001$, which is a part of the pump $P-001$ is connected to the transformer $PTr-001$. If the SPIN inference engine does not detect any constraint violation, the electrical motor response, which is an output of the gPROMS model, is stored in the JPS knowledge graph. The ElChemo framework then runs SPARQL query for the pump motor active power data in the JPS knowledge graph, which is used as an input for the corresponding electrical model to study the power quality effect. The pump motor electrical response is almost identical to the feed change as the electrical system responds faster than its chemical system. The sudden surge in pump motor power requirement will impact the electrical system and cause fluctuations in frequency, voltage, and current.

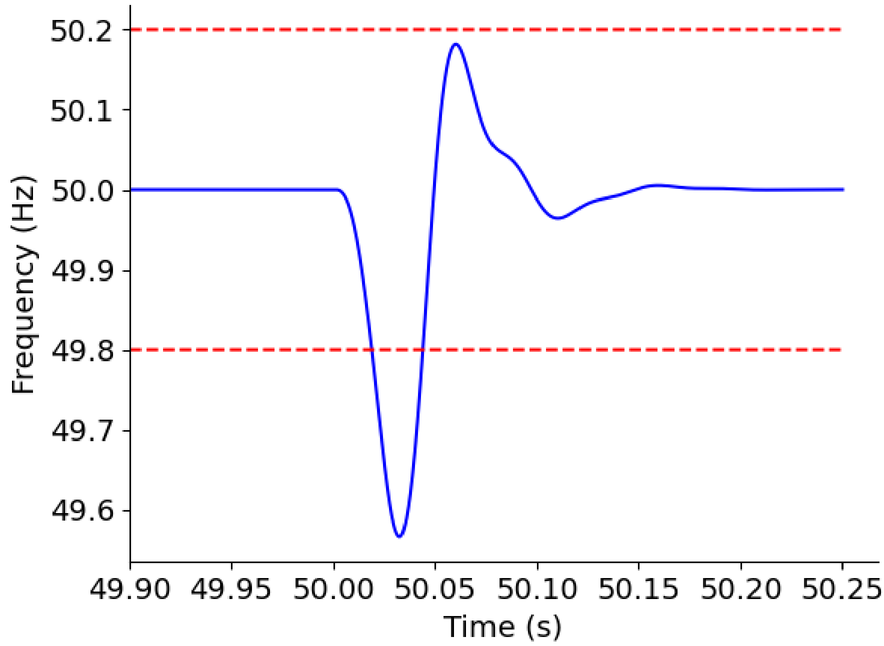


**Figure 10:** *Frequency response of the electrical system measured at the LV side of transformer for case 1. The red dotted lines represents the allowable limits for frequency fluctuations.*

Figure 10 represents the frequency response due to the change in flow rate, and data are stored in the JPS knowledge graph expressed as Abox assertions listed in Table 4.

**Table 4:** *Abox assertions for frequency response to change in feed flow rate.*

| S.No | Individual assertions |
|---|---|
| 1 | PowerTransformer(PTr-001) |
| 2 | RatedFrequency(RFreq-001) |
| 3 | Frequency(Freq-001) |
| 4 | ScalarValue(V-RFreq-001) |
| 5 | ScalarValue(V-Freq-001) |
| 6 | SI_DerivedUnit(Hz) |
| 7 | hasRatedFrequency(PTr-001, RFreq-001) |
| 8 | hasFrequency(PTr-001, Freq-001) |
| 9 | hasValue(RFreq-001, V-RFreq-001) |

Continued on next page

Table 4 – continued from previous page

| S.No | Individual assertions |
|---|---|
| 10 | numericalValue(V-RFreq-001, 50) |
| 11 | maximumValue(V-RFreq-001, 50.20) |
| 12 | minimumValue(V-RFreq-001, 49.80) |
| 13 | hasUnitOfMeasure(V-RFreq-001, Hz) |
| 14 | hasValue(Freq-001, V-Freq-001) |
| 15 | numericalValue(V-Freq-001, 50) |
| 16 | hasUnitOfMeasure(V-Freq-001, Hz) |
| 17 | TimeInstant(T-V-Freq-PTr-001) |
| 18 | hasTime(V-Freq-001, T-V-Freq-PTr-001) |
| 19 | second(T-V-Freq-PTr-001, 49.90) |

The frequency response of the electrical system measured at the LV side of the transformer is validated by the SPIN inference engine to detect any frequency deviation more than the allowable limit of $\pm$ 0.2 $Hz$ as specified by Energy Market Authority (EMA) [1]. It can be seen that at the beginning of the step-change (around 50 $s$), the frequency dips below the allowable limit of $\pm$ 0.2 $Hz$ and falls to 49.6 $Hz$ at around 50.05 $s$ and continues to be below the nominal value for a period of 3 $ms$. At this instant, the SPIN inference engine detects a constraint violation, *i.e.* , value more or less than the specified limit. The ElChemo framework will abort the process, and the values will not be stored in the JPS knowledge graph.

Similarly, the other constraints listed in the Appendix section A.2 are implemented using the SPIN framework to detect any fluctuation in the voltage in the electrical system, as shown in Figure 11. The voltage sag goes beyond the allowable 3% limit set by EMA [16]. Figure 12 shows the corresponding surge in the current due to the dip in the voltage.

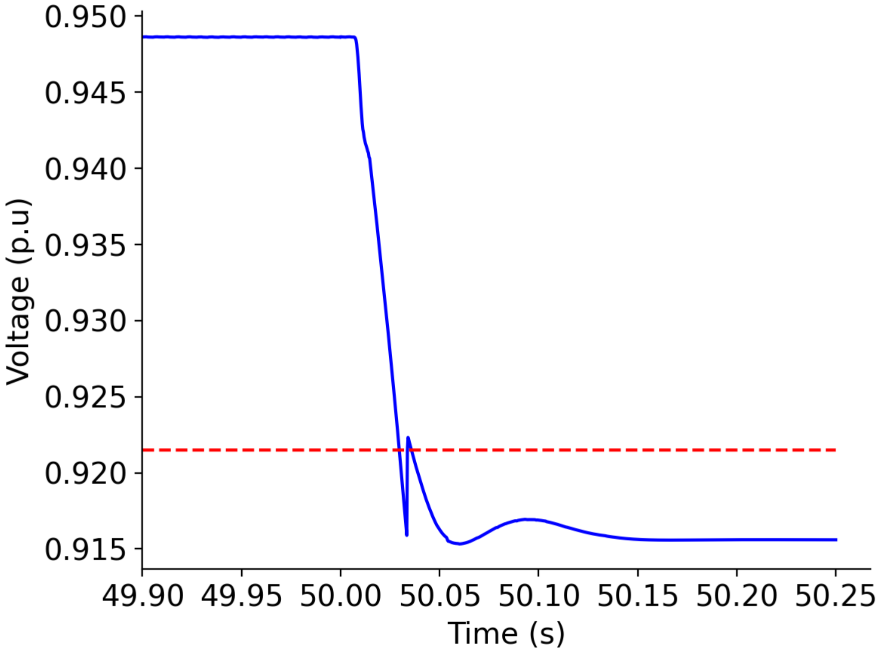


**Figure 11:** *Voltage response of the electrical system measured at the LV side of transformer for case 1.*

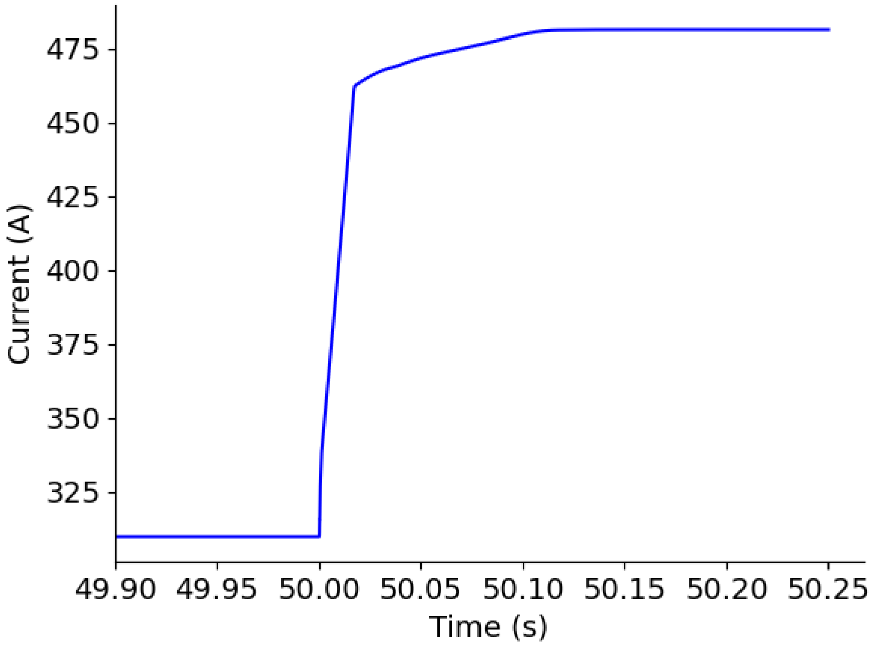


**Figure 12:** *Current response of the electrical system measured at the LV side of transformer for case 1. The red dotted lines represent the maximum allowable dip in voltage.*

The resulting response from the chemical system is shown in Figure 13. It is also observed that the product quality of the distillate never falls below the required 0.973. It is observed that the change in the feed flow rate as a single step function, as mentioned in the case 1 does not violate the constraints for the chemical system, but it is in clear violation of the electrical system parameters and therefore not recommended.

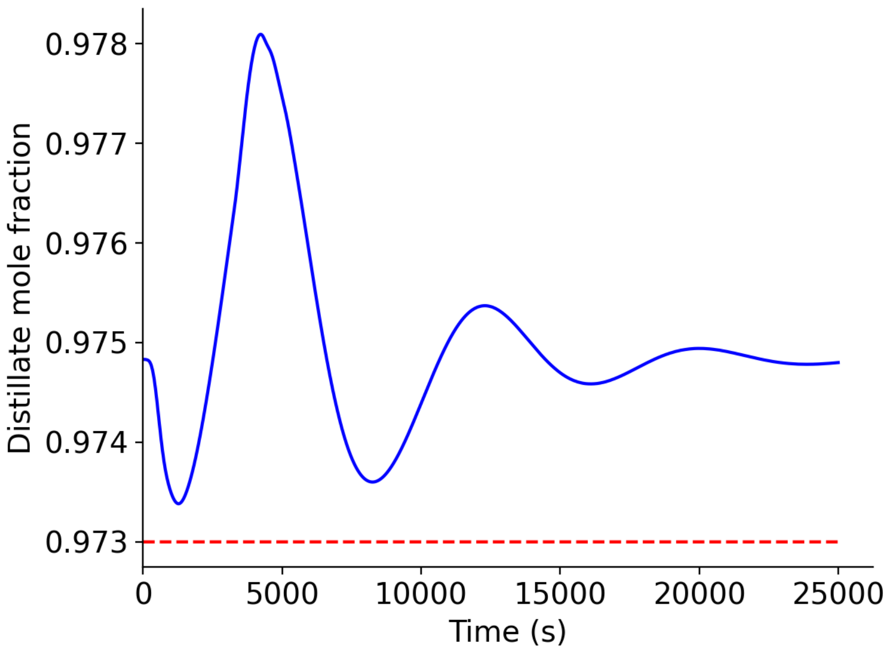


**Figure 13:** *Distillate product quality for case 1. The red dotted line represents the minimum distillate product quality that needs to be maintained.*

#### 7.1.2 Case 2

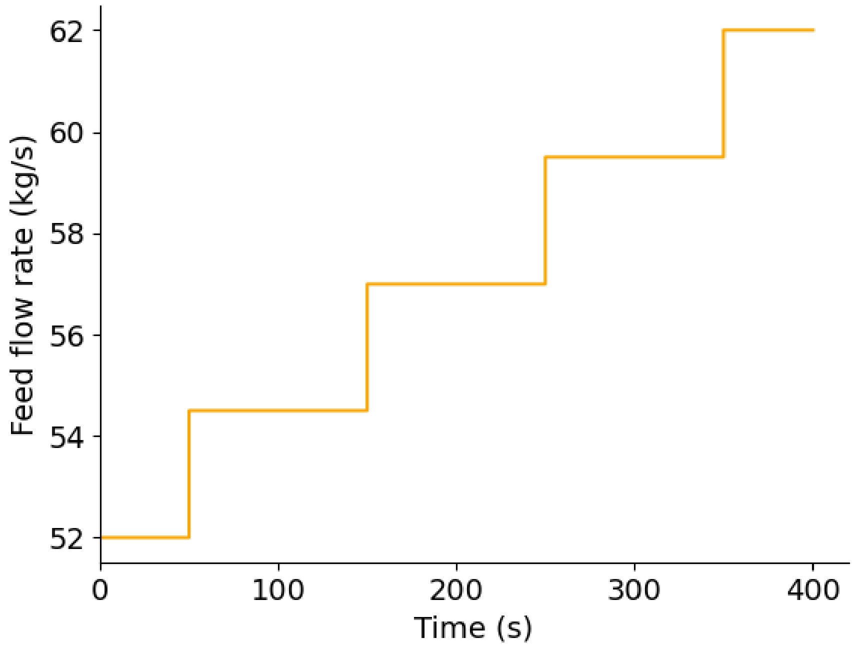


**Figure 14:** *Feed flow rate curve for case 2.*

For the second case, the feed flow rate change is introduced as a series of step changes with a magnitude of 2 $kg/s$ at regular intervals of 100 $s$ as shown in Figure 14. The corresponding active power fluctuations in the motor are shown in Figure 15.

Figure 16 shows the frequency response, and it can be seen that throughout the entire duration of the step changes, the frequency fluctuations are within the allowable limits. The rate at which frequency changes is dependent on the size of the imbalance between supply and demand, the energy stored within the system (in the form of rotating machines), any natural response to frequency, and any control action taken in response to frequency. Each step change introduced for the feed flow rate in case 2 corresponds to 7.5% increase in the pump motor's active power with respect to the rated active power of the transformer. Whereas in case 1, the single-step change introduced in the feed flow rate corresponds to 26% increase in the pump motor's active power with respect to the rated active power of the transformer. Since the change in the active power demand with respect to the rated active power of the transformer is lower for case 2, it is therefore within the specified limits. This is because the system is connected to an infinite grid network that helps to restore the frequency to the nominal operating value of 50 Hz. Similarly, the voltage fluctuations shown in Figure 17 are also within the limits. Figure 18 showcases the corresponding surge in current due to the dip in voltage.

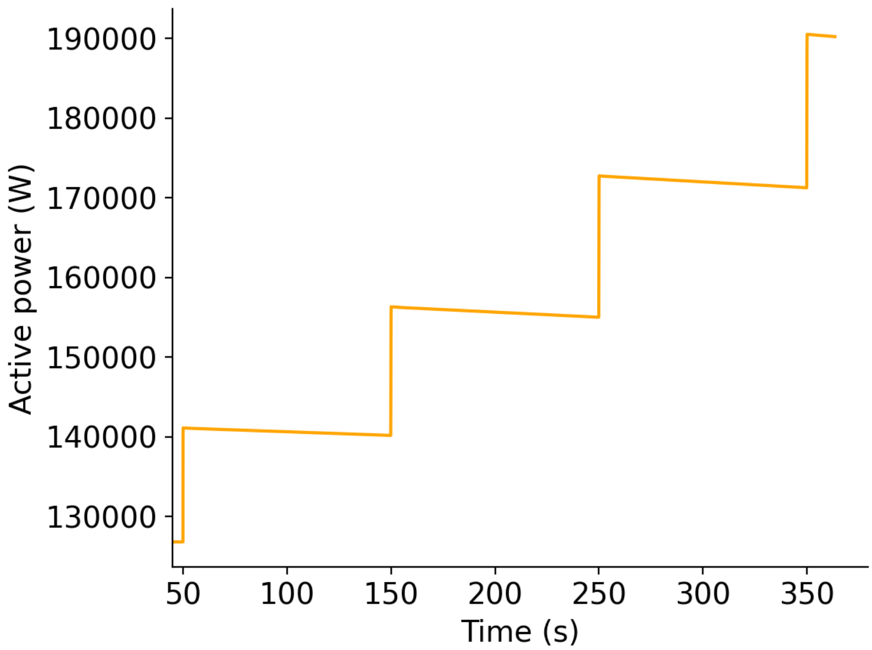


**Figure 15:** *Motor power response to change in feed flow rate for case 2.*

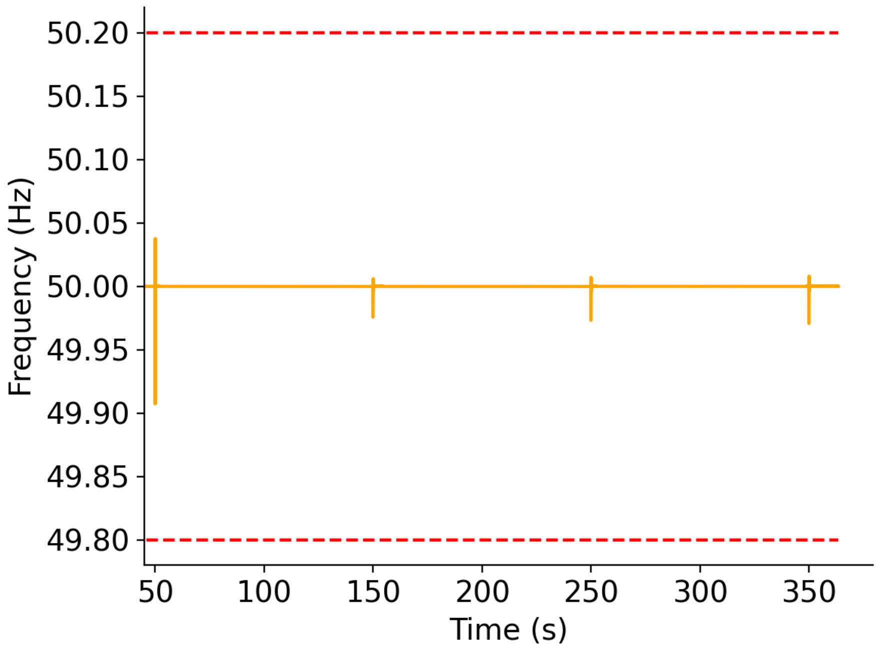


**Figure 16:** *Frequency response of the electrical system measured at the LV side of transformer for case 2. The red dotted lines represent the allowable limits of frequency fluctuations.*

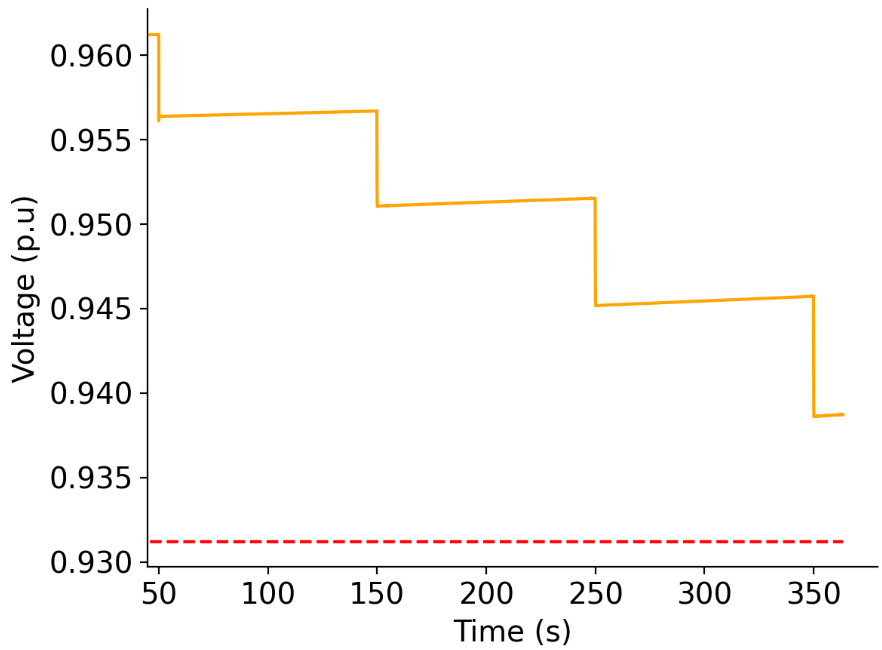


**Figure 17:** *Voltage response of the electrical system measured at the LV side of transformer for case 2. The red dotted lines represent the maximum allowable dip in voltage.*

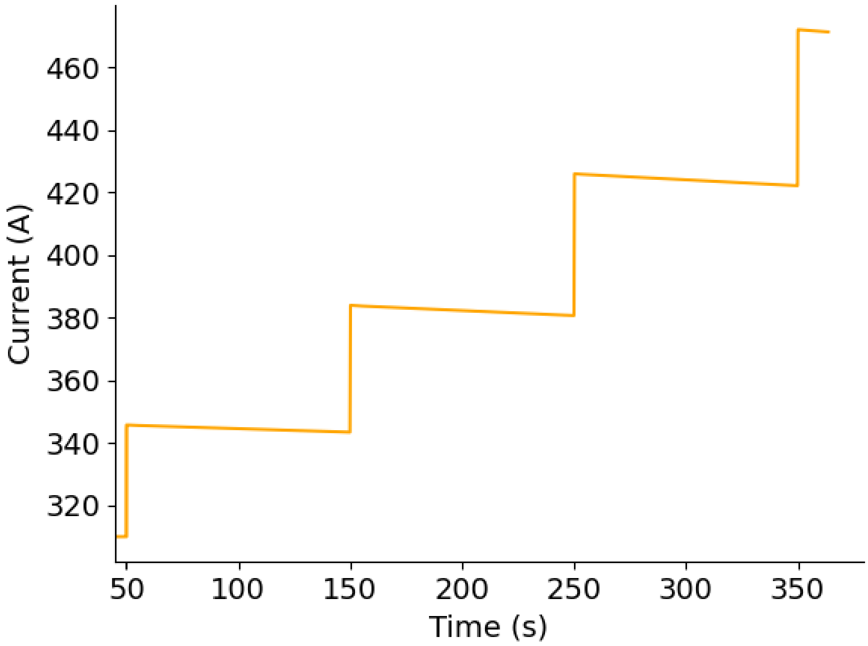


**Figure 18:** *Current response of the electrical system measured at the LV side of transformer for case 2.*

Figure 19 shows the distillate quality for the chemical system. It can be seen that the curve is almost identical to the product quality for case 1 (see Figure 13). This is because the response time for the chemical system is longer compared to the electrical system. It means that change in the feed flow rate for both cases are almost identical from the chemical system's perspective due to the short duration of time in which it happens. Therefore, it is recommended to increase the feed flow rate as a series of step changes, as mentioned in case 2 to adhere to the constraints in both the chemical and electrical domains due to the increase in the demand for the final product.

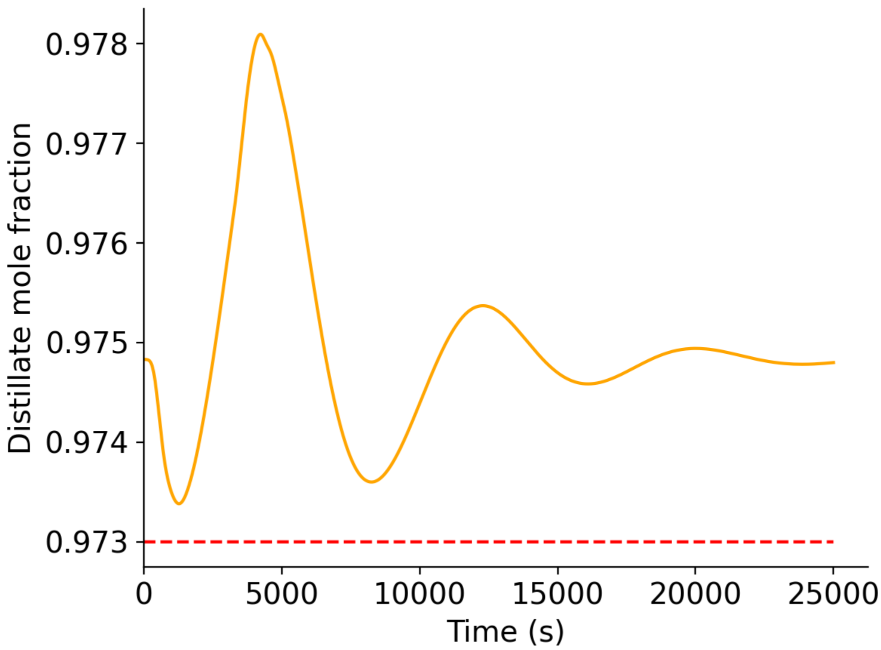


**Figure 19:** *Distillate product quality for case 2.*

## 7.2 Design Optimisation: Electrical System

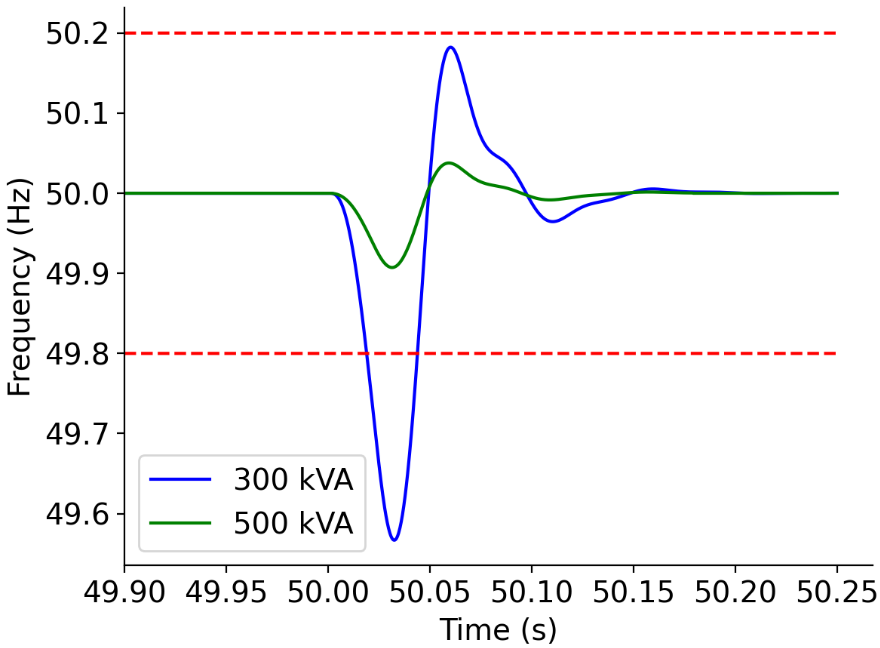


**Figure 20:** *Frequency responses of the electrical system measured at the LV side of transformer for 300 kVA and 500 kVA ratings of transformer. The red dotted lines represent the allowable limits of frequency fluctuations.*

In this section, a comparative study is made between two different transformers' ratings to determine the optimum design of the transformer for the electrical system based on the best operating decision derived in the previous section, which will result in the cost-savings.

The transformer chosen for this case study has a rating of 300 $kVA$ as opposed to the standard design, which would have been 500 $kVA$. The cost difference between the two systems is around \$ 50,000. Figure 20 provides a comparison of the frequency response for both the ratings of the transformers due to a single step-change in the feed flow rate as discussed in case 1. It is observed that the frequency fluctuation for the 500 $kVA$ transformer is within the limit throughout the disturbance in the chemical system. Similar effects can be seen for the voltage response as shown in Figure 21.

It can be observed that the frequency and voltage deviation can be significantly reduced by using a higher rating transformer. This is because the change in the active power demand with respect to the rated active power for the transformer rated at 500 $kVA$ is 15.55%, which is much lower than the value of 26% for the transformer rated at 300 $kVA$. Most industries are willing to pay for this over-design as they lack the knowledge in the electrical system response due to the disturbances or changes in the other domains.

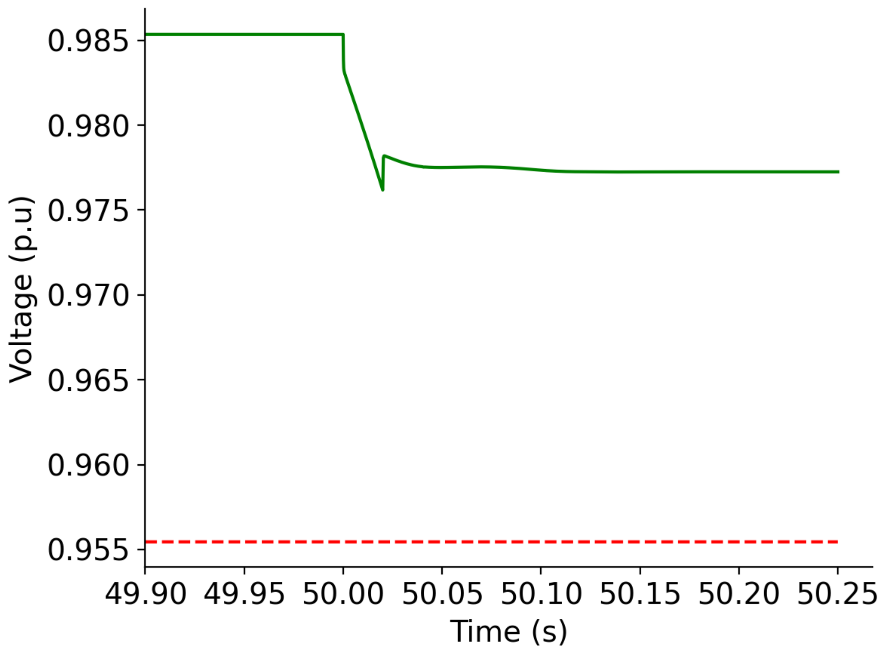


**Figure 21:** *Voltage responses of the electrical system measured at the LV side of transformer for 500 kVA transformer. The red dotted lines represent the maximum allowable dip in voltage.*

The ElChemo framework implemented in the JPS helps to address this challenge by establishing cross-domain communication between the chemical and electrical domains in a chemical plant. The digital coupling of the electrical and chemical systems will help the industries to select equipment with a lower rating, resulting in cost savings. It can be observed from Figure 16 and 17, for the 300 $kVA$ transformer, with a multiple-step change in the feed flow rate, both the frequency and voltage do not violate the specified limit. In Figure 20 and 21, for the 500 $kVA$ transformer, both the frequency and voltage deviations for the electrical system are within the specified limits even with the single-step change in the feed flow rate. Since the product quality does not change with the type of step changes introduced in the feed flow rate, it is recommended to choose a 300 $kVA$ transformer for the presented electrical system. The best operating decision discussed in the previous subsection needs to be adopted to increase the final product demand.

# 8 Conclusions

An ontology for cross-domain interoperability between various heterogeneous silos, named OntoTwin, has been proposed within the JPS. DL syntax has been used to describe the OntoTwin ontology in this paper. The OntoTwin ontology establishes interactions between the chemical and electrical systems in a plant. The major contributions of this paper are:

- Introduction of the OntoTwin knowledge base implemented as OntoTwin ontology that extends the JPS knowledge graph.

- Development of ElChemo framework for autonomous operational optimisation of interactions between chemical and electrical systems.
- Implementation of DL reasoning and SPIN inference to detect any logical inconsistency and constraint violation.
- Discussion of a possible agent composition approach for formalising the ElChemo framework.
- Operational optimisation for the equipment in the electrical system.

All of these contributions allow semantic interoperability between tools in chemical and electrical engineering domains such as gPROMS [2] and MATLAB [26]. OntoTwin ontology will implement all the functionalities that describe the behaviour of the chemical process and electrical system models in the near future. We aim to increase the reusability and interoperability between data, models, and software from different domains to perform cross-domain analysis.

# Acknowledgements

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# List of abbreviations

| | |
|---|---|
| **M2M** | **M**achine-to-**M**achine |
| **JPS** | **J**-**P**ark **S**imulator |
| **EIP** | **E**co-**I**ndustrial **P**ark |
| **HPC** | **H**igh **P**erformance **C**omputing |
| **SFTP** | **S**SH **F**ile **T**ransfer **P**rotocol |
| **OWL** | **W**eb **O**ntology **L**anguage |
| **XML** | e**X**tensible **M**arkup **L**anguage |
| **DL** | **D**escription **L**ogics |
| **SWRL** | **S**emantic **W**eb **R**ule **L**anguage |
| **SPIN** | **SP**ARQL **I**nference **N**otation |
| **PQ** | **P**ower **Q**uality |
| **KMS** | **K**nowledge **M**anagement **S**ystems |
| **EMA** | **E**nergy **M**arket **A**uthority |
| **MSM** | **M**inimal **S**ervice **M**odel |
| **PMU** | **P**hasor **M**easuremnet **U**nit |
| **LV** | **L**ow **V**oltage |
| **ONAF** | **O**il **N**atural **A**ir **F**orced |
| **kW** | **k**ilo **W**att |
| **kV** | **k**ilo **V**olt |
| **kVA** | **k**ilo **V**olt **A**mpere |
| **kVAR** | **k**ilo **V**olt **A**mpere **R**eactive |

# A Appendix

## A.1 Properties of the equipment in the chemical and electrical system

**Table 5:** *Feed properties*

| Property | Value |
|---|---|
| Design flow rate | 65 $kg/s$ |
| Temperature | 270 $K$ |
| Pressure | 3 $atm$ |
| Mole fraction of propane | 0.4 |
| Mole fraction of isobutane | 0.6 |

**Table 6:** *Feed pump properties*

| Property | Value |
|---|---|
| Pump model | KSB Multitec ABCD |
| Pump type | Multi stage centrifugal pump |
| Motor design rating | 200 $kW$ |
| Design RPM | 2900 $rpm$ |
| Flow rate | 1500 $m^3/h$ |
| Maximum head | 1000 $m$ |
| Set point pressure | 14 $atm$ |

**Table 7:** *Distillation column properties.*

| Property | Value |
|---|---|
| No. of trays | 32 |
| Feed tray | 14 |
| Column diameter | 5.91 $m$ |
| Allowed flooding factor | 0.8 |
| Tray spacing | 0.61 $m$ |

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Table 7 – continued from previous page

| Property | Value |
|---|---|
| Tray efficiency | 0.4 |
| Active area fraction | 0.8 |
| Weir height | 0.025 *m* |
| Tray thickness | 0.002 *m* |
| Hole diameter | 0.0045 *m* |
| Flow coeff. per stage | $3x10^{-8}$ |
| Reflux ratio | 0.77 |
| Hole area fraction | 0.1 |

**Table 8:** *Design properties of equipment in the chemical system.*

| Property | Value |
|---|---|
| **Pump controller** | |
| Controller gain | 1 |
| Integral time constant | 2.56 *min* |
| Derivative time constant | 04 |
| Discharge pressure set point | 14 *atm* |
| **Feed pre-heater** | |
| Outlet temperature | 330 *K* |
| Pressure drop | 0.1 *bar* |
| **Reboiler** | |
| Diameter | 5.08 *m* |
| Length | 10.16 *m* |
| Liquid level | 6.35 *m* |
| **Reboiler level controller** | |
| Controller gain | 1 |
| Integral time constant | 20 *min* |
| Derivative time constant | 0 |

Continued on next page

Table 8 – continued from previous page

| Property | Value |
|---|---|
| **Condenser** | |
| Diameter | 4.08 $m$ |
| Length | 8.16 $m$ |
| Liquid level | 2 $m$ |
| **Condenser level controller** | |
| Controller gain | 1 |
| Integral time constant | 20 $min$ |
| Derivative time constant | 0 |

**Table 9:** *Rating of the transformer connected in the electrical system.*

| Property | Value |
|---|---|
| Power rating | 300 $kVA$ |
| Rated voltage | $6.6/0.4$ $kV$ |
| Winding connection | $Y_g/Y_g$ |
| Frequency | 50 $Hz$ |
| Impedance | 14.5 % |
| Cooling | ONAF |

**Table 10:** *Rating of the motor connected in the electrical system.*

| Property | Value |
|---|---|
| Type | Squirrel cage induction motor |
| Rated power | 200 $kW$ |
| Rated voltage | 400 $V$ |
| Frequency | 50 $Hz$ |
| Full load speed | 2900 $rpm$ |
| Pole | 2 |

## A.2 Constraints

- If the distillate's mole fraction of propane and bottoms' mole fraction of isobutane is greater than or equal to 0.973 then the chemical system model is acceptable.
- If the change in flow rate is more than 1% within a second, then the electrical model should be executed to detect any power quality disturbance.
- Voltage Fluctuation: The voltage difference from nominal is within $\pm 3\%$ of nominal value for step changes.
- Voltage Supply: The allowable voltage variation for transmission and distribution network is $\pm 6\%$.
- Frequency Deviation: A deviation of $\pm 0.2\ Hz$ is allowed in the frequency.

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