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Final Report:

Characterizing Hydraulic Fracturing Fluid Greenness: Application of a Hazard-based Index Approach

Phase II: An Integrated Hazard Screening and Indexing System for Hydraulic Fracturing Chemical Hazard Assessment

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Executive Summary

The use of chemicals in hydraulic fracturing has raised many environmental and human health (EHH) concerns regarding water resources contamination. The unconventional gas industry has begun to transition toward the use of chemicals with minimum EHH hazard for reasons of responsible gas production and public confidence. Various methods have been developed to measure the EHH hazard of hydraulic fracturing chemicals. The methods can generally be divided into hazard screening and hazard indexing approaches. Each approach is associated with different advantages and limitations.

Sponsored by the Canadian Association of Petroleum Producers (CAPP), British Columbia Oil and Gas Commission (BCOGC), British Columbia Oil and Gas Research and Innovation Society (BC OGRIS), and Mitacs Accelerate Program, a project was initiated at the School of Engineering, University of British Columbia Okanagan in 2016, with an aim to develop a universally applicable method to assess the EHH hazard potential of various chemicals used in hydraulic fracturing. The new method was developed to combine the features of pre-existing chemical hazard assessment methods. In the first phase of the project, two representative methods, including a hazard indexing system (HyFFGAS) and a hazard screening system (Intrinsik), were discussed and applied to assess the EHH hazard of the representative chemicals used in BC. The assessment results were also compared. From the first phase of the project, the features of the two types of hazard assessment systems were well understood.

In light of the results of the first phase study, an integrated hazard screening and indexing system (ICHSIS) was developed by combining the strengths of the two chemical hazard assessment methods. The development of the ICHSIS was elaborated regarding its designed purpose, hazard endpoints and criteria selection, hazard screening and indexing procedures, results aggregation and interpretation, and data uncertainty evaluation. The ICHSIS was applied to assess the EHH hazard potential of the representative chemicals used in hydraulic fracturing in British Columbia. The hazard screening results show that more than half of the ingredients and additives can be grouped into high hazard designations, suggesting that the use of chemicals with lower EHH hazard is necessary. The hazard indexing results were consistent with those from the previously developed indexing system, but the data confidence of the results was significantly improved. The integrated system can also help with decision-making related to the hazard mitigation and reuse of fracturing fluids from a perspective of EHH hazard potential. The integrated system offers a useful tool to monitor and communicate chemical hazards between industry, regulatory organizations, and the public. The hazard assessment results can identify the potential for chemical hazard mitigation and promote more sustainable unconventional gas production.

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1. Introduction

Unconventional natural gas production has significantly redrawn the energy landscape in Canada over the past years. The total remaining natural gas resource size in Canada is 30.8 trillion m^3, with 72% coming from unconventional gas formations in Alberta and British Columbia (NEB, 2017). By 2040, Canadian natural gas production is projected to increase 18%, and the increase will be primarily attributed to unconventional natural gas production (NEB, 2017). The rapid growth of the unconventional gas industry is mainly owing to the advent of novel natural gas production technologies such as horizontal drilling and hydraulic fracturing (HF), which allow for the economic extraction of natural gas from low permeability formations such as gas-bearing shales, sandstones, and coal beds (Myers 2012; Vidic et al. 2013; Soeder et al. 2014).

Despite the promising resource potentials and economic benefits, the rapid expansion of the unconventional gas industry has triggered considerable public debate regarding possible environmental and human health (EHH) impacts caused by HF (Vengosh et al. 2014; Boudet et al. 2014; Jenner and Lamadrid 2013; Soeder et al. 2014). One of the major concerns involves the chemicals used in HF, which could potentially contaminate ground and surface water supplies and pose health risks to surrounding aquatic ecosystems and water resource users (Akob et al., 2016; Ferrer and Thurman, 2015; Hurley et al., 2016; Kahrilas et al., 2014; Orem et al., 2014, 2017; Stringfellow et al., 2014, 2017). In the HF process, various additives are mixed with the base fluid (typically water) and proppants (commonly quartz sands) to produce fracturing fluids, which are pumped into underground under high pressures to initiate fractures in the low-permeability formations. The additives are designed to have different downhole functions, such as inhibiting the growth of undesirable microbes, adjusting the viscosity of fracturing fluids, preventing corrosion of well casing and pipelines, and improving the transportation of proppants (Hurley et al. 2016; Stringfellow et al. 2014). According to the downhole functions, additives can be divided into several functional categories including gelling agents, friction reducers, crosslinkers, breakers, biocides, corrosion inhibitors, scale inhibitors, iron control agents, clay stabilizers, surfactants, and demulsifiers (Hurley et al. 2016; Stringfellow et al. 2014).

In HF operations, chemicals are used at three different levels, including ingredient, additive, and fracturing fluid levels. An additive normally consists of several ingredients at different concentrations. The species and concentrations of ingredients can vary significantly among different additives (FracFocus, 2014). A typical fracturing fluid may use three to twelve additives, depending on the geological characteristics of the target formations and the requirements of the HF operators (Soeder et al. 2014). Additives may only account for a small fraction (e.g., < 2%) of the fracturing fluid; however, the use of millions of gallons of fracturing fluid for a single HF operation still involves a substantial

amount of additives (Soeder et al. 2014; All consulting, 2008). More critically, some of the ingredients are potential carcinogens, mutagens, and substances with acute and chronic toxic effects on human health and aquatic ecosystems (Cozzarelli et al., 2017; Finkel and Hays, 2013; Hu et al., 2017; Kassotis et al., 2017, 2016; Orem et al., 2017; Rogers et al., 2015; Soeder et al., 2014; Stringfellow et al., 2014). Additionally, since fracturing fluids usually contain a set of additives consisting of one or more ingredients, the composite hazard of additives is difficult to calculate, increasing the complexity and uncertainty in hazard assessment (Hurley et al. 2016).

The HF chemical use depends not only on geological characteristics and operational conditions but also on other factors, such as chemicals' efficacy, availability, cost, and EHH hazard potentials. Although there are various government regulations, industry codes-of-practice, and company standard operating procedures in place to prevent or minimize the likelihood of unintended releases of HF fracturing fluids, the risk posed by HF chemicals to surrounding ecosystems and resource users cannot be neglected. The use of chemical additives with minimized EHH effects is, therefore, encouraged by both the regulatory organizations and industries for reasons of responsible production and public confidence (Brannon et al. 2012; Kargbo et al. 2010; Gordalla et al. 2013; CAPP 2012; Hurley et al. 2016). The transition towards more environmentally responsible HF chemical use has presented several challenges, such as developing frameworks and methodologies which can provide meaningful and reliable chemical hazard assessment results in a context of unconventional gas production.

Various chemical hazard assessment systems have been developed to systematically evaluate EHH hazards and generate outcomes for informed decision-making in HF chemical management. The representative systems include the Quantitative Ranking Measure of Oil Field Chemical Environmental Impacts (QRM) by Baker Hughes Inc. (Jordan et al. 2010), Chemical Hazard Rating System (CHRS) by Sanjel Corporation (Hepburn, 2012); Chemical Scoring Index (CSI) by Halliburton Inc. (Verslycke et al. 2014); Intrinsik Screening-level Assessment System (Intrinsik Screening system) by Intrinsik Environmental Consulting Inc. (Intrinsik, 2013), Hydraulic Fracturing Fluid Greenness Assessment System (HyFFGAS) by Hurley et al. (2016), and GreenScreen system by the Clean Production Action (CPA, 2016). It should be noted that the GreenScreen system was not specifically designed for HF chemical hazard evaluation; rather, it has been widely used for general hazard assessment of various ingredients from house-hold chemical products to industrial reagents, including chemicals used in oil and gas field productions (CPA, 2016). These systems assess different types of chemical hazards (e.g., physical, environmental, and human health hazards) and generate assessment results for HF chemicals at different levels (e.g., ingredient, additive, and fluid levels). Hurley et al., (2016) has comprehensively reviewed these chemical hazard assessment systems regarding their objectives, hazard criteria, indexing approaches, and aggregation

techniques and developed the HyFFGAS based on the review results. Generally, the existing HF chemical hazard assessment systems can be divided into two main categories including hazard screening systems and hazard indexing systems, and thus they are inherently linked with different advantages and limitations. It is of great importance to develop an integrated chemical hazard assessment system that combines the strengths of the two categories for a more effective HF chemical hazard evaluation.

In this study, the advantages and limitations of hazard screening and indexing systems are discussed in a context of HF chemical hazard assessment. Based on the discussion of the two categories of systems, an integrated chemical hazard screening and indexing system (ICHSIS) was developed. The objective defining, parameters selection, data uncertainty analysis, and chemical hazard weighting, aggregation, and classification of the ICHSIS were elaborated. The ICHSIS was used to assess the representative additives used in HF operations in British Columbia, Canada, and the assessment results were compared with HyFFGAS. The developed system provides a useful framework for an effective chemical hazard assessment in the unconventional gas industry.

2. Hazard screening and indexing systems

Both the hazard screening and indexing systems being used for HF chemical hazard assessment are qualitative methodologies, either use descriptive terms or numerical rating scales to evaluate chemical hazard (Ferrari et al., 2016). The systems are separately developed to describe HF chemical hazard using different hazard metrics at different HF chemical levels (Hurley et al., 2016). These systems share a common feature that the assessment processes are all ingredient-driven. In other words, the chemical hazard assessment processes all begin at the ingredient level since ingredients are the essential elements of an additive and a fracturing fluid. However, hazard screening and indexing systems use different approaches to present ingredients' hazard and aggregate the hazard to the additive/fracturing fluid level. The assessment results from the two categories are also associated with different hazard implications and data uncertainties.

2.1 Hazard screening systems

Chemical hazard screening aims to select an appropriate hazard designation for a given chemical, whether it is in the form of an ingredient, additive, or fracturing fluid. The hazard designations are assigned based on qualitative hazard description and potency consideration, rather than numerical scales. Two representative chemical hazard screening systems, including the Intrinsik Screening system and GreenScreen system, are being used for HF chemical hazard evaluation. The two systems operate at screening level with a focus on the defined series of endpoints (e.g., carcinogenicity, aquatic toxicity, and human acute oral toxicity) relevant to a chemical's EHH hazard profile. The hazard endpoints selected are representative of the major EHH hazard concerns in a

context of unconventional gas production. The chemical toxicological data (CTD) of an ingredient is screened against the selected hazard endpoints to determine whether the concerned hazard exists or not, and the severity of the hazard if it exists. The ingredient's hazard profile is presented in the form of qualitative hazard designations, such as the three hazard categories used by the Intrinsik Screening system and the four hazard benchmarks used by the GreenScreen (CPA, 2016; Intrinsik, 2013). Different hazard designations represent different severity levels of EHH hazard. The concentrations of ingredients in an additive/fluid are also screened against the cut-off concentrations of various hazard endpoints to determine whether the hazard is in-effect or not.

The chemical hazard screening systems can generate descriptive hazard designations reflective of the EHH hazard concerns of various chemicals, without involving any numerical conversion and aggregation algorithm. Thus, the results from hazard screening systems are relatively objective and easy for hazard communication. Nonetheless, the hazard screening systems are less applicable when comparing two chemicals with the same hazard designation. Also, the ingredient concentration evaluation mechanism is Boolean (i.e., yes/no) in the hazard screening systems, neglecting the fact that the higher concentration of a hazardous ingredient contained in an additive/fluid, the higher EHH hazards that the additive/fracturing fluid might have.

2.2 Hazard indexing systems

Various indexing systems were developed as tools to translate information regarding the properties of HF chemicals to a single measure reflective of overall chemical hazard (Hurley et al. 2016). The single measure (i.e., index) allows for the comparison of the EHH hazard of different chemicals. The QRM, CHRS, CSI, and HyFFGAS are the representative HF chemical hazard indexing systems (Hurley et al. 2016; Verslycke et al. 2014; Hepburn, 2012; Jordan et al. 2010). These indexing systems were developed based on various hazard endpoints, scoring rules, and score aggregation approaches. The chemical property on the selected hazard endpoints and their concentrations are transformed to a numerical scale using specific sub-index functions, scoring rule sets, or implicit rating curves (Hurley et al., 2016). The resultant sub-indices or scores are weighted and aggregated to produce a single meaningful value. Various weighting techniques, such as the weighted sum aggregation and ordered weighted averaging aggregation, were used in the aggregation process to embed the relative importance of each sub-index in the final index (Sadiq and Tesfamariam, 2007). Qualitative hazard descriptions are established based on the scales of the final indices to facilitate hazard interpretation and decision-making on chemical selection. It is important to know that hazard interpretation varies among the different indexing systems, depending on index formulation and degree of field validation (Hurley et al., 2016).

In the application of indexing systems, a few issues are expected as a result of the abstraction of information and data. Indexing systems are not entirely successful in providing a true picture of a system due to diverse types of input data and partly because they are insufficient to aggregate diverse data properly (Sadiq et al., 2010). The improper aggregation could generate eclipsed, exaggerated, and ambiguous results (Sadiq et al., 2010; Swamee and Tyagi, 2000). For instance, eclipsing occurs when a chemical being assessed is associated with one or more critical EHH hazard, yet the derived hazard index comes out at a moderate level, failing to show any critical hazard due to improper aggregation. The eclipsed result would present an underestimated hazard and thus lead to an impractical decision support. Moreover, sub-index weightings, similar to the selection of hazard endpoints, are subjective depending on assessor and system developers' opinions. Different system developers may have different insights regarding the importance of hazard endpoints, so it is possible that different indexing systems generate different EHH hazard assessment results for the same chemical. Therefore, it is difficult to develop a widely applied, commonly agreed indexing system for chemical hazard assessment within the oil and gas industry (Hurley et al., 2016). There is a great need to develop an integrated system, which combines the strengths of hazard screening and indexing systems, for a more accurate and efficient chemical hazard assessment and communication among unconventional gas industry stakeholders, governmental regulators, and the public.

Sponsored by the Canadian Association of Petroleum Producers (CAPP), British Columbia Oil and Gas Commission (BCOGC), British Columbia Oil and Gas Research and Innovation Society (BC OGRIS), and Mitacs Accelerate Program, a research project was initiated at the School of Engineering, University of British Columbia Okanagan in 2016. The project aims to develop a universally applicable method to assess the EHH hazard potential of various chemicals used in HF by combining current existing chemical hazard assessment methods.

3. Project objectives

The project titled "Characterizing Hydraulic Fracturing Fluid Greenness: Application of a Hazard-based Index Approach" includes two internship units (i.e., phases). The specific objectives of each internship unit are given below:

Internship unit 1 (Phase I):

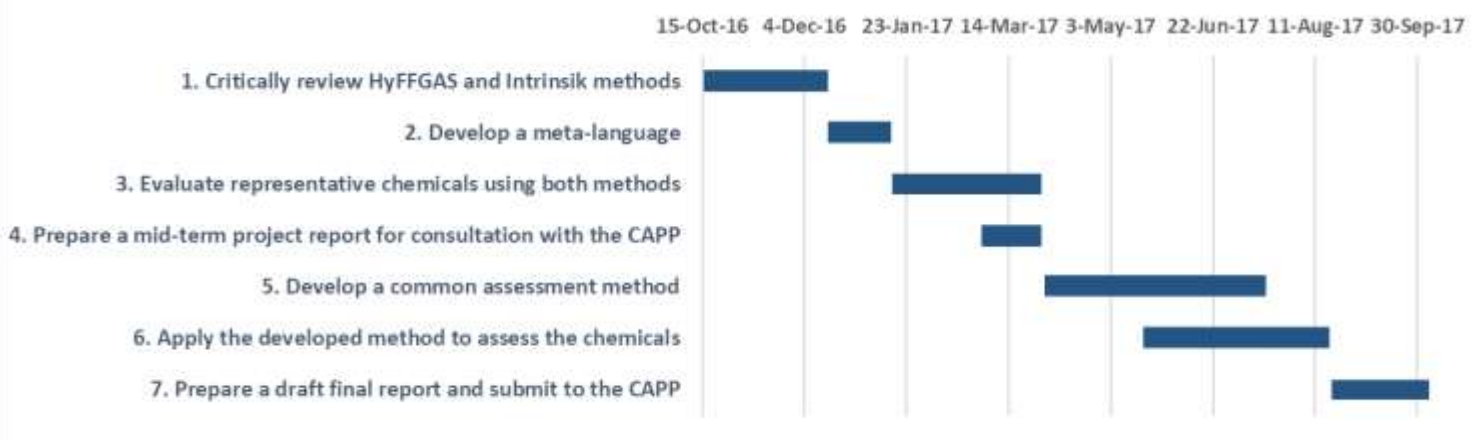
1) Compare and discuss the underlying concepts used in the HyFFGAS and Intrinsik methods
2) Develop a meta-language of common terms used in the evaluation of HF fluid EHH hazards toxicity

3) Evaluate the representative HF chemical additives using the HyFFGAS method and the Intrinsik method and compare the results

Internship unit 2 (Phase II):

4) Develop a common HF chemical additives EHH hazard assessment method
5) Use the developed method to assess the EHH hazard of the representative HF chemicals

4. Project timeline



5. Retrospect of Project Phase I

In the first phase of the project, the underlying concepts, terminologies of different hazard parameters, and hazard assessment procedures of two systems, including the hydraulic fracturing fluid greenness assessment system (HyFFGAS) and the Intrinsik Screening System, were reviewed and compared. The two systems were also used to assess the hazard potential of representative additives used in HF operations in BC. The HyFFGAS generated numerical assessment results on additives regarding EHH toxicity, allowing for the comparison of additives' hazard potential. The Intrinsik system categorized additives into appropriate groups representing different hazard levels for effective chemical management. The comparison of the two systems found that fewer additives recorded in the FracFocus database can meet the assessment requirements by the Intrinsik system. That is because the Intrinsik system relies partially on obtaining chemicals' information directly from the supplier to enable the assessment. The assessment results from the two systems also showed discrepancies, despite the fact that the assessments were conducted on the same additives. The results analysis suggested that the differences in chemical toxicological data sources, the definition of hazard parameters, and uncertainty evaluation approaches, are responsible for the discrepancies.

A mid-term report generated from the Phase I of the project was submitted to the project sponsors. Valuable feedback and recommendations were received from the Shale Water Steering and Technical Committee at CAPP for the development of the new method. The feedback and suggestions are summarized in Appendix A1.

6. Development of ICHSIS

Informed by the results from the Phase I study and the feedback from the project sponsors, an integrated chemical hazard screening and indexing system (ICHSIS) was developed in Phase II of the project. The ICHSIS is intended to characterize the EHH hazard potential of HF chemicals at the ingredient, additive, and fluid levels through an integrated hazard screening-indexing approach. The assessment results generated by the ICHSIS can be used to guide the selection, handling, and use of HF chemicals with the minimum EHH effect by HF practitioners and to facilitate the development of chemical management policies by regulators. In the ICHSIS, the EHH hazard potential is defined as the properties and characteristics of a HF chemical, either an ingredient or a composite additive/fracturing fluid, that render it capable of causing an adverse effect on the EHH. The ICHSIS does not assess the hazard exposure frequency that determines whether or not the hazard potential to cause adverse effect will be realized. Since risk is defined as exposure to undesirable consequences (e.g., hazard) (Li et al., 2007; Piver et al., 1998), the assessment results of ICHSIS is not indicative of the actual EHH risk, but rather reflects only the chemical's hazard potential. The ICHSIS does not consider the cumulative effect of a chemical mixture or degradation products or incorporate chemical fate and exposure in the environment. The EHH hazard potential of HF chemicals is primarily evaluated through a water exposure as there is substantial concern regarding the potential for HF production to contaminate water sources.

The designed function of the ICHSIS is similar to that of the HyFFGAS. The HyFFGAS is intended to characterize relative HF fluid system chemical greenness based on critical human health and environmental health hazards/impact potentials through water exposure (Hurley et al., 2016). Nonetheless, the terminology "*greenness*" used by the HyFFGAS has a broader meaning than the EHH hazard potential (Manahan, 2006). A chemical product may have low EHH hazard potential but it might not green due to the low rating on other greenness criteria. There is also no global conformance to a definition of greenness. Although the assessment endpoint of HyFFGAS is a subset of the holistic greenness, using this ambiguous terminology may lead to confusion for stakeholders, scrutiny of service providers, and lack of trust in the rating system. As a result, the ICHSIS has abandoned the terminology "*greenness*" and uses the EHH hazard potential as the assessment outcome to avoid ambiguity.

The ICHSIS is designed to accommodate HF chemical data from two sources, including chemical data provided directly by chemical suppliers and the online FracFocus Chemical Disclosure Registry database (FracFocus, 2017). The first data source is available to industrial stakeholders and governmental regulators through several databases. The FracFocus database is publicly accessible to a wide range of users for hazard monitoring from a public perspective.

6.1 Assessment framework

The general assessment procedure of ICHSIS is outlined in Figure 1. The assessment process begins with the chemical data acquisition. That is, the Chemical Abstract Service Registration Numbers (CASRN) and concentrations of the ingredients within an additive/fracturing fluid are identified, and then the ingredients' CTD are searched. The CTD and concentrations are processed through a hazard screening and a hazard indexing approach, respectively. In both approaches, the CTD of an ingredient is assessed against the selected EHH hazard endpoints and criteria to generate a hazard screening outcome (e.g., hazard designation) and a hazard indexing outcome (e.g., hazard index), coupled with indicators of data confidence levels, respectively. The ingredients' hazards are then aggregated by their respective concentrations in the additive/fracturing fluid to generate a hazard screening outcome and a hazard indexing outcome at the additive/fracturing fluid levels, respectively. Based on the hazard assessment outcomes, decision to use a chemical can be made for the purpose of chemical hazard mitigation. The EHH hazard endpoint and criteria selecting, CTD searching, hazard screening and indexing, and assessment outcome interpretation are discussed in the following sections.

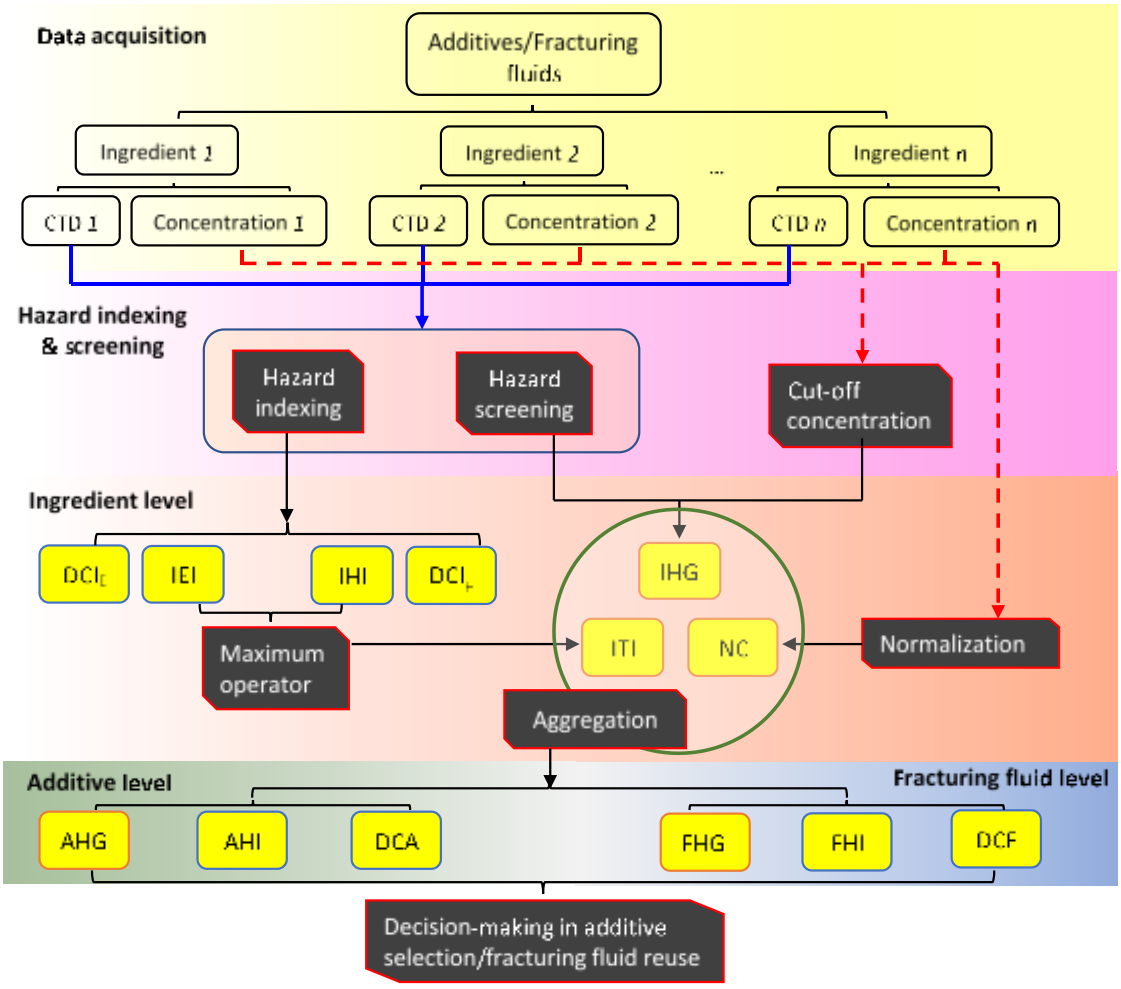


Figure 1 Chemical hazard assessment procedure of ICHSIS

6.2 Hazard endpoints and criteria selection

The CTD is evaluated against the hazard endpoints and criteria of interest. In ICHSIS, the hazard endpoint denotes the type of the EHH adverse effect, such as carcinogenicity, mutagenicity, acute aquatic toxicity (Table 1). The hazard criteria refer to the hazard levels within each hazard endpoint, representing the severity of a particular type of adverse effect. For example, Category 1 to 3 carcinogens as three hazard criteria were included under the hazard endpoint carcinogenicity. The selection of hazard endpoints involves subjective decision-making; however, some general guidelines that should be

followed to ensure an effective selection process. For instance, the selected hazard endpoints should represent a combination of environmental health and human health impacts that are considered to be relevant and significant. Each endpoint should be accepted as an important determinant of a chemical's hazard profile and suitable for indexing and screening purposes. The selected hazard endpoints should also be a balanced consideration between the scope boundaries of chemical hazard evaluation and adequate coverage of the potential chemical hazards that could be posed to the EHH (Hurley et al., 2016; Intrinsik, 2013). In ICHSIS, the hazard endpoints were determined based on the review of existing hazard indexing/screening systems, emerging chemical hazard regulatory and initiatives, and the input gathered from consultation with industry representatives and regulatory authorities.

The selected hazard endpoints and criteria are shown in Table 1. The definitions of hazard endpoints and criteria can be found in the Globally Harmonized System of Classification and Labelling of Chemicals implemented by the United Nations (UN, 2013). In addition to the conventional human health hazard endpoints defined in the GHS, an emerging hazard endpoint, namely endocrine disruptor (E), was included in the ICHSIS based on the relevant environmental strategy of the European Commission (European Commission, 2017). This endpoint was introduced because there is a growing concern about the extent of risk posed by endocrine disruptors to human and wildlife health and therefore calls for an action to reduce the risks (European Commission, 2017; Kassotis et al., 2016, 2017). Moreover, the EHH hazard potential is assessed in a context of the unintended release of HF chemicals caused by spill accidents, equipment failure, or the loss of well-bore integrity. Thus, physical hazards (e.g., flammability, explosiveness, corrosiveness, reactivity) are not included in the ICHSIS because these hazards are more applicable to the workplace safety and less relevant to the EHH risk posed by an unintended release of HF chemicals. Since the likelihood of exposure to the physical hazards is minimized by the existing industry codes-of-practice and standard operation procedures, assessing these hazards could result in duplication of work by the ICHSIS. As shown in Table 1, hazard scores (HS) ranging from 0 to 10 were assigned to the hazard criteria under each endpoint. A higher HS indicates that a higher EHH hazard potential concerning the hazard endpoint. The HSs were intended to differentiate and scale the hazard criteria, and they were designed based on the authors. Since the HSs were assigned subjectively, they can be modified to suit different hazard assessment requirements.

Table 1 EHH Hazard endpoints, criteria, and scores inclusive in ICHSIS

Environmental health hazard			Human health hazard		
Endpoints	Criteria	Score	Endpoints	Criteria	Score

Environmental persistence (P)	Rapidly/ready biodegradable	10	Carcinogenicity (C), mutagenicity (M), reproductive toxicity (R), and endocrine disruptor (E)	Cate. 1 (A, B)	10
	Inherently biodegradable	5		Cate. 2 (A, B)	5
	Not rapidly/inherently biodegradable	0		Cate. 3	0
Bioaccumulation potential (B)	High	10	Chronic human oral toxicity (ChT)	Yes	10
	Low	0		No	0
Acute/chronic aquatic toxicity (AT)	Cate. 1	10	Acute human oral toxicity (AhT)	Cate. 1	10
	Cate. 2	6		Cate. 2	6
	Cate. 3	3		Cate. 3	3
	Cate. 4	0		Cate. 4	0

Note: Cate. = Category

The HyFFGAS has a different list of EHH endpoints as compared with that of the ICHSIS. For example, the HyFFGAS does not assess the chronic human oral toxicity and endocrine disruptor but evaluate the dermal toxicity of chemicals (Hurley et al., 2016). Since the hazard endpoints and criteria in the HyFFGAS were also selected based on the Globally Harmonized System of Classification and Labelling of Chemicals, their respective definitions are the same as these in the ICHSIS; However, it is important to note that the Category 1 and 2 carcinogenic, mutagenic, and reproductive toxic effect are considered to have the same hazard effect in the HyFFGAS, but they are treated differently in the ICHSIS.

3.3 Chemical toxicological data (CTD)

The hazard screening and indexing rely on the CTD of ingredients. The quality and availability of CTD greatly affect the data confidence performance of the hazard assessment results. A variety of data sources, including peer-reviewed chemical toxicity databases, material safety data sheets, suitable ingredient analogs, and chemical toxicity model simulations, are used by ICHSIS to increase the availability of CTD. In comparison, the HyFFGAS uses material safety data sheets as the only CTD source, and thus the assessment results are expected to have lower data confidence. As shown in Table 2, the data sources are divided into four tiers based on their data confidence implications. A data confidence score (DCS) is assigned to each tier of data sources for indexing purpose. The DCS is in a range of 0 to 10, and the higher value indicates a higher data confidence level of the data source.

As shown in Figure 2, a CTD searching rule was established to ensure that the assessment results will be generated with the highest possible data confidence. The ingredients within an additive/fracturing fluid are identified by their respective CASRNs, and then the tier 1 data sources are searched according to the CASRNs. If the CTD cannot be found in the tier 1 data sources, then the tier 2 data sources will be searched. Similarly, the tier 3 data sources will be used if the CTD searching in tier 2 data sources is

not successful. When using the tier 3 ingredient analogs, the data confidence level is compromised. Thus, a lower DCS was assigned to the tier 3 data sources because the derived CTD is not directly related to the target ingredient. If the CTD lacks in tier 1 to 4 data sources, then a data gap can be identified for the target ingredient concerning the hazard endpoint. In that case, a moderate-level hazard criteria and HS will be assigned to the data-missing endpoint. If there are no moderate-level hazard criteria or HS exist in the endpoint, then the most conservative result (i.e., the highest hazard) of the endpoint will be used to generate an assessment outcome. The assessment results with data gaps are marked with an indicator "*" to differentiate them from the assessment results without data gaps.

Table 2 Chemical toxicological data (CTD) sources inclusive in ICHSIS

Ingredient	Tier	Data source/gap	DCS
Target ingredient	Tier 1	Chemical toxicity databases	10
	Tier 2	Material safety data sheets	8
Analog ingredient	Tier 3	Chemical toxicity databases	6
		Material safety data sheets	4.8
		Model simulation	3.6
Target ingredient	Tier 4	Model simulation	6
	-	Data gap	0

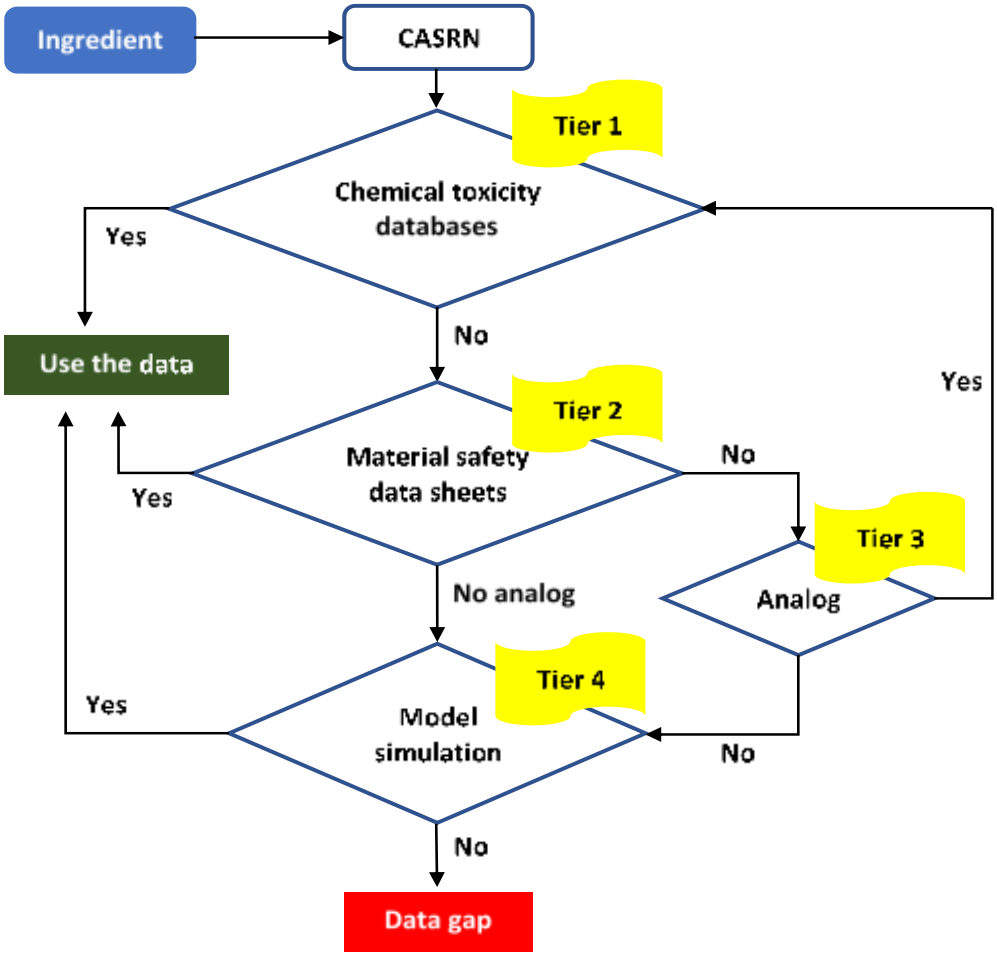


Figure 2 Chemical toxicological data searching rule

The information regarding the naturel of an ingredient and its environmental persistence (P) can be found in the Environment and Climate Change Canada (ECCC) database and TOXNET-HSDB (sub-category "Environmental fate & exposure"). If the ingredient is not listed in ECCC or TOXNET databases, then searching for the ingredient's material safety data sheets in chemical suppliers' material safety data sheets libraries. If there is no material safety data sheet available for the ingredient, then using Analog Identification Methodology (AIM) to find an analog ingredient and repeat the CTD searching process from the tier 1 databases. The tutorial of AIM can be found in its user manual. Also, whether to include a "pass 2" in searching the analog ingredient process or not should be decided by the assessor. If the AIM fails to find an analog ingredient, then using the US EPA Suite Biowin software to model the environmental behavior of the ingredient. If all attempts fail to generate a result, then a data gap is identified for the endpoint P. A moderate hazard category "inherently biodegradable" will be assigned to the data-

missing endpoint and the CS for endpoint P will be zero. An indicator "*" will be added to show that a data gap exists for the endpoint.

For an environmentally persistent ingredient, its chronic human oral toxicity (ChT) must be evaluated. The data of ChT effect can be collected from the US EPA Integrated Risk Information System (IRIS) database, Agency for Toxic Substances & Disease Registry (ATSDR) database, the Risk Assessment Information System (RAIS)-Chemical Toxicological Values, and TOXNET-HSDB. A Reference Dose for Chronic Oral Exposure (RfD) of 10 mg/kg/day is used as the threshold value to determining whether there is a chronic toxic effect or not.

The databases available for searching CTD are shown in Table 3. The modeling tools are also included in the table. The chemical toxicity databases have equal importance, so there is no order of using different data sources under the same tier. It is recommended to search all available databases for each endpoint to check data consistency. If there is a data conflict between different databases, then the most conservative data should be used for hazard assessment. It is important to note that the list of databases should be updated periodically (e.g., every year) to ensure that all the databases are accessible. Also, if new database has been established, which can provide useful information to chemical hazard assessment, then the database is recommended to be included in ICHSIS.

Table 3 Chemical toxicity databases and modeling tools for different hazard endpoints

Hazard endpoints	Databases	Weblinks
P	• ECCC • TOXNET-HSDB • (Modeling) EPA Suite-Biowin	ECCC: http://www.ec.gc.ca/lcpe-cepa/default.asp?lang=En&n=5F213FA8-1&wsdoc=D031CB30-B31B-D54C-0E46-37E32D526A1F TOXNET-HSDB: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm (Modeling) EPA Suite-Biowin: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface
B	• ECCC • TOXNET-HSDB • (Modeling) EPA Suite-Kowwin	ECCC: http://www.ec.gc.ca/lcpe-cepa/default.asp?lang=En&n=5F213FA8-1&wsdoc=D031CB30-B31B-D54C-0E46-37E32D526A1F TOXNET-HSDB: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm
AT	• ECCC • TOXNET-HSDB • ECHA • (Modeling) ECOSTAR	ECCC: http://www.ec.gc.ca/lcpe-cepa/default.asp?lang=En&n=5F213FA8-1&wsdoc=D031CB30-B31B-D54C-0E46-37E32D526A1F TOXNET-HSDB: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm ECHA: https://echa.europa.eu/search-for-chemicals

		(Modeling) ECOSTAR: https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model
C	• IARC • TOXNET-CCRIS • TOXNET-CPDB • (Modeling) EPA Oncologic	IARC:http://monographs.iarc.fr/ENG/Classification/ClassificationsCASOrder.pdf TOXNET-CCRIS: https://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?CCRIS TOXNET-CPDB: https://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?CPDB (Modeling) EPA Oncologic: https://www.epa.gov/tsca-screening-tools/oncologictm-computer-system-evaluate-carcinogenic-potential-chemicals
M	• ECHA • TOXNET-CCRIS • TOXNET-GENE-TOX	ECHA: https://echa.europa.eu/search-for-chemicals TOXNET-CCRIS: https://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?CCRIS TOXNET-GENE-TOX https://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?GENETOX.htm
R	• ECHA • Cali.OEHAA • TOXNET-HSDB	ECHA: https://echa.europa.eu/search-for-chemicals Cali.OEHAA: https://oehha.ca.gov/media/downloads/proposition-65//p65single01272017.pdf TOXNET-HSDB: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm
E	• European Commission (EUC) -EDS Annex I	EUC: http://ec.europa.eu/environment/chemicals/endocrine/strategy/substances_en.htm#priority_list
AhT	• ECHA • TOXNET-HSDB • OECD	ECHA: https://echa.europa.eu/search-for-chemicals TOXNET-HSDB: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm OECD: http://webnet.oecd.org/hpv/ui/Search.aspx
ChT	• IRIS • ASTDR • TOXNET-HSDB • RAIS	IRIS: https://www.epa.gov/iris ASTDR: https://www.atsdr.cdc.gov/mrls/mrllist.asp TOXNET-HSDB: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm RAIS: https://rais.ornl.gov/

6.4 Hazard screening

The acquired CTD of an ingredient is screened against the hazard endpoints to generate a descriptive hazard designation for the ingredient. As shown in Table 4, four hazard groups (HG) as hazard designations were established for chemical classification regarding the EHH hazard potential. Each HG has several hazard classification criteria, and each hazard classification criteria is the combination of different environmental health and human health hazards. An ingredient will be assigned a HG designation based

on its CTD on the selected hazard endpoints. For example, if an ingredient is associated with high environmental persistence (P) and high bioaccumulation potential (B), then it will be classified as a HG1 chemical according to the HG classification criterial shown in Table 4. This ingredient should be avoided to use due to its high EHH hazard potential. In comparison, if an ingredient only has high environmental persistence (P) but without any other EHH adverse effect, then the ingredient will be considered a HG3 ingredient, and it is allowed to use but there are opportunities for improvement. The four HGs were developed in light of the four benchmarks used by the GreenScreen system (CPA, 2016), which is being widely used by various industry associations as well as governments and non-governmental organizations for chemical hazard screening. An informed chemical use suggestion was also established for each HG.

The ingredient EHH hazard screening process is shown in Figure 3. The nature (organic/inorganic) of a given ingredient is examined first. Inorganic ingredients are required to be assessed differently because they are inherently environmentally persistent. It is apparently questionable to label a natural occurring inorganic ingredient as high environmental health hazard due to its high P. If an inorganic ingredient has no significant EHH toxicity, it will still be classified as a HG4 ingredient. Also, the chronic human oral toxicity (ChT) was selected to accommodate the possibility of a long-term exposure of human to an ingredient present in potable water resources as a result of spill accidents. This endpoint is reserved for ingredients that are identified to be highly persistent in the environment, causing potentially chronic exposure (Intrinsik, 2013). Hence, the rapidly and inherently biodegradable organic ingredients are exempted from the ChT screening.

Table 4 Four hazard groups (HG) of the ICHSIS

HG	Classification criteria [a]	Use implication	Numeralized value
HG 1	• P: Inherently biodegradable ∧[b] B: High ∧ AT: Category 2 • P: Not rapidly/inherently biodegradable ∧ B: High • P: Not rapidly/inherently biodegradable ∧ AT: Category 1 ∨[c], M, R, or E: Category 1 ∨ AhT: Category 1 ∨ ChT: Yes • B: High ∧ AT: Category 1 ∨ C, M, R or E: Category 2 ∨ AhT: Category 2 ∨ ChT: Yes • C, M, R or E: Category 1	The use of HG 1 chemicals should be avoided	10
HG 2	• P: Inherently biodegradable ∧ AT: Category 3 ∨ C, M, R, or E: Category 2 ∨ AhT: Category 3 • P: Inherently biodegradable ∧ B: High	HG2 chemicals are allowed to use but substitutes of lower EHH	6

	• P: Not rapidly/inherently biodegradable ∧ AT: Category 3 ∨ C, M, R or E: Category 2 ∨ AhT: Category 3 • B: High ∧ AT: Category 3 ∨ C, M, R or E: Category 2 ∨ AhT: Category 3 • C, M, R or E: Category 2 • AT: Category 1 ∨ AhT: Category 1 ∨ ChT: Yes	hazard potential should be searched	
HG 3	• P: Not rapidly/Inherently biodegradable ∨ Inherently biodegradable • B: High • AT: Category 2 ∨ 3 • AhT: Category 2 ∨ 3	HG3 chemicals have lower EHH hazard potential than HG2 chemicals, but there are opportunities for improvement	3
HG 4	• P: Rapidly biodegradable ∧ B: Low ∧ AT: Category 4 ∧ C, M, R, and E: Category 3 ∧ AhT: Category 4 ∧ ChT: No	HG4 chemicals have no significant EHH hazard potential, so they are recommended to use	0

[a] Based on the combination of hazard endpoints and criteria in Table 1
[b] ∧: Mathematical operator "and"
[c] ∨: Mathematical operator "or"

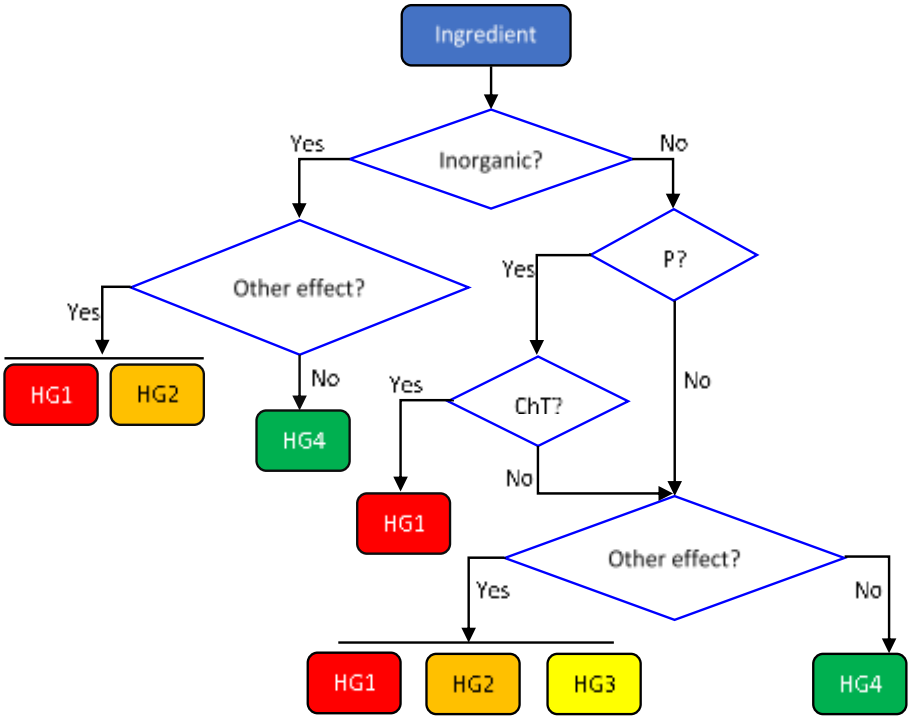


Figure 3 Hazard screening at the ingredient level

The HG designation of an additive depends on the HG designations and concentrations of its ingredients. As shown in Figure 4, determining the HG for an additive is a hierarchical screening process starting with the search of HG1 ingredients in the additive. If a HG1 ingredient is found in the additive, then its concentration present in the additive is required to be determined against the cut-off concentrations of the concerned hazard endpoints (Table 5). The cut-off concentrations indicate that the potential EHH hazard potential of an additive will depend not only on the properties of its ingredients but also on their concentrations. The ICHSIS considers ingredients that are present at concentrations below the cut-off values and have negligible EHH hazard. The cut-off concentrations that apply vary by the hazard endpoints, and are consistent with those used as part of other chemical hazard classification systems, including the Health Canada's Workplace Hazardous Materials Information System and the Globally Harmonized System of Classification and Labelling of Chemicals (Health Canada, 2015; UN, 2013).

As shown in Figure 4, if the HG1 ingredient's concentration is higher than the cut-off concentrations of the concerned hazard endpoints, then the additive will be classified as a HG1 additive since it contains at least one in-effect HG1 ingredient. If the HG1 ingredient's concentration is lower than the cut-off concentrations, then the concerned endpoints will be considered as not been triggered. However, there is an exceptional situation. For example, if a HG1 ingredient characterized by high P and high B, then the additive containing this ingredient will be classified into HG1 regardless the cut-off concentrations screening results. This is because if the additive is spilled, the high P and B properties could make the ingredient long-lasting in the environment and consequently accumulate in the receptors' bodies to cause an adverse effect. In this case, the additive will still be labeled HG1 with an indicator (e.g., HG1!) to differentiate itself from other ordinary HG1 additives. If no HG1 ingredient contained in the additive, then search for HG2 ingredients and screen the concentrations of ingredients in the same approach. Screening ingredients from HG1 to HG4 and their concentrations to determine the HG for the additive. The use implications of additives in different HGs are the same as ingredients.

Figure 4 Hazard screening at the additive/fracturing fluid level

Table 5 Cut-off concentrations of different hazard endpoints

Hazard	Endpoints	Cut-off concentrations (%)
Environmental health	AT	≥ 1.0
	P	≥ 1.0
	B	≥ 1.0
Human health	C	≥ 0.1
	M	≥ 0.1
	R	≥ 0.1
	E	≥ 0.1
	AhT	≥ 1.0
	ChT	≥ 1.0

In the ICHSIS, the EHH hazard assessment at the fracturing fluid level is the same as the additive level. A fracturing fluid can be regarded as an additive which contains a large number of ingredients diluted in millions of gallons of water (Kargbo et al., 2010). The species and concentrations of ingredients vary significantly in different fracturing fluids, implying that every assessment at the fracturing fluid level will generate a unique result. The hazard screening result of a fracturing fluid represented by the four HGs. A HG1 fluid indicates that at least one HG1 ingredient presented in the fluid and its concentration in the fluid is higher than the cut-off concentrations. A HG2 fluid has two implications: (i) there is no HG1 ingredient in the fluid, but there is at least one HG2 ingredient in the fluid, the concentration of which is high enough to trigger the endpoint; and (ii) there might be one or more HG1 ingredients contained in the fluid, but their concentrations are too low to trigger the hazard endpoints. The second implication allows a recovered flowback fluid can be reused as the base fluid as long as the concentrations of high-hazard ingredients are lower than the cut-off thresholds. If a fluid consists of two or more additives containing the same ingredient, then the concentration of this ingredient in the fluid must be calculated as a sum. Similar to the additive assessment, there is an exception related to the special ingredients characterized by high P and B. That is, if any ingredients of high P and B is present in a fluid, then the fluid will be classified as a HG1 fluid regardless of the concentrations.

6.5 Hazard indexing

Although the hazard screening results can objectively reflect the inherent EHH hazard potential of various ingredients, additives, and fracturing fluids, they are less informative when comparing two chemicals within the same HG. It is important to use the hazard indexing approach in addition to the hazard screening approach for a more versatile chemical hazard assessment system.

The conversion of multi-dimension non-commensurate chemical hazard data into numerical indices involves several steps such as scoring hazard criteria, weighting hazard endpoints, aggregating scores to generate an index, scaling and interpreting the index. Subjective opinions are incorporated in these steps. Thus, hazard indexing should be used as a supplement to the hazard screening to minimize the influence of subjective opinions on the chemical hazard assessment. The HSs of hazard criteria (Table 1) are the indicators of the severity of hazards related to various hazard endpoints, and they need to be aggregated to generate a numerical value reflective of the overall environmental health and human health hazards. The aggregation of HS requires weighting of the relative importance of different hazard endpoints. A set of weights of n endpoints can be written as:

$$W = (w_1, w_2, \dots, w_n) \text{ where } \sum_{j=1}^{n} w_j = 1 \qquad (1)$$

The Analytical Hierarchy Process (AHP) is used for assigning weights to different hazard endpoints. The AHP is a useful technique for organizing and analyzing complex decisions and has widely been used in group decision-making (Saaty, 2008). The AHP generates a weight for each evaluation criterion according to the decision maker's pairwise comparisons of the criteria. The higher the weight, the more important the corresponding criterion is. The relative importance of two criteria (i.e., j and k) is measured according to a numerical scale from 1 to 9, as shown in Table 6, where it is assumed that the j^{th} criterion is equally or more important than the k^{th} criterion. The phrases in the "Interpretation" column of Table 6 are only suggestive and may be used to translate the decision maker's qualitative evaluations of the relative importance of two criteria into numbers.

Table 6 Relative importance value in AHP

Importance value [a]	Interpretation
1	j and k are equally important
3	j is moderately more important than k
5	j is strongly more important than k
7	j is very strongly more important than k
9	j is extremely more important than k

[a] Importance value of 2, 4, 6, 8 in-betweens

The ICHSIS assesses ingredients' environmental health hazard and human health hazard separately, enabling HF stakeholders to know the most concerned hazard, whether is to environmental health or human health, of an ingredient more intuitively. As a result, two matrices (i.e., J_E and J_H) of the pairwise comparison of the environmental health and human health hazard endpoints regarding their relative importance were established, respectively (Table 7). The importance values were assigned by the author, and they can be modified as required if better information becomes available. For example, in matrix J_E, endpoint AT has been assigned importance values of 5 and 3 compared to endpoints P and B, respectively. That means endpoint AT is 5 and 3 times more important than endpoint P and B regarding the environmental health hazard implication, respectively. Each element in the lower triangle of the matrix is the reciprocal of an element in the upper triangle. The geometric mean of each row of the matrix is calculated, and then the weights of each endpoint (i.e., w_j) can be derived by normalization of the geometric means.

Table 7 Matrices of relevant importance of environmental health and human health hazard endpoints

Matrix	Pairwise comparison of endpoints			w_j	Rank
J_E	P	B	AT		

	P	1.00	0.50	0.20				0.12	3
	B	2.00	1.00	0.33				0.23	2
	AT	5.00	3.00	1.00				0.65	1
		C	M	R	AhT	ChT	E		
	C	1.00	5.00	5.00	3.00	5.00	5.00	0.44	1
	M	0.20	1.00	3.00	0.33	3.00	3.00	0.14	3
J_H	R	0.20	0.33	1.00	0.33	3.00	3.00	0.10	4
	AhT	0.33	3.00	3.00	1.00	3.00	3.00	0.22	2
	ChT	0.20	0.33	0.33	0.33	1.00	1.00	0.54	5
	E	0.20	0.33	0.33	0.33	1.00	1.00	0.54	5

It is the author's opinion that endpoint aquatic toxicity (AT) should be assigned the highest importance in environmental health hazard since 27% of the ingredients have been identified as of Category 1 and 2 aquatic toxicity in a comprehensive HF chemical hazard assessment in British Columbia (Hu et al., 2017). Also, the acute aquatic toxic effect is immediate, and the response to this type of hazard is time-critical. If ingredients of high AT toxicity are accidentally released into the aquatic ecosystem, serious consequences (i.e., loss of aquatic organisms) could happen within a short time (i.e., < 96 hours). Endpoint B was ranked as the second important since a high B ingredient can be accumulated in the receptors' bodies and cause a long-term adverse effect. Endpoint P was assigned the lowest importance in environmental health hazard. This is because if a highly persistent ingredient without significant AT or B effect is released into the environment, it will not cause immediate health hazard to the environment.

Among the human health hazard endpoints, endpoint carcinogenicity (C) was assigned the highest importance since about 22% of the ingredients have been identified as Category 1 and 2 carcinogens in the previous study (Hu et al., 2017). Endpoint C also has a serious human health hazard implication to the public. Endpoint acute oral toxicity (AhT) was assigned the second-high importance since the toxic effect is immediate and lethal. Endpoints mutagenicity (M) and reproductive toxicity (R) were assigned moderate importance because their effect is not lethal and immediate as compared to endpoint C and AhT. Endpoint chronic oral toxicity (ChT) was assigned a relatively low importance since the adverse effect only becomes positive after repetitive exposures for a long period. Also, ChT is dependent on the environmental health hazard endpoint P. Only a high P ingredient can pose a chronic health risk to the receptors. Endpoint E was also assigned a low importance value since it is an emerging hazard endpoint. Few chemical toxicity databases have the data for the evaluation of endpoint E.

An environmental hazard index (IEI) and a human hazard index (IHI) are calculated for each ingredient through a weighted sum aggregation:

$$IEI/IHI = \sum_{i=1}^{n} w_i \times HS_i \quad (2)$$

Where w_i and HS_i are the weights and HS of hazard endpoint i, respectively, and n is the total number of environmental health and human health hazard endpoints, respectively. Based on the combinations of w_i (Table 7) and HS_i (Table 1), the possible IEIs and IHIs can be calculated. Figure 5 shows the cumulative percentage distribution function of the calculated IEIs (i.e., 24 IEIs) and IHIs (i.e., 684 IHIs). Five hazard levels (Table 8) can be established to describe environmental health and human health hazard potential according to the IEI/IHI values corresponding to different percentiles of the cumulative percentage distribution function.

Table 8 Ingredient hazard levels classification based on IEIs and IHIs

IEI	IHI	Hazard level	Implication
(7.17, 10]	(6.73, 10]	High (H)	The ingredient is a serious threat (e.g., immediate toxic and/or lethal effect) to environmental/human health
(5.54, 7.17]	(5.48, 6.73]	Medium-to-high (MH)	The ingredient is an environmental/human health threat (e.g., sub-lethal effect)
(4.14, 5.54]	(4.41, 5.48]	Medium (M)	The ingredient is of moderate environmental/human health hazard concern
(2.51, 4.14]	[3.16, 4.41)	Low-to-medium (ML)	The ingredient is harmful to environmental/human health (e.g., adverse effect from long-term exposure)
[0, 2.51)	[0, 3.16)	Low (L)	The ingredient is of low harm to environmental/human health

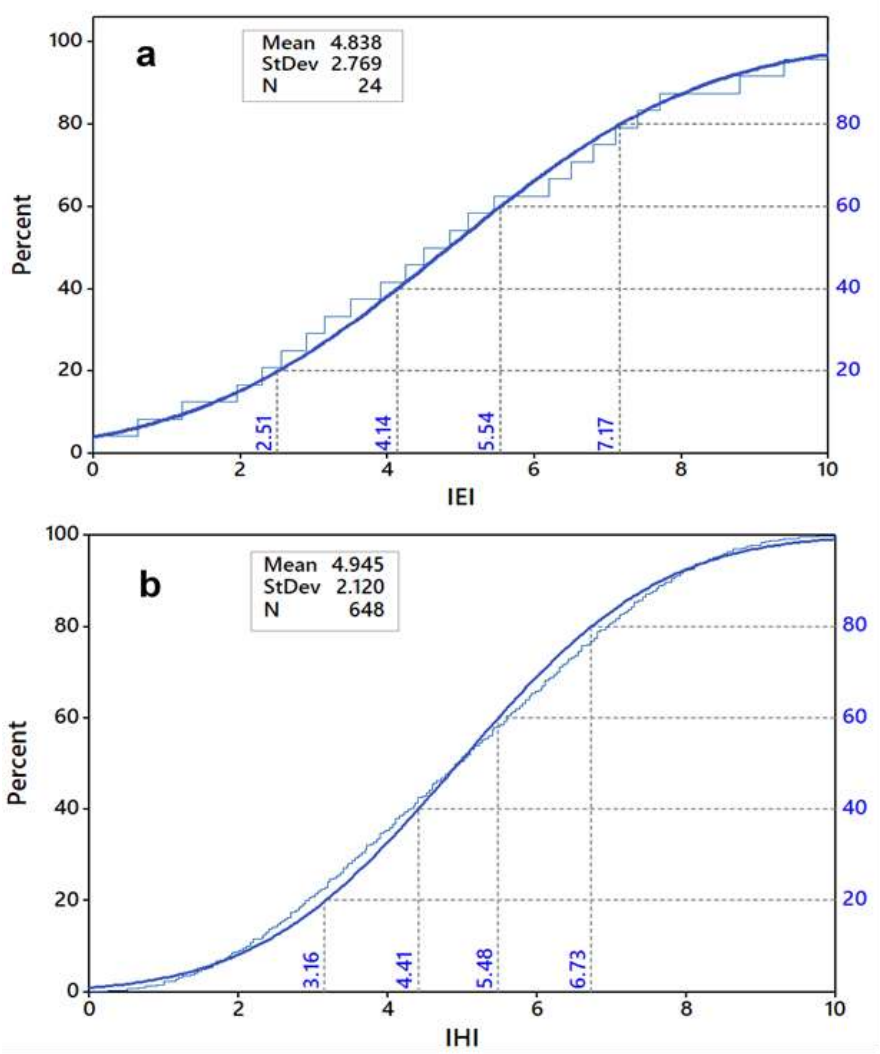


Figure 5 Cumulative percentage distribution function of possible (a) IEIs and (b) IHIs

An ingredient total hazard index (ITI) is determined using the maximum operator function, by which the higher value between the IEI and IHI will be selected (i.e., ITI = max (IEI, IHI)). The ITI reflects the highest hazard potential that an ingredient has, either to environmental health or human health. The hazard aggregation at the ingredient level is different from the HyFFGAS, in which equal weights (i.e., 0.5) are assigned to the environmental health score and human health score, respectively, and then the weighted scores are summed to generate an ingredient greenness index (IGI) (Hurley et al., 2016). The HyFFGAS generates a neutralized EHH hazard assessment result that might underestimate the hazard implications due to the improper aggregation. For example, if an ingredient is associated with very high environmental health hazard (e.g., environmental health score of 0) but no significant human health hazard (e.g., human health score of 10), then the HyFFGAS will generate an IGI of 5, showing the ingredient

has medium-level EHH hazard (Hurley et al., 2016). Based on the IGI, HF practitioner would treat the ingredient as a substance of moderate EHH hazard, ignoring the fact that if this ingredient is released into the environment, it might cause serious environmental consequences. In comparison, the ICHSIS generates an ITI of 10 for the same ingredient, indicating that the ingredient is highly hazardous to the EHH. Thus, the ingredient will be handled more carefully.

The EHH hazard potential of an additive is determined by the hazard potential and concentrations of its ingredients. As stated in previous sections, ingredients' hazard potential is embodied in HG designation and ITI. The HG designation shows the inherent EHH hazard of an ingredient objectively, while the ITI is the maximum hazard value of the ingredient no matter whether the hazard is related to environmental health or human health. The ITI also incorporates assessors' subjective opinions on the importance of different hazard endpoints. Therefore, both the HG and ITI should be considered in the hazard aggregation from the ingredient level to the additive level. The four HGs are numeralized (Table 4), and then weights are assigned to the numeralized HGs values and ITIs for hazard aggregation. Because HG can reflect the EHH hazard more objectively than ITI, a higher weight (or importance) was assigned to HG. In this study, mathematical weights of 0.7 and 0.3 have been assigned to HGs and ITIs, respectively. An ingredient's hazard vector (IHV) can be calculated as:

$$IHV = 0.7 \times Numeralized\ HG + 0.3 \times ITI \quad (3)$$

For an additive consists of n ingredients, its additive hazard index (AHI) is calculated as:

$$AHI = \sum_{i}^{n} IHV_i \times NC_i \quad (4)$$

Where NC_i is the normalized concentration of ingredient i. If the concentration of an ingredient is reported in a range, then the maximum value will be selected. In case of an additive that only has a partially disclosed ingredient list, the undisclosed ingredients will be considered as non-hazardous to the EHH (CCOHS, 2017). Similarly, a fracturing fluid hazard index (FHI) can be calculated using Eq. (4) because a fracturing fluid is considered as an additive by the ICHSIS.

6.6 Data confidence evaluation

It is important to evaluate the data confidence levels of the assessment results since they can affect chemical management decision-making. A data confidence index is calculated for each ingredient (DCI), additive (DCA), and fracturing fluid (DCF) as a measurement of data certainty/uncertainty of the hazard assessment results. The DCI is presented

separately by the data confidence of environmental health (DCI_E) and human health (DCI_H) hazard indexing results. DCI is calculated based on the DCSs (Table 2) of different CTD sources for endpoint i using Eq. (5):

$$DCI = \frac{\sum_i^n DCS_i}{Maximum \sum_i^n DCS_i} \quad (5)$$

The maximum sum of DCS for IEI is 30 and for IHI is 60, respectively. The resultant DCI is in a range from 0 to 1, and higher value means higher data confidence of the assessment results. According to the four percentiles of the cumulative percentage distribution function of DCIs shown in Figure 6, four data confidence levels (Table 9) were established to describe the data certainty/uncertainty of the ingredient hazard assessment results. Similarly, the data confidence index for the additive/fracturing fluid assessment results (i.e., DCA for additive, DCF for fracturing fluid) can be calculated using Eq. (5), and the interpretation of different data confidence levels is shown in Table 9.

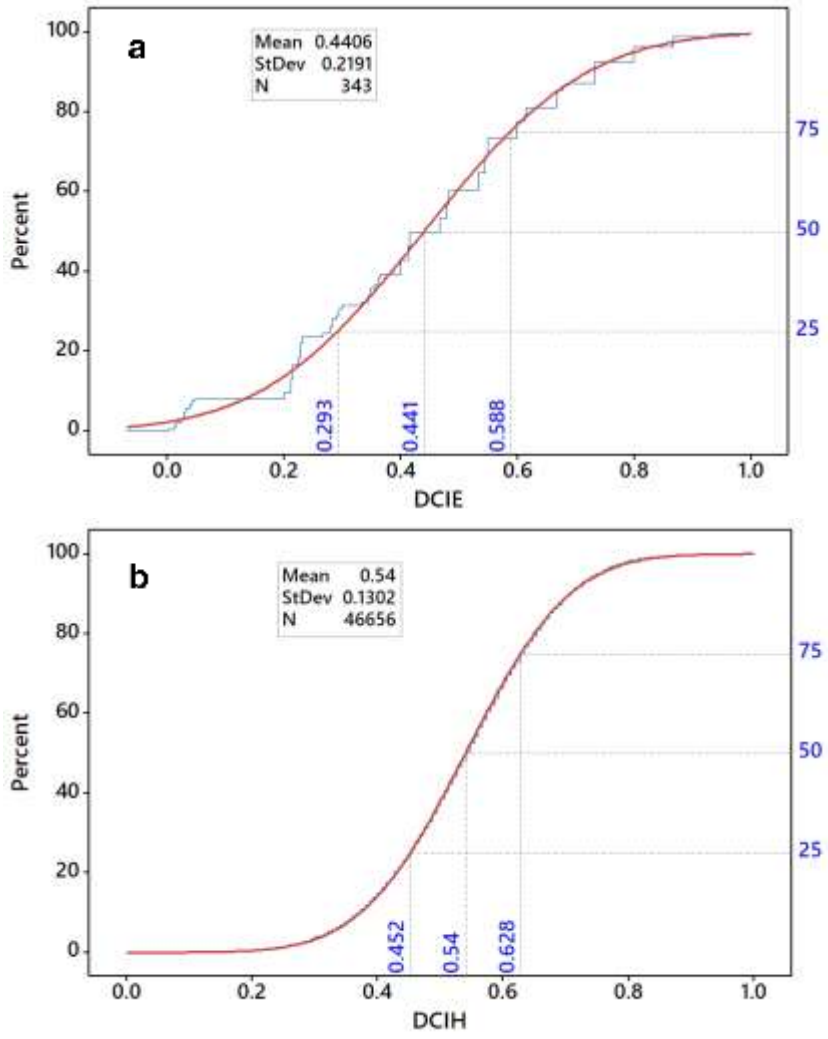


Figure 6 Cumulative percentage distribution function of possible (a) DCI_E and (b) DCI_H

Table 9 Data confidence levels of chemical hazard assessment results

DCI_E	DCI_H	DCA/DCF	Level	Interpretation
[0.59, 1.00]	[0.63, 1.00]	(0.75, 1.00]	High (H)	Signals that a substantial amount of credible CTD exists for the ingredient(s) across the EHH hazard endpoints. Uncertainty with respect to the assessment result is low.
[0.44, 0.59)	[0.54, 0.63)	(0.50, 0.75]	Medium-to-high (MH)	Signals a lower, but still appreciable amount of CTD exists for the ingredient(s) across the EHH hazard endpoints. The credibility of data is also lower. Uncertainty of the assessment result remains relatively low.
[0.29, 0.44)	[0.45, 0.54)	[0.25, 0.50)	Low-to-medium (ML)	Signals a lower amount of CTD exists for the ingredient(s) across the EHH hazard endpoints. Also, the data credibility is not high. Uncertainty surrounding the assessment result is increased. Further review is recommended.
[0, 0.29)	[0, 0.45)	[0, 0.25)	Low (L)	Signals both the amount of CTD and the data credibility are low for the ingredient(s) across the EHH hazard endpoints. Uncertainty surrounding the assessment result is high. Further review is strongly recommended.

6.7 Assessment outcome interpretation

A series of assessment results is produced for an ingredient, including the qualitative HG and numerical ITI, IEI, DCI_E, IHI, and DCI_H. For example, the assessment result of a non-hazardous ingredient A can be presented as:

Ingredient	HG	ITI	IEI	DCI_E	IHI	DCI_H
A	4	0	0(L)	1(H)	0(L)	1(H)

A series of codes is used to present the assessment result of the ingredient A: **IHG4-0-0^EL(1H)-0^HL(1H)**. The first code is the overall HG designation of the ingredient A, the second number is the ITI of the ingredient A, which is the maximum value out of the IEI and IHI, and the third code is the IEI result (the superscript "E" represents "Environmental health") coupled with the data confidence result DCI_E. The IEI result 0^EL(1H) can be interpreted as the environmental health hazard potential is low (i.e., IEI = 0, L: a low level environmental health hazard), and the data confidence index is the maximum (i.e., 1, the highest data confidence level). The human health hazard assessment result can be presented in the same format, which is shown as the last code.

The ingredient's EHH hazard should be interpreted by considering all resultant codes generated from the assessment. Using the code series to present hazard assessment result has several advantages. Firstly, the overall HG qualitative description allows for the public and chemical users to easily understand the hazard designations of the assessed ingredients and make the informed decisions, such as whether the use of the ingredient should be avoided or recommended. A HG4 ingredient has a lower EHH hazard potential than a HG3 ingredient, and the HG1 ingredients have the highest hazard potential. The ITI allows for the comparison between two ingredients that have the same HG designation. The ingredient has the higher ITI is associated with higher EHH hazard potential. By evaluating the IEI and IHI, chemical users can understand the main hazard concern of the ingredient, such as whether the ingredient is an environmental health hazard concern or a human health hazard concern or both. Also, the associated DCIs can provide a data certainty measurement for each hazard class rather than the overall EHH hazard. For example, if an ingredient scored a high DCI_E but a low DCI_H, then it can be concluded that the environmental health hazard assessment result is of high data certainty, but the human health hazard assessment result suffers from high data uncertainty.

The assessment result of an additive is also presented using combined hazard designation and index. For example, the assessment result of a non-hazardous additive can be presented as AHG4-0(1H). The first part "AHG4" is the additive HG designation, and the latter part "0(1H)" means that the AHI is 0 and the DCA is 1 (H: high data confidence level). If an additive has been classified as a HG1 (or 2) additive because one of the ingredients has a data gap, then the HG designation of that additive will be presented with an indicator "*" to show the additive is not a regular HG1 (or 2) additive (e.g., AHG1*). The hazard potential of an AHG2* additive is estimated conservatively, so the actual hazard potential might be lower than the assessed. However, the actual hazard potential will only be known until the data gap is filled. If a special HG1 ingredient (e.g., an ingredient that has high P and high B) is contained in an additive, then the additive will be classified as a HG1 additive with an indicator "!" (i.e., AHG1!), suggesting that the cut-off concentrations are not in-effect in hazard assessment for the additive. An application example is shown in Table 10 to illustrate the AHIs of different additives. Additives A1 and A2 contain similar ingredients, but the concentrations of the ingredients present in the two additives are at different magnitudes. Also, additive A1 has one or more undisclosed ingredients, shown as ingredient x. Additives B1 and B2 contain different ingredients, but the ingredients have the same HG designations and concentrations.

Table 10 The AHIs of four hypothetical additives

Additives	Ingredients	Concentrations (%)	Normalized Concentrations	AHIs

A1	a1 (HG1, ITI = 10)	3	0.03	0.585
	a2 (HG3, ITI = 5)	5	0.05	
	a3 (HG4, ITI = 0)	2	0.02	
	x (undisclosed)	90	0.9	
A2	a1 (HG1, ITI = 10)	30	0.3	5.85
	a2 (HG3, ITI = 5)	50	0.5	
	a3 (HG4, ITI = 0)	20	0.2	
B1	b1 (HG2, ITI = 5)	10	0.1	1.08
	b2 (HG2, ITI = 3)	10	0.1	
	b3 (HG4, ITI = 0)	80	0.8	
B2	b4 (HG2, ITI = 6)	10	0.1	1.15
	b5 (HG2, ITI = 4.3)	10	0.1	
	b3 (HG4, ITI = 0)	80	0.8	

The resultant AHIs can well reflect the EHH hazard potential of different hypothetical additives. Additive A1 and A2 both are HG1 additives since both contains the HG1 ingredient a1. However, the AHI of A1 is ten times lower than that of A2 because of the lower ingredient concentrations. Also, the undisclosed ingredient x is automatically classified as a HG4 ingredient and scores an ITI of 0. Thus, the effect of ingredients' concentrations on additive assessment result can be reflected in the AHI. Moreover, when comparing the EHH hazard potential of two additives with the same HG, the AHI can be used to facilitate the comparison. For instance, both additive B1 and B2 are HG2 additives, and both additives have similar ingredients (i.e., b1 is similar to b4, b2 to b5, and b3 to b6, respectively). The similar ingredients are also present at the same concentrations in the two additives, respectively. Additive B2 scores a higher AHI than B1 because of the higher ITI of its ingredients, indicating that B2 has a higher EHH hazard potential. Assuming A1 and B1 has the same downhole function, B1 is more preferred since it has a lower hazard designation (HG2) compared to A1 (HG1), despite the fact that A1 has a lower AHI.

The hazard assessment result of a fracturing fluid is similar to that of an additive. The assessment results of three hypothetical fluids are shown in Table 11 as an example. Fluids F1 and F2 contain the same ingredients at different concentrations, thus different FHIs are calculated for the two fluids. It should be noted that even a HG1 ingredient, a1, is found in F1 and F2, its concentrations present in the two fluids are lower than the minimum cut-off concentration (i.e., 0.1%) of the human health hazard endpoints. Therefore, both fluids will not be classified as HG1 fluids. Moreover, the concentrations of ingredient a3, a HG3 substance, are also lower than the minimum cut-off concentration, and there is no HG2 ingredient present in the two fluids, and thus both F1 and F2 can be considered as HG4 fracturing fluids, which are relatively safe to the EHH and reusable. Fluid F2 has a higher EHH hazard potential because of the higher FHI, so F1 is more preferred to use in HF operations.

Fluid F3 contains ingredients with the similar IHGs and ITIs as these contained in fluid F1. Assuming ingredient b1 contained in F3 is a special HG1 ingredient (i.e., high P and B), fluid F3 will be classified as a HG1 fluid even that the concentration of b1 is lower than the minimum cut-off concentration. Ingredient b1 will be marked with a superscripted "!" to indicate that it requires special attention. The FHG of F3 will also be marked with the superscripted "!" to show that it contains as least one special HG1 ingredient. The final assessment result of a fracturing fluid is presented in a same format as an additive. For example, a fluid assessment result of FHG4-0.058(1H) can be generated for fracturing fluid F1.

Table 11 The assessment results of three hypothetical fluids

Fluids	Ingredients	IHG	ITI	Concentration (%)	NC [a]	FHI	FHG
F1	a1	1	10	0.005	0.005	0.058	4
	a2	3	5	0.003	0.003		
	a3	4	0	0.0004	0.0004		
	Water	4	0	0.9916	0.9916		
F2	a1	1	10	0.008	0.008	0.094	4
	a2	3	5	0.005	0.005		
	a3	4	0	0.001	0.001		
	Water	4	0	0.986	0.986		
F3	b1$^{!}$	1	8	0.005	0.005	0.057	1$^{!}$
	b2	3	4	0.003	0.003		
	b3	4	0	0.0004	0.0004		
	Water	4	0	0.9916	0.9916		

[a] NC: normalized concentration

7. Application of ICHSIS

The developed ICHSIS was applied to assess the representative HF additives used in British Columbia. The additive data was collected from the FracFocus database from November 2011 to August 2014. Different additives were grouped into 13 functional categories such as gelling agent, crosslinker, and biocide, and so forth, according to their designed functions (Hu et al., 2017; Hurley et al., 2016). The representative additives were selected for the assessment according to their use percentage within each functional category. Additives with at least one reported ingredient and a use percentage higher than 10% were selected. As a result, a total of 25 additives were considered representative. It is noteworthy that the most commonly used friction reducers were reported without any known ingredients and concentrations, thus they were not eligible for the hazard assessment. Moreover, friction reducer is the most frequently used functional category in British Columbia due to that a large portion of HF treatments in this province involved slick-water fracturing (Hu et al., 2017). The lack of information

about friction reducers' chemical compositions increases the uncertainty of HF chemical's impact to the EHH.

7.1 Ingredient hazard assessment

The selected additives comprise of 43 different ingredients. Among these ingredients, twelve were reported without CASRNs; Thus, analog ingredients were used for hazard assessment. Suitable analog ingredients were generated using the Analog Identification Methodology developed by the US EPA (USEPA, 2017). As shown in Figure 7, about 21% of the assessed ingredients were categorized as HG1 ingredients, and their use should be avoided in HF operations. No special HG1 ingredient (i.e., ingredients marked as HG1! due to high P and B) was found during the hazard screening. Nearly half of the assessed ingredients are HG2 substances, suggesting that substitutes with lower EHH hazard potential should be searched for hazard mitigation. Only 9% of the ingredients can be labeled as non-hazardous HG4 ingredient. Among all the ingredients, no confirmed or suspected endocrine disruptor was found. Environmental persistence and high aquatic toxicity are the main environmental health concerns. This finding is generally consistent with the results from the comprehensive chemical hazard assessment, in which the environmental persistence (e.g., 30%) and high aquatic toxicity (e.g., 27%) were confirmed as the cause of high environmental health hazard (Hu et al., 2017). About 20 to 25% of the assessed ingredients are associated with Category 1 or 2 adverse human health effects (i.e., C, M, and R). Acute human oral toxicity does not seem to be a significant hazard concern due to the majority of ingredients (e.g., about 80%) falls into Category 4 acute oral toxicity. Nevertheless, roughly 21% of ingredients were confirmed with chronic human oral toxicity, which has the potential to cause a long-term adverse effect on human health.

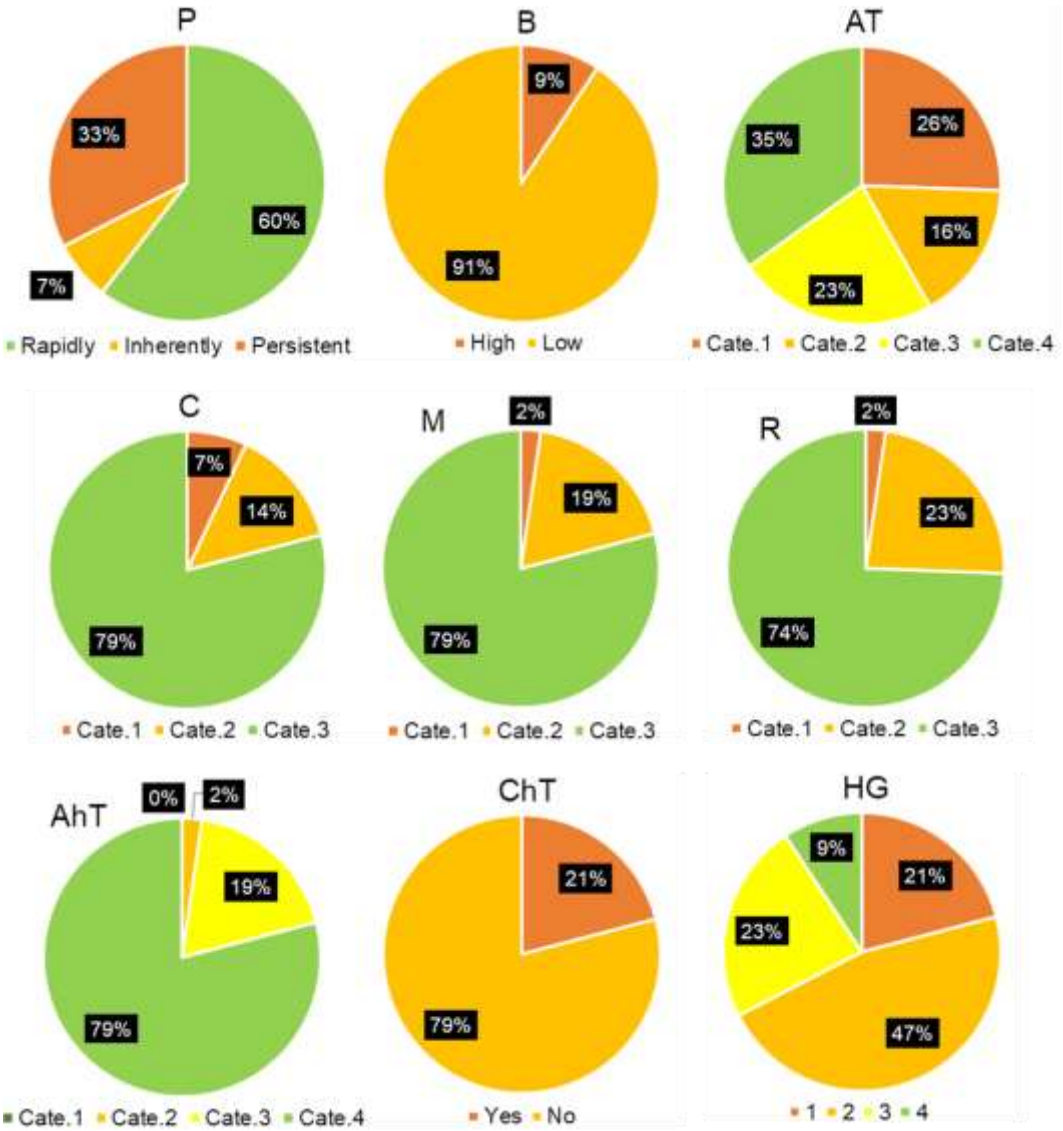


Figure 7 General results of ingredient hazard assessment (N = 43)

The ingredients assessment results from ICHSIS were compared with those from HyFFGAS. Since HyFFGAS generates ingredient greenness scores on a scale from 0 to 10 and a higher greenness score indicates a lower EHH hazard, the greenness scores were subtracted by ten to generate a hazard index (i.e., HyF) for comparison. As shown in Figure 8a, the ITI distributes more evenly than HyF, and both the mean and median values of ITI are lower than those of HyF. Since both ITI and HyF were not normally distributed, a nonparametric test (i.e., the Mann-Whitney test) was applied to check the statistical difference between the indices generated by the two systems. The result shows that there is no significant difference ($p > 0.05$) between ITI and HyF. Thus, the ingredient hazard assessment results from ICHSIS are considered consistent with those from

HyFFGAS. However, the median value of the hazard indices generated by HyFFGAS indicates a medium-to-high level EHH hazard due to the different hazard index scaling (Hurley et al., 2016). It is noteworthy that environmental health hazard is a cause of concern because the mean value of IEI suggests that the ingredients are associated with low-to-medium environmental health hazard (Table 8), while the mean value of IHI shows that the human health hazard is low. The difference between IEI and IHI is significant ($p < 0.05$).

The data confidence performance of the assessment results from the two systems is shown in Figure 8b. Since HyFFGAS does not have a function for data confidence evaluation, the data confidence level of the results generated from HyFFGAS was processed using the same approach (Eq. 5) as used by ICHSIS. It can be seen that the data confidence performance was significantly ($p < 0.05$) improved by ICHSIS. The ingredient assessment results from ICHSIS can be characterized as high data confidence level, while results from HyFFGAS were associated with overall medium-to-high data confidence. The improvement is owing to the diverse CTD sources used by ICHSIS. In comparison, HyFFGAS uses material safety data sheets as the main CTD source, which is defined as a tier 2 data source in ICHSIS. Using tier 1 authoritative chemical toxicity databases not only can increase the availability but also can improve the credibility of the CTD. Moreover, ICHSIS uses analog ingredients to simulate the CASRN-missing ingredients, which can also significantly reduce the uncertainty of the assessment results.

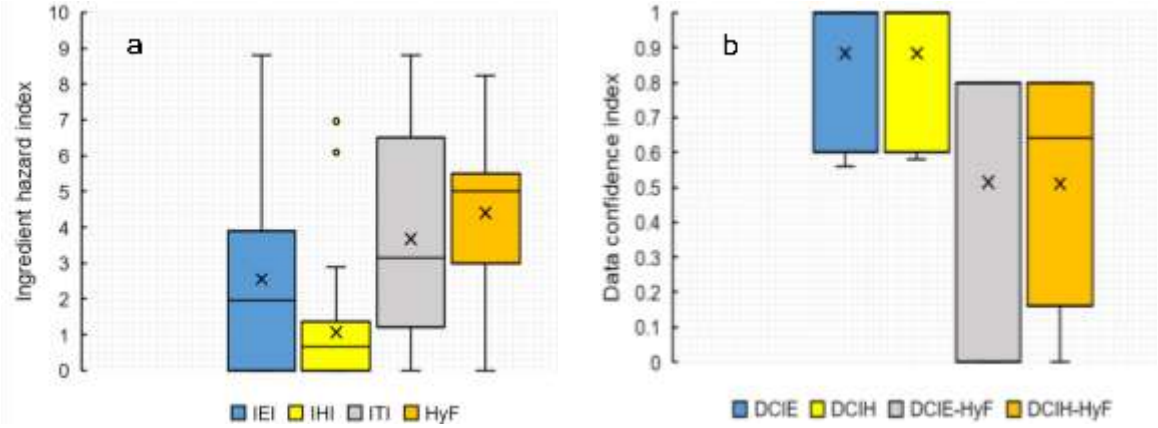


Figure 8 Comparison of (a) ingredient hazard indices and (b) data confidence indices (N = 43)

The hazard aggregation method can affect the final hazard assessment outcome. The ICHSIS uses the maximum operator to aggregate environmental health and human health hazard, while HyFFGAS uses weighted sum aggregation by assigning equal

weights to environmental health and human health. The weighted sum aggregation will generate a compromised total hazard and lead to an underestimated hazard evaluation. For example, ingredient Benzene, C10-16-alkyl derivatives (CASRN: 68648-87-3) has a high environmental health hazard because of its high bioaccumulation potential (ECCC, 2017) and Category 1 aquatic toxicity (ECHA, 2017), but it has no significant human health hazard potential. The IEI and IHI of this ingredient are calculated as 8.8 and 0, respectively, representing high environmental health hazard and low human health hazard. An ITI of 8.8 is generated for this ingredient using the maximum operator by ICHSIS. In comparison, HyFFGAS generates an environmental health hazard score of 9 and a human health hazard score of 2 for the same ingredient. An ingredient hazard score of 5.5 can be calculated using the weighted sum aggregation. The ingredient hazard score indicates a medium-to-high level hazard according to the hazard scale of HyFFGAS (Hurley et al., 2016), neglecting the fact that if the ingredient is accidentally released into the environment, severe environmental health consequence can be caused.

7.2 Additive hazard assessment

Among the selected representative additives, about 28% are HG1 additives. These HG1 additives contain at least one HG1 ingredient, and the concentrations of HG1 ingredients are higher than the cut-off values. A relatively large percentage of HG1 additives indicates that the need for additives with lower EHH hazard potential is imperative. About 44% and 16% of additives are HG2 and HG3 additives, respectively, suggesting a significant potential for hazard mitigation. Only 12% of the additives are non-hazardous HG4 additives. The hazard screening results of additives are generally similar to those of ingredients since ingredients are the basic components of additives.

As shown in Figure 9a, the AHI distributes in a wider range than the hazard index from HyFFGAS, allowing for a higher-resolution comparison between different additives on their EHH hazard potential. Similar to ingredients' hazard assessment, both the mean and median values of AHIs are lower than those of additive hazard index generated from HyFFGAS; However, the difference in the index distribution patterns of the two systems is not significant ($p > 0.05$). As shown in Figure 9b, the DCAs from ICHSIS are much higher than the DCAs from HyFFGAS, and the improvement is significant ($p < 0.05$). The data confidence level of the AHIs from ICHSIS are primarily high, while those of the results from HyFFGAS fall within the range from low-to-medium to medium-to-high. The high data confidence of the results from ICHSIS can be attributed to the diversity of the tier 1 CTD sources.

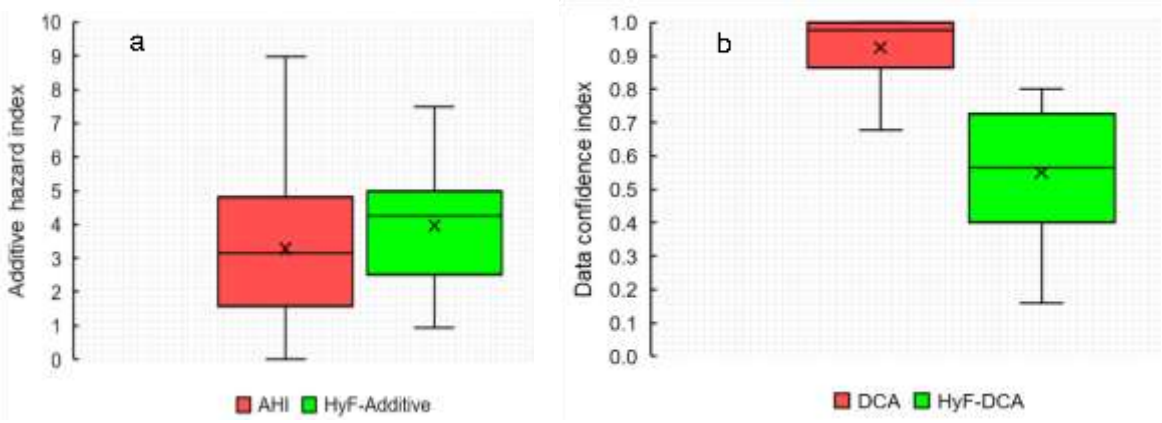


Figure 9 Comparison of (a) additive hazard indices and (b) data confidence indices (N = 25)

7.3 Fluid hazard assessment

Three hypothetical fracturing fluids (i.e., F1, F2, and F3) were designed for hazard assessment. The representative additives in different functional categories were randomly selected to compose the hypothetical fracturing fluids. As shown in Table 12, the fracturing fluids contain the same additives/ingredients from different functional categories, but the concentrations of the ingredients are different. Fluid F1 contains the lowest concentrations of ingredients among all three fluids. The ingredients' concentrations in F2 are ten times higher than the concentrations of the respective ingredients in F1. Fluid F3 contains several additives such as iron control agent, activator and biocide at high concentrations, while the concentrations of the remain additives are the same as those in F1. The total concentration of ingredients is lower than 1% in each fracturing fluid. that the total concentration of ingredients is reasonable as additives only account for less than 2% of a fracturing fluid (All Consulting, 2012; Soeder et al., 2014). The assessment results show that the fluid F1 can be labelled as a HG4 fluid, which has no significant EHH hazard potential even that it contains several HG1 ingredients. The low hazard designation is because the concentrations of ingredients in F1 are lower than the cut-off concentrations of various hazard endpoints. Therefore, the recovered fluid F1 is recommended for reuse as long as the concentrations of HG1 ingredients are lower than the cut-off values. The reuse of recovered fracturing fluid would significantly reduce the consumption of freshwater resource and increase the sustainability of HF treatment. In comparison, fluid F2 is labeled as a HG1 fluid due to the high concentrations of HG1 ingredients. For instance, the concentration of a HG1 ingredient, phenol formaldehyde resin, present in F2 is higher than 0.1%. This ingredient is a significant EHH hazard concern because of the high environmental persistence, high aquatic toxicity (ECCC, 2017), and Category 1 carcinogenicity (ECHA, 2017). Also, the FHI of F2 is higher than

that of F1 because of the increased concentrations of HG1 ingredients. Fluid F2 needs to be reformulated for use due to the high concentration of the HG1 ingredient. Moreover, fluid F3 was classified as a HG2 fluid. The concentrations of all the HG1 ingredients in F3 are lower than the cut-off values, so the HG2 ingredients were screened following the hierarchy shown in Figure 4. The concentrations of HG2 ingredients such as the alkyl benzene sulphuric acid (contained in the anti-sludge agent) and methanol (contained in the activator) exceed the cut-off values, resulting in a positive HG2 designation for fluid F3. The reuse of fluid F3 is possible as long as the concentrations of the HG1 ingredients are lower than the cut-off values.

Table 12 Hazard assessment results of three hypothetical fracturing fluids

Additive	Ingredient	CASRN	Conc. (%) in additive	Conc. (%) in fracturing fluid			Assessment results				
				F1	F2	F3	Ingredient	Additive	F1	F2	F3
Iron control agent	2-Mercaptoethanol	60-24-2	90	2.40E-03	2.40E-02	2.40E-03	IHG1-7.7				
	Cupric chloride	7447-39-4	10	2.60E-04	2.60E-03	2.60E-04	IHG1-7.7	AHG1-7.7			
	Monoethanolamide	141-43-5	30	8.00E-04	8.00E-03	8.00E-04	IHG3-0.7				
Anti-sludge agent	Alkyl benzene sulphuric acid	68584-22-5	85	2.05E-03	2.05E-02	2.05E-02	IHG2-1.0				
	Methanol	67-56-1	10	2.41E-04	2.41E-03	2.41E-03	IHG3-3.9	AHG1-4.6			
	Benzene, C10-16-alkyl derivatives	68648-87-3	5	1.20E-04	1.20E-03	1.20E-03	IHG1-7.7				
	Sulphuric acid	7664-93-9	5	1.20E-04	1.20E-03	1.20E-03	IHG3-1.2				
Activator	Methanol	67-56-1	50	5.00E-03	5.00E-02	5.00E-02	IHG2-0.5	AHG2-5.4			
	Alcohols, C12-14 secondary, ethoxylated	84133-50-6	70	8.00E-03	8.00E-02	8.00E-02	IHG2-6.5				
Scale control agent	Ethylene glycol	107-21-1	60	8.29E-04	8.29E-03	8.29E-03	IHG2-0.5	AHG2-2.2			
	Non-hazardous ingredients	-	60	8.29E-03	8.29E-02	8.29E-03	IHG4-0				
Biocide	Glutaraldehyde	111-30-8	20	1.95E-04	1.95E-03	1.95E-03	IHG2-6.5		FHG4-2.8	FHG1-5.7	FHG2-2.5
	Methanol	67-56-1	10	1.60E-06	1.60E-05	1.60E-05	IHG2-0.5	AHG2-1.7			
	Non-hazardous ingredients	-	70	1.12E-05	1.12E-04	1.12E-04	IHG4-0				
Breaker	Ammonium persulfate	7727-54-0	5	4.24E-04	4.24E-03	4.24E-04	IHG3-3.2	AHG3-0.2			
	Non-hazardous ingredients	-	95	8.05E-03	8.05E-02	8.05E-03	IHG4-0				
Clay control agent	1,6-Hexandiamine, dihydrochloride	6055-52-3	40	7.47E-03	7.47E-02	7.47E-02	IHG4-0	AHG4-0			
	Non-hazardous ingredients	-	60	1.12E-02	1.12E-01	1.12E-01	IHG4-0				
Gelling agent	Phenol formaldehyde resin	9003-35-4	95	6.11E-03	6.11E-01	6.11E-03	IHG1-7.7	AHG1-9.0			
	Phosphoric Acid	7664-38-2	5	3.21E-04	3.21E-02	3.21E-04	IHG3-1.2				
Crosslinker	Monoethanolamide	141-43-5	60	8.75E-04	8.75E-03	8.75E-04	IHG3-0.7				
	Boric acid	10043-35-3	13	1.17E-03	1.17E-02	1.17E-03	IHG1-3.2	AHG1-2.4			
	Non-hazardous ingredients	-	27	1.02E-03	1.02E-02	1.02E-03	IHG4-0				

8. Conclusion

The rapid growth of the unconventional gas industry has triggered considerable concerns regarding the EHH impacts posed by HF and associated activities. To help mitigate such concerns, the use of HF chemicals with lower EHH hazard potential is encouraged. Despite some government legislation regulating chemical use in HF, the transition to more sustainable chemical use has been an industry-level response to internal and external demands. In response to the transition, many chemical hazard assessment methods have been developed to measure the hazard profiles of HF chemicals. The existing methods can generally be divided into hazard screening and indexing categories. The representative methods, including HyFFGAS and Intrinsik, of the two categories were applied to assess the HF chemicals, and the assessment results from the two methods were compared. By reviewing the advantages and limitations of the two methods, an integrated system named ICHSIS was developed to assess the EHH hazard potential of HF chemicals at ingredient, additive, and fracturing fluid levels. The development of ICHSIS was further discussed regarding its designed purpose, hazard endpoints and criteria selection, hazard screening and indexing process, sub-index aggregation, and final outcome interpretation. The ICHSIS was validated by assessing the representative chemicals used in HF in British Columbia, and the results were compared with those generated from the previously developed indexing system (i.e., HyFFGAS). The results generated from ICHSIS show that more than half of the ingredients and additives were grouped into high EHH hazard designations such as HG1 and 2, suggesting that the need for hazard mitigation is necessary. The indexing results from ICHSIS can be used to compare the hazard potential of chemicals within the same hazard designation. The indexing results from ICHSIS were generally consistent with those from HyFFGAS, but the data confidence level of the results was significantly improved. The fluid hazard assessment results indicate that ICHSIS can aid decision-making on the reuse of recovered fracturing fluid to increase the sustainability of HF production. The ICHSIS represents an improved chemical hazard monitoring, decision-making, and communication methodology, which can promote progress toward more sustainable unconventional gas production. The developed integrated chemical hazard assessment system can also serve as a useful reference to chemical hazard management in other industries.

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Appendix A1

Summary of Technical Feedback & Recommendations on UBCO Mid-term Project Report.

Summary of Technical Feedback & Recommendations on UBCO Mid-term Project Report

	Technical Feedback	Recommendation for Final Assessment Approach
1.	Lack of context for hydraulic fracturing chemical use	Add context to final approach and published research paper: • Existing federal regulatory oversight • Use of chemicals in other everyday applications • Lack of exposure opportunities (thus risk) • Dilution in final product mixture -> thus assessment results at additive level should be interpreted as ultra-conservative • Additive selection considers cost, efficacy, availability • Sound wellbore construction practices to protect groundwater resources
2.	Terms 'hazard' and 'risk' used interchangeably	Make clear distinction of these terms. Risk = hazard times exposure. Both systems are hazard-based not risk-based.
3.	"Greenness" is an ambiguous term and not clearly defined.	Avoid the terminology 'green' and 'sustainable chemical use'.
4.	Description of Intrinsik system appears to be inadequate and doesn't recognize that supplier either conducts assessment in-house or third party does it under C.A. Simply states fewer chemicals meet Intrinsik's assessment requirements and thus its capability is limited. That augmented data set was not available for UBCO to compare.	Fully describe the Intrinsik system; rather than attempting to augment the data set, suggest screening only chemicals with CAS #'s. If there is no CAS # (and no HMIRC #) reported FracFocus, the ingredient is likely non-hazardous, thus not required to be reported on the SDS/to FracFocus. By excluding non-hazardous components and keeping the assessment at the chemical level, process is simplified and hazard uncertainty due to missing data is mitigated. Alternatively, prefer to screen individual components instead of the fluid blend. It is easier to identify the "problem chemicals" and change them out. This will mitigate the issue and not discourage the use of produced/recycled water use.
5.	HyFFGAS relies on MSDSs, which are based on workplace H&S and contain limited environmental hazard data.	Use Government toxicology databases as primary source of hazard information. Use MSDSs as secondary source.
6.	Limited data produces greenness indexes with wide range, indicating high level of hazard uncertainty with no means to address it. Intrinsik addresses uncertainty through calculation of Data Availability Index (DAI) and offers guidance on how to fill data gaps.	Adopt Data Availability Index.
7.	Numerical scores to express hazard imply precision that does not exist. Numerical values in HyFFGAS can only be referenced to one another.	Assessment results should convey uncertainty/variability. Consider category approach (like Intrinsik's method does), or benchmarking against other well-understood chemicals in the environment (like GreenScreen does). Recommend to compare HyffGas scoring to commonly used products like RoundUp or household bleach for example. This will provide a comparison of scores against a product familiar to the public. Preferably the implementation of additional categories; as this can actually have some more distinction between chemicals. A numerical might be workable, however, clearing the decimal points would be similar to other systems.
8.	AGI score ranges are not interpreted consistently in report.	Establish clear and consistent interpretation of scoring.
9.	HyFFGAS assigns equal weight to environmental and human health hazards, and cannot determine which influenced score.	Weighting should reflect relevant exposure pathways and stakeholder concerns. A toxicologist should make this recommendation. Dr. Davies provided his opinion in the review of the mid-term report. A separate human health and environment score would increase the importance of the outcome; as currently stating that a product fails is not being clear why it fails. Having separate scores would indicate where the issue may be.

10.	Two systems differ in their consideration of specific toxicity endpoints and exposure routes.	Toxicology SMEs to determine whether the following endpoints/exposure routes should be included or not: • Category 2 carcinogens, mutagens, reproductive toxins • Dermal exposure route in acute toxicity endpoint • Chronic oral toxicity endpoint A toxicologist should make this recommendation. Dr. Davies provided his opinion in the review of the mid-term report. UBCO may seek out other toxicologists' opinions if their project timeline permits.
11.	HyFFGAS does not use cut-off concentrations for ingredients present at too low of a concentration to affect a product's hazard potential. Intrinsik's system does.	Adopt cut-off concentrations.

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