OnE:
An Ontology Evaluation Framework

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Abstract: A comprehensive set of evaluation criteria, named OnE, for evaluating ontologies has been proposed in this paper. Each criterion of OnE has been defined in a way such that together they are capable of evaluating any ontology from all aspects. The process of using OnE for evaluation has been demonstrated by evaluating chemical ontologies. Also, for this purpose, an ontology on the domain of agricultural chemicals has been constructed by following the human-centric faceted approach for ontology construction (HCFOC) and has been evaluated using OnE. The results obtained after the evaluation has provided insights about the ontologies. The constructed ontology aims to support any information system trying to support farmers in the process of decision making while selecting chemicals for use in agriculture. Also, it is envisaged that the demonstrated ontology and the set of evaluation criteria named OnE will redefine ontology evaluation and make it easy while making a strong impact on ontology developers.

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1.0 Introduction

Decision making is important to achieve the desired goals and objectives in any domain. Ontologies are being increasingly used to support decision making systems. An ontology is a formal, explicit specification of a shared conceptualization (Studer et al. 1998). It helps in querying a dataset for getting appropriate results and making decisions. There exist different kinds of ontology construction methodologies. Among them the faceted approach has gained quite prominence with contributions from the field of library and information science. The HCFOC methodology by Ghosh et al. (2020) makes use of the facet analysis and the analytico synthetic classification approach. Vickery (1968) has defined "faceted classification" as "the sorting of terms in a given field of knowledge into homogeneous, mutually exclusive facets, each derived from the parent universe by a single characteristic of division." In the field of library and information science, it is particularly used for constructing thesauri, information retrieval schemes, cataloging, etc. An analytico-synthetic scheme is any scheme in which a compound subject is first analyzed into its facets in the idea plane and later synthesized in the verbal plane and in the notational plane respectively (Ranganathan 1937). In addition to these, the HCFOC methodology also makes use of the human centric approach and the selective dissemination of information (SDI) approach to deal with context. Both these models help in increasing the precision of information retrieval systems. The human centric approach analyses a domain keeping a human at the centre. The theory of SDI propounded by Luhn (1961) advocates dissemination of items to those users who need it the most. In this paper, construction of an ontology on the agricultural chemicals domain, named AgriChem, following the HCFOC methodology has been demonstrated.

Agriculture deals with chemicals that are used in preparing pesticides, insecticides, fungicides as well as fertilizers. Proper execution of tasks like selection of pesticides to protect the crops, selection of fertilizers to enhance the fertility of the soil, etc., requires proper determination of the context of a farmer's information requirement. A farmer is the primary information seeker in the agricultural chemicals domain, and the demonstrated ontology has been modeled keeping the farmer at the centre. The domain of agricultural chemicals was chosen purposefully since India is an agriculture-based country, and it is the major source of income for more than 80% of the population of rural India. It also provides employment to 52% of labor approximately. It is envisaged that the demonstrated ontology will be able to support any agriculture-based information system for helping farmers in making decisions regarding the selection of the chemicals according to their requirements.

While building ontologies, a lot of unintentional errors might occur. Some of the errors have been mentioned in Gomez-Perez (1996, 2004). Incompleteness and redundancy are the most common. An ontology is evaluated with the aim to find the errors and lacunas and improve it. Jarosław (2018) states that the ontology evaluation process involves the identification of the criteria based on which the effectiveness of an ontology is measured. In this paper, a new set of more accurate evaluation criteria, named OnE, has been proposed. OnE has been used to evaluate CHEBI, CHEMINF and AgriChem. Chemical Entities of Biological Interest (CHEBI) is a structured classification of molecular entities of biological interest focusing on small chemical compounds (Degtyarenko, K, et al. 2007). Chemical Information Ontology (CHEMINF) includes terms for the descriptors commonly used in cheminformatics software applications and the algorithms that generate them. CHEMINF has introduced atomic concepts and roles, transitive roles, conjunction, disjunction, existential and value restriction, role hierarchies, inverse roles, number restrictions and data types (Hastings, J, et al. 2011).

2.0 Literature review

Lopez (1999) has developed the methontology framework, which specifies an ontology developmental process while detailing the steps for performing activities, techniques used, output and evaluation of ontologies. This framework was later used, as has been mentioned in Sankar (2006), for the development of chemical ontologies applied for representing the chemical reactions for organic compounds. Feldman (2005) designed a chemical ontology for categorization of small molecules. While searching chemical databases like PubChem, this ontology served as a powerful tool. Also, main functional groups accountable for biological activities could be specified. Degtyarenko (2007) has compared established commercial chemistry resources and CHEBI. In Adams (2009), the design of a set of individually maintained, interoperating and integrating ontologies collectively called ChemAxiom, has been shown. Hastings and Janna (2011) have developed a chemical information entities' ontology. Their aim was to create a list of calculated properties of chemical entities driven by data. A chemical ontology for assistance in automated compound classification in chemical databases or textual documents has been developed by Bobach (2012). Use of established chemical ontologies and XML schema for the encoding of fundamental chemical entities like AtomEntity, MolecularEntity, etc., has been demonstrated in Vijayasarathi (2015). Jiang (2015) and Wang (2019) have developed a chemical ontology for identification of toxic chemicals while formulating life saving drugs. Meshalkin (2017) developed two methodologies for developing an ontology of chemical technology for reagents and pure substances. The first methodology was for constructing the ontology and the second one was for using the ontology in interactive intelligent systems for semantic processing of science and technical text documents. Lauser (2006) has proposed a methodology for conversion from existing controlled vocabulary AGROVOC to Agricultural Ontology Service Concept Server (AOS/CS). Sanchez-Alonso (2009) has proposed an AGROVOC based ontology. The purpose of the ontology was to serve the purpose of learning resources available in the organic agricultural domain. Joo (2016) has also proposed an agricultural activity ontology using AGROVOC for standardizing the agricultural activities like purpose, means, crop and field. La Barre (2006) has demonstrated the use of faceted analytico-synthetic theory for construction of websites. Prieto-Diaz (2003) has demonstrated the use of a faceted approach for constructing an ontology.

There exist many ontology evaluation strategies. Some criteria for ontology evaluation proposed by Gruber (1995) are clarity, coherence, extendibility, minimal encoding bias and minimal ontological commitment. Uschold (1996) propounded that going middle out and handling ambiguity are two techniques to correct an ontology. Gomez Perez (2004, 1996) mentioned some basic criteria for ontology evaluation based on which many ontology evaluation processes have been performed. Different levels and underlying criteria have been mentioned. Fox and Gruninger (1998) have proposed functional completeness, generality, efficiency, perspicuity, precision granularity and minimality as the evaluation criteria. Burton-Jones (2005) has recommended a framework, which states that if any ontology can be seen then it must be present. If any ontology can be read then it must be seen. If any ontology can be understood then it must be read. If any ontology can be useful then it must be understood. If any ontology can be trusted then it must be useful. Here the formulae are well explained. Syntactic quality, semantic quality, pragmatic quality and social quality are considered as the evaluation criteria. The criteria for ontology evaluation mentioned in Gangemi (2005) are cognitive ergonomics, transparency, computational integrity and efficiency, meta-level integrity, flexibility, compliance to expertise, compliance to procedures for extension, integration, adaptation, etc., generic accessibility and organizational fitness are the proposed criteria. Tartir (2005) has introduced relationship, inheritance, class and attribute richness as the evaluation criteria. Stvilia (2007) has explained each criterion with suitable formula. The proposed criteria are accuracy/validity, cohesiveness, complexity, semantic consistency, structural consistency, currency, redundancy, naturalness, precision/completeness, verifiability, volatility and authority. Yu (2007) has also provided formulae to evaluate an ontology using different criteria such as depth/breadth/fanout, degree distribution/density, cohesion/modularity, importance/connectivity, tangledness, class richness and circularity error. Obrst (2007) has introduced two new criteria, namely adaptability and mappability. Other criteria are coverage, intelligibility, validity and soundness, specific use cases, consistency, completeness and inferences. Kehagia (2008) has recommended layers, which are structural/architectural layer, representational/semantic layer, application layer, philosophical layer, usability layer and lexical/vocabulary layer. Each layer further consists of different evaluation criteria. Zhu (2009) has proposed concept orientation (intrinsic), consistency, non-redundancy, soundness and comprehensive coverage (extrinsic) as the evaluation criteria. The parameters by which the proposed criteria are measured have also been mentioned. The ontology evaluation criteria mentioned in Vrandecic (2009) are accuracy, adaptability, clarity, completeness, computational efficiency, conciseness, consistency and organizational fitness. Duque-Ramos (2011) has considered formalization, formal relations support, cohesion, tangledness, schema and value reconciliation, consistent search and query, knowledge reuse, knowledge acquisition, reliability, operability, modularity, reusability and analyzability as the evaluation criteria. Intrinsic (correctness) and extrinsic (usefulness) evaluation criteria of ontology have been mentioned in Bright (2012). Clarity, consistency or coherence, conciseness, completeness, coverage, expendability/extendibility, correctness and minimal ontological commitment are the major criteria for ontology evaluation as has been stated in Haghighi (2012). Terminology, natural languages, external resources, size and breadth of the ontologies and encoding information have been considered as the evaluation criteria in Trokanas (2015).

3.0 Construction of an agricultural chemicals ontology

As defined in Lakel (2015), "Ontology construction or Ontological engineering is a research methodology which gives us the design rationale of a knowledge base, kernel conceptualization of the world of interest, semantic constraints of concepts together with sophisticated theories and technologies enabling accumulation of knowledge which is dispensable for knowledge processing in the real world." The construction of an ontology on agricultural chemicals using the HCFOC methodology and the open-source ontology editor Protégé 5.5.0 (https://protege.stanford.edu) has been demonstrated here. Data was collected from reliable sources of agricultural sciences and chemical sciences for creation of a knowledge base for testing this ontology. Since the agricultural chemicals domain is multi faceted, the HCFOC methodology is one of the best to deal with it. It includes eight steps, which have been discussed below.

3.0.1 Step 0: domain selection

The HCFOC methodology recommends that an area of research or domain is to be selected for constructing the ontology. The demonstrated ontology has been constructed on the agricultural chemicals domain. The reason for choosing this domain is that demand for information regarding agriculture is always high as the Indian economy is primarily based on agriculture and it is still the main source of income of many Indians according to Arjun (2013).

3.0.2 Step 1: focus map creation

This is one of the key steps of this methodology as it helps in understanding the context of the primary information seeker for providing them with more accurate results based on their queries. A prospective map of the primary information seeker's context is to be constructed, which will also represent the purpose and scope of the demonstrated ontology. For this purpose, competency questions were acquired after interacting with farmers, chemists, chemical suppliers, researchers and heads of agricultural research institutes from different parts of India in their native language. Also, farmers' associations' activities available on the internet were closely followed to get a grasp of the possible essential requirements of the farmers. Some of the frequently asked questions are as follows: a) Which chemical is used to control weed?; b) Which type of fertilizer fertilizes paddy?; c) What is the molecular formula of Urea?; d) What helps to regulate plant growth?; e) By which pest food crops are affected?; f) Which herbs are controlled by herbicide?; g) Which pesticides and fertilizers are used for cereals?; and, h) Which chemicals attract pollination agents? The terms that need to be considered as key for answering the aforementioned questions are pesticide, pest, fertilizer, crop, molecular formula, agricultural chemicals, plant growth regulator, food crop, herb, herbicide, pollination agent, attractant, etc. An analysis of all the competency questions helped in carrying out a user-centered needs assessment for identifying some key characteristics for AgriChem. Thus, a focus map of the whole domain was formed.

3.0.3 Step 2: information acquisition

Information for constructing the agricultural chemicals ontology has been obtained from various chemical information databases, government and non-government research institutes' and agricultural associations' websites, websites of pesticides, fertilizers and information blogs where farmers, agriculture scientists share their experiences about new inventions and their working experiences. The beginners in the field have shared their difficulties in various websites as well as in social media. All are rich sources of information about this domain. According to the HCFOC methodology, all such information was considered that were intersecting with the prospective map formed in the previous step. Next, the acquired information was compiled to construct an information base.

3.0.4 Step 3: term identification

In this step, suitable terms were chosen to represent the concepts (which have been identified in the previous step) belonging to the domain. The terms were so chosen such that all the required concepts get represented. The HCFOC methodology recommends that in this step controlled vocabulary must be consulted for ruling out the chances of ambiguity creation. For example, while trying to choose a term for representing a chemical that is used to repel harmful insects in plants one has many options between "repellent," "offensive," "rebarbative," "repugnant," etc. But the definition of the term "repellent" only has been found to be appropriate with the context and was used in the ontology. In another case, the terms "defoliant," "fungicide," "pesticide," "paraquat," "weedkiller," etc., were found to be synonymously used with "insecticide." But, according to the consulted controlled vocabularies (refer Appendix A), "fungicide" and "weedkiller" have different purposes than "insecticide." "Paraquat" is one type of "herbicide." "Defoliant" is a different chemical used to destroy or cause widespread loss of leaves. According to WordNet, "insecticide" is a chemical to control insects only. This definition also matches the context. So, in this case, use of controlled vocabularies ruled out creation of ambiguities. Some of the other identified terms are "pesticide," "herbicide," "attractant," "kharif," "rodent," "nematode," "mollusca," "pest," "plant growth regulator," etc.

3.0.5 Step 4: analysis

The terms which have been identified in the previous step were analyzed. It was decided whether a term can be used as a class/sub-class/instance/relation/attribute (of object or of data). This step was carried out keeping in mind the objective, scope, purpose and the context of the primary information seeker. The basic purpose of term analysis is to find out the similarities and differences between each term. For understanding the context of a farmer, the principle of context and canon of relevance of Ranganathan (1989) proved to be very useful while constructing the ontology. Terms having similar features were grouped together for better classification. For example, the terms "attractant," "repellent," "plant growth regulator," "pesticide" and "fertilizer" were grouped together under agricultural chemical, taking into consideration the fact that all of them were representing chemicals used in agriculture, having similar physical properties like molecular formula, weight, boiling and melting points, density, etc. The class "Agrochemical" consists of five main classes. Further, its subclasses "Fertilizer" and "Pesticide" consist of three and ten subclasses respectively. Some of these subclasses were further divided into many more subclasses. Thus, under the class "Agrochemical," more than eighteen concepts were grouped. Also, in this way, complex and compound concepts were broken into more elementary concepts.

3.0.6 Step 5: knowledge synthesis

According to the HCFOC methodology, the first-link-downwards and last-link-upwards approach ingrained in the analytico-synthetic classification method was used in this step. In the last-link-upwards approach, concepts were approached starting from the specific ones and proceeding towards the generic ones. While in the first-link-downwards approach, concepts were approached starting from the concrete ones and proceeding towards abstractness. For example, the top-level facet "Fertilizer" was broken down into "Nitrogenous," "Phosphate" and "Potassic." Similarly, the top-level facet "Insecticide" was broken into Inorganic_Insecticide and Organic_Insecticide. Again, it was checked whether all the sub-facets combined exhaust their respective top-level facet. This mitigated the chance of leaving out and misplacing of concepts. In this way, Insecticide got listed under Pesticide and Pesticide got listed under Agricultural chemical. In this step, relation between the concepts was also established. The "principle of context" and "principle of helpful sequence" as proposed in Ranganathan (1989) helped in facet discovery and listing.

3.0.7 Step 6: knowledge representation

This step consists of three sub steps, which have been described below:

Term Standardization: In this step, existing standard vocabularies on the domain were consulted to choose the correct terms (from among existing synonyms representing various context) to represent the concepts. It is expected that the use of correct terminology will increase the user friendliness and interoperability of the ontology. In the demonstrated chemical ontology, the concept "pesticide" represents chemicals used to kill pests. Thus, under "pesticide," all other pest killing chemicals have been included where pests represent any kind of insects, herbs, fungi, bacteria, algae or rodents, i.e., any type of living being that destroys crops. But Attractant, Plant growth regulator and Fertilizer have not been included under Pesticide as their roles are not similar with Pesticide.

Ordering: The terms representing the concepts were ordered and inserted in the ontology. The ordering criteria were chosen from those stated in the HCFOC methodology and while ordering primary focus was on the purpose of the ontology. The result of ordering can be seen in the Figures 1 and 2.

Modelling: The HCFOC methodology recommends the use of DERA (domain, entity, relation, attribute) framework mentioned in Giunchiglia and Dutta (2011) for structuring the facets of the domain. Here in the agriculture domain D, the set of facets Agricultural_chemical, Crop, Pest, belong to the element E, the set of facets kills, damages, controls, attracts, regulate_growth, fertilizes, etc. belong to the element R and the set of facets has_name, has_usage, applied_on, has_type, has_category, has_type, has_scientific_name belong to the element A. Urea, cereals, esfenvalerate and beetle are instances of members belonging to E. The following example in Table 1 shows how relationships have been established between the concepts in the ontology.

Here, bonfire cauliflower is an instance of the class Fungi, which damages cauliflower, an instance of the class Horticulture crop. Similarly, propazine is an instance of the class Herbicide, which controls Broadleaf dock, an instance of the class Weed.

3.0.8 Step 7: evaluation

An initial round of evaluation of AgriChem was carried out as has been detailed in HCFOC. A set of evaluators consisting of farmers, students, research scholars and professors of agriculture were asked to enlist the questions that they would like to be answered if they think of cultivating their own land. The concepts present in the queries were extracted and it was looked into whether AgriChem contained those concepts or not. Based on that, the queries were classified as "fully answerable," "partially answerable" or "not answerable" as has been shown in Tables 2, 3 and 4.

Class	Subject	Predicate	Object	Class
Fungi	Bonfire Cauliflower	damages	Cauliflower	Horticulture crop
Herbicide	Propazine	controls	Broadleaf dock	Weed

Table 1. Relationships between the concepts.

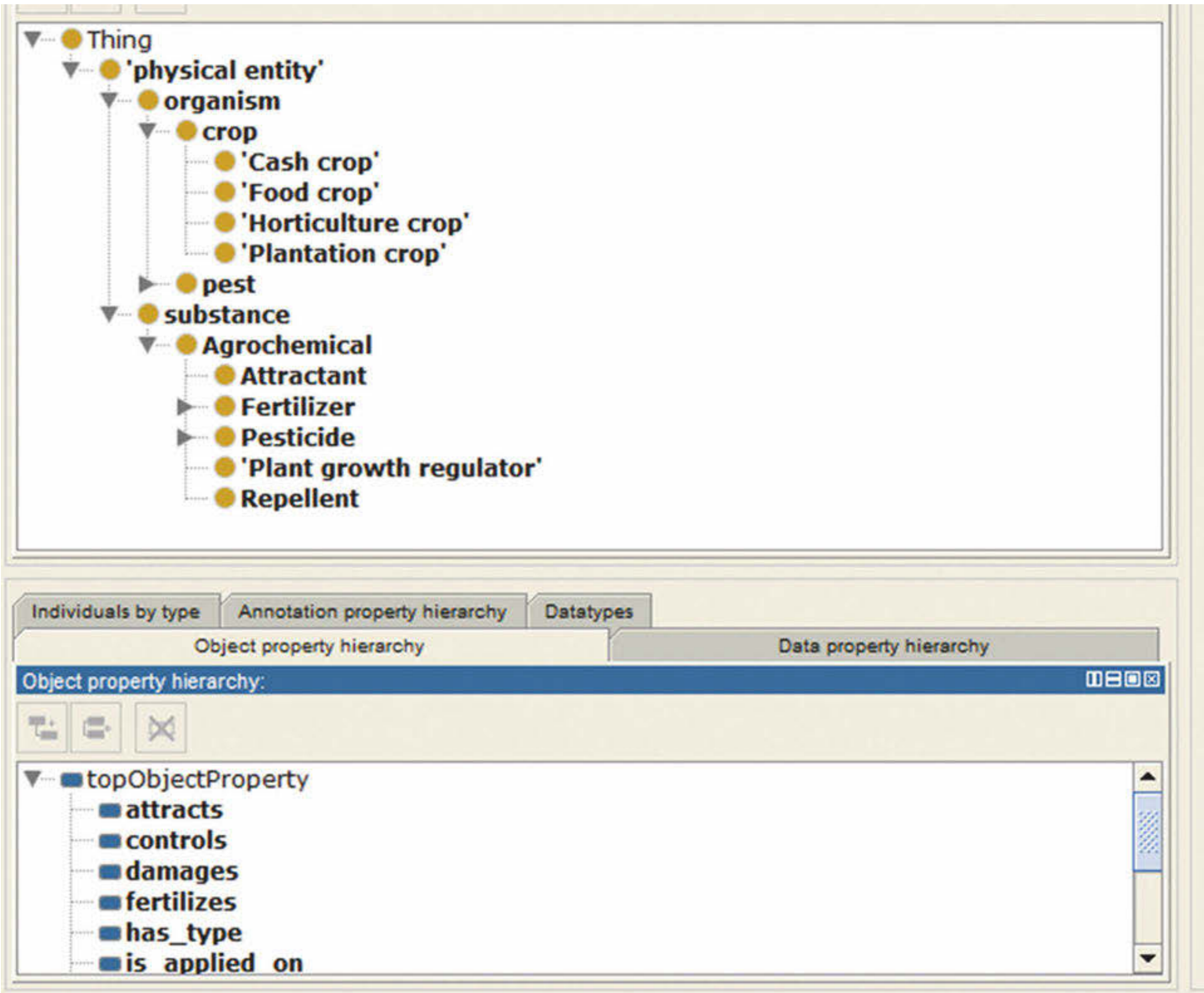

Figure 1. Partial list of classes and properties from AgriChem.

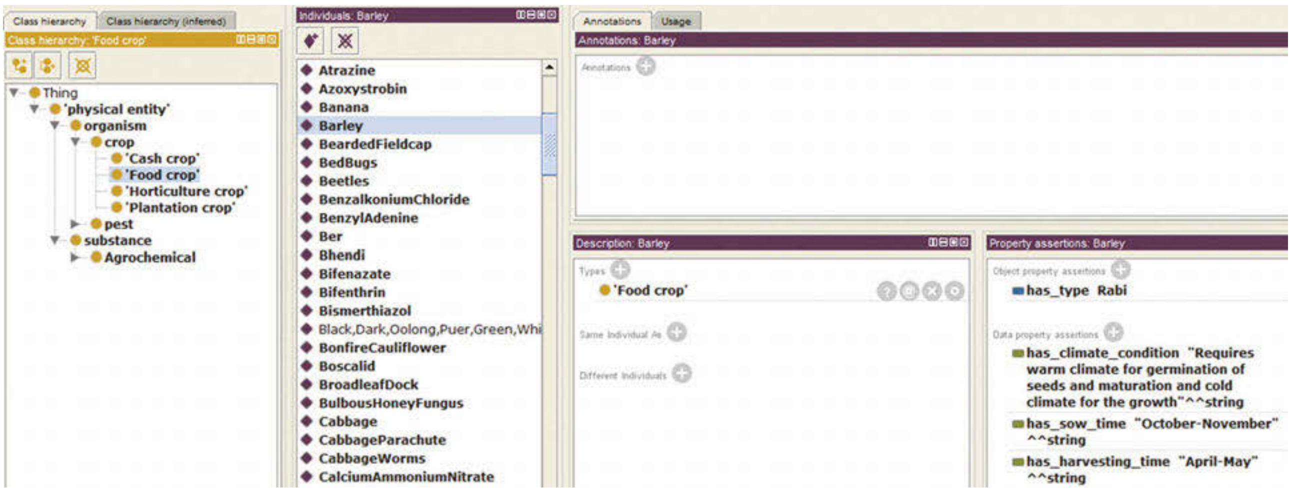

Figure 2. A typical representation of an entity and its attributes in AgriChem.

Insecticide	has_molecular_formula	has_melting_point	has_boiling_point	has_molecular_weight	has_density	has_vapour_pressure
Acetamiprid	C10H11ClN4	101-103°C	352.4°C at 760 mmHg	222.6741	1.17g/cm3	3.85E-05mmHg at 25°C
Amitraz	C19H23N3	86-87°C	450.7°C at 760 mmHg	293.406	0.98g/cm3	2.57E-08mmHg at 25°C
Acephate	C4H10NO3PS	93°C		183.1659	1.263g/cm3	
Bifenthrin	C23H22ClF3O2	68-71°C	744.4°C at 760 mmHg	422.8718		4.95E-22mmHg at 25°C
Diazinon	C12H21N2O3PS	120 °C	decomposes	96.0874	1.116-1.118 g/cm3 at 20 °C	0.000228mmHg at 25°C
Dichlorvos	C4H7Cl2O4P	60°C (-)	176.8°C at 760 mmHg	220.9757	1.435g/cm3	1.45mmHg at 25°C
Dieldrin	C12H8Cl6O	143-144°C	416.154°C at 760 mmH	380.9093	1.849g/cm3	0mmHg at 25°C
Diflubenzuron	C14H9ClF2N2O2	230-232°C		310.68		
Endosulfan	C9H6Cl6O3S	106°C	449.7°C at 760 mmHg	406.9251	1.94g/cm3	7.42E-08mmHg at 25°C
Esfenvalerate	C25H22ClNO3	59°C	538.9°C at 760 mmHg	419.9001	1.21g/cm3	1.11E-11mmHg at 25°C
Methamidophos	C2H8NO2PS	44.5°C	208.7°C at 760 mmHg	141.1292	1.286g/cm3	0.211mmHg at 25°C
Phosmet	C11H12NO4PS2	72.5°C	412.6°C at 760 mmHg	317.321	1.473g/cm3	5.11E-07mmHg at 25°C
Pyridaben	C19H25ClN2OS		429.9°C at 760 mmHg	364.9326	1.12g/cm3	1.35E-07mmHg at 25°C
Abamectin	C48H72O14		940.9°C at 760 mmHg	873.0769	1.24g/cm3	0mmHg at 25°C
Tebufenozide	C22H28N2O2	191 to 191.5 °C		352.4699	1.074g/cm3	
Dimethoate	C5H12NO3PS2	52-52.5°C	117 °C	229.2574	1.304g/cm3	
Demethon-S-methyl	C6H15O3PS2	<25 °C				0.0004 mmHg
Chlorpyriphos	C9H11Cl3NO3PS	42-44°C	395.8°C at 760 mmHg	350.5863	1.49g/cm3	4.09E-06mmHg at 25°C
Phosalone	C12H15ClNO4PS2	47.5 to 48 °C	446.7°C at 760 mmHg	367.8086	1.443g/cm3	3.57E-08mmHg at 25°C
Fenthion	C10H15O3PS2	7.5°C	360.4°C at 760 mmHg	278.3281	1.25g/cm3	4.61E-05mmHg at 25°C
Monocrotophos	C7H14NO5P	55 °C	120 °C	223.1635	1.195g/cm3	0.000446mmHg at 25°C
Malathion	C10H19O6PS2	2.85°C	385.1°C at 760 mmHg	330.358	1.272g/cm3	3.9E-06mmHg at 25°C

Insecticide / Fungicide / Herbicide / Rodenticide / Bactericide / Nematicide / Algicide / Larvicide / Molluscicide / Miticid

Figure 3. A snapshot of the test dataset used for testing AgriChem.

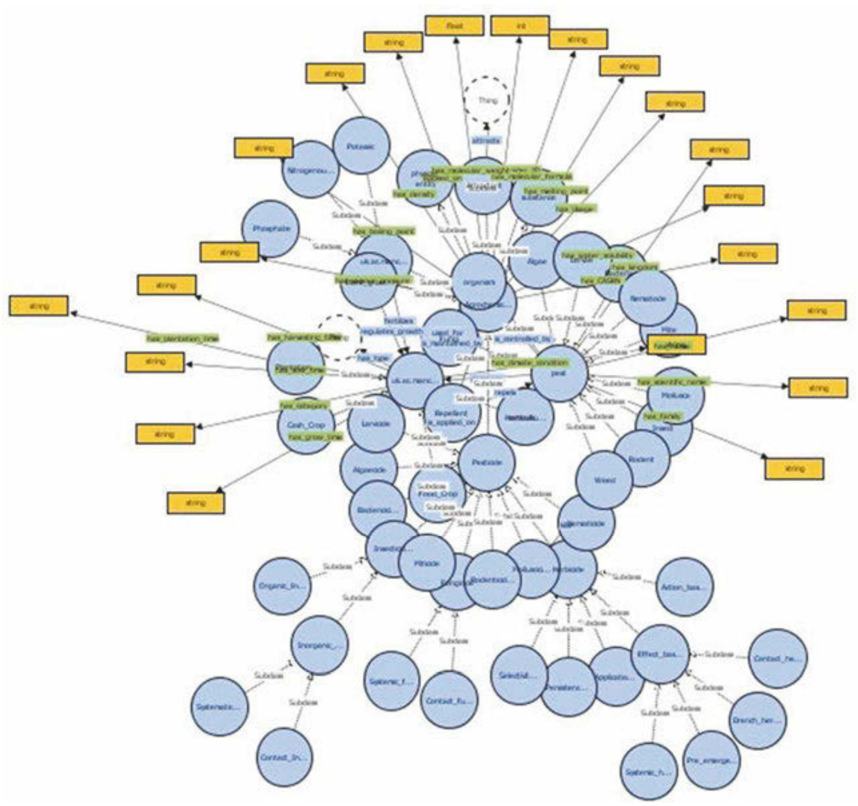

Figure 4. Visualization of AgriChem.

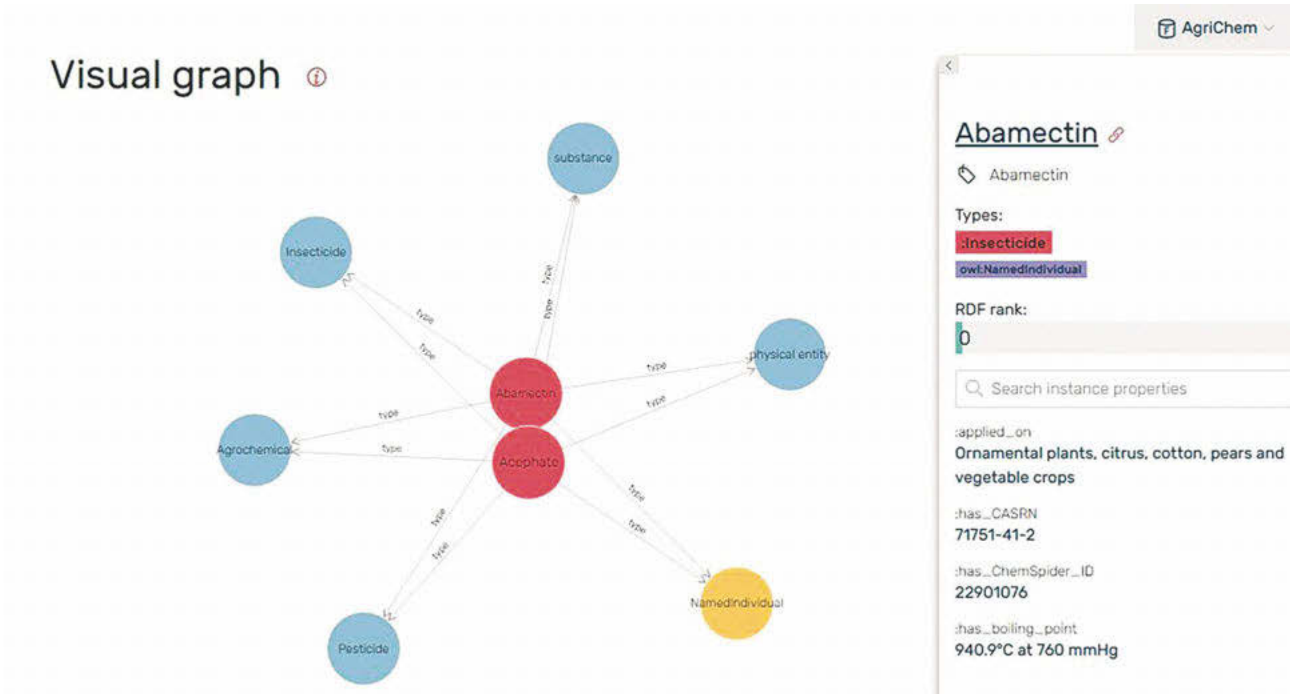

Figure 5. Visualization of "abamectin," an instance of an entity belonging to AgriChem.

Queries	Key terms
Make a list of fungicides contain less than 22 carbons.	<fungicide, molecular formula>
What are the fertilizers used for rapeseeds?	<fertilizer, crop>
Required climate condition of tomato?	<crop, climate condition>
Make a list of a weed belongs to the family Phytolaccaceae	<weed, family>
By which insects cash crops are affected?	<insects, crop>

Table 2. Examples of fully answerable queries and the extracted key terms.

Queries	Key terms
What are the scientific techniques for pest control and uses of fertilizers?	<pest, pesticide, technique, fertilizer>

Table 3. Examples of partially answerable queries and key terms.

Queries	Key terms
Safety measures taken by farmers while using chemicals	<pesticide, fertilizer, safety, farmer>
Who are the suppliers of the used chemicals and what is the market price of the chemicals?	<pesticide, fertilizer, supplier, price>
Are there any organic fertilizers instead of chemical fertilizers?	<organic fertilizer, substituent>

Table 4. Examples of unanswerable queries and key terms.

Figure 6. Fertilizers used for paddy and potato retrieved from AgriChem using SPARQL Query.

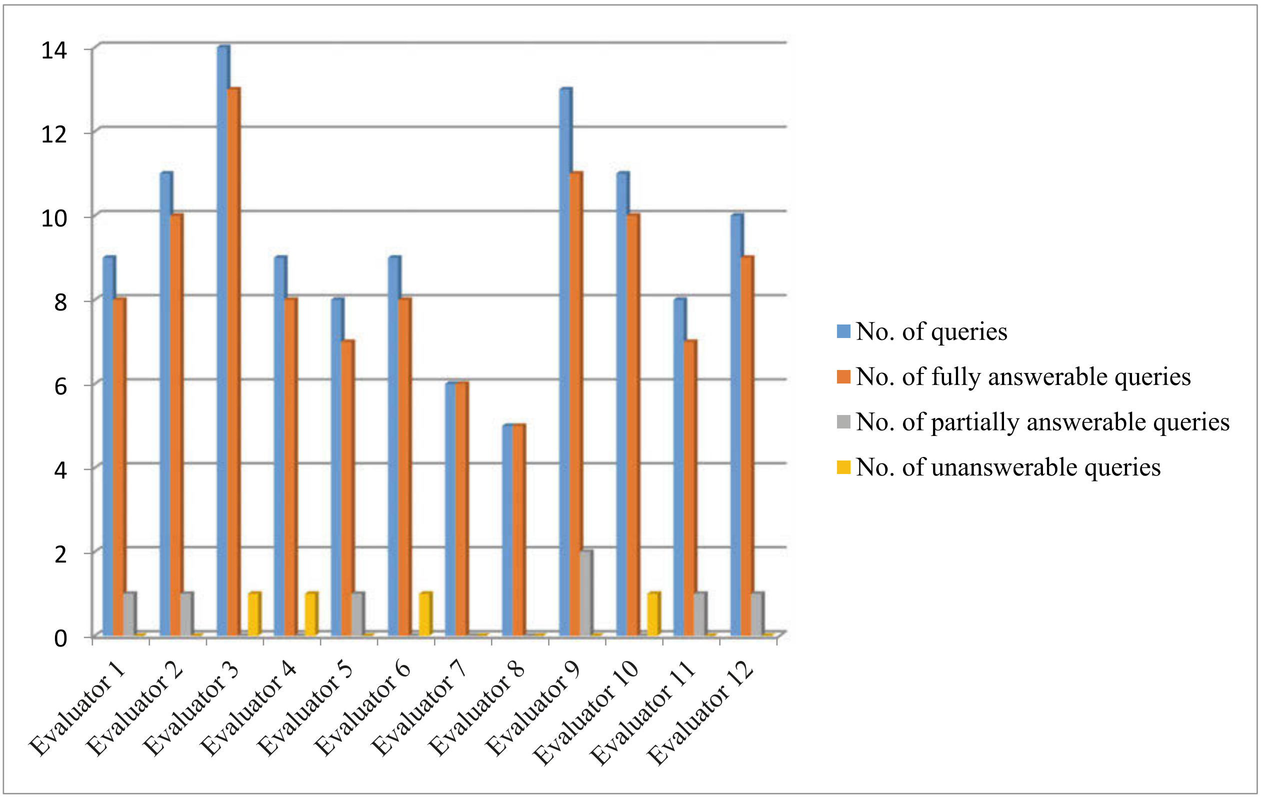

Figure7. Graphical representation of the statistics of the queries posed by the evaluators.

Out of 113 queries posed by the evaluators, 102 (i.e., more than 90%) were fully answerable, seven were partially answerable and four were unanswerable. More technical queries involving names of chemicals were put forward by students and researchers. Many questions put by the farmers were found to be common. The queries of the farmers were relatively straight forward, mostly concerning pest and related remedies. The queries have been listed in Appendix B. The concepts extracted from the unanswerable and partially answerable questions were analyzed. After the initial phase of evaluation, the concepts like safety measures, storage strategies, supplier, market price of chemicals, major crop producing regions, soil type, substitutes of fertilizer, cultivation technology, agronomic practices and techniques and physical properties of chemicals (color, hardness, electrical conductivity) were not present in AgriChem. Only a few popular chemical identifiers, i.e., CASRN, ChemSpider have been included. Though pest control technique has not been included in the ontology, it is clear from AgriChem which pesticide is to be used to control which pest. Out of the extracted concepts some were found to be out of the scope of the ontology and some have been considered for addition into the ontology for enhancing the purpose and scope of AgriChem.

4.0 OnE and its critera

Ontology evaluation is a very important step where the ontologies are examined based on different evaluation criteria (Hastings 2011). Ontology evaluation specifically aims at measuring the quality of ontologies, either to provide feedback to ontology developers and knowledge engineers or to give insights on the adequacy of ontologies to their users (Vrandecic 2005). Different types of criteria have been mentioned as has been discussed in the literature review section. But no single set of criteria covers all those sections that need to be considered for evaluating an ontology. A comprehensive study of the existing ontology evaluation criteria was done. Intent of each criterion and strategy mentioned in the ontology evaluation methodologies were identified. Criteria having similar purpose were grouped together. Some of them were selected and some new ones were proposed and a new set of criteria named OnE has been proposed. This set of criteria along with a definition of each criterion has been discussed. Also, based on this set of criteria, the constructed and existing ontologies have been evaluated.

4.0.1 Accuracy

This criterion is to check whether an ontology is able to represent the concepts belonging to a domain correctly. Statements that can be inferred should be correct. The defining axioms should be logically consistent. Coherence should exist between the natural language documentation and formal statements. The intended meaning of defined terms should be communicated. So, it is to be checked whether the terms have been chosen in a way that the concepts are getting concisely represented with no compromise on clarity. Satisfactory answers of competency questions and conceptual clarity has been considered as the ultimate test for determination of accuracy.

4.0.2 Interrelatedness

The existence of cohesion in the ontology is to be gauged using this criterion. The more the classes are connected the more the cohesiveness symbolizes the high expressive power of the ontology. A larger number of disjoint categories indicates less cohesiveness. An ontology that contains more relations (other than class-subclass relations) is richer. Ontology statistics, i.e., number of classes, object and data properties, connectedness of classes and ability to perform complex queries are considered while checking interrelatedness in an ontology.

4.0.3 Consistency

This criterion checks the extent to which the same values (vocabulary control) or elements (classes, properties) have been used to convey the same concepts and meanings or have been represented with the same structure, format and precision in an ontology. Consistency is also influenced by modularity. The more modular an ontology is, the less is the chance of creation of inconsistencies by changes in the ontology.

4.0.4 Exhaustiveness

This criterion is to test whether the ontology has necessary inputs (explicitly stated or otherwise) for all the knowledge that is expected to be inferred from the ontology. Richness of relationships and attributes helps in exhaustively covering the domain knowledge. An ontology which is expandable grows with time and can be exhaustive. Percentage of partially answerable and non answerable queries (made to the ontology) at a point of time can point out how exhaustive it is. An analysis of these queries may suggest new concepts that should be further added in the ontology if they fall within the scope and purpose of the ontology. Existence of mailing and editing facilities for suggesting new concepts show the intent to make the ontology exhaustive.

4.0.5 Reusability

This criterion is to test the degree to which the ontology or parts of it can be used to build other ontologies. Alignment with upper level ontologies increases interoperability and hence increases reusability. Minimal encoding bias also increases reusability. Availability of ontologies in a multi-language platform, i.e., internationalization, web services of ontologies, universal accessibility, ability to retrieve data from remote end point through SPARQL queries and free availability of licensed ontologies contribute in making an ontology reusable.

5.0 Evaluation of ontologies using OnE

Three ontologies namely, CHEBI, CHEMINF and AgriChem have been evaluated using the criteria mentioned in OnE. This revealed whether the selected criteria are best suited to their defined purpose. The observations made after the evaluation will be discussed in detail in the subsequent sections. The evaluation was primarily based on the authors' observations.

5.0.1 Evaluation of CHEBI

Accuracy: From the beginning, CHEBI aimed to standardize biochemical terminology. Also, the need to store and

Criteria	Inspired from
Accuracy	Correctness (Gomez-Perez (1996, 2004), Bright (2012), Haghighi (2012)), Conciseness (Gomez-Perez (1996, 2004), Vrandecic (2009), Haghighi (2012)), Pragmatic quality (Burton-Jones 2005), Clarity (Gruber (1995), Uschold (1996), Vrandecic (2009), Haghighi (2012)), Semantic quality (Burton-Jones 2005), Relationship richness and Attribute richness (Tartir 2005), Local correctness (Stuckenschmidt 2009), Evaluation of correctness and identification (Jarosław 2018).
Interrelatedness	Cohesion (Gruber (1995), Yu (2007), Duque-Ramos (2011), Haghighi (2012)), Coherence (Tartir 2005), Relationship richness (Tartir 2005), Connectivity (Tartir (2005), (Yu (2007)), Module cohesion (Stuckenschmidt (2009), Oh (2012)).
Consistency	Consistency (Gomez-Perez (1996, 2004), Uschold (1996), Vrandecic (2009), Zhu (2009), Haghighi (2012), Oh, (2012), Semanticness (Burton-Jones 2005), Semantic consistency and Structural consistency (Stvilia 2007), Consistent search and query, Modularity (Duque-Ramos 2011), Inconsistency (Jarosław 2018).
Exhaustiveness	Completeness (Gomez-Perez (1996, 2004), Obrst (2007), Vrandecic (2009), Haghighi (2012)), Expandability (Gomez-Perez 1996, 2004), Functional completeness (Gruninger, 1998), Attribute richness, Relationship richness (Tartir 2005), Precision/completeness (Stvilia 2007), Coverage (Obrst (2007), Haghighi (2012)), Comprehensive coverage (extrinsic)(Zhu 2009), Local completeness (Stuckenschmidt 2009), Incompleteness (Jarosław 2018).
Reusability	Minimal encoding bias (Gruber 1995), Expandability (Gomez-Perez 1996, 2004), Generic accessibility (Gangemi 2005), Alignment and Formal relations support, Reusability and Knowledge reuse (Duque-Ramos 2011).

Table 5. Criteria in OnE and the criteria by which they are inspired.

represent the 2D chemical structures was recognized. A lot of effort to retain consistency is visible. To formalize the differences between the terms that are often incorrectly and inappropriately used in the biochemical literature, cyclic relationships have been introduced. For example, many times "lactate" is used as a synonym of "lactic acid," but in CHEBI, lactic acid (CHEBI: 28358) has a conjugate base lactate (CHEBI: 24996). Thus, CHEBI performs well in terms of accuracy.

Interrelatedness: Most of the relationships defined in CHEBI are new and are specifically required by CHEBI. Two of them, "is a" and "is part of," used in CHEBI are defined by the Relations Ontology. In CHEBI, the relationship "X is conjugate acid of Y" means that the relationship "Y is conjugate base of X" is true. Again, for the relationships "A is tautomer of B" and "C is enantiomer of D" also means that "B is tautomer of A" and "D is enantiomer of C" are always true. Members of these cyclic relationships are placed at the same hierarchical level of the ontology. Currently, the following statistics are available about CHEBI: class – 132,780, object properties – ten, annotation properties – thirty-six.

Consistency: CHEBI follows open standards for chemical structure representation, such as the International Chemical Identifier (InChI), International Union of Pure and Applied Chemistry (IUPAC). It has also incorporated the Chemical Markup Language (CML). The majority of the small organic molecules in CHEBI (including isotope-labeled ones), connectivity and stereochemistry (2D structure) can be unambiguously represented as InChI strings. The terminology of CHEBI is explicitly endorsed, where applicable, by international bodies such as IUPAC, Nomenclature Committee of the International Union of Biochemistry and Molecular Biology (NC-IUBMB) and Joint Commission on Biochemical Nomenclature (JCBN), etc.

Exhaustiveness: CHEBI has 132,780 classes. There is a forum for reporting bugs, discussing annotation issues and to request new CHEBI terms and entries. Also, there is a mailing option. The default structures of molecular entities from CHEBI are deposited into PubChem (an open repository of chemical structures established at the National Center for Biotechnology Information) monthly.

Reusability: CHEBI does not contain proprietary items or items that have been derived from a proprietary source. CHEBI is freely available and is the most reusable biochemical information source. In the form of MySQL table dumps and Open Biomedical Ontologies (OBO) format flat file, the entire data is available to all without constraint. Programmatic access to its database is provided by CHEBI Web Services. This is to aid the users in integrating CHEBI into their applications. This also provides a standard means of interoperating between different software applications. CHEBI's home page is available in French, German, Russian and Spanish besides English; the User Manual and Frequently Asked Questions are available in English and German. Thus, accessibility, interoperability and internationalization have made CHEBI reusable.

5.0.2 Evaluation of CHEMINF

Accuracy: CHEMINF includes atomic concepts and roles, transitive roles, conjunction, disjunction, existential and value restriction, role hierarchies, inverse roles, number restrictions, identifiers, labels (rdfs:label) and definitions (dc:description). CHEMINF resources are linked data nodes, with de-referencable URIs. Algorithmic or procedural information can be distinguished from declarative or factual information. The expressivity and the conceptual clarity of CHEMINF are very high.

Interrelatedness: Integration of calculated properties (descriptors) of chemical entities within a semantic web context is the primary focus of CHEMINF. The following statistics about CHEMINF is available: class – 792, object properties – 106, data properties – seven, annotation properties – seventy-three.

Consistency: CHEMINF is linked with standard vocabularies and top-level ontologies. The tactic that has been followed to preserve consistency is to maintain separate files for the ontology and reference them from the primary ontology file cheminf.owl using the OWL import mechanism. These separate files have been mapped with other top-level ontologies, for example, the Blue Obelisk Descriptor Ontology. A high-level framework for the development of domain ontologies is provided by Basic Formal Ontology (BFO) (an upper level ontology which has been adopted by the OBO (Open Biological and Biomedical Ontology) Foundry). For establishing the fundamental relations between the entities, BFO uses the Relation Ontology (RO). Due to the alignment with BFO, CHEMINF reaps these benefits. Also, it has inherited from BFO the capability of making foundational distinctions between continuants and occurrents; and between dependent and independent entities. CHEMINF developers have considered the alignment of CHEMINF with alternative upper level ontologies to be the subject of future work.

Exhaustiveness: CHEMINF includes chemical graphs (including different formats for encoding them), chemical descriptors (including definitions, specifications and axioms describing the intended purpose), algorithms (including software implementations), chemical data representation, formalisms and formats. Thus, it is evident that necessary effort has been put to make CHEMINF exhaustive.

Reusability: CHEMINF is licensed as creative commons share-alike by attribution and is freely available from the Google Code project site. In the recently introduced RDF version of the CHEMBL database (labeled as CHEMBL-RDF), the annotation of SMILES and InChI strings has been standardized using CHEMINF. Due to this, softwares such as Bioclipse can now automatically discover molecular structure information available via SPARQL end points.

5.0.3 Evaluation of AgriChem

Acccuracy: AgriChem uses the HCFOC methodology for ontology construction. This methodology compromises the analytico-synthetic approach which ensures clarity. Also, this methodology has helped in choosing correct terms for representing different concepts according to the scope and purpose of the ontology. Some of the SPARQL queries made to AgriChem have been given below

Interrelatedness: The following statistics about AgriChem are available: class – fifty-four, object properties – twelve, data properties – twenty-two. From the statistics it is evident that the ratio between the number of classes and the number of object properties is balanced. Also, the sufficient number of data properties will certainly help in describing the classes properly.

Consistency: Standard vocabularies like WordNet, online agricultural thesaurus, dictionaries and other digital reference tools on agriculture have been used to define the concepts and choose contextual terms to represent them. This has helped in preventing the creation of inconsistencies. The ontology has been aligned with the top-level ontology DOLCE. The ontology is modular. Also, the faceted approach ingrained in the HCFOC methodology makes the ontology flexible. Thus, addition or deletion of concepts will not create inconsistencies.

Exhaustiveness: The modular nature of the ontology and use of the faceted approach helps in deletion and addition of concepts easily. After the initial phase of construction of AgriChem was over, many partially answerable and non answerable questions were discovered. Many useful concepts such as cultivation technology, pest control technique, replacement of fertilizer, storage procedure of chemicals, safety measures while handling chemicals, etc., were found. These concepts will be analyzed and if they fall within the scope of the ontology will be represented in the ontology. Thus, AgriChem possesses the necessary features for becoming exhaustive.

Reusability: AgriChem has been aligned with the top-level ontology DOLCE. Besides this, CHEBI, CHEMINF, AGRO and AGROVOC were consulted for incorporating relevant and standard terms within the ontology. It is envisaged that this will help in increasing reusability and interoperability. No local level encoding has been used. The ontology is available at https://webprotege.stanford.edu/#projects/9edb68ae-0cd6-4740-a2f5c3b1c282da22/edit/Classes.

6.0 Conclusion and future work

As of now, AgriChem will be able to support any agricultural information system focusing on agricultural chemicals by exposing the semantics related to use of agricultural chemicals explicitly. As the faceted approach is ingrained in the HCFOC methodology, it will be extremely effortless and straight forward to insert concepts into the ontology. After inserting the concepts obtained after the initial evaluation phase, the precision of answers returned will further increase. Successive updates and evaluation of AgriChem will make it truly exhaustive of its domain. Devising the criteria of OnE helped in understanding the process of evaluating ontologies. Also, the process of manipulating ontology after evaluation was understood. Two criteria namely, volatility and authority have not been included in OnE. Volatility represents the amount of time the concepts of an ontology remains valid. It can be measured by the average update rate of the ontology. Authority represents the degree of reputation of an ontology in a given community or culture. It can be measured by citations or by measuring its usage. Both of these criteria are important but can be used to evaluate an ontology only over a long period of time. They might be included in future revisions of OnE. Each criterion of OnE has been designed in such a way that they could be utilized to evaluate ontologies irrespective of domain. Future work involves creation of a tool for evaluating ontologies based on the criteria of OnE. It is envisaged that the results demonstrated here will be utilized to produce and evaluate better domain models.

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Appendix A: List of consulted controlled vocabularies and databases on the domain

Resource	*URI*
AGROVOC | Agricultural Information Management System	http://aims.fao.org/vest-registry/vocabularies/agrovoc
Agricultural Thesaurus and Glossary	https://agclass.nal.usda.gov
National Agricultural Library Thesaurus	http://agroportal.lirmm.fr/ontologies/NALT
National Portal of India	https://www.india.gov.in/topics/agriculture
Crop | agriculture | Britannica	https://www.britannica.com/topic/crop-agriculture
ICAR-Central Plantation Crops Research Institute	https://www.iari.res.in/
agritech.tnau.ac.in	http://agritech.tnau.ac.in/agriculture/agri_index.html
Pest | vermin | Britannica	https://www.britannica.com/science/pest-vermin
Types of Pests | Fort Pest Control	http://fortpestcontrol.com/types-of-pests
A-Z Animals – Animal Facts, Pictures and Resources	https://a-z-animals.com
Weed Killer Crisis 2020	https://www.weedkillercrisis.com/
Indian Farmers; One family One Voice	http://indianfarmers.org
OFAI – India's biggest network of organic farmers	https://ofai.org
What are agricultural chemicals? – famic	http://www.acis.famic.go.jp/eng/chishiki/01.htm
Agricultural chemical users' manual	ISBN: 0734503210
PubChem	https://pubchem.ncbi.nlm.nih.gov/
Empowering Innovation & Scientific Discoveries	https://www.cas.org/
ChemSpider | Search and share chemistry	http://www.chemspider.com
Chemistry – LC Linked Data Service	http://id.loc.gov/authorities/subjects/sh85022986.html
ChEMBL Database	https://www.ebi.ac.uk/chembl/
CHEMnetBASE Search	http://www.chemnetbase.com/faces/search/SimpleSearch.xhtml
Agricultural Chemicals	https://www.iari.res.in
Pesticides in agriculture | European Commission	https://ec.europa.eu/info/food-farming-fisheries/sustainability-and-natural-resources/biodiversity-and-land-use/pesticides_en
WordNet Search – 3.1	http://wordnetweb.princeton.edu/perl/webwn

Appendix B: List of unique questions posed by evaluators

Queries	*Key Terms*
For cultivation of seasonal fruits which insecticides should be used?	<season, crop, agrochemical, usedFor>
What is the use of Diazinon?	<agrochemical, usedFor>
To control yellow and brown rust which fungicide is used?	<disease, agrochemical>
By which pest food crops are affected?	<pest, affect, crop>
What is harvesting time of Soybean?	<crop, harvestingTime>
What is the scientific name of Mushroom flies?	<pest, scientificName>
By which pests the vegetable crops are affected?	<pest, crop>
What is the molecular weight of Urea?	<agrochemical, molecularWeight>
What is the use of Pendimethalin?	<agrochemical, usedFor>
What is harvesting time of Rabi crop?	<crop, harvestingTime, season>
To which family and kingdom does Chickweed belong to?	<crop, family, kingdom>
Why Methyl eugenol is being used?	<agrochemical, usedFor>
What is the chemical formula of Bismerthiazol?	<agrochemical, chemicalFormula>
What are the pesticides and fertilizers that are used for cereals?	<agrochemical, crop>
Which herbs are controlled by herbicide?	<agrochemical, usedFor, crop>
What are the insecticides available for horticulture crop?	<agrochemical, crop>
What climate should be required for plantation crop?	<climate, crop>
Why copper sulphate is used?	<agrochemical, usedFor>
What are the fertilizers used for rapeseeds?	<agrochemical, usedFor,crop>
What is the time of sowing of Kharif crop?	<crop, sowingTime, season>
What are affected by rodents and how are they controlled?	<pest, affects, crop, controls>
What the pesticide is mostly used for the tomatoes?	<agrochemical, usedFor,crop>
What is the use of IR-3535?	<usedFor, agrochemical, chemSpiderId>
What herbicide is used for Carrot?	<agrochemical, usedFor,crop>
To control fruit flies which insecticide is used?	<agrochemical, pest>
What is the technique of pest control?	<pest controlling_technique>
Which fungicide is used for fruits?	<agrochemical, crop>
For indoor greenhouse vegetables which miticides are used?	<crop, climate, agrochemical>
Why attractants are used?	<agrochemical, usedFor>
List all the chemical identifiers of Acetamiprid.	<agrochemical, identifier>
What are the main elements of Paclobutrazol?	<agrochemical, constituents>
What is the solubility of fertilizers?	<agrochemical, solubility>
What is applied on tobacco to control nematode?	<crop, pest, agrochemical, usedFor>
What is used to control Mosquito larvae?	<pest, agrochemical, usedFor >
What is the sow time of Peanut?	<crop, sowingTime>
Which insecticide is used to control Semilooper attacking Bhendi?	<pest, agrochemical, usedFor, crop>
Which insecticide is applied on Potato?	<agrochemical, usedFor, crop>
By which insects cash crops are affected?	<pest, affects, crop>
What are the scientific techniques for uses of fertilizers?	<agrochemical, scientificUseTechnique>
Are there any organic fertilizers instead of chemical fertilizers?	<agrochemical, replacement>
Which types of weeds are controlled by Tebuthiuron?	<agrochemical, controls >
Which fertilizers are used for cereals?	<agrochemical, usedFor,crop>
Nitrogenous Fertilizers are used for which type of soil?	<agrochemical, appliedOn>
Which fertilizers are used for food crops?	<agrochemical, crop>

Queries	*Key Terms*
What is the replacement of fertilizer?	<agrochemical, replacement>
What is the water solubility of Nitrogenous fertilizers?	<agrochemical, solubility>
Which fertilizer is used for Potatoes?	<agrochemical, crop>
What is the chemical formula of Monocalcium phosphate?	<agrochemical, chemicalFormula>
What is the market price of the chemicals?	<agrochemical, price>
Are the used chemicals safe enough?	<agrochemical, safety>
How to store the used chemicals?	<agrochemical, storageProcedure>