Modelling Decision Support Systems using Conceptual Constraints

Linking Process Systems Engineering and Decision Making Models

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Abstract: This paper presents the use of a Conceptual Constraint (CC) Domain to systematize the construction of Decision Making Models (DMMs). The modelling systematics include the integration between the CC Domain and production systems as well as an identification procedure which contains some steps aimed at constraint identification using the CC Domain. The CC Domain consists of different modelling elements such as Conceptual Constraints (generic constraint types), Conceptual Components (pieces of a constraint), and Conceptual Component Elements (pieces of a conceptual component that may be connected to production systems). In this instance, the CC Domain is integrated with the Process Systems Engineering (PSE) Domain as a production system domain. The PSE Domain contains information from the multi-level functional hierarchical in an enterprise and it will be used to cover a wide range of scenarios related to hierarchical integration of DMMs. In addition, an integration step between the CC and PSE Domains is illustrated. The focus of the work is to show how these models should be developed in order to be properly integrated, and how they are used by different functionalities with an identification procedure.

1 INTRODUCTION

Process Systems Engineering (PSE[1]) may be described as the art of decision-making for engineering disciplines such as design, operation, and control of chemical, physical, and biological processes through the aid of systematic computer based methods and optimization tools (Grossmann and Westerberg, 2000). The PSE community uses conceptualized modelling in order to support systematic problem solving. Recently, ontological modelling has been used to build semantic structures, while Knowledge Engineering (KE) foundations have been implemented as a new modelling paradigm with the purpose of supporting chemical process engineering (Morbach et al., 2007), managing chemical batch processes (Muñoz et al., 2010), data reconciliation (Roda and Musulin, 2014), pharmaceutical product engineering (Remolona et al., 2017), etc. In addition, there are other communities working on similar issues that PSE attempts to solve (e.g. planning & scheduling (Palacios et al., 2016), failure prevention (Rajpathak et al., 2001)).

Ontologies use semantic structures, which aim to represent an abstraction of a domain as well as support KE applications in many applications such as Decision Support Systems (DSSs), Artificial Intelligence, etc. DSSs contain a big range of functionalities and connections to different domains (Shim et al., 2002). While the conceptualization of Decision Making Models (DMMs) in information systems is crucial, its systematization remains an open research field. There are many types of DMMs that may be used rather than mathematical programming (e.g. dynamic programming or simulations). Addi-

Table 1: Abbreviations.

Abbr	Explanation
BaPron	Batch Process Ontology
CC	Conceptual Constraint
CComp	Conceptual Component
CCompEl	Conceptual Component Element
DMM	Decision Making Model
DSS	Decision Support System
ISA88	Batch Control Standard from International Society of Automation
KE	Knowledge Engineering
PSE	Process Systems Engineering

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[1] Complete list of abbreviations are given in Table 1.

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tionally, the PSE Domain structure may vary from multi-level hierarchical systems to other systems (e.g. multi-scale systems, systems of systems, interwoven systems). However, this work considers (i) multi-level hierarchies in order to model the information presented in production systems and (ii) DMMs based on mathematical programming.

2 BACKGROUND

2.1 DMMs Related Background

The DSSs based on mathematical programming, have been a topic of great interest in recent years; moreover, mathematical programming has been used to tackle modelling issues in the solution stage of decision-making procedures.

Mathematical programming has been used to support strategic, tactical, and operational decisions based on the production and distribution activities of a production system. However, a hierarchical integrative approach can represent an alternative to mathematical programming. Under this approach, relevant information is aggregated to develop proper mathematical models (Bradley et al., 1977). DMMs based on mathematical programming mainly consist of following items (Williams, 2013):

Sets: include indices for certain classes of variables, indicating the size/complexity of the model to be solved.

Parameters: coefficients of the model (defined as a scalar or matrix).

Variables: decision variables of the model.

Constraints: relation between parameters and variables which have to be considered to ensure feasibility of the proposed decision.

Objective: expression to be minimized or maximized during the decision-making procedure.

Traditionally, DMMs in production systems are constructed manually according to the existing data and problem features (e.g. time horizon, decision variables and parameters, definition of constraints, and selection of objective functions). However, there is a lack of generic systematics for the construction of such models (Gani and Grossmann, 2007).

The previous classification of the DMM elements is generally used for demonstration purposes and the systematic development of general formulations aiming to solve a domain problem in a generic way. However, the connections among constraints and other elements (such as sets, parameters and variables) are not straightforward inside a formulation and these connections do not appear among different formulations. Some of the main types of constraints are (Williams, 2013):

- productive capacity constraints or manpower,
- raw material availability,
- marketing demands and limitations,
- balance constraints (e.g. energy and material),
- quality stipulations,
- hard and soft constraints that can be violated or can be violated by means of an extra cost,
- chance constraints related to probability, and
- simple and generalized upper bounds.

These constraints are generally used to create the DMMs by selecting and revising according to the analysis of the process. However, this constraint classification is not enough to support the automated construction of DMMs. For this reason, the CC Domain has been proposed and patterns of constraints are suggested to be used during the conceptual modelling of the CC Domain (Dombayci and Espuña, 2018).

2.2 PSE Related Background

Over the last decades, ontology development and usage have been important subjects in applications related to KE, Artificial Intelligence, Natural Language Processing, etc. In the case of PSE, the extensive exploitation of general PSE ontologies to support the development and maintenance of models, as well as their integration and coordination with system/models from the related areas/domains is object of growing interest (Morbach et al., 2007, Muñoz et al., 2010,Roda and Musulin, 2014,Remolona et al., 2017). The research on these application has supported the management of the great amount of information related to the problem statement and the new exploitations has supported development and (re)used of conceptual models.

The need of a generic model to support PSE activities has been recognized from the very beginning of the PSE. A reference model for computer integrated manufacturing has been developed (Williams, 1989) as a conceptual representation of the system and it has evolved to a widely used ANSI standard on batch control as ISA88 (ISA, 2010). The interdisciplinary area of PSE and KE, different methodologies have been developed which centre on the creation of domain knowledge. The batch process ontology (BaPrOn) is built from the concepts of a batch control standard (ISA88) and used in order to monitor and control the scheduling in a pilot plant (Muñoz et al., 2010). The intention of not just communicating but also supporting the integration of different software tools and exploitation of plant database information are also considered (Muñoz et al., 2012). Additionally, integration between planning and scheduling activities in batch processes have been modelled using ontology modelling techniques (Vegetti and Henning, 2015).

The ISA88 standard has supported the background of the PSE Domain with the main model representations: process, procedural, and physical models. These models contain the hierarchical representation of production systems and connections between these model elements. The ISA88 has also been used to build another ontology which is a result of a systematic approach for the construction of domain ontologies (Dombayci et al., 2015). The methodology has two main steps: (i) a procedure for extraction of concepts and class-subclass pairs from a technical document (Farreres et al., 2014) and (ii) a systematic procedure for solving inconsistencies and contradictions arisen from the first step. These two steps constitute a semi-automatic ontology construction methodology. In addition, the semi-automatic procedure produces a list of suggestions for improving technical documents by analysing the conceptual model that is semi-automatically constructed from the source (Dombayci et al., 2017). But more importantly basic concepts related to the standard are extracted and the multi-level hierarchical structure of ISA88 has been introduced with its concept and relations.

3 METHODOLOGY

The basic structure underlying the system and concepts in CC Domain is detailed in Section 3.1. The integration of PSE Domain is suggested to enhance the CC Domain functionalities and the integration using ontological elements such as concepts, object properties, data properties, and instances are presented in Section 3.1.

In addition, the general steps are introduced related to the functionalities that can be used to demonstrate the domain applications is detailed in Section 3.3. The identification procedure related steps are introduced in Section 3.3.1 and the last step related to the identification is presented in Section 3.3.2 with a case study.

3.1 The Conceptual Constraint Domain

The conceptualization of DMMs in a Conceptual Constraint (CC) Domain is important for the automated building of DMMs using a knowledge-based system. Therefore, the construction of integrated ontological models and their usage in order to provide conceptualized models for the CC Domain functionalities are studied. This work demonstrates the modelling, the integration, and the connection of DMMs and knowledge models from the PSE point of view in order to maintain a complete DSS. The main aim is to link these two domains together in order to develop systematic strategies for supporting decision-making procedures.

The basic design of the CC Domain is the abstraction of the DMMs that are constructed through constraints, sets, parameters, and variables; ontological modelling techniques are adopted to model the domain with ontological model elements. There are 3 main types of concepts that belong to this ontological model: the Conceptual Constraint (CC), the Conceptual Component (CComp), and the Conceptual Component Element (CCompEl). A relational demonstration of these elements is shown in Figure 1 and this figure is adapted for the case study in Figure 5(see Section 3.3.2).

The CCs represent the semantic models of the main types of constraints, which are built from the main publications containing DMMs related to production systems. The first step is to build a taxonomy that captures the main constraints such as 'BalanceCC', 'ResourceAllocationCC', 'TimingCC', 'SizingCC', 'SequencingCC', and 'EconomicalCC'. Then, the taxonomy is detailed considering these main types of constraints, as depicted in Figure 2. The CCs are separated into fundamental constraint types, then the CC taxonomy is deepened with subclasses. For instance, the 'BalanceCC' has the 'MaterialBalanceCC' and the 'EnergyBalanceCC' concepts as subclasses, which share the balancing as a common element as well as the same CComps such as the 'StoredAmount'. Depending on characteristics of the CC the 'StoredAmount' CComp may change from energy to material and the CCompEls that are connected to the PSE Domain change from a concept connected to an energy to material.

The CComps represent the concepts that construct the CCs. The partOf relation connects CCs and CComps in order to construct the patterns of each CC; each CComp may be connected to more than one CC. The elements in the DMMs (parameters, variables) are represented through CComps. The representation of these elements is straightforward, for example, the

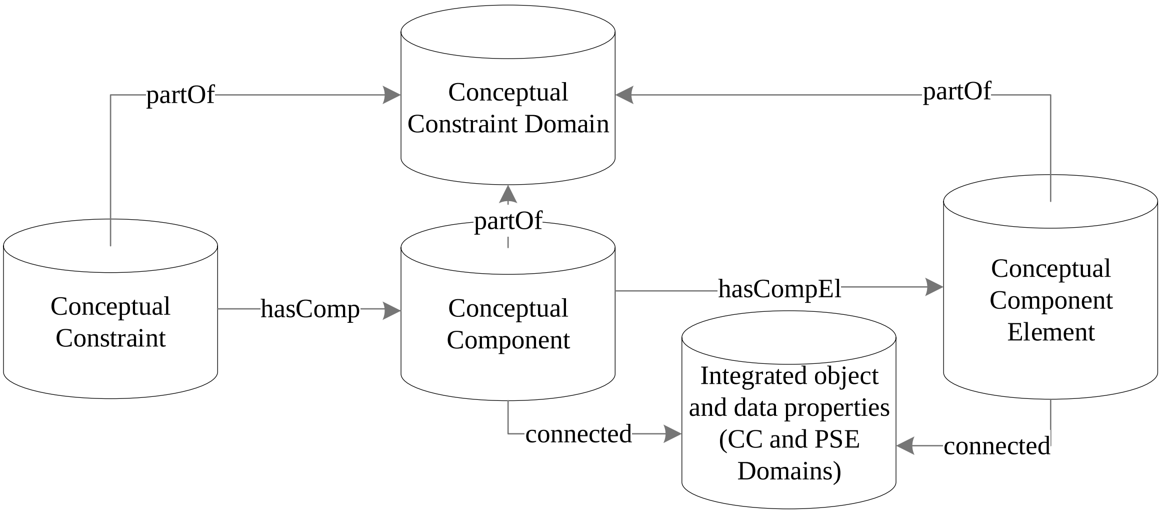


Figure 1: Relations in the CC Domain.

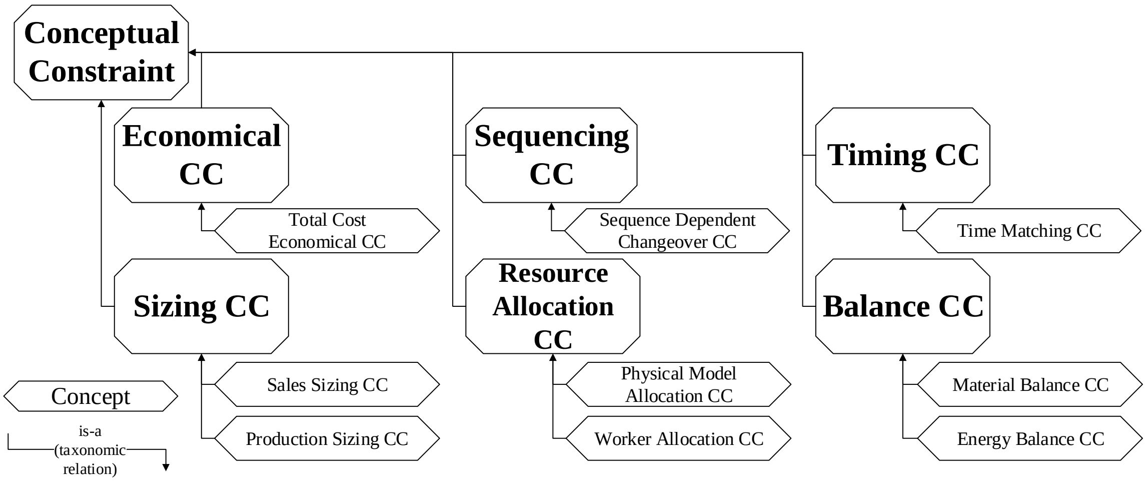


Figure 2: Part of the Conceptual Constraint Taxonomy in the CC Domain.

CComp 'ProducedMaterial' may present a variable. On the other hand, the 'ProducedMaterial' CComp may present an expression that is constructed from a variable and a parameter. For instance, the 'ProducedMaterial' may present a proportion (parameter) of the input material (variable).

The CCompEls represent the connections of the CComps to the different concepts, which appear in the conceptual domain (i.e., the PSE Domain) in order to carry out the applications. Therefore, the CComps are connected to the CCompEls for the definition of a DMM. For instance, the 'ProducedMaterial' CComp may be defined with a unit in one DMM and with a process cell in another DMM.

3.2 Integration of the CC and PSE Domains

The Material Balance CC example is depicted in Figure 3 containing the 'ProducedMaterial' CComp and its relations. Two separate sections are used for the CC and PSE Domains. The CC Domain section the CCs are connected to CComps. In the CC Domain section the CCs are connected to CComps, while the CCompEls are connected to their specific concepts in the PSE Domain. Then, each CComp is connected to the CCompEls that exist in PSE Domain. The example shows that *'a MaterialBalanceCC has ProducedMaterial as a CComp'* and *'ProducedMaterial CComp may be linked to 4 different CCompEls depending on the DMM-formulation (F1, F2, F3, F4)*. These formulations represent different DMMs

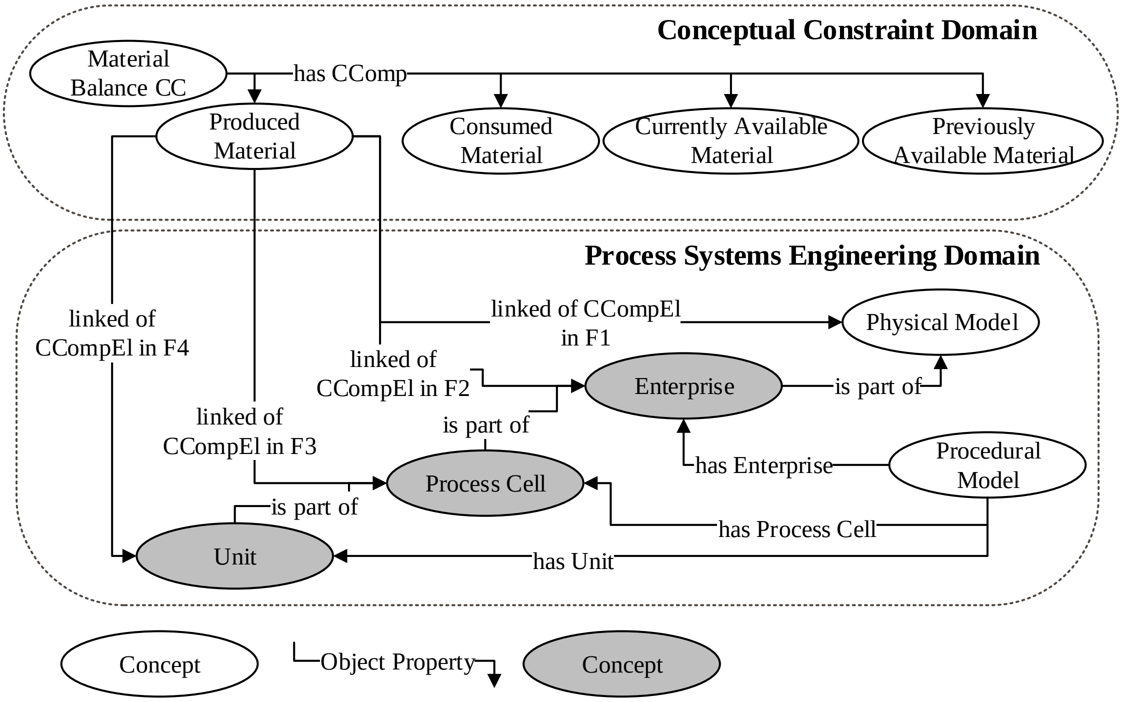


Figure 3: Connections between CC and PSE Domains.

in the multi-level hierarchies. However, these elements appear in the PSE Domain where another taxonomy exists. In this sense, the 'PhysicalModel' concept has different sub-concepts and the 'ProceduralModel' is connected to these elements of physical model through the 'ProceduralModel'. In addition, a 'partOf' relation is depicted in the PSE Ontology that contains the hierarchical model representation of an enterprise.

3.3 Functionalities

The integration between the CC and PSE Domains brings these domains together for the applications; for example, extending the DMMs arisen in a specific hierarchical level to another level or using an already constructed DMM for a specific problem instead of constructing a new DMM from the beginning. In this section, 5 steps required for the constraint prediction application are explained. The first 3 steps are the steps that are general steps to be used in many functionalities include parsing and matching from sets, parameters, variables and equations to the CC Domain elements. Afterwards, Section 3.3.1 introduces the fourth step that is a network construction from the DMMs. The fourth step is required for the explanation of the functionality explained in Step 5 in order to predict the CC type.

Here, the basic steps required in order to identify a constraint within the framework, starting from a constraint that is written using a high level syntax are explained:

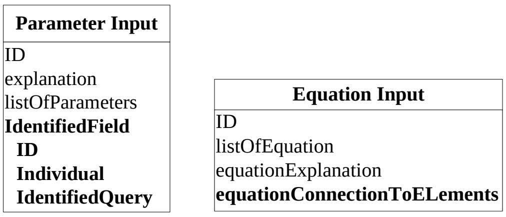
Step 1: The first step is to parse the source containing a constraint that is to be identified within the pre-determined structure. The DMM equations are decomposed into elements by automatically parsing a source file into set, variable, parameter and equation inputs.

Step 2: The DMM elements found in the previous step are matched in a list of CComps and CCompEls. For instance, set inputs are matched to the CCompEls, whereas parameter and variable inputs are matched to the CComps. The matching step can be performed in two ways: (i) direct user interaction and/or (ii) based on a dictionary that stores user decisions for previous matching procedures. The information coming from a user interaction or the dictionary are used in the Step 3 for matching the connections between equations. Inputs are stored in a structure contains IDs, explanations, list of parameters and corresponding identified fields as depicted in Figure 4(a).

Step 3: The equation inputs are connected to the CC Domain elements (CComps and CCompEls) through the set, parameter and variable inputs. These connections are stored as 'equation connections to the elements' in enriched equation input structure as illustrated in Figure 4(b).

Table 2: Connections of Equation 1.

Symbol	Explanation from the source paper	CC Domain connection (CComp)	PSE Domain connection (CCompEl)
K	**Set:** energy storage systems ($k \in K$)		PhysicalModel
TRH	**Set:** time intervals included in the current prediction horizon ($t \in TRH$)		Time Model
η_k^{in}	**Parameter:** charging efficiency of energy storage system k	ChargingEfficiency	PhysicalModel
η_k^{out}	**Parameter:** discharging efficiency of energy storage system k	Discharging Efficiency	PhysicalModel
$Ld_{k,t}$	**Variable:** energy supplied to load system k during interval t (kW h)	SuppliedDemand	PhysicalModel, TimeModel
$SP_{k,t}$	**Variable:** energy supplied by storage system k during interval t (kW h)	SuppliedDemand	Physical Model, TimeModel
$SE_{k,t}$	**Variable:** electricity storage level of system k at the end of the interval t (kW h)	CurrentlyAvailable Amount	PhysicalModel, TimeModel



(a) Parameter Input. (b) Equation Input.

Figure 4: Enriched Input Structures.

3.3.1 The Network Construction

This section illustrates how constraint identification is managed in the domain by exploiting the already established connections between the CC and PSE Domains. The Step 4 introduces complete and consistent DMMs containing known constraints as input.

Step 4: A network is built through the CC Domain using the CC Domain model information that was previously developed using the Machine Learning Toolbox of Matlab. A Bayesian network is build using CComp and CCompEls as features of each class (CCs) so that the network can be used to predict the type of the introduced constraint.

3.3.2 The Constraint Identification and the Case Study

The Step 5 is the core step that uses the general steps (1-3) and network construction and predicts the type of the constraint.

Step 5: This step combines all the connected-identified elements of an equation and the CC Domain network in order to predict the type of the CC in the domain. As a result, a set of probability values are received corresponding to the unknown constraint.

Constraint Identification Case Study: In order to demonstrate the constraint identification, an energy balance equation from an energy supply and demand planning DMM is used (Silvente et al., 2015):

$$SE_{k,t} = SE_{k,t-1} + \eta_k^{in} * Ld_{k,t} - \frac{SP_{k,t}}{\eta_k^{out}}, \forall k \in K, t \in TRH \tag{1}$$

Equation 1 has been parsed and paired through the same procedures explained in Section 3.3 (Step 1-3). Table 2 shows the full list of symbols, nomenclature explanations of these symbols from the source paper and connected elements in the CC and PSE Domains. The connected elements of the sets (K and TRH) are the CCompEls and the rest of the symbols belong to the CComp type of concepts. Accordingly, while sets have the same concept in the PSE Domain column, the CComps (variables and parameters) have connected CCompEls.

Relations in the CC Domain are shown in Figure 5. The connections of elements in the CC Domain are depicted with the example including the relations between the models. The demonstrative example is used as an instance of the domain where the parsed and matched information are shown. For instance, Equation 1 is depicted as a 'BalanceCC' since there are many CComp connections with the hasComponent relation. After the implementation of Step 5, the prediction probabilities are obtained as in Figure 6. As a result, the constraint in Equation 1 is predicted as a 'BalanceCC' with 0.64 probability and an 'EnergyBalanceCC' with a probability of 0.07 (the remaining predictions are less than 0.03); note that the classification is made by evaluating 41 types of CCs. The domain model can be continuously improved as new formulations are reviewed. The results are expected to have higher probability value while the domain model

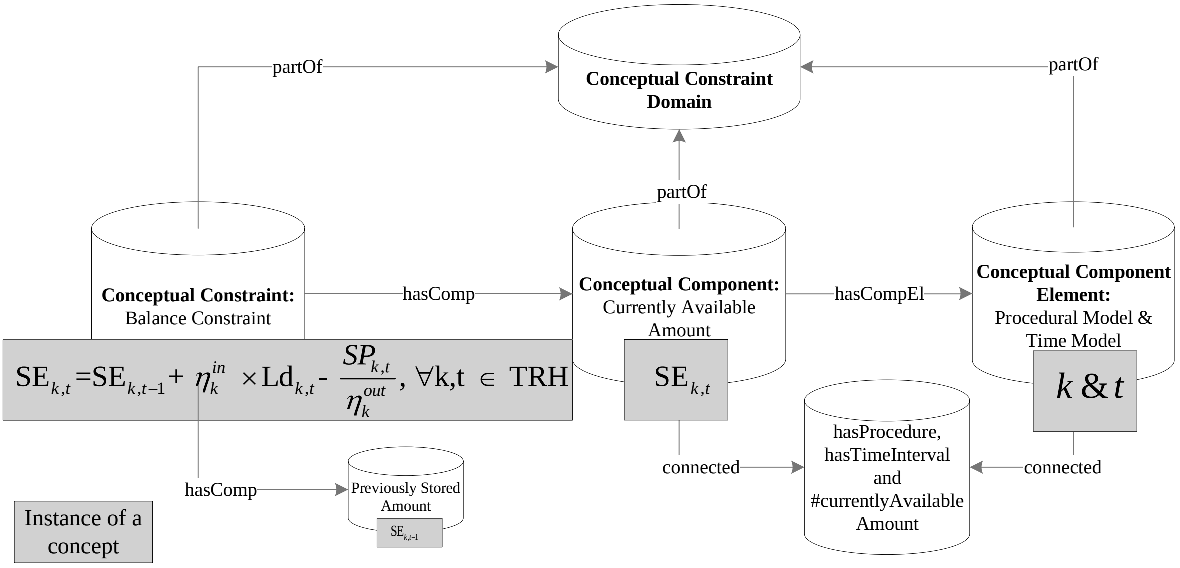


Figure 5: Connections of Conceptual Models with the Example.

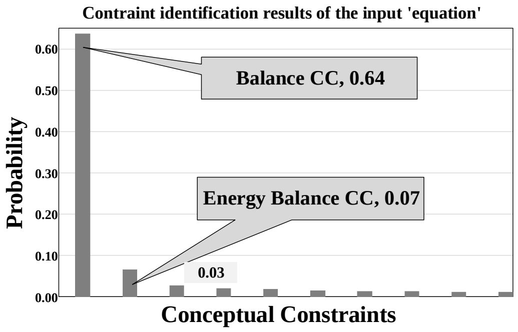


Figure 6: Result of Identification of Equation 1 (x-axis represents each CC and y-axis gives the probability of being in the same CC).

is getting more accurate and larger in terms of different formulations introduced.

The purpose of the identification procedure is not only to predict the type of the constraint but also to fully identify the constraint connections to the domain. Therefore, all connections related to the constraint have been introduced to the system. The constraint is defined as a Balance CC with the connections to the specific physical model used but it can be expected to be used in any extension procedure by simply changing the connections in the PSE Domain.

4 CONCLUSIONS

This paper has presented a framework aiming to support construction of Decision Making Models (DMMs) using the Conceptual Constraint (CC) Domain. The construction of DMMs requires a procedure that involves a DMM abstraction and the integration with domains connected to the main purpose. The CC Domain contains the generic/abstract model information of DMMs and conceptualized patterns of constraints. Therefore, the CC Domain is adequate for representation of constraints. A production system domain, the Process Systems Engineering (PSE) Domain, containing multi-level hierarchies, is selected to be integrated into the CC Domain to illustrate its main features. The paper presented a procedure that allows the identification of constraints in the CC Domain. The procedure was demonstrated using an example from energy systems in order to show some aspects of the framework. This identification procedure may be used as the basis of an integration procedure that integrates DMMs at multi-level hierarchies. The CC Domain is continuously improved by considering different DMMs; however, it is important to consider automated processing of the DMMs to improve the CC Domain. Further developments should be devoted to explore the potential use of classification algorithms.

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