A Clustering Analysis of Codes of Conduct and Ethics in the Practice of Chemistry

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Abstract

Up until recently, the international disarmament and non-proliferation community lacked a universal code of conduct. The use of chemical weapons triggered a series of discussion at Organization for the Prohibition of Chemical Weapons to explore the development of a unified set of ethical guidelines for chemistry professionals with the goal of preventing the re-emergence chemical weapon stockpiles.

Following calls by various member states of the Chemical Weapons Convention for a culture of greater responsibility exemplified through a professional code of ethics binding on all member states, we used Natural Language Processing algorithms to investigate governing documents across different communities of chemistry practitioners. This paper presents a quantified lexical approach including TFIDF to find the most differentiating attributes of codes of conduct and ethics.

The result was used by the representatives from academia, industry, and chemical societies. As a result, in October 2015 The Hague Ethical Guidelines were published to provide a framework for promoting the debate on the vital dimension of ethics in relation to chemical disarmament and non-proliferation on all levels of education, research, and practice of the chemical sciences and industries.

1 Introduction

Scientific discovery along with the innovations and technologies that follow has been transformative. A wealth of knowledge and capabilities are integrated into our day-to-day lives in such a way that we do not recognize them as a benefit from science. Reflecting on the many scientific discoveries that have led to improvements in quality of life and health, how much do we know or think about the scientific research from where they came?

One thing about science however, is that the channeling of its power for harm, whether intentional or by accident, often draw considerably more attention and discussion. Particularly when the discussion turns to what the future will bring based on the scientific research we see today. Owing to this, it is common in security communities concerned about emerging technologies and the proliferation of new types of weapons, to question how aware scientists are of the potential harm their work may bring (Shang, Dando, and Crowley 2018). In the realm of disarmament and non-proliferation of chemical weapons, these issues are continually debated, with calls for a culture of responsibility amongst

Note: All necessary data and codes to replicate the analysis in this paper can be found at: https://github.com/Amirosimani/topic_analysis_ethics practitioners (Rodda 2018), and where acknowledgement of such awareness could usefully be exemplified through professional codes of ethics (Frank, Forman and Cole-Hamilton 2018, Brown 2018).

When the discussion of ethics in chemistry turns to the dangers of weaponized chemicals, the Chemical Weapons Convention (OPCW 1993a), an international disarmament and non-proliferation treaty with a membership of 193 of the World's States (OPCW 2019a), established norms and values for peaceful and ethical practices for the science of chemistry, and more broadly across the larger scientific landscape where chemistry converges with other scientific fields to bring forward innovation (Forman et al 2018).

There is an unfortunate consequence of a discourse that focuses exclusively on a need for ethics in science because of the potential for harm without acknowledging the benefit and need for science in support of addressing security issues – a narrative that suggests science cannot be trusted. For disarmament and non-proliferation of chemical weapons, such distrust can discourage promoting and maintaining scientific literacy in decision making. The discourse on ethics in chemistry while intended to bolster norms in support of instruments such as the Chemical Weapons Convention, provides a means for non-technical stakeholders to avoid discussing technical information pertinent to treaty implementation. As the implementation of the Chemical Weapons Convention requires sound scientific and technical expertise, distrust of science can challenge effectiveness (Forman, Timperley, Sun and van Earton, 2018; Forman and Timperley 2018).

With the recognition of the importance of science for treaty implementation, as well as the need to promote the norms enshrined in the Chemical Weapons Convention, the Organisation for the Prohibition of Chemical Weapons (OPCW), the organisation that implements the Chemical Weapons Convention, hosted two workshops in 2015. Scientists from academia, government laboratories and chemical industry participated and The Hague Ethical Guidelines were developed (OPCW 2019b). These guidelines serve as elements for ethical codes and starting points of the discussion of ethical issues relevant to the practice of chemistry. The guidelines promote responsible conduct and the prevention of misuse of chemistry, and they also callout the need for chemistry and where it serves to benefit us all (Husbands and Suárez 2016).

The Hague Ethical Guidelines were developed by chemistry practitioners coming together from more than 20 countries, it is noteworthy that with two workshops held over a six-month period (OPCW 2015a and 2015b), these scientists were able to come to a consensus on key elements of ethical codes that support chemical disarmament and non-proliferation. The guidelines have been acknowledged by the states parties of the Chemical Weapons Convention as an "important step to advance understanding among chemistry practitioners of the importance of nurturing responsible and ethical norms for scientific research and development" (OPCW 2018). In contrast, discussions on the development of codes of conduct and/or ethics at the policymaking levels in international disarmament treaties often move forward much more slowly. In this context, discussions of a code of conduct for biological sciences undertaken within the policymaking organs of the Biological Weapons Convention (an international biological weapons disarmament treaty), have been on-going without a consensus (Biological Weapons Convention 2018a and 2018b).

Within the discussions that produced the Hague Ethical Guidelines, it was recognized that the discourse around ethics (Kovac 2018 and 2015) and responsible conduct (Pearson and Mahaffy 2006) has been a long standing thematic discussion in chemistry communities. A collection of 142 codes, including both codes of conduct (rules to follow) and codes of ethics (principles to aspire to) was assembled and reviewed during the workshops (OPCW 2015c). This too is noteworthy, as within the policymaking organs of the Chemical Weapons Convention, the existence of this many codes (which actually represent just a fraction of what is likely to exist) was largely unknown – suggesting that there are certainly opportunities to enable more productive discussions between scientific and security communities.

Discussing ethical issues within scientific communities is valuable for bringing forward concerns about scientific discovery and preventing the misuse of science. Yet there is also a need to appreciate the role of "atoms, molecules and math" outside scientific communities. The ethics discussion amongst the scientists helps to build trust from those that ultimately need science to accomplish their goals. Conversely, a lack of science discussion by those asking for scientists to take on ethical issues can discourage dialogue between scientific and non-scientific communities. The Hague Ethical Guidelines workshops brought to light both of these issues.

The existence of a rich collection of existing codes of ethics and codes of conduct related to chemistry raises some interesting questions. If so many codes already exist what distinguishes one from another? Are there already core elements within these codes that have relevance to address the concerns of chemical disarmament and non-proliferation? With such a wealth of existing documents, does chemistry need another code? The collection of codes from the Hague Ethical Guidelines workshops serves as an interesting dataset from which insights into these questions might be drawn. We have used the dataset to perform a text based analysis to look further into these questions and their potential implications for the discourse on ethics in chemistry and supporting the norms of the Chemical Weapons Convention.

2 Implementation and norms of the Chemical Weapons Convention

States parties of the Chemical Weapons Convention are obligated to uphold a prohibition on the development, production, acquisition, stockpiling, retention, transfer or use of chemical weapons. Treaty implementation covers four primary operations. 1) The destruction of chemical weapons, where any state possessing chemical weapons stockpiles must declare and destroy them (OPCW 2017a). To date more than 96% of the 72,000 metric tonnes of declared chemicals weapons across the states parties of the Chemical Weapons Convention have been verifiably destroyed (OPCW 2019c). 2) The non-proliferation and prevention of re-emergence of chemical weapons. This obligates the states parties to comply with a verification regime and allow international inspectors to visit their territories to inspect industrial chemical production facilities (OPCW 2017b) and requires the implementation of national laws to regulate the production and transfer of certain chemicals (OPCW 2017c and 2017d). 3) Assistance and protection is the provision which obligates states parties to assist one another if requested in response to a chemical incident (OPCW 2017e). The OPCW also facilitates capacity building and training programmes to build response capabilities within the States Parties (OPCW 2019d). And 4) supporting and promoting international cooperation for peaceful uses of chemistry (OPCW 2017f), which includes programmes to enhance laboratory skills, provide research grants and support conference attendance for scientists from developing countries (OPCW 2019d). Operationally, destruction of stockpiles and implementation of the verification regime are the most visible aspect of the Chemical Weapons Convention. The inclusion of capacity-building obligations and promoting international cooperation through science (a form of science diplomacy), while less visible are just as important, for the success of international treaties relies on building trust and facilitating cooperation across geopolitical borders. It follows that norms of the Chemical Weapons Convention by supporting and promoting the elimination of chemical weapons, preventing the re-emergence of chemicals as weapons, eliminating the desire to use chemicals to do harm through building capabilities that minimize the impact of a chemical event and promoting international cooperation.

Additionally, the Chemical Weapons Convention calls upon each State Party to "assign the highest priority to ensure the safety of people and to protect the environment" and cooperate appropriately with other States Parties (OPCW 1993b). Such an obligation would seem to align with the aspirational principles and norms found across the chemical sciences, and especially in fields such as green and sustainable chemistry (Forman and Timperley 2019). It follows that in the many codes of ethics and codes of conduct found in chemistry, even if there is no specific mention of chemical weapons, calls for protection of health and environment would also be supported by the norms of the Chemical Weapons Convention (and conversely such codes would support these same norms).

3 A collection of codes of ethics and codes of conduct in chemistry

In order to perform an inclusive analysis in the context of the Chemical Weapons Convention, a corpus was needed that includes representative documents across different communities of chemistry practitioners (defined by types of organisations) and world regions (as defined by United Nations regional groups (Sidhu, 2008)), Both codes of conduct and codes of ethics are relevant.

For our research, 143 documents were collected. These were identified through open access web based searches in English, and through reaching out to chemistry practitioners. We should remark that many non-English speaking institutions like chemical societies or science associations share the same code of conduct or ethics with their umbrella international organization. We recognize that our collection is far from being comprehensive for what codes exist. It does however contain documents coming from professional scientific and engineering societies, academies of sciences, chemical industry, government and international organisations.

Each document in the collection had the following six attributes:

1. The organisation (identified by name): to which the code belongs (or had been drafted by).

2. The country ("State Party") that the organisation which developed the code is located. For international or multinational organisations the country where the headquarters is located was used to define this attribute. United Nations agencies were classified as "International" for this attribute.

3. The region from where the code originated. This is the OPCW regional group to which the country attribute belongs. These regions are the African Group, the Asian Group, the Eastern European Group, the Group of Latin America and the Caribbean (GRULAC), and Western European and Other States Group (WEOG) (OPCW 2019a). The regional group for United Nations agencies was classified as "Worldwide".

4. The type of organisation from which a code was developed were classified as chemical industry, chemistry, science (including chemistry), government, chemical engineering and engineering (including chemical). Each organisation was assigned a "type" based on its function. Chemical companies and chemical industry organisations were assigned as chemistry industry. Chemistry societies and associations were assigned as chemistry. Scientific organisations that include more than chemistry, such as an academy of science, were assigned as science (including chemistry). Codes issued by government ministries and agencies were assigned as government. Codes for chemical engineers were assigned as chemical engineering, and broader engineering organisations were assigned as engineering (including chemical). International ogranisations (e.g. UN agencies) were specified as "international organisation".

5. Each document was also assigned as a code of conduct, a code of ethics or combination of the two types of code. The assignment was based on the stated purpose of the code from the organisations which had developed it.

6. The Code itself was defined as the text in the body of the document.

The composition of the corpus and the breakdown of the attributes across the 143 documents are provided in Table 1.

Attribute	Value	Count
Region	African Group	8
	Asia-Pacific Group	35
	Eastern European Group	12
	GRULAC	6

Attribute	Value	Count
	WEOG	68
	Worldwide	14
Total		143
Organization Type	Chemistry	32
	Chemistry - Industry	64
	Chemical Engineering	10
	Engineering	7
	Government	11
	International	2
	Science	17
Total		143
Document Type	Conduct	74
	Ethics	64
	Mixed	5
Total		143

Table 1 – Overview of collected documents

4 Measuring similarity and clustering

The 143 documents were placed in a data frame where rows denoted individual documents and columns the six respective attributes. A pipeline was created to apply the following steps on the body of documents. First, numbers and special characters were removed. Second, words were transformed into their lemmas. Finally, stop words were removed. These are important steps to reduce the feature space dimension and improve the clustering. (Das & Chakraborty 2018).

To represent similarity of the documents, a commonly used vector representation of text in the field of information extraction called Term Frequency Inverse Document Frequency (TF-IDF) is used. TD-IDF is essentially a numeric measure of relevancy of a given word in a given document. As “TF-IDF works by determining the relative frequency of words in a specific document compared to the inverse proportion of that word over the entire document corpus” (Ramos 2003). The TF-IDF weights are used to evaluate how important a word is to a document in the corpus. The importance increases proportionally to the number of times a word appears in the document but is offset by the frequency of the word in the corpus.

The default Term in TF-IDF is a single word token or unigram. While using unigrams are simple and powerful, it doesn’t keep contextual word order. For example, in a unigram model, the word “Chemical Weapons Convention” will be transformed to 3 separate tokens [“Chemical”, “Weapons”, “Convention”]. Using n-grams that take n consecutive sequences of words, will address that problem. For this study, we used 1-3 n-grams which results in [“Chemical”, “Weapons”, “Convention”, Chemical Weapons”, “Weapons Convention”, “Chemical Weapons Convention”]. Additionally, only n-grams that are repeated more than 5 times in the corpus were kept. The result is a 143x6227 sparse matrix with 90867 tokens. Parameters for the preprocessing pipeline is shown in figure 1.

Once TF-IDF vectors for all documents had been calculated, the angle between two vectors was used as an indicator of their divergence. The cosine of the angle between the vectors has been suggested as metric to determine numeric similarity of two vectors (Singhal 2001). Furthermore, Cosine similarity is a standard approach in the field of information extraction to get a baseline result (Mihalcea et al, 2006) (Gomaa & Fahmy, 2013).

A benefit of the approach to measure topical similarity in documents is that it is language-independent and doesn’t need any prior information about the content or language. In addition, simple vector operation and linear algebra can be utilized to calculate and sort document similarity (Grossman & Frieder, 2012)

The next step was the clustering of documents based on their similarity score. There are many approaches to find good clusters in machine learning. While a standard parametric approach is to learn a mixture density, it requires making assumptions on the density of each cluster (e.g. each cluster is Gaussian). A suggested alternative are spectral methods that use top eigenvectors of distance matrix between points (Ng et all 2018). Spectral clustering is a widely used algorithm due to its simplicity of implementation and high performance comparing to other clustering algorithms like k-means (von Luxburg, 2007).

Since clustering is an unsupervised machine learning approach, there is no grand truth on the number of clusters. To determine the optimal number of clusters, we iterated through one to twenty clusters and assessed the "goodness" of the algorithm using V-measure. V-measure is the harmonic mean between homogeneity and completeness as shown below (sklearn metrics, 2019).

$$V = 2 \times \frac{(homogeneity \times completeness)}{(homogeneity + completeness)}$$

The advantage to using v-measure is its ability to overcome many problems that affect previously defined cluster evaluation measures. These include1) dependence on clustering algorithm or data set, 2) accurate evaluation and combination of homogeneity and completeness in the clustering, and 3) symmetry in the measurement to help with interpretation (Rosenberg & Hirschberg, 2007).

The v-measure for each cluster based on type of document, region, and type of organization is shown in Figure 2.

It is immediately clear that clusters are more complete and homogenous if documents from the same type of organizations are grouped together. It is also observed that the optimal number of clusters is 7 (Figure 3) which is coincidently the number of types of organization type in the corpus.

5 Findings and Discussion

The corpus of codes on which the analysis is based is certainly far from comprehensive across all existing codes related to the practice of chemistry, yet it revealed some very informative observations about how ethical considerations are formalized by chemistry practitioners from a range of national, regional, and international scientific, engineering, industry, and governmental organisations.

When discussing codes, it is common to distinguish between codes of conduct and codes of ethics, the former providing rules and guidelines to follow and the latter reflecting values to aspire to. From the text analysis, the word choices and associations found in codes of conduct were similar enough to those in codes of ethics that a separation of code types within the cluster analysis was not observed (Figure 2). This result is not unexpected, as the conduct advocated for chemistry practitioners would reflect the values of the profession (which would reflected by words found in codes of ethics).

Perhaps not completely unexpected, but an interesting finding from the analysis, is that the clusters were not reflective of the regional origin of the codes within the corpus (Figure 2). The significance of this finding is that it counters a narrative that suggests codes might be or even should be unique based on the region or country from where they originate (Biological Weapons Convention 2018a and 2018b). As each cluster contains similar codes from organisations located in countries from different regional groups, the analysis suggests that internationally, those thinking through the values of the profession address similar concepts and issues.

In the end, the most distinguishable characteristic of the codes falling into similar clusters of the analysis is the type of organisation the code was developed by and/or for (Figure 2). Figure 3 illustrates a two dimensional projection of documents similarity. Each cluster has a unique color. Additionally, type of organizations is shown using different shapes.

Relevant to the practice of chemistry, the analysis does show that independent of their purpose, the many codes have much in common with one another and these areas of commonality would usefully provide guidelines on topical areas of importance to include within the drafting of any new codes.

These observations bring us back to the question of a need for a unifying and global code. It could be argued that the common elements and values promoted by the codes could be usefully disseminated by a single code made available in multiple languages. Conversely, it could be argued that the rich variety of codes is a useful approach in initiating and maintaining productive dialogue on ethical issues amongst chemistry practitioners.

The purpose of The Hague Ethical Guidelines (OPCW 2015a and 2015b) is to provide a set of elements that could provide a basis for developing new codes. The Global Chemists Code of Ethics is an example of a code that was formulated using The Hague Ethical Guidelines as a starting point (Brown 2018). The value of developing new codes, even if the content may be reflective of what already exists would appear to be the exact reason we have so many codes available to us already – if we wish to encourage discussion of ethical issues in chemistry, encouraging individual organizations to draft and develop their own codes could provide a sense of ownership, which may make the aspirations of the code (independent of how similar it is to other codes) more familiar and supported by those within that organization.

It is also recognized that codes are not static documents (OPCW 2015a and 2015b), to make codes valuable they need to be discussed and nurtured, so that they continue to reflect core ethical values and the representation of these values within the fields that the codes are adopted within.

The analysis has also shown that ethical issues discussed within chemistry do share commonality with the norms of chemical disarmament and non-proliferation. In the on-going engagement between security and scientific communities, this observation might be valuable to make more visible. The increased visibility might serve as a means to raise awareness about the Chemical Weapons Convention amongst chemistry practitioners, and give security communities more insight into those they look to engage with on chemical security issues and the role the scientific community has always played in preserving international norms.

6 Future Work

The analysis presented in this paper is intended to provide further insight into the core elements of the discussion of ethical issues within the field of chemistry, and in so doing to help nurture and maintain dialogue on these issues helpful to chemistry practitioners and those who might question commitments within the science of chemistry to follow responsible practices alike.

To further support the discussion, a topic analysis over the corpus can help identify the core elements of an ethical guide for ethical and responsible practice of chemistry, specifically in reference to the Chemical Weapons Convention. This would enable further analysis to investigate if the ethical issues considered by chemistry practitioners have always reflected the norms that were set under the Convention over two decades ago.

Additionally, current method of using TF-IDF to measure similarity, ignores semantic information of text documents. We are planning to implement the same analysis using word embeddings in order to capture the semantic relationships among different documents.

```
Pipeline(memory=None,
     steps=[('vect', CountVectorizer(analyzer='word', binary=False, decode_error='strict',
        dtype=<class 'numpy.int64'>, encoding='utf-8', input='content',
        lowercase=True, max_df=0.5, max_features=None, min_df=5,
        ngram_range=(1, 5), preprocessor=None,
        stop_words=['i', 'me',...y=None)), ('tfidf', TfidfTransformer(norm='l2', smooth_idf=True, sublinear_tf=False,
use_idf=True))])
```

Figure 3 - Text Vectorization pipeline

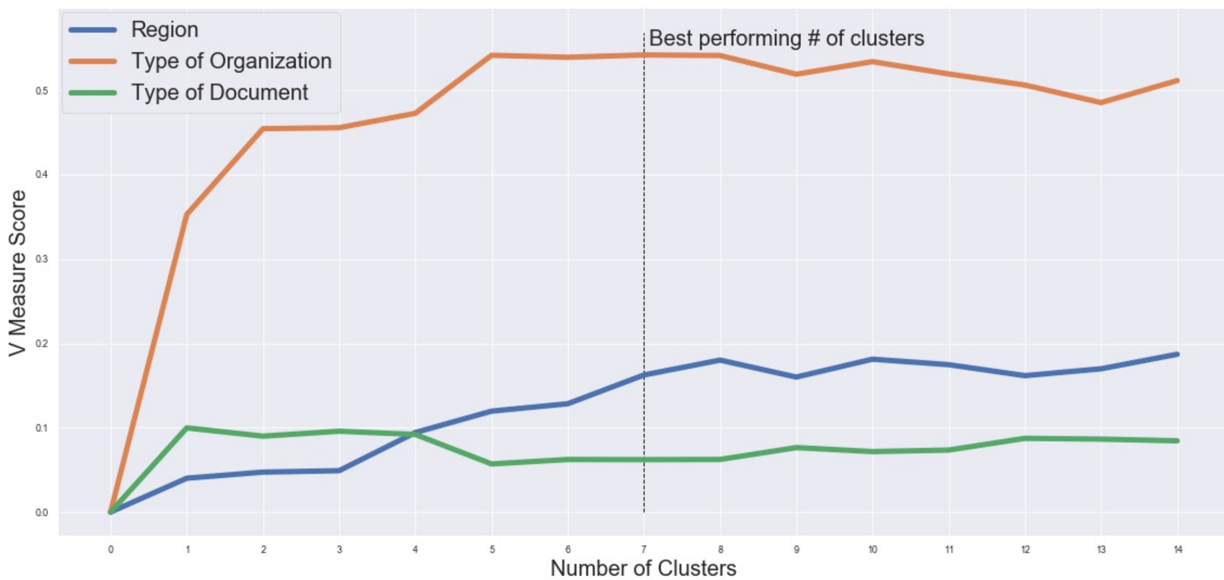

Figure 1 - Clustering performance for different attributes of documents

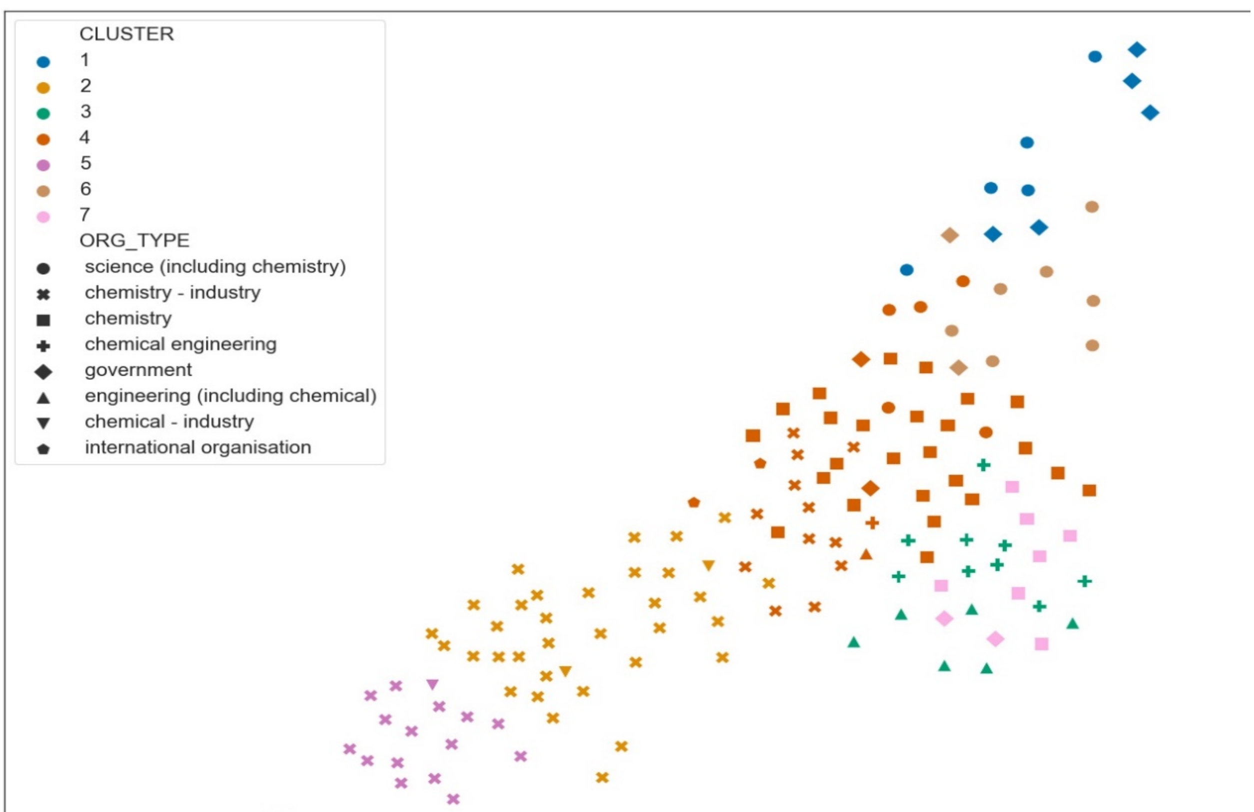

Figure 2-Documents clusters - organisation type

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