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An Ontology for Process Safety

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Safety engineering is a cross-domain discipline that requires knowledge and information of different kinds. Process safety engineering for example needs knowledge of fields like mechanical engineering, chemistry, chemical engineering, control and automation, etc. Knowledge of these domains along with the specific concepts related to the safety discipline allows to perform process safety design, analysis and management. In order to increase the efficiency of these processes and use and reuse information available from the safety community a common understanding of the concepts and its relations is needed. In this work, a chemical process safety ontology, OntoSafe, is presented. It has concepts of very different topics related to safety, from toxicology to safety instrumented systems. It is intended to be a live project that is available to the safety community.

1. Introduction

The philosophical definition of ontology is that it is a systematic way of explaining "being" – essence of a thing Gomez-Perez et al. (2007). The engineering view of an ontology is that is a formal description of concepts and its relations. As stated by Gruber (1994), it is defined as, "an explicit specification of a conceptualization". An ontology is composed of classes of objects, their hierarchy, relations, and axioms. A class represents a set of things that share a set of properties. Class hierarchies are defined with the use of the subclass relation (also known as the is-a relation), which states that every member of a subclass is also a member of the superclass, inheriting all the characteristics of the superclass.

Ontologies are software elements and as such they are encoded in machine-readable languages, being OWL (web ontology language) (McGuinness and Harmelen, 2004) probably the most widely used ontology language. Ontologies allows to have a common and shared understanding, which has the additional benefit of being reusable as indicated by Uschold and Jasper (1999). They proposed that an ontology contributes in communications between human agents, to achieve inter-operability among computer systems via the process of translating, using ontology as an interchange format.

Ontologies have been used in process systems engineering for the las three decades, Muñoz et al. (2013) or Silvente et al. (2013). There has been a growth of publications since 1990 to 2016 as stated in Batres (2017). But, related to safety, the ontological descriptions are just focused on some safety aspects, Kwang et al. (2012). An ontology covering all (or most) of the aspects regarding to process safety is a valuable asset for the community and it is the main purpose of this work.

Safety engineering is multi-disciplinary in nature, requiring many kinds of information. In the case of process safety knowledge about chemistry, mechanical engineering, process engineering, control and automation, waste management, risk analysis and management among others is needed besides the specific safety knowledge. The specific definition of safety concepts and their relationships with these other fields can be of great use to those practitioners that are not so familiar with many of the concepts and the implications of the relations. Regarding the reuse of information, a particular use can be, for example, in the identification of accident scenarios. The existence of an ontology allows the computational integration of different sources of information and the location of information of past accidents thanks to the support of automated reasoning capabilities, Batres et al. (2014). Another use of ontologies, which are "formal models that use mathematical logic to clarify and define" things (Madin et al., 2008), is to enhance the sharing and exchange of the HAZOP results between computer systems. For example, when a HAZOP produces scenarios that can be reached

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from several deviations (Limb, 2009), an ontology-based tool can be used to check for consistency and identify missing parts of a given scenario. Information is more easily exchanged with ontologies because ontologies provide an agreement of the meaning of the terms that are communicated providing the structure and semantics that ensures the validation of the information. Finally, another example where the ontology is suitable to be applied is in the Process Safety Management (PSM) process, Tan et al. (2012). It helps in the integration of the various elements, facilitates the maintenance and produces a more reliable procedure.

As it has been said, ontologies are in the end software programs, different tools exist to develop and build ontologies. One of the most used is the Protégé ontology editor which is a software application for editing, browsing, and deploying ontologies (Tudorache et al., 2008). Protégé has a graphic user interface with which classes, relations and logical axioms can be defined. Ontologies can also be integrated with other ontologies. In this work the Protégé tool has been used to develop the process safety ontology.

In this paper we present the developed chemical process safety ontology (OntoSafe). In the next chapter the main ontology components and their functions are described. In chapter 3, Ontosafe contents are described and an indication of its possible usage is also presented. Finally, chapter 4 draws some conclusions and comments on future work.

2. Process Safety Ontology Components

A chemical process safety ontology (OntoSafe) has been developed in order to have a common repository with the main concepts for the process safety community. This ontology has 513 classes (concepts), 80 object properties 70 data types and 58 individuals that complement the classes. Although it is an important amount of concepts, the relationships between them are as (or even more) important as the classes themselves.

2.1 Classes

All the concepts in the ontology have a definition, relationships with other classes, references (which is a very important part of an ontology as a shared conceptualization needs the source of those definitions). Figure 1 shows an example of a concept, Fireball. Besides the description, its references and the relations with other classes, there are additional annotations for the concept with its own references. These annotations explain the relationships with other classes, in this case, they explain the relation between Fireball and Boilover.

Annotations	2080	20		Annotations: FireBall
First addition 2014 The effects of the bollover are assentially the generation of a fireball, which is the most serious effect, and, to a minor extent, the ejection of a fireball, which is the most serious effect, and, to a minor extent, the ejection of a fireball, which is the most serious effect, and, to a minor extent, the ejection of a fireball, which is the most serious effect, and, to a minor extent, the ejection of a fireball, which is the most serious effect, and, to a minor extent, the ejection of a fireball, which is the most serious effect, and, to a minor extent, the ejection of a fireball, which is the most serious effect, and, to a minor extent, the ejection of a fireball, which is the most serious effect, and, to a minor extent, the ejection of a fireball, which is the most serious effect, and, to a minor extent, the ejection of a fireball, which is the most serious effect, and, to a minor extent, the ejection of a fireball, which is the most serious effect, and, to a minor extent, the ejection of a fireball, which is the most serious effect, and, to a minor extent, the ejection of a fireball, which is the most serious effect, and, to a minor extent, the ejection of a fireball, which is the most series and the effects and Consequences of Major Accidents in findustrial Plants iscausedBy some BalEVE Joaquim Casal Image: Constraint of Chemical Image: Constraint of Chemical ispontentiallyCausedBy some BLEVE Constraint of Sublegical Risk Department of Chemical Image: Constraint of Chemical Image: Constraint of Chemical	Image: Constraint of the second se	2 I o S an inside the doud the fire- and increases. Large (but sh 2 II 2 III 2 II 2 II 2 III 2 II 2 II 2 II 2 II 2 III 2 III 2 II	te explosion of a vessel containing a superheated flammable liquid. Since there is no oxyg trong thermal radiation, the density of the mixture decreases and the diameter of the fire Annotations for SubClassOf FireBall SubClassOf isCausedBysome Bollover Annotations The effects of the bollover are essentially the generation of a fireball, which is the most serious effect, and, to a minor extent, the ejection of ignited fuel around the tank. In Effects of the Effects and Consequences of Major Accidents in Industrial Plants Joaquim Casal Centre for Studies on Technological Risk Department of Chemical Englished the Order of the Effect and consequences of Major Accidents in Industrial Plants	Annotations: FireBall Annotations: FireBall Ignition of a mass of liquid/yapour mixture that is typically associated with only burns on the outside of the fireball. As droplets evaporate due to the duration) fireballs can also occur in tank fires in the event of a boilover. rdf:seeAlso Less' Process Safety Essentials Hazard Identification, Assessment and Control Sam Mannan Butterworth-Heinemann is an imprint of Elsevier The Boulevard, Langford Lane, Kidlington, Oxford, OX5 1GB, UK 225 Wyman Streek, Waltham, MA 02451, USA Eiset action 2014 Pescription: FireBall SubClass Of fire isCausedBy some FlashVaporizatingFuelSource isPotentiallyCausedBy some BLEVE
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Figure 1. Fireball class of the ontology. Annotations help to explain the relationships with other classes.

2.2 Object properties and data properties

Relations are represented in OWL through the use of properties. There are two main types of properties, object and data properties. Object properties relate two classes (or individuals of the classes). Object properties can have hierarchies as well (as it happens with classes) and they also have characteristics (transitive, symmetric, inverse, etc). For example, a property can have its inverse, if a property that relates two individuals a to b is has Consequence then the inverse (relating b to a) is IsConsequenceOf.

Data properties relate a class (or an individual of the class) to a data type. Properties (or relations) are a really valuable and important part of every ontology as the rules engine or Reasoner (usually a first-order predicate

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logic that can infer consequences using the information in the ontology) uses them to infer logical consequences about what has been encoded in the ontology. Figure 2 shows some of the object properties (left) and data properties (right) implemented in this work. Besides these two main properties, there is another interesting property which is the Annotation property. This one allows to attach metadata to other classes, individuals or even other properties.



Figure 2. Object properties (left) and data properties (right) implemented in OntoSafe

2.3 Individuals

Individual are resources that have been placed in a class, they are instances of the class, so they are not classes themselves. Individuals help to describe some classes or to perform logical inferences, they are not necessary in an ontology. Figure 3 shows some of the individuals built for this ontology.

Individuals:	Individual Annotations Individual Usage		
◆ ※	Annotations: ClassDFireExtinguisher		2080
B_Stability BusinessLosses C_Stability CarbonDioxideFireExtinguisher Catalytic Catalytic ClassDFireExtinguisher ClassKWetChemicalFireExtinguisher CleanAgentFireExtinguisher CleanAgentFireExtinguisher Condenser	Annotations () rdfs:comment [language: en] (2) Class D Fire is one that involves combustible metals or combustible metal alloys. There are basically two types o Class D fire extinguishers. The extinguishing agent for type 1 Class D is Sodium Chloride. The extinguishing agent for type 2 Class D is a copper based dry powder.		
Critical CWTank	Description: ClassDFireExtinguisher	? = ×	Property assertions: ClassDFireExtinguisher 🂵 🗉
D_Stability E_Stability Electrochemical EnvironmentDamage	Types 🕂 FireExtinguisher	0000	Object property assertions 🕀
Functions F_Stability Fatalities	Same Individual As 🕀		Negative object property assertions
Fines Fireproofing Flame Flare Frequent	Different Individuals	0000	Negative data property assertions 🕀
Improbable InfraredDetector Injuries IonizationDetector KoDrum V			

Figure 3. Individuals of Ontosafe

3. Ontology description

The ontology has been built considering the following main blocks:

- Chemical process safety fundamental concepts
- Chemical process safety system
- Industrial Hygiene
- Safety standards, regulations and organizations
- Mathematical (emision and dispersión) models

Following is a description of the content of the main superclasses.

- 1. Chemical Process Safety System. Under this class all the layers of protection (prevention and mitigation layers) and their management are included. For example, one important subclass in the protection layer management is the Human Factor class, under this class concepts like operator role, training, job design, allocation of operator functions, etc. are further described.
- 2. Chemical Process Safety Fundamental Concepts. This is a very important superclass as it includes fundamental concepts related to risk prevention, process safety, accidents, hazards, toxicology etc. Figure 4 shows the main subclasses (many of them are also superclasses) and in this example Toxicology subclass is shown with its own subclasses and relationships with other classes (out of the scope of Fundamental Concepts) like Industrial Hygiene or Chemical Hazard.



Figure 4. Superclass Fundamental Concept and its subclasses, and Toxicology class and its subclasses.

- Industrial Hygiene. This class is devoted mainly to hazardous chemical substances management and hazardous waste management and disposal. Information related to storage, handling, containment, substance identification, safety data sheets is included under this main topic.
- 4. Safety standards, regulations and organizations. This is an important part of the ontology which many times is considered as a minor issue. International organizations like REACH, ISO, WHO, AICHE, OSHA, HSE, AENOR, ... safety standards as NFPA, GHS, ANSI-ISA 18.2 or some safety regulations (in this case regulations from Spain and the UK) are defined in the ontology.
- 5. Mathematical models. Emission and dispersion models (like the Pasquill.Gifford for example) are described under this class of the ontology.

Although not properly a safety superclass, the ontology also includes the Chemical Process Control System class, where the main concepts related to control are introduced. This has been included as there are several safety concepts that refer to these elements. Ideally, another ontology (a Process Control Ontology) should exist and the relations would be with elements of that ontology.

In Figure 5, Fire class is depicted. In the top of the figure it can be shown the annotations related to the concept. In the middle the description tab shows the relationships with other classes, it can be observed the necessary and sufficient conditions for a fire to happen (relation isCausedBy) or some potential consequences through the property isCauseOf.

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The bottom right of the figure shows how Fire concept is related to other classes, the arrows indicate also the type of relationship. For example, Fire is a subclass of Major Accident and superclass of class A Fire, class B Fire, and so on.

Annotations: Fire	
Annotations 🕒	
rdfs:comment [language: en] Combustion or fire is a chemical reaction in which a substance combines with an oxidant and releases energy. Part of the energy releases	ased is used to sustain the reaction
In safety ontext it refers to accidental or uncontroled combustion	
rdfs:comment [language: en]	
Chemical Process Safety	
Fundamentals with Applications	
Prentice Hall International Series in the Physical and Chemical Engineering Sciences	
Description: Fire	208
SubClass Of 🕂	
isCausedBy only	0000
(FuelSource and IgnitionSource and OxydizerSource)	0000
(FuelSource and IgnitionSource and OxydizerSource)	0000
isCauseOf some BLEVE	0080
isCauseOf some FireEffect	0000
isMitigatedBy some FireAndGasProtectionLayer	0080
isPotentialCauseOf some DominoEffect	0000
MajorAccident	
General class axioms 🕰	* DominoEffect
SubClass Of (Anonymous Ancestor)	* RiskOfFire
isPotentiallyCausedBy some Incident	
isPotentiallyCausedBy some Hazard	* BLEVE TankFire
isCauseOf some Consequence	1
isPotentiallyCausedBy some Risk	ClassE-Fire
Usage: Fire	ctionLayer
Show: V this V disjoints V named sub/superclasses	Te FireBall
Fire SubClassOf isPotentialCauseOf some DominoEffect	* MajorAccident
Fire SubClassOf isCauseOf some BLEVE	Charles Fire
Fire SubClassOf isCauseOf some FireEffect	Cassering
Gids: nice Fire Sub-ClassOf MajorAccident	A
Fire SubClassOf isCausedBy some	PoolFire
(FuelSource and IgnitionSource and OxydizerSource)	
	ClassD-Fire
	FireEffect
	* ClassA-Fire
	* JetFire

Figure 5. Fire class annotations, description, usage and relations with other classes.

OntoSafe is a public ontology available at Webprotege (https://webprotege.stanford.edu/#projects/07323336-09a8-4baf-b33c-eff91cb9b249/edit/Classes?selection=Class(owl:Thing)). It is a live project so it is expected to be update several times a year.

4. Conclusions

In this work an ontology for chemical process safety has been presented. Although some previous approaches exist towards safety ontologies they are focused on some specific parts or applications of the safety domain. The developed ontology, Ontosafe, pretends to cover all the aspects related to process safety from toxicology to hazardous substances handling, to human factors, to risk analysis, to emission dispersion models, etc. The ontology has 513 classes, 80 object properties, 70 data properties and 58 individuals.

To develop an ontology takes a lot of time and resources which can be easily compensated through the use and reuse over time. Another important issue is that they have to be alive and updated every now and then which means resources for maintenance. Besides, ontologies have to be publicly accessible and be easy to use in order to foster the participation of the community.

Ontologies can be very useful if properly used. Different ontologies exist for different domains in engineering but they are not widely used. It is important not only to have ontologies for a specific domain but to relate them to other existing ontologies. OntoSafe is a live and ongoing project which is public and available to the process safety community. Next steps include its relation with ontologies of other domains like OntoCape (a chemical engineering ontology) concepts.

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