SYSTEMIC ANALYSES AND INDICATORS FOR ASSESSING RISKS TO DRINKING

WATER RESOURCES FROM HYDRAULIC FRACTURING CHEMICALS

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The Supervisory Committee certifies that this ***disquisition*** complies with North Dakota

State University's regulations and meets the accepted standards for the degree of

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ABSTRACT

Hydraulic fracturing (HF) is a disruptive technology that has unlocked a vast amount of hydrocarbon resources, but presents risks to drinking water resources. Applying systemic risk assessment approaches to environmental and public health risks created by onshore unconventional oil and gas development (OUOGD) has not been explored and there are research gaps in system dynamics related to HF chemical transparency, variety, and hazard levels.

The first objective of this research is to advance the application of systemic causation models to assess environmental and public health risks associated with OUOGD. A critical review of systemic causation models and their application for assessing these risks is presented. Holistic conceptual OUOGD process and control structure models are elucidated to provide a catalyst for future research.

The second objective is to improve techniques and metrics used to measure and monitor systemic HF chemical transparency and feedback loops. After a comprehensive review of existing transparency indicators, two new metrics are developed and applied. The percent of wells with publicly disclosed ingredients increased from ~0% to 95%, and the average percent of HF fluid mass withheld on chemical disclosure forms decreased ~46.8%.

The third objective is to provide context and analyze changes in HF chemical variety and influencing factors. A methodology for processing public HF chemical disclosure data into an updated unique HF chemical list is provided. The annual unique HF chemical counts were found to have dropped 32.3%. Identified HF chemicals are compared with reference chemical lists, including known food, cosmetics, and water-related additives and contaminants, for system and risk context. Approximately 70.0% of the HF chemicals are found in the reference chemical list.

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The last objective is to develop and apply a repeatable methodology for reporting relative HF chemical hazard levels to drinking water resources and characterize system dynamics. New individual parameters and aggregated risk indicators with associated approaches are provided. The aggregated metric indicated a 42.6% risk reduction. Overall, this research reveals past progress and methods for fostering future improvements related to HF chemical stewardship that can potentially be applied toward safer chemicals and transparency across all industries.

DEDICATION

To my awesome wife, Kathryn,

and incredible mother, Renate.

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1. GENERAL INTRODUCTION

It is appropriate to classify managing environmental and public health risks associated with onshore unconventional oil and gas development (OUOGD) as a "wicked problem" (most regulators and policymakers will agree). Rittel and Webber (1973) define a problem as "wicked" when insurmountable challenges associated with solving the social aspect of the problem exist due to the differences in individual stakeholders' values. Balancing OUOGD benefit and risk perceptions during policy-making has proven to be a challenging endeavor. Some researchers have suggested that potential impacts caused by OUOGD are too significant to proceed with the industrial activity (de Melo-Martín et al., 2014; Grasso, 2020). Other stakeholders have acknowledged that OUOGD benefits are critical to every aspect of the United States (U.S.) economy, national security, energy transition efforts, and overall quality of life without fully recognizing associated risks (U.S. DOE, 2020). Regardless, as long as society requires hydrocarbon resources, they should be prudently and safely developed and produced, deploying the best tools and methods to monitor and manage associated environmental and health risks. Adopting systemic risk analyses, causation models, and indictors can potentially improve the OUOGD industry and stakeholders' ability to address environmental and public health hazards. This dissertation research investigates system dynamics related to drinking water resources quality risk from hydraulic fracturing chemicals as a case study. It examines hydraulic fracturing chemical disclosure, variety, and hazard-levels changes over the past decade in the U.S.

1.1. Background

1.1.1. Systemic Risk Analyses

"Wicked problems" require systemic and comprehensive approaches for problem formulation and solution creation because decisions based on inadequate system conceptual

models can lead to unintended consequences and negative risk-return trade-offs (Leveson, 2012; McGarity, 2004). Sociotechnical systems, including those encompassing OUOGD, are defined by human, physical, and digital functions and their relationships, which can be documented in a control structure abstraction based on control theory. Systemic hazard analysis methods consider complex and non-linear functional relationships within sociotechnical systems and differ from traditional linear analysis approaches that primarily consider the linear failure of components. Despite significant attention and research regarding OUOGD environmental and health risks (Adgate et al., 2014; Annevelink et al., 2016; Guo et al., 2020; Hill et al., 2019; Kaden and Rose, 2016; Ma et al., 2018; Maloney et al., 2017; McKenzie et al., 2012; NAS, 2018; Saunders et al., 2018; Torres et al., 2018, 2016; U.S. EPA, 2016a; Vengosh et al., 2014; Vidic et al., 2013) and significant progress in developing collaborative, integrated, and systemic risk management frameworks (Bravo and Hernandez, 2020; Linkov et al., 2018), the usage of systemic hazard analysis methods in OUOGD is limited. However, the need and value of expanding research and practice in these areas have recently been acknowledged (Small et al., 2014).

1.1.2. Hydraulic Fracturing Chemicals

Hydraulic fracturing has occurred in the U.S. since 1947, but the technology reached broad commercialization in the 21st century (Gallegos and Varela, 2014; King, 2012). The objective of the process is to increase the permeability of tight geologic formation (e.g., shale) by injecting large quantities of water, sand, and additives at pressures high enough to fracture the target hydrocarbon formation. Water is the typical carrier fluid, but other fluids (e.g., nitrogen, carbon dioxide, propane) have been used in rare cases. The sand acts as a proppant to ensure the formations remain open after the imposed pressure is removes. Hydraulic fracturing additives, composed of one or more chemicals, serve specific and deliberate purposes primarily designed to

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improve well performance, mitigate risk, or both. Chemical categories include, but are not limited to, acids, biocides, breakers, stabilizers, crosslinkers, friction reducers, gels, iron controls, non-emulsifiers, pH-adjusting agents, scale inhibitors, and surfactants (GWPC, 2021). These chemicals have diverse levels of hazardous characteristics (e.g., toxicity, mobility, persistence).

In general, information availability is critical for all risk assessment and decision-making processes, and hydraulic fracturing chemical information is no exception. After considerable attention from public, government, and regulatory stakeholders, in 2011, FracFocus (FF) became the primary repository for oil and gas (O&G) companies to disclose hydraulic fracturing chemical information to stakeholders in the U.S. Initial research on hydraulic fracturing chemical transparency, characteristics, and hazards quickly followed this data availability effort (Konschnik and Dayalu, 2016; U.S. EPA, 2016a; Yost et al., 2016a, 2016b, 2017). However, there has been limited peer-reviewed research to define the system(s) controlling these variables and their dynamics over time. In addition, approaches and tools successfully applied to assess hydraulic fracturing chemicals and fluid hazard levels have not been extrapolated to investigate system and functional behaviors (Hu et al., 2019, 2018; Hurley et al., 2016; Shen and Somasundaran, 2019; Xu et al., 2019; Yost et al., 2017).

1.2. Research Problem Statement

Analysis methods based on linear causation models used in traditional and integrated frameworks to date have failed to fully characterize the sociotechnical system, control structure, and system states (or behaviors) influencing OUOGD environmental and public health risks. There is a need to evaluate the applicability of systemic causation models to assess and manage these risks. Consistent and understood approaches for measuring and reporting systemic hydraulic fracturing chemical withholding rates, risk factors, and other related context are

lacking, which could lead to ineffective policy decisions, unproductive public concerns, research limitations, and chemical risk reduction constraints. Hydraulic fracturing chemical policies and analytical trends over the past decade present a unique opportunity to gain knowledge and insights that could foster greater alignment on chemical information availability and decisions in and beyond the oil and gas industry.

1.3. Research Objectives

1. To advance the application of systemic causation models to assess environmental and public health risks associated with OUOGD.

    a. To critically review the feasibility of applying systemic causation models to assess environmental and public health risks associated with OUOGD.

    b. To provide a catalyst for future research by synthesizing novel holistic conceptual OUOGD process model and control structure.

2. To improve techniques and metrics used in measuring and monitoring systemic hydraulic fracturing chemical transparency.

    a. To critically review existing hydraulic fracturing chemical transparency indicators.

    b. To identify and apply new metrics for assessing hydraulic fracturing chemical transparency at system and associated functional levels.

3. To provide context and analyze changes in hydraulic fracturing chemical variety and influencing factors.

    a. To produce a methodology for processing public hydraulic fracturing chemical disclosure data into an updated unique hydraulic fracturing chemical list.

b. To compare hydraulic fracturing chemicals with reference chemical lists, including known food, cosmetics, and water-related additives and contaminants, for system and risk context.

4. To develop and apply a repeatable methodology for reporting relative hydraulic fracturing chemical hazard levels to drinking water resources and characterize system dynamics.

1.4. Dissertation Organization

This dissertation contains 6 chapters. Chapter 1 (this chapter) includes a brief review of the research background, problem statement, objectives, and dissertation organization (this section). Chapter 2 focuses on applying systemic causation models to OUOGD and developing holistic OUOGD process and control structure models, which align with objective 1. It is based on a critical review manuscript titled "Systemic risk analyses for potential impacts of onshore unconventional oil and gas development on public health and the environment : A critical review" published in *Science of the Total Environment* (Hill et al., 2021a). The exploration and development of hydraulic fracturing disclosure metrics and trends are provided in Chapter 3 to achieve objective 2. Investigating chemical transparency is an essential step in the research process because information availability is critical to performing risk assessments. The chapter is primarily extracted from a manuscript titled "Hydraulic Fracturing Chemical Disclosure Policy and Data Analysis: Metrics and Trends in Transparency." published in *Environmental Science & Technology* (Hill et al., 2021b). Chapter 4, relating to objective 3, presents a method for processing public and proprietary hydraulic fracturing additive information to examine the variety of chemicals used over time and factors impacting chemical selection. In addition, Chapter 4 provides risk context in the form of a comparative analysis between hydraulic

fracturing and non-hydraulic fracturing reference chemical list, including reported food, cosmetics, and water-related additives and contaminates. A manuscript titled "Examining Hydraulic Fracturing Chemicals with the Potential to Impact Drinking Water Resources: A Temporal and Comparative Analysis" based on research described in Chapter 4 is under submission for publication in a peer reviewed journal. In Chapter 5, a repeatable approach for investigating systemic and relative hydraulic fracturing chemical risk factors is developed, corresponding to objective 4. The contents of Chapter 5 will be used to prepare a manuscript for submission to a peer reviewed journal. Chapter 6 summarizes research accomplishments and recommendations for future research.

2. CRITICAL REVIEW OF SYSTEMIC RISK ANALYSES ON THE POTENTIAL IMPACTS OF ONSHORE UNCONVENTIONAL OIL AND GAS DEVELOPMENT ON PUBLIC HEALTH AND THE ENVIRONMENT [1]

2.1. Introduction

The primary objectives of this chapter are to highlight the distinctive value proposition of leveraging systemic risk analysis and causation modeling techniques, as well as to further the application of these methods to OUOGD environmental and health risk management. These objectives are founded on the assumption that society's goal is to minimize the risk and maximize the return of emerging technologies through comparative, collaborative, and integrative risk governance (Linkov et al., 2018). The chapter starts with a unique conceptualization of OUOGD environmental impacts before quickly transition to insights gained from reviewing the evolution of popular sequential and systemic accident hazard assessment theories, practices, and methods in parallel with the emergence of unconventional hydrocarbon production. Original OUOGD process model and control structure are synthesized from an exhaustive and multi-disciplinary (i.e., engineering, risk analysis, business, policy, etc.) literature review. The benefits of incorporating systemic hazard analysis approaches throughout the OUOGD process model and control structure are evident and will gain value with the continued integration of new digital technologies (e.g., robotics, big data analytics, artificial intelligence,

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[1] The material in this chapter was co-authored by Christopher Hill, Dr. Om Yadav, and Dr. Eakalak Khan. Christopher Hill had primary responsibility for the literature review and synthesis. Christopher Hill was the primary developer of the conclusions that are advanced here. Christopher also drafted and revised all versions of this chapter. Dr. Om Yadav and Dr. Eakalak Khan served as advisors and proofreaders for the work conducted by Christopher Hill.

machine learning, internet of things) (Anderson, 2017; Hanga and Kovalchuk, 2019; Li et al., 2020; Mohammadpoor and Torabi, 2020; Shukla and Karki, 2016a, 2016b).

2.2. What are the Potential Environmental and Public Health Risks and Benefits Associated with OUOGD?

Society's understanding and perception of OUOGD environmental and public health risks and benefits are critical inputs into finding solutions to this "wicked problem." Figure 1 summarizes potential causes of ecological and health implications commonly found in the literature (Adgate et al., 2014; Gill et al., 2017; Kaden and Rose, 2016; McKenzie et al., 2012; Small et al., 2014; U.S. EPA, 2016a; Vengosh et al., 2014; Vidic et al., 2013). Although the OUOGD process and associated control structure are unique, similar possible adverse effects are present in most industrial activities, except for direct subsurface pollution through migrations and induced seismicity. Due to the nature of hydrocarbons, energy release (e.g., fire, explosion) is always associated with their production and management. The relatively high quantity of water and sand used in hydraulic fracturing are the primary resource management concerns. Minimizing surface disturbance, surface pollution (e.g., spills), and waste generation require continuous monitoring and management. Air quality and climate change risks have also been associated with OUOGD. Nuisances with the potential to impact the quality of life of stakeholders in the vicinity of operations include view and noise disturbance. Threats to water sources (quality and quantity) appear to have received the most attention in peer-reviewed research and policy discussions, followed by air quality and climate change. Although potential OUOGD environmental and public health impacts have been well reported, understanding the sociotechnical system and system states leading to these impacts has not been well characterized.
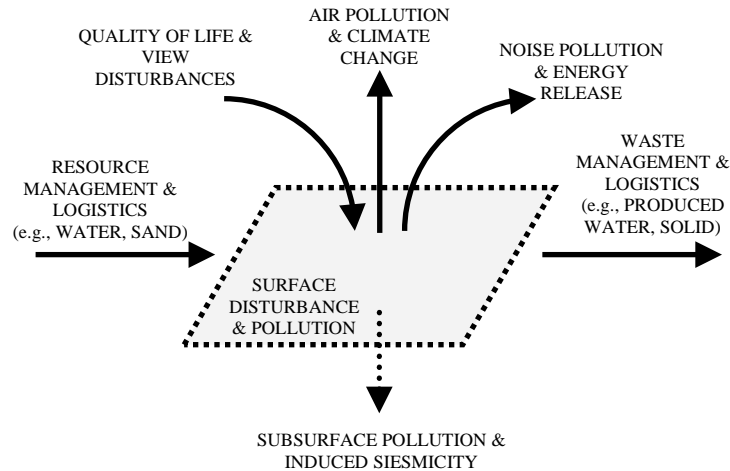
Figure 1. Summary of potential causes of OUOGD ecological and health impacts commonly found in the literature.
(Adgate et al., 2014; Kaden and Rose, 2016; Small et al., 2014; U.S. EPA, 2016a)

Most environmental and health research focuses on natural gas development because it was the first wave of U.S. unconventional hydrocarbon production, and these types of resources have been found near more populated areas. This has led to more public experience and awareness of unconventional natural gas relative to oil resources. However, risks associated with unconventional natural gas development can, for the most part, be assigned to unconventional oil development and vice versa. In addition, these resources are, in some cases, found together. Further, most environmental and public health risks attributed to OUOGD can also be applied to conventional hydrocarbon development. Policymakers, researchers, and public stakeholders have and continue to weigh OUOGD risks in conjunction with their social benefits.

The positive implications of OUOGD on the U.S. economy and national security, both of which can impact public health, are clear and prominent (U.S. DOE, 2020). The proliferation of hydraulic fracturing and directional drilling technologies has contributed to the increase in domestic supply and reduction in prices of hydrocarbon commodities, which have previously led to Middle Eastern oil embargos, $140 per barrel oil, and $4 per gallon of gasoline. In addition,

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the increased production of natural gas using these disruptive technologies has had one of the most material impacts on the reduction in greenhouse gas emissions in the U.S. Since 2000, the U.S. has seen the most significant per capita emission reductions (tCO2e/capita), relative to other developed nations, partly due to the replacement of coal with natural gas for power generation (Crippa et al., 2020; United Nations Environmental Program, 2020; U.S. DOE, 2020). Enhancing society's ability to objectively debate and analyze risks and benefits at all levels (i.e., policy to field execution) on this topic will lead to improved risk-based decision-making.

2.3. Why Are Stakeholders Relying Solely on Old Linear Causation Models in OUOGD?

2.3.1. Major Accident Risk Management

Society strives to understand accidents using causation models so it can prevent them from occurring. Causation models are abstractions of the events and factors leading to accidents, like an explosion or release of toxic chemicals. These models can be applied prospectively (i.e., risk management) or retrospectively (i.e., accident investigations). Major industrial accidents with significant environmental and public health impacts have occurred since the start of the industrial age, and unfortunately, they continue to happen. Notable upstream (i.e., exploration and production) and downstream (i.e., refined products) oil and gas incidents include the Union Carbide Bhopal chemical plant (1984), Love Canal (1980s), Piper Alpha offshore platform (1988), Exxon Valdez oil spill (1989), Longford gas plant (1998), and Deepwater Horizon oil spill (2010) (Cullen, 1990; Hopkins, 2000; Khan and Abbasi, 1999; Pereira et al., 2015). Khan and Abbasi (1999) provided a comprehensive review of major process-related accidents and causes between 1926 and 1997. Examples of recent considerable environmental and public health incidents commonly associated with OUOGD include Dimock, Pennsylvania gas migrations; Pavilion, Wyoming, U.S. water quality; Dish, Texas, U.S. air quality; Blackpool,

Lancashire, United Kingdom induced seismicity; and Fox Creek, Alberta, Canada induced seismicity incidents (Hildenbrand et al., 2020; Prpich et al., 2016; Stephens, 2015; Texas Department of State Health Services, 2010; Zhou et al., 2017). Fortunately, researchers and practitioners (e.g., operators, service companies, regulators) continue to learn from real and perceived OUOGD failures. Despite substantial risk assessment and management efforts, public trust and perception related to the governance of unconventional oil and gas activities is low, and expectations are high (Mazur, 2016).

Both acute (i.e., rapid, short-duration, easy to detect) and chronic (i.e., slow, long duration, difficult to detect) ecological and public health accidents have been attributed to OUOGD. However, chronic incidents caused by a combination of latent physical and human failures appear to be the primary concern of researchers and policymakers because there is more uncertainty in the fate, transport, exposure, dose, and effect of these incidents. For example, an undetected hydraulic fracturing chemical leak or spill is an example of a chronic incident. Figure 2 illustrates this type of chronic incident and a general causal chain of events leading to a potential environmental or public health impact. It is worth noting that there have been documented hydraulic fracturing chemical spills with ecological impacts (U.S. EPA, 2016a). However, limited epidemiological research has been published tracing chronic public health impacts to the release of hydraulic fracturing chemicals in the environment, and most of this research has been found inconclusive (HEI Energy, 2019). Regardless, this type of risk is real, and all stakeholders must continue to explore novel and more effective tools for hazard characterization, monitoring, and management.

Occupational Safety Impact		Environmental Release		Environmental and Public Health Impact			
Loss of Primary Containment	Loss of Secondary Containment	Release to the environment (Spill or Leak)	Spill not detected and cleaned up	Fate and transport under chemical and environment properties	Exposure of environmental or human receptor	Receptor unable to detect and respond to hazard	Dose causes adverse outcome in environmental or human receptor

Decreasing Likelihood of Occurrence

Figure 2. Hydraulic fracturing chemical spill accident scenario leading to environmental and public health impacts.

Risk, or uncertainty on objectives, can be measured quantitatively (i.e., absolute values) and semi-quantitatively (i.e., index or rating values) as the product of likelihood and impact. Risk management is a process used to reduce the likelihood and impact of accidents to an acceptable level through planning (i.e., scope, context, criteria, objective), risk identification, risk analysis, risk evaluation, and risk treatment with appropriate reviewing, monitoring, and communicating throughout (International Organization for Standardization, 2018). Prospective accident causation models are critical tools used in risk identification and analysis. Formal risk identification and analysis are emerging sciences younger than the oil and gas industry (Aven et al., 2018).

2.3.2. The Parallel Emergence of OUOGD and Accident Causation Theories, Perspectives, and Models

The evolution of accident causation theories, perspectives, and models has been driven by public and government reactions to major accidents and risk perceptions, as discussed above. Coincidently, the progress of these risk management tools has occurred temporally in parallel with the emergence of OUOGD. The first popular causations model debuted, in 1931, just sixteen years before the first known hydraulic fracturing application in 1947 (Ashton, 2013; Gallegos and Varela, 2014; Underwood and Waterson, 2013a). Although industrial risk identification and management are well rooted in energy development through some of the

unfortunate major accidents discussed above, the scientific literature on applying causation

models specifically to the development of unconventional hydrocarbon resources has been

limited. Figure 3 depicts a synthesis of the evolution of popular accident causation theories,

perspectives, and models in chronologically parallel with the emergence of OUOGD. These two

topics are interacting and interdependent components of a broader sociotechnical system.

Key U.S. Onshore Unconventional Resource Development Events

1975: U.S. DOE started funding hydraulic fracturing research

2005: Energy Policy Act of 2005 general excluded hydraulic fracturing from the Safe Drinking Water Act

2018: U.S. regains its spot as top oil producing country in the world

1973: U.S. loses its spot as the top oil producing country in the world and OPEC oil embargo

2016: U.S. EPA releases multi-year study on HF's potential impacts to drinking water sources

2003: Continental Resources started acquiring acreage in North Dakota's shale oil-rich Williston Basin

2011: First year more oil wells were hydraulically fractured in the U.S. than gas wells

1953: Increase in the amount of water and sand used in fracturing fluids

1998: Mitchell Energy SH Griffin #4 "slickwater" hydraulic fracturing in the Barnett Shale (Dish, TX) started the gas shale boom

2008: EOG Resources started acquiring acreage in South Texas's shale oil-rich Eagle Ford Basin the oil shale boom

1947: First hydraulically fractured vertical well

Key Accident Causation Theory and Practice Events

1976: "Domino Theory" for accident causation

1993: Layer of Protection Analysis

2012: Prospective system-theoretic process analysis (STPA) and retrospective causal analysis based on STAMP (CAST)

1974: Event Tree Analysis

1991: High Reliability Organizations

1969: Comparative Risk Analysis

1984: Normal Accident Theory

2006: Resilience Engineering Concept

1963: Hazard and Operability Studies

1981: "Swiss Cheese" Causation Model

2004: Systems-Theoretic Accident Model and Processes (STAMP) and Functional Resonance Analysis Method (FRAM)

1962: Fault Tree Analysis

1980: Energy-Barrier Perspective

1940: Failure Mode and Effect Analyses

2000: Man-Made Disasters Theory

1979: Bowtie Diagram

1931: "Domino Theory" for accident causation

1997: Sociotechnical system causation model, AcciMap accident analysis technique, and Conflicting Objectives Perspective

1978: Inherently Safer Design

Figure 3. The emergence of OUOGD and the evolution of popular accident causation theories, perspectives, and models.
(Al-shanini et al., 2014; Enverus, 2021; Fu et al., 2020; Gallegos et al., 2015; Gallegos and Varela, 2014; Hasan et al., 2020; Hill et al., 2021b; Hollnagel, 2004; Hollnagel et al., 2006; Katsakiori et al., 2009; Leveson, 2012, 2004; Rasmussen, 1997; Underwood and Waterson, 2013a)

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The linear causation paradigm maintained a monopoly in risk management until 1997, when Rasmussen introduced the concept of system thinking into the process (Rasmussen, 1997). Coincidentally, one year later, Mitchell Energy "cracked the code" on "slickwater" hydraulic fracturing at its SH Griffin #4 gas well, starting the Shale Revolution (Yergin, 2020). Katsakiori et al. (2009) and Underwood and Waterson (2013) reviewed advancements in accident causation models and concluded that the application of models is transitioning from sequential to systemic models. However, based on a literature review, the transition is not occurring quickly in the onshore unconventional oil and gas industry. A reasonable hypothesis on the causes of slow adoption is that regulatory and industry stakeholders may have been too busy applying traditional risk analysis methods while regaining U.S. energy independence to notice the simultaneous transition to systemic approaches. Researchers and other stakeholders also do not appear to have readily adopted systemic practices to characterize the OUOGD systems and associated hazards. However, the emergence of OUOGD occurred quickly, challenging researchers to understand new technologies (i.e., hydraulic fracturing, direction drilling), associated impacts, and apply conventional linear models and reductionist thinking. Past performance and methods may not indicate future trends because OUOGD and risk management both continue to evolve rapidly. The recent relative reduction in OUOGD activity and increased transparency present a unique opportunity to redirect resources to research and apply novel holistic risk analysis approaches to identify and mitigate environmental and public health risks and accident causal factors.

2.3.3. Limitations and Strengths of Traditional Linear Causation Models

Linear causation accident models have strengths and weaknesses (Lehto, 1991; Leveson, 2012). A brief review of linear hazard identification techniques currently popular in OUOGD is

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provided to help readers understand their limitations and strengths in contrast with systemic methods. "What if" analyses, hazard and operability studies (HAZOP), failure mode and effect analyses (FMEA), bowtie models, and layer of protection analyses (LOPA) are the most common prospective hazard management tools used in the oil and gas industry (Chastain et al., 2017; Stemn et al., 2018). "What if" analysis captures scenarios development by team generated questions regarding process errors and failures.

HAZOP is a more systematic type of study conducted by dividing physical processes into individual nodes and reviewing each node and associated operational parameters for potential losses using process deviation guide words. Like HAZOP, FMEA focuses on possible failure modes (i.e., man, material, machine, measurement, method, and environment) of physical components (e.g., equipment parts or units). Bowtie diagrams (a combination of a fault tree and event tree) illustrate and quantify sequential event scenarios and probabilities, respectively. LOPA quantitatively assess hazard barriers to determine safety criticality and the need for additional action (e.g., add barriers, increase reliability of existing barriers to meet desired risk tolerance) (Center for Chemical Process Safety, 1993; Chastain et al., 2017). Bayesian networks have also been used to model complex dependencies between factors (Kanes et al., 2017). For a more comprehensive review of risk identification and assessment methods based on linear causation or probabilistic models found in the unconventional oil and gas research and practice, Torres et al. (2016) is recommended.

A principal assumption of the tools and techniques discussed above is that accidents and associated consequences result simply from a chain of events. This perspective is helpful in the creation of simplistic mental models for straightforward systems. However, cause-effect models do not typically capture linear and non-linear component interaction and dependencies with

broad cascading consequences. Sociotechnical systems are complex in nature and can be prone to unexpected events. Therefore, accidents associated with these systems are challenging to characterize with linear events and barrier failures. Leveson provided a comprehensive review of linear event-based accident model limitations (Leveson, 2012, 2004). In summary, most modern advancements in technology (e.g., energy, transportation, communication, information, computers, software) have increased the complexity, dynamics, and speed of sociotechnical systems, presenting modeling challenges for understanding hazards, controls, and accidents. In addition, sequential models do not consider the value of feedback loops and information transfer to functions not directly managing physical components. Those attempting to solely use linear causation models to manage risk in these systems have a significant potential for large understanding gaps, leading to substantial accidents or lost opportunities.

Hasan et al. (2020) recently stressed the need to shift away from sequential causation models in the offshore oil and gas space for similar reasons, and the review presented in this chapter echoes this sentiment for OUOGD. Despite sequential accident model limitations, they still appear to have a monopoly in OUOGD. This is the case most likely because they have a proven (although not perfect) track record, identify "root causes" ("someone to blame"), and are challenging, costly, and risky to deviate from in fast-paced environments. Regardless, OUOGD stakeholders can and should overcome this inertia to adopt causation accident models and risk assessment techniques found in system theory. Doing so would help overcome linear model limitations, which it is believed can lead to safer OUOGD designs/operations and improvements in stakeholder communication.

2.4. Are Systemic Risk Analysis Techniques Applicable To OUOGD?

The aims of this section are to provide a general overview of the most prevalent systemic

causation models found in research and practice (AcciMap, Functional Resonance Analysis

Method [FRAM], Systems-Theoretic Accident Model and Processes [STAMP]) (Underwood and

Waterson, 2012) and critically review the feasibility of applying these models to assess

environmental and public health risks associated with OUOGD. A brief description of AcciMap

and FRAM is provided before exploring the STAMP methodology in greater detail. Although

popular in research, there has been limited practical application of these powerful techniques in

proactive oil and gas risk management (Davis et al., 2014; Underwood and Waterson, 2013b).

Potential causes of slow practitioner adoption include a lack of awareness and experience with

these new procedures; time and resource constraints (training and change management);

differences relative to traditional methods leading to cognitive dissonance; and they are not

designed to identify "someone to blame." This review addresses some of these impediments and

provides a catalyst for applying systemic risk assessment methods in OUOGD to mitigate

potential environmental and public health impacts.

2.4.1. Benefits of Systemic Risk Analysis Techniques

Sociotechnical systems are constantly evolving. It is necessary to use tools that

appropriately capture the complexity and dynamics of these systems and the interaction and

interdependencies of components (i.e., physical, human, digital hardware, software). The system

perspective moves beyond immediate causes and "finding someone to blame" to look at design

iterations, accident contributing factors, and emergent behaviors at all levels of the system. This

line of thinking is counter to the reductionist approach used in linear accident causation models,

which typically focuses on understanding components separately and assumes that they can be

chained together to describe the system or accident completely. Systemic models replace linear cause-effect component abstractions with interconnected functional networks and loops containing feedback and non-linear relationships.

Underwood and Waterson (2012) conducted a literature review to identify available systemic models and their popularity. Thirteen models were identified from 449 articles, and STAMP (52%), FRAM (19.9%), and AcciMap (17.9%) were found to be the most common models referenced. All three of these models are generic in nature. Therefore, they can be applied to most system abstraction levels (i.e., government, company, team, process, etc.) and any industry, including OUOGD. STAMP, FRAM, and AcciMap approaches were compared using the Chevron Richmond refinery accident, and STAMP was found to provide a more complete understanding of accident causes (Yousefi et al., 2019). It is believed that these findings translate to OUOGD and, therefore, recommended to prioritize STAMP method research and application.

2.4.2. Brief Exposure to Sociotechnical Systems and AcciMap

Rasmussen (1997) identified earlier than most that industrial risk was shifting in terms of the speed, scale, competition, and flow of information. His early realization of the importance of human and social risk factors led him to advocate for a multi-disciplinary approach to incorporate political, economic, legal, management, engineering, psychological, and other sciences into safety science and risk management. To help model systems using a cross-functional approach, Rasmussen (1997) pioneered the use and characterization of the safety control structure based on control theory and feedback loops. The AcciMap accident analysis technique, which is part of a broader proposed risk management framework, embodied Rasmussen's safety control structure (Figure 4). The method maps system interactions,

decisions, and accident contributing factors across six defined system levels (i.e., government,

regulatory bodies, local government/company management, technical/operational management,

physical process, and equipment/surroundings). However, it still relies on sequential causation at

its lowest hierarchical level. The model can be used proactively to understand accident scenarios;

however, most of its oil and gas application in literature appears to be toward accident

investigation (i.e., Esso Gas Plant and Richmond Refinery) (Hopkins, 2000; Yousefi et al.,

2019). Salmon et al. (2020) provided a comprehensive review of published AcciMap analyses

and extracted relationships between common contributory factors.

Government

Public Opinion

Judgement ← Safety Review, Accident Analyses

Laws

Regulators, Associations

Judgement ← Incident Reports

Regulations, Industry Practices

Company

Judgement ← Operations Reviews

Company Policy, Practices

Management

Judgement ← Logs, Work Reports

Plans

Staff

Judgement ← Observations, Data

Action

Work

Hazardous Process

a → b → c
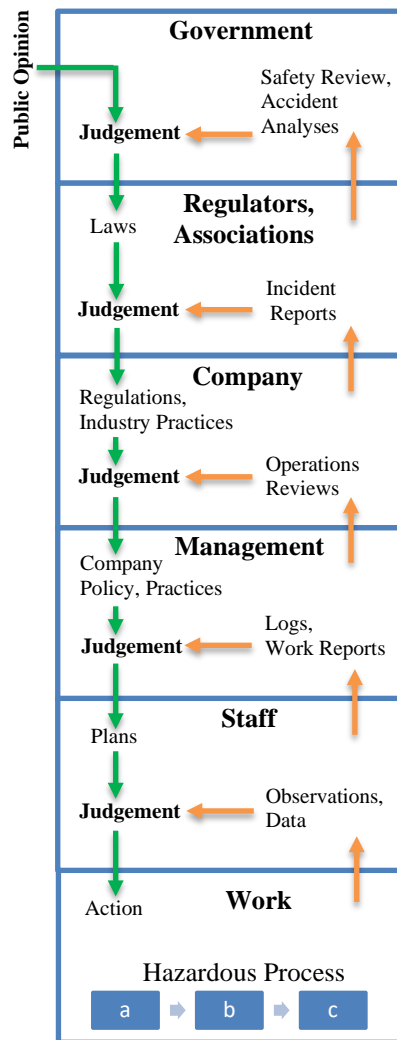
Figure 4. General sociotechnical system.
(adapted from Rasmussen, 1997)

2.4.3. Brief Exposure to Functional Resonance Analysis Method

FRAM is established on resilience engineering principles focusing on maintaining system safety under dynamic operational conditions (Hollnagel, 2004). The concepts behind FRAM successes and failures are equivalent, systems adapt to system conditions, accident causes are typically emergent in nature, and understanding dependencies and relationships is critical. In functional resonance, individual system function variability is believed to have a broad impact on system performance (successes and failures). System technical, human, and organization

functions are characterized and coupled together using six parameters: inputs, preconditions, time, resources, controls, and outputs (Figure 5). The analysis technique is comprised of five primary steps: 1) define purpose and scope of analysis 2) establish functions of the system necessary to meet system objective, 3) understand individual functional output variability, 4) describe system variability caused by individual functional variability, and 5) establish function management approaches for system variability outside of allowable tolerances. FRAM is still maturing and being explored for risk analysis across various industries, including oil and gas (Cabrera Aguilera et al., 2016). Unlike AcciMap, FRAM does not pre-define control structure hierarchy levels, and the method is primarily concerned with day-to-day rather than higher functions (e.g., government, regulations).
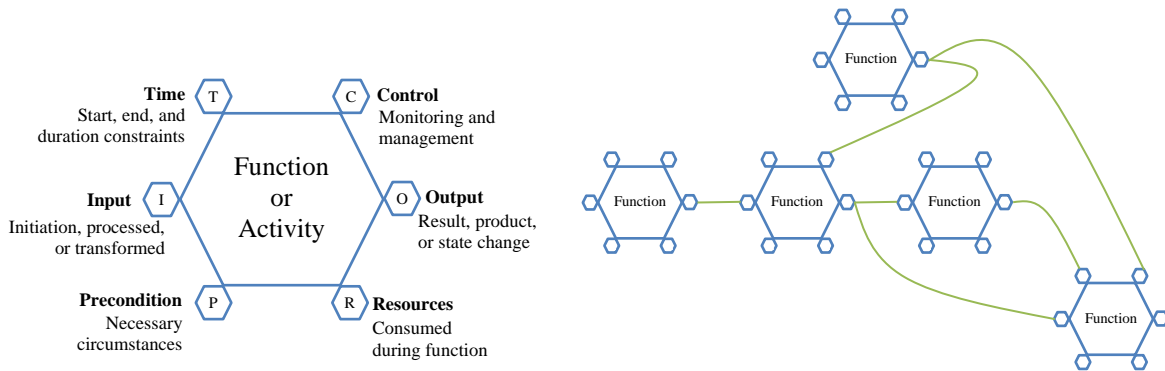
Figure 5. General FRAM function diagram.
(adapted from Hollnagel, 2012)

2.4.4. Brief Exposure to Systems-Theoretic Accident Model and Processes

Like AcciMap, STAMP is founded on systems and control theory. The technique strives to capture proximal events and causal factors leading to accidents (Leveson, 2004). Although STAMP is based on Rasmussen's legacy, the approach differs from AcciMap by having a more comprehensive control structure, completely excludes linear causation models, and extends beyond operating phases to include design phases as well (Leveson, 2017). A brief review of STAMP and system-theoretic process analysis (STPA) is given below because they are

foundational to understanding the hierarchical OUOGD control structure in Section 2.6 and viable replacements for HAZOP analyses commonly used in OUOGD.

STAMP focuses on ensuring system safety constraints (passive or active) are defined and enforced in the context of well-defined control structures and process models. A control structure is an abstraction of relevant real-world functions using interconnected and interacting control loops consisting of controllers, process models, actuators, sensors, and the controlled process of interest. A general control loop with failure modes is provided in Figure 6. Controllers (i.e., human, physical, digital) rely on a process model (i.e., how they interpret the controlled process, environment, and system) and provide direction to other controllers or process actuators. Accidents are expected when the control structure fails to adequately maintain safety constraints. For example, a public health organization must ensure the public is not exposed to toxic chemicals, and an oil and gas company must always be under the positive control of chemicals. Regarding the environment and public health, these safety constraint examples illustrate that hazards (i.e., toxic chemical exposure to the public) are being controlled by multiple interacting control structures with complex interactions. However, in Section 2.6, an industry perspective is used to synthesize the general control structure based on a comprehensive literature review.
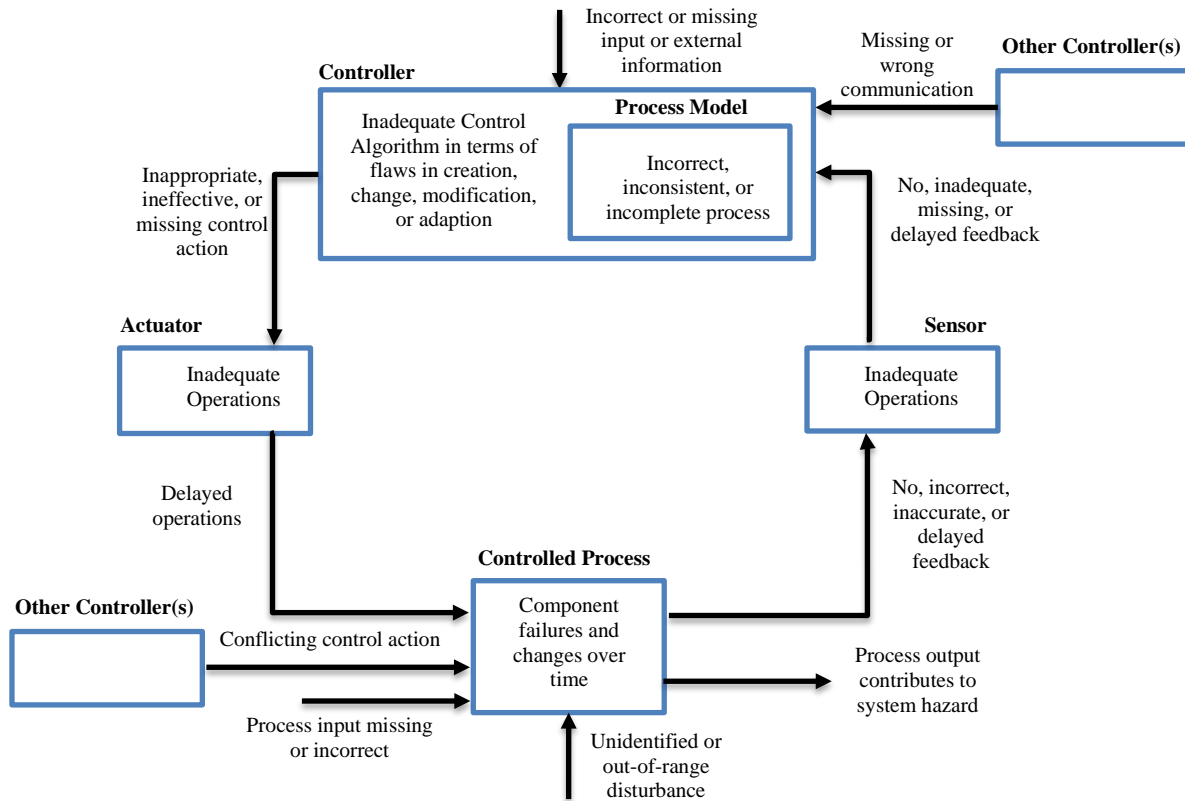
Figure 6. STAMP general control loop and control failure causes.
(adapted from Leveson, 2012)

The STPA methodology used in research and practice for proactive risk management is
founded on STAMP theory. STPA, like HAZOP analyses, systematically reviews components,
failure modes, and consequences to provide recommendations to reduce risk. STPA
accomplishes this using a four-step process: 1) define analysis purpose, system boundaries,
losses, and hazards; 2) model control structure, 3) identify unsafe control actions (UCA), and
develop controller requirements and constraints to prevent UCA, and 4) identify loss scenarios,
and set design recommendations and operational requirements to avoid loss scenarios. System
hazards are used to define general system constraints. Safety constraints are lost when one or
more control loops (e.g., function) fail or execute UCA. UCA occurs when an action is not
provided, inappropriately provided, or incorrectly timed (i.e., early, late, out of sequence, too

long, too short) by a controller. System and functional safety constraints are generated to prevent

UCA. Loss scenarios define the causes of UCA or system hazards. Figure 6 has general

examples of UCA causes. A specific OUOGD example is the release of hydraulic fracturing

chemicals into the environment because an operator believed the chemical hose was connected to

the tank. STPA is a novel and powerful tool for risk management that has been successfully

applied to the oil and gas sector (Altabbakh et al., 2014; Gong and Li, 2018; Kim et al., 2018;

Leveson, 2012; Meng et al., 2018; Pereira et al., 2015). However, the application of STAMP or

STPA to OUOGD environmental and public health risks could not be identified in peer-reviewed

literature. The extensive body of research, practical handbooks, and available trained consultants

make STAMP and STPA ideal for quick adoption into OUOGD (Leveson and Thomas, 2018;

STAMP Engineering Services, 2020).

2.4.5. Limitations of Systemic Risk Analysis Techniques

Like linear techniques, systemic hazard analyses have their challenges, limitations, and

weaknesses. Underwood and Waterson (2012; 2013) identified "model validation, usability,

analyst bias, and the implications of not apportioning "blame" the need to close the existing

significant research-practice gap. Despite these limitations, systemic accident models have

proven to "exceed conventional accident causation method" in a head-to-head oil and gas case

study by identifying additional risk factors (Altabbakh et al., 2014). Although this comparison

was not specific to OUOGD, there appears to be an opportunity for similar contributions of

systemic risk assessments in this space. The rapid adoption of new digital technologies (e.g.,

robotics, big data analytics, artificial intelligence, machine learning, internet of things)

(Anderson, 2017; Hanga and Kovalchuk, 2019; Li et al., 2020; Mohammadpoor and Torabi,

2020; Shukla and Karki, 2016a, 2016b) in OUOGD may demand the adoption of these novel and

holistic techniques for the adequate management of financial, health, safety, and environmental risks. Therefore, it is concluded that systemic risk analysis techniques are applicable and potentially critical to prudent OUOGD.

2.5. Why Is the OUOGD Process Model So Hard to Define?

Accidents can be caused by incorrect, inconsistent, or incomplete process models. The U.S. Environmental Protection Agency (EPA)'s concept model of the hydraulic fracturing water cycle from its 2016 study of the potential impacts of hydraulic fracturing on drinking water resources focuses strictly on the following five phases: water acquisition, chemical mixing, well injection, produced water handling, and wastewater (U.S. EPA, 2016a). Although the U.S. EPA's comprehensive multi-year study significantly improved communication and understanding of OUOGD among stakeholders, its process model is incomplete and lacks a system perspective. Specifically, the U.S. EPA's model is limited to a single well phase (i.e., completion), does not capture process functions beyond field activities, and fails to illustrate each well is part of a broader field development strategy. These types of process model issues are not unique to U.S. EPA's research. Incorrect, inconsistent, and incomplete OUOGD process models, based on reductionist approaches or linear thinking, frequently appear in environmental and public health research to date (McKenzie et al., 2012; Vengosh et al., 2014; Vidic et al., 2013). However, these abstraction steps are essential and necessary on a path to more holistic models and, it is worth noting that all models are subjective and have limits. With that said, a comprehensive OUOGD process model that encompassed the current state of knowledge could not be identified in peer-reviewed literature, so a synthesize systemic abstraction was developed in this study for researchers and practitioners to build and improve upon.

A standard system development life cycle model can be applied as a starting point for abstracting the OUOGD process and levels. However, it is essential to acknowledge the social, technological, and subsurface uncertainty within the highly competitive and iterative upstream oil and gas industry. These complexities require highly adaptive management approaches and result in non-linear behaviors, iterations, and interactions within the process. Figure 7 illustrates a conceptual model for a three-level (i.e., field development, pad-well, and well-phase) hierarchical OUOGD process based on a synthesis of literature and personal experiences. The presented model is provided from an operator perspective. However, it can be used by stakeholders to describe multiple operators in a basin as well.

Level 1. Field Development
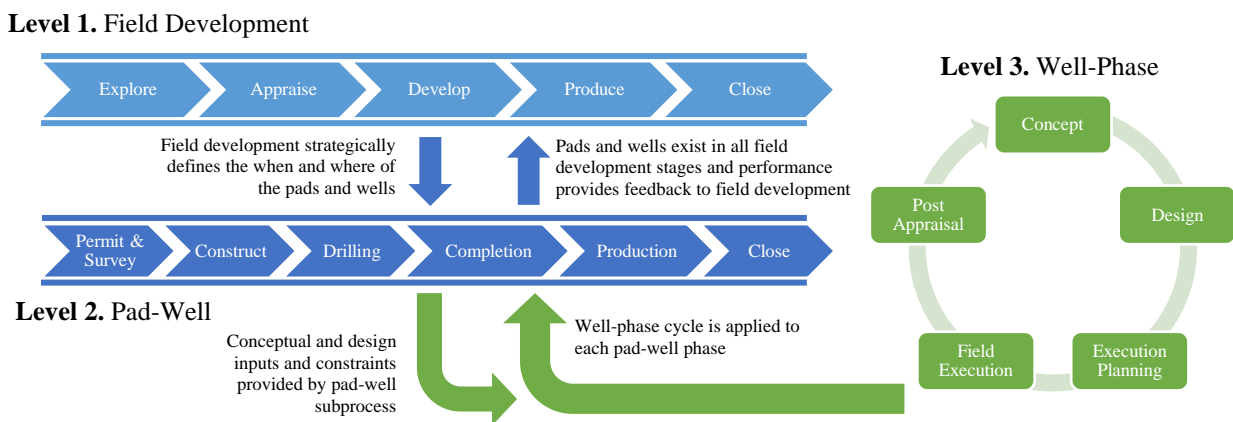
Figure 7. General hierarchical OUOGD process model.

The highest level of the process is "Field Development," which encompasses all activities associated with economically recovering hydrocarbon resources from a particular basin or play. Many factors can influence field duration or lifespan, which can extend decades or be halted prematurely due to economics (e.g., commodity prices, regulatory changes). The second level, the "Pad-Well" level, is the most common perspective found in research. Pads and wells are constructed and utilized throughout all stages of field development. Although the pad-well "Production" phase can last decades, the other pad-well phases are measured in days and weeks

(U.S. EPA, 2016). It is a common semantic mistake in the literature to classify most of the well lifecycle as hydraulic fracturing. However, hydraulic fracturing is only conducted in the "Completion" well-phase. Although not common, well recompletions can occur. The last level, the "Well-phase" level or cycle, is applied to each pad-well phase (e.g., drilling, completion) by different expert teams specializing in that particular phase. Recognizing the relationships between these process model levels and stages is critical for understanding the OUOGD system and managing associated environmental and public health risk and stakeholder behaviors. For example, an operator may use more fresh water and chemicals during hydraulic fracturing activities during "Exploration" to test and characterize the hydrocarbon reservoir. The results and feedback from exploration and appraisal wells can be used to design infrastructure, optimize chemicals, and plan water recycling efforts for future wells. Using information gained early in field development to extrapolate risks over the life of a field or across OUOGD can be misleading (in both positive and negative directions).

It is worth acknowledging, like most projects, the opportunity and cost to influencing risk decreases and increases, respectively, at all levels as the development process progresses (Green and Perry, 2008). It is easier and more cost-effective to control, influence, or plan to manage risk early, and the difficulty and cost of doing so increase over time. The likelihood of unintended adverse consequences can also increase when unplanned or ad hoc risk mitigation activities are attempted late in a development or project. Understanding the OUOGD process and earlier application of systemic risk analyses will lead to fewer accidents.

Not surprisingly, the field execution and operational aspects of the "Pad-well" and "Well-phase" levels are typically the focus of environmental and public health impact research because this is where the hazards and direct causes exist. However, systemic risk analysis methods and

the presence of risk controls beyond fieldwork boundaries lead one to believe there is value in an expanded perspective. Understanding the higher field development level and lateral components within the other two aspects is critical for managing OUOGD environmental and public health risks. Similar field activities can have different risk profiles depending on when they occur in the process. This section briefly describes each of the hierarchical levels and essential components synthesized from literature with identified gaps. Below, emphasis is provided on the characterization of the field development level and other process aspects that are not typically acknowledged in environmental and public health risk publications.

2.5.1. Field Development Level

The field development process is initiated by geologists and engineers typically located in a corporate office and continuously evolves during desktop and field activities. The presented field development outline, generated from petroleum engineering, business, and finance references (Darko, 2014; Herrmann et al., 2013; Suslick et al., 2009), is combined with practical experience and ecological and public health risk resources below.

The "Explore" and "Appraise" stages are focused on gathering information to make informed investment decisions. These steps are incredibly confidential due to competition from other operators and the associated business risk. Historic well logs and 3D seismic testing are used to map subsurface formations. During these phases, the field activity is relatively low, but pads and wells are necessary to test and characterize reservoirs. There are potentially higher environmental risks or impacts per well relative to other field development phases because of limited infrastructure and significant surface uncertainty. For example, truck traffic and flaring may be higher without oil and gas gathering systems in place, and additional hydraulic fracturing chemicals may be used to understand which chemicals are most effective in stimulating

hydrocarbon reservoirs. Surface use agreements and leasehold acquisition from land and mineral

owners are necessary to conduct all field activities. Operators typically start by evaluating a

small area or leasehold. If the economics are determined to be favorable in the "Appraisal" stage,

a significant leasehold position is acquired for full-scale development. Operators strive to

develop oil and gas fields safely and economically. Therefore, there is a general self-imposed

requirement and belief that this is possible before moving forward and operating in a basin.

Operator and service companies have internal controls and management systems, as discussed in

Section 2.6, to monitor and manage environmental and public health risks from "Concept" to

"Close."

Practical and rational changes to environmental and public health regulations or other risk

control measures before the significant capital deployment for land acquisition are more likely to

be accepted by industry stakeholders because they can be factored into investment decisions. The

industry appears hesitant to support command-and-control, bureaucratic, redundant, or arbitrary

regulations that do not have a clear, measurable, or conclusive risk reduction benefit (American

Petroleum Institute, 2012a). There seems to be a conflict between the preferred collaborative risk

governance approach and confidential dynamics created by oil and gas law in the "Explore" and

"Appraise" field development stages (Hill et al., 2021b; Linkov et al., 2018; Lowe, 2014). This

disconnect may be the critical source of tension and misunderstanding between public and

industry stakeholders. However, if most U.S. unconventional hydrocarbon basins have been

discovered and development initiated, this is expected to be less of an issue moving forward.

The "Develop" and "Produce" stages of OUOGD have similar activities but deferring

priorities. During the "Develop" stage, operators deploy a significant amount of resources and

capital to strategically ensure that profitable leaseholds do not expire and establish infrastructure.

Infrastructure examples include oil and gas gathering pipelines, produced water gathering systems, electrical distribution systems, access roads, and other infrastructure to minimize risks, impacts, and costs. The "Produce" stage strives to optimize the development plan to maximize cash flow and return on capital deployed. During both stages, surface and subsurface information continues to be gathered while executing work at the pad-well and well-phase levels (e.g., construct, drilling, completion). This information is used to further reduce environmental and public health risks. For example, with more knowledge and confidence, operators may have the option to decrease chemical volumes and consider "greener" chemicals while maintaining or even increasing reservoir productivity (Harry et al., 2020; Thomas et al., 2019). With infrastructure, reduced uncertainty, and improved understanding of hydrocarbon resource boundaries, operators can optimize risk and return in the "Produce" stage more confidently. Most of the environmental impacts and public health risks associated with OUOGD found in research appear to be concentrated in the "Develop" and "Produce" stages because this is where the highest field activity concentration occurs.

When the field production has declined or economic circumstances (e.g., commodity price, production expenses) have deteriorated to a level at which it is not financially viable to continue operating, fields are closed (i.e., decommissioned and reclaimed). The reclamation process is focused on managing environmental and health risks and impacts. It includes plugging the wellbores to prevent fluid migration to drinking water sources, removing surface equipment, restoring the field to its original state, and clean-up any pollution found during the process. Although the "Close" stage is the end of the field development process, it is worth acknowledging that significant acquisition and divestiture activity occurs in the oil and gas industry. A field asset or well may be bought or sold at any point during the process. When

assets, wells, or leasehold change hands, the purchasing operator will conduct due diligence to fully understand associated liabilities. Understanding environmental and public health impacts and risks are a critical aspect of acquisition due diligence.

2.5.2. Pad-Well Level

Other researchers have adequately characterized the stages of a typical unconventional well from a field execution perspective (U.S. EPA, 2016). Therefore, the highlights and discussion below are limited to key points related to environmental and public health hazards. Note that a pad can have one or more wells, which may be drilled at the same or different times. Once a well location is determined, operators conduct permitting and survey activities before construction begins. Permission from mineral owners, surface owners, and regulatory agencies is required. Oil and gas companies conduct surveys for wetlands, endangered species, archaeological evidence, baseline groundwater quality, and other site conditions as required by regulators and surface owners (in surface use agreements), as well as defined by best practices. At this stage, vulnerable receptors and unacceptable impacts are intended to be identified to mitigate or minimize impact and risk. The "Construct" phase includes all surface civil (i.e., pad), mechanical (i.e., facilities), and electrical (i.e., power and instrumentation) installation activities. Under some circumstances, mechanical and electrical construction can take place between or after drilling and completions. During the "Construct" phase, primary risks of concern are ecological impacts caused by surface disturbance and erosion, pollution caused by equipment fuel or oil leaks, and traffic accidents caused by logistics.

The "Drilling" phase encompasses the mobilization/demobilization of rigs, drilling the well to the target depth, installing multiple layers of cement and casing, and testing the integrity of the well. The sight and sound of drilling rigs over a few weeks have been known to disturb

communities. Significant risks include drilling mud/chemical releases, naturally occurring radioactive material (NORM) found in drill cuttings, and well blowout (i.e., loss of well control) incidences. The "Completion" phase, and more specifically hydraulic fracturing, has been the most researched aspect of OUOGD due primarily to the associated water consumption, toxic chemical usage, and increased formation water production. Subsurface migration and induced seismicity are known public concerns. Also, during completion activities, noise, traffic, and flaring can present environmental and health risks. The "Drill" and "Completion" phases are the most capitally intensive aspects of OUOGD, and they have also been characterized as the most hazardous. (Adgate et al., 2014; Hays et al., 2017; Kaden and Rose, 2016; Small et al., 2014; U.S. EPA, 2016a)

During "Production," operators and other stakeholders realize a return on their investment (e.g., capital, permitted impacts, risk, etc.) in the form of cash flow, royalties, taxes, and domestic energy. Workover activities (e.g., well cleanout) and surface equipment maintenance are typically required to maintain and optimize production. "Production" phase hazards include flaring (i.e., air quality, energy), produced water management, surface spills (i.e., facility integrity), NORM, fire/explosion, and subsurface pollution (i.e., well or gathering system integrity). As discussed in Section 2.5.1., when production has declined or economic circumstances (e.g., commodity price, production expenses) have deteriorated to a level at which it is not financially viable to continue production, wells are decommissioned and reclaimed. Closure activities include plugging and abandoning the well, decommissioning surface equipment, and site restoration, which presents similar hazards to those found in the "Construct" and "Production" phases.

2.5.3. Well-Phase Level

Recall, each well-phase is typically managed by a team of experts specializing in that particular phase. The well-phase subprocess defines a general project management cycle used by these teams to manage all risks, including environmental and safety hazards. It is beyond the scope of this review to comprehensively discuss the project management cycle. However, acknowledging this subprocess and associated steps is necessary to fully understand and characterize the control structure proposed in the next section.

Risk analysis and management activities are not exclusively conducted during field execution. On the contrary, the goal is to analyze and mitigate as much risk as possible before field activities begin in OUOGD. Therefore, engineering and operations professionals leverage the tools discussed in Section 2.3 (e.g., HAZOP, FMEA, Bowtie Model, LOPA) to assess risks in the concept, design, and execution planning steps. Plans, procedures, and specifications generated in these steps are referenced during field execution. General hazards are disclosed and contingency plans are developed in collaboration with first responders (e.g., fire department). Regular project/operations meetings and field-specific hazard identification assessments, like job safety analyses (JSAs), are conducted before work by all personnel on-site. Linear causation models are used in accident post-appraisal reviews and root-cause failure analyses with the expectation of learning from these failures. Concept, design, and planning steps incorporate these lessons learned into future projects.

Research to date has focused on field execution and operations aspects of OUOGD because this is where the hazards and apparent sequential causes of risks exist. Expanding the discussion to encompass the full planning, execution, and learning project cycle for each phase of a well provides a more comprehensive perspective of the control structure, opportunities, and

issues. In addition to well phases, this project cycle is typically applied to infrastructure projects (e.g., saltwater disposal wells, gathering systems, network, electrical distribution systems).The OUOGD process model can be challenging to define because it encompasses a complex system that spans decades, and very few individuals/groups have the opportunity to observe its multiple levels from a meaningful, holistic perspective.

2.6. How Are Environmental and Public Health Risks Associated with OUOGD Controlled?

Oil and gas operators are the primary owners of the hierarchical OUOGD process; however, external factors and critical stakeholders (e.g., public, policymakers, regulators, land and mineral owners) significantly influence risk and control activities. In this section, a general OUOGD control structure using the STAMP model is elucidated, essential risk assessment and control activities in this structure are discussed, and examples of risk governance enhancements by using a systemic and holistic perspective are provided. General and other oil and gas STAMP safety control structures have been published (Altabbakh et al., 2014; Gong and Li, 2018; Kim et al., 2018; Leveson, 2012; Meng et al., 2018; Pereira et al., 2015), which are used as a starting point for the abstraction provided and useful references for additional context. Figure 8 is the OUOGD safety control structure that was conceptually developed in this review. The goal of the content below is to highlight unique OUOGD control functions, interactions, and insights related to environmental and public health risk management, not describe the OUOGD control structure in detail. It is suggested that readers reference other STAMP resources for additional information that is not specific to OUOGD (Leveson, 2012) and acknowledged that particular regulatory and industry functions will vary depending on the field operating processes and hazards of interest. Therefore, the general OUOGD control structure should be considered a starting point for researchers and practitioners to develop their own models for circumstances and risks of interest.
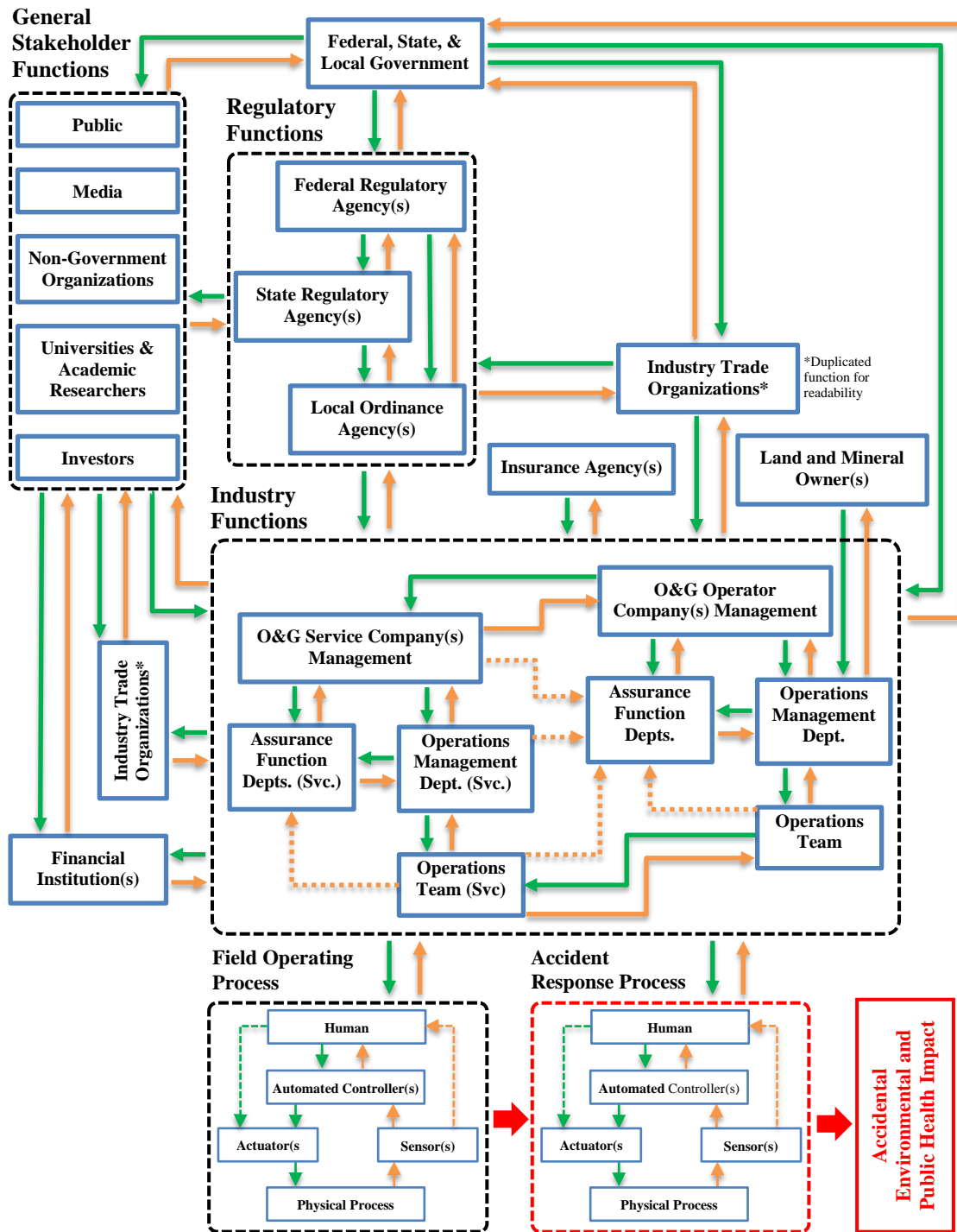
Figure 8. General OUOGD control structure.

The "Field Operations Process" represents field activities that take place in each pad-well

phase (e.g., construct, drill, completion). There are operating process handoffs between pad-well

stages that are not represented in Figure 8 because it would deteriorate readability. The

"Accident Response Process" is triggered when an accident occurs. At which point, the control structure shifts to solely responding to a loss of primary containment and preventing/mitigating environmental and public health impacts. During major acute accidents, the hazard propagates the system and environment too quickly for response efforts to prevent effects. Accidental consequences occur when the "Field Operations Process" and "Accident Response Process" do not maintain control of safety constraints.

2.6.1. Political and Regulatory Functions

Political and regulatory functions at the federal, state, and local levels are the most common control functions references in literature. Stakeholders have lobbied federal, state, or local governments to ban OUOGD related activities (e.g., hydraulic fracturing, pipelines), and some governments have accepted these requests (Soeder, 2018). Although banning industrial activities can eliminate environmental and public health risks, it also removes the associated public benefits. Federal, state, and local regulations designed to protect the environment and public safety are not typically unique to OUOGD. Applicable major U.S. federal environmental and health laws pertain to OUOGD, but existing scope exemptions have caused stakeholder concern (Fink, 2019; Willie, 2011; Zirogiannis et al., 2016). It is worth noting that a positive influence on risk management and safety practices in OUOGD can be traced to laws where exemptions exist. For example, the Occupational Safety and Health Act 29 CFR 1910 regarding process safety management, passed in 1992, does not apply to most OUOGD activities. However, this regulation has provided a catalyst for hazard and risk analysis method development and application throughout the oil and gas industry, which have percolated into OUOGD. Prudent oil and gas operators apply applicable best practices to the onshore exploration and production activities and sites.

For the most part, the state has primacy over permitting oil and gas activities while adhering to federal regulations and agency oversight, unless the well is drilled on federal land. State agencies have been in close coordination throughout the "shale boom" through interaction within legacy multistate non-governmental organizations (e.g., Groundwater Protection Council [GWPC], Interstate Oil and Gas Compact Commission [IOGCC]). Collaboration and coordination between federal and state agencies appear to be increasing in the OUOGD space (U.S. EPA and NM EMNRD, 2018). The relationship between state regulations and local ordinance presents challenges because the oil and gas pursuits can be nearby communities typically governed by local zoning laws. It is worth noting that formal agency actions at all levels are conducted in a transparent manner in the U.S. that allows for public participation. The critical role of risk analysis in policy and regulatory decision making is well known and accepted (National Research Council, 2009). Using systemic models (e.g., STAMP) can enhance federal, state, and local agencies' risk management efforts and improve collaboration with each other and stakeholders.

2.6.2. General Stakeholder Functions

The public, non-government organizations, universities/academic researchers, and investors are classified as general stakeholders. These groups continue to have a significant influence on OUOGD risk perception and management. Their feedback to political, regulatory, and industry functions has been captured in policy comments, documentaries, shareholder proxies, countless peer-review publications, and other formats (Mazur, 2016). Regardless of the argued legitimacy of some general stakeholder function claims by industry stakeholders, this group has served a vital system role, ensuring an open dialog regarding OUOGD environmental and public health risks and impacts. Finding ways to improve transparency and communication

with these groups while protecting trade secrets and confidential business information is a system challenge that requires additional attention. Systemic risk analysis techniques may be part of the solution.

2.6.3. Land and Mineral Owner Functions

The land and mineral owner function of the system is unique to U.S. onshore oil and gas exploration (Lowe, 2014). This function does not exist in offshore development or in most other hydrocarbon-producing countries. Lease agreements define the contractual arrangement between the operators and mineral owners. Although there are standard lease forms, the mineral owners have the right to make non-standard contractual language requests at the risk of losing the operator's interest and investment. Similarly, the surface use agreement, which defines the contractual arrangement between the operator and surface landowner, has the flexibility to incorporate hazard transparency and mitigation requirements. These two types of contracts may present opportunities to define and document safety constraints rarely discussed in environmental and public health research. At the very least, they appear to provide an opportunity for discussion and fostering a shared mental model through existing feedback pathways. In addition, there may be unintended environmental risks or consequences caused by the incorporation of some contractual terms that economically favor the land or mineral. For example, an operator may be required to procure fresh water from the land or mineral owner for hydraulic fracturing on a lease disincentivizing produced water reuse.

2.6.4. Industry and Trade Organization Functions

Industry trade organizations (e.g., American Petroleum Institute [API], International Association of Oil and Gas [IOGP], International Petroleum Industry Environmental Conservation Association [IPIECA]) serve a vital role in facilitating and formalizing shared

recommended practices (RP), standards, and frameworks for the management of environmental and public health risks. API's (2012b) RP 51R Environmental Protection for Onshore Oil and Gas Production Operations and Leases is an example. Although industry members have more control over these activities, the formal process for developing these resources is open to other stakeholders.

Like the rest of the control structure, the industry functions are general and highly simplified. Oil and gas operators direct OUOGD permitted by government agencies and assisted by various vendors and service companies. The structure and operating models of these types of entities are specifically designed to maximize returns and minimize risk, including environmental and public health risks. IPIECA and IOGP's (2014) Operating Management System Framework for Controlling Risk and Delivering High Performance in the Oil and Gas Industry is an example of a prudent operating model used by operations management teams. From a corporate governance perspective, assurance departments are additional and independent (from Operating Departments) functions specifically designed to maintain control of safety constraints. These functions included internal audit, enterprise risk management (ERM), ethics, and compliance departments. For more information on these functions, review the Committee of Sponsoring Organizations of the Treadway Commission guidance resources (2021). In addition to supplementing linear causation methods currently used in process risk management (e.g., HAZOP, LOPA), the application of systemic risk analysis approaches in ERM (corporate and government entities) is an intriguing opportunity that appears in need of further research (Jagoda and Wojcik, 2019; McShane, 2018).

It is common for operators and service companies to transfer and share risk to insurance companies or other non-operated partners, respectively (Sustainability Accounting Standards

Board, 2018; Wetherell and Evensen, 2016). In addition, companies typically rely on financial institutions for capital (IPIECA et al., 2020). Therefore, insurance companies, financial institutions, and non-operating partners have a unique opportunity to promote the adoption of systemic risk analysis techniques in OUOGD while defining system control structures, hazards, and constraints.

OUOGD environmental and public health risks are controlled by a complex sociotechnical system comprised of interconnected functions, not a linear chain of components. The further refinement and application of systems thinking to improve the characterization of these risks and control structures is recommended.

2.7. Summary

This chapter discusses the value of hazard assessment tools with a foundation in systems thinking. These techniques have incremental value when used throughout the OUOGD system in conjunction with standard linear causation models. Readers and practitioners should use caution when adopting new approaches to risk management and understand that these changes can have unintended consequences in complex systems. The presented general development process model and control structure have limitations based on extensive research and personal experiences. Given these limitations, in combination with their general nature, the intent and expectation are that these models will be adapted for specific applications and circumstances with critical thinking by users. The body of knowledge related to applying systemic hazard analysis techniques to OUOGD environmental and public health risks is limited, if not nonexistent. The groundwork for advancing this practice and area of study has been provided in this review. The original hierarchical development process model and control structure presented fill critical knowledge gaps, which should help accelerate research and practice. The current

opportunity for the broad adoption of sociotechnical hazard analysis approaches in the

unconventional oil and gas industry is evident. It is acknowledged that OUOGD information

gaps exist, and data limitations can increase uncertainty in a risk assessment regardless of the

approach taken (e.g., linear or systemic). However, risk-based decisions are typically made in

uncertain environments with information limitations. Existing OUOGD information limitations

should not prevent the application of the methods discussed in this chapter. The need and value

will continue to increase with the integration of new digital technologies (e.g., robotics, big data

analytics, artificial intelligence, machine learning, internet of things).

3. HYDRAULIC FRACTURING CHEMICAL DISCLOSURE AND TRANSPARENCY POLICY-LEVEL METRICS AND TRENDS [2]

3.1. Introduction

Chemical risk management is a critical aspect of public policies, industrial activities, and daily lives (Fu et al., 2019; Torres et al., 2016; Wang et al., 2020). Disclosure is a fundamental component of chemical risk management, and policymakers are struggling to balance public transparency with protecting commercial rights and innovation investments (Weil et al., 2006). The lack of consistent and understood approaches for measuring and reporting chemical withholding rates could lead to ineffective policy decisions, unproductive public concerns, research limitations, and chemical risk reduction constraints. Chemical disclosure is an essential public health and safety issue (Kinchy and Schaffer, 2018) with national economic and security implications related to the prudent development of all technologies and unconventional hydrocarbon resources in the U.S. (U.S. EIA, 2020, 2019). Hydraulic fracturing chemical disclosure policies, at federal and state levels, and analytical trends over the past decade present a unique opportunity to gain knowledge and insights that could foster greater alignment on chemical information availability in and beyond the oil and gas industry.

In general, chemical disclosure policies in the U.S. allow for the withholding of information under "trade secret," "confidential business information (CBI)," "proprietary," or other similar claims, with appropriate processes for challenging the legitimacy of these claims

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[2] The material in this chapter was co-authored by Christopher Hill, Dr. Om Yadav, and Dr. Eakalak Khan. Christopher Hill had primary responsibility for data collection and analysis. Christopher Hill was the primary developer of the conclusions that are advanced here. Christopher also drafted and revised all versions of this chapter. Dr. Om Yadav and Dr. Eakalak Khan served as advisors and proofreaders for the work conducted by Christopher Hill.

and providing workers and emergency first responders necessary information to perform their duties (Applegate, 1991; GWPC, 2021; U.S. EPA, 2020a). Despite the allowance for information withholding, chemical transparency has resulted in positive behaviors reducing chemical-related human health and environmental risks. For example, between 1988 and 1995, the U.S. EPA found an approximate 45% reduction of toxic chemicals reported in its Toxic Release Inventory (TRI) (U.S. EPA, 1997), indicating that information sharing, even when limited and imperfect, can lead to significant public health and environmental risk reductions (Jobe, 1999).

Regulators worldwide and at all levels continue to embrace disclosure, with trade secret protection, as a vital tool in chemical risk governance and reduction (GWPC, 2021; Ingre-Khans et al., 2020; U.S. EPA, 2020a). Over the past decade, during the expansion of OUOGD across the U.S., the O&G industry has endured considerable encouragement and rulemaking to increase hydraulic fracturing ingredient information accessibility (Liroff et al., 2019; U.S. DOE, 2014; Waxman et al., 2011). However, following the path of continuous improvement utilizing the FF Register, state regulations, and trade secret claims remain in doubt and debate (Fink, 2019; Trickey et al., 2020). Two primary perspectives dominate the ongoing discussion around this topic: 1) allow for an appropriate level of chemical information withholding to promote innovation and protect related research investments, and 2) require complete transparency without allowing for withholding of any chemical information. Most state O&G regulations have adopted the first perspective with the opportunity to verify trade secret claims and ensure first responders have access to necessary information (Dundon et al., 2015).

There is a lack of context, definition, understanding, and innovation in system or policy-level chemical transparency measurement techniques, leading to ambiguity and confusion

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regarding progress to date on this issue. The study presented in this chapter seeks to provide

clarity on this topic by answering the following primary research questions:

1. What metrics are most effective for measuring and monitoring hydraulic fracturing

   chemical transparency?

2. Has hydraulic fracturing chemical transparency increased over the past decade?

3. Has the system chemical disclosure form approach increased transparency and

   reduced withholding rates?

To answer these questions, first, key events, metrics, and trends in public chemical

disclosure policies are assessed, focusing on hydraulic fracturing, through a qualitative

retrospective analysis of regulations and research. Second, new metrics to improve

understanding and characterization of well-stimulation component information availability are

developed. Using existing and newly developed metrics, a retrospective quantitative analysis and

demonstrate the usefulness of these metrics is conducted. Lastly, a summary of the policy and

practical implications of this study is given. Attempts to resolve the ongoing "chemical

withholding" policy debate are not addressed; however, the context provided does inform

objective public discourse and policymaking. Chemical management, risk, and transparency are

not unique to hydraulic fracturing or the O&G industry. Learnings from the evolution of

chemical disclosure in the O&G sector over the past decade and contributions from this study

can be adapted and applied to similar challenges in other industries and the global chemical

ecosystem.

3.2. Materials and Methods

Qualitative and quantitative analyses of HF chemical transparency are combined in this

study to enrich understanding from both perspectives. The qualitative evaluation focuses on

crucial general and hydraulic fracturing chemical-specific disclosure events and research from 1947 (first hydraulically fractured well) (Gallegos and Varela, 2014) to 2019. The quantitative analysis seeks to understand trends in well stimulation chemical transparency between 2010 and 2019 using public and proprietary datasets.

3.2.1. Qualitative Analysis

The qualitative aspect of the study aims to understand vital regulatory and research context before conducting a quantitative analysis by examining state and federal oil, gas, and environmental regulatory websites for rules, reports, and research. The FF website was also an essential resource for understanding the evolution of hydraulic fracturing disclosure policies and practices. The study queried the Web of Science and Google Scholar databases for the following search terms to identify related research; 'chemical risk*,' 'chemical disclosur*,' 'chemical transparen*,' 'chemical withhold*,' 'withheld chemical*, 'hydraulic fracturing,' 'oil and gas,' 'unconventional oil,' 'unconventional gas,' 'petroleum,' 'hydrocarbon resources,' 'shale oil,' and 'shale gas.' Knowledge gained from the literature review together with the quantitative analysis are synthesized and summarized.

3.2.2. Quantitative Analysis

Figure 9 is an overview of the quantitative analysis workflow. Appendix A provides examples of acquiring, processing, and analyzing a FF chemical disclosure form for reference. The study limited the quantitative analysis scope from January 1, 2010, to December 31, 2019. The starting date coincides with a tipping point in public interest determined in the qualitative analysis and approximately one year before FF' opening (April 2011) (Groundwater Protection Council, 2021). The end date allows for a full 10-year evaluation and mitigates the risk of data quality issues arising from the timing of information availability in 2020. When appropriate, the

evaluated years were limited further for increased quality and reduced uncertainty in reported metrics. In addition to Microsoft Excel (2008 32 bit), the following data science analysis tools were utilized in the quantitative analysis; Spyder (v 4.0.1) and Python (v 3.7.6) along with Numpy (v 1.18.1), Pandas (v 1.0.1), Matplotlib (v 3.1.3), Scipy (v 1.4.1), and Seaborn (v 0.10.0) packages.
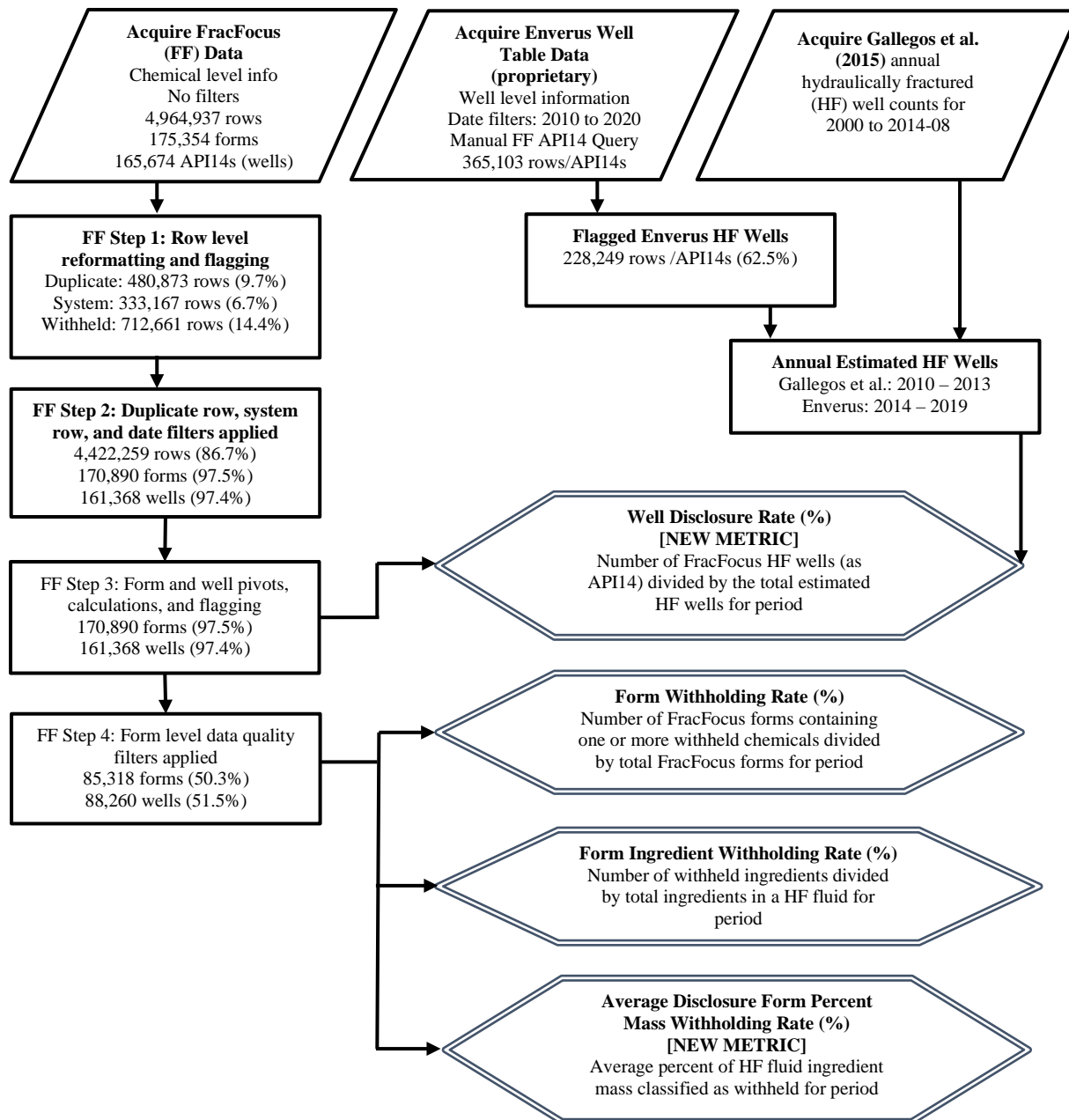
Figure 9. Quantitative data acquisition, processing, and analysis workflow.

3.2.2.1. Data Sources

Hydraulic fracturing additives, composed of one or more chemicals, serve specific and deliberate purposes primarily designed to improve well performance, mitigate risk, or both. Chemical categories include, but are not limited to, acids, biocides, breakers, stabilizers, crosslinkers, friction reducers, gels, iron controls, non-emulsifiers, pH-adjusting agents, scale inhibitors, and surfactants (GWPC, 2021). It is worth noting that the types and amounts of chemical used in a hydraulic fracturing job vary based on subsurface characteristics (e.g., pressures, temperatures), resource type (e.g., oil, gas), carrier fluid used (e.g., fresh water, recycled produced water), and other factors. Section 3.3.1 provides a more comprehensive discussion regarding the evolution of hydraulic fracturing disclosure; however, it is essential to understand that FF has become the primary repository for O&G companies to disclose hydraulic fracturing chemical information to regulatory and public stakeholders. These companies submit forms containing fracturing job information to the FF Register: company, well identifiers, well location, job dates, and ingredient (e.g., name, supplier, purpose, identifiers) information. There are two types of disclosure approaches: traditional and system. The system approach disclosure form differs from the traditional approach by decoupling additives from its chemical ingredients, as shown in Figure 10. This approach encourages O&G companies to be more transparent by protecting CBI and making it more difficult to reverse engineer proprietary blends. Examples of traditional and system approach forms are provided in Appendix A.

Traditional Approach		System Approach	
Additive 1	Chemical 1	Additive 1	
	Chemical 2	Additive 2	
	Chemical 3		Chemical 1
	Chemical 4		Chemical 2
Additive 2	Chemical 1		Chemical 3
	Chemical 2		Chemical 4
			Chemical 5
			Chemical 6

Figure 10. Quantitative data acquisition, processing, and analysis workflow.

The FF is the primary repository for hydraulic fracturing chemical disclosure form information. The dataset used in this study was obtained from the FF website on Sunday, August 23, 2020, in comma-separated values (CSV) format. This dataset has approximately 4,964,937 rows of chemical level information associated with 165,674 unique wells, identified by the 14-digit American Petroleum Institute number (API14). This information was left unchanged and unfiltered before downloading. Regarding data quality, FF has known data quality issues that are discussed in the Uncertainty and Data Quality section of this chapter (Allison, 2020; Konschnik and Dayalu, 2016; Trickey et al., 2020; U.S. EPA, 2016a). Enverus' (previously DrillingInfo) proprietary dataset (Enverus, 2021) was acquired from its desktop application by downloading wells with a spud and first treatment date between January 1, 2010, or later. The study also attempted to capture all unique FF API14s through a manual search of the Enverus database. Approximately 2,409 (1.5%) of the 165,674 FF API14s could not be identified in the Enverus desktop application after further investigation. Unidentified FF well numbers are assumed to be caused by FF API14 data quality issues. In total, 365,103 rows of well-level (identified by API14 numbers) information were obtained from Enverus.

Gallegos et al. (2015) developed an estimated annual hydraulically fractured well frequency for January 2000 through August 2014 based on an analysis of proprietary IHS data

because there was no known information source providing this information at the time. The research pulled annual hydraulically fractured well frequencies between 2000 and 2013 directly from this manuscripts' supplement materials, discarding the 2014 frequency because it was a partial year ending in August.

3.2.2.2. Data Processing

The Enverus dataset was used to produce an estimated the annual hydraulic fractured well frequency from 2014 to 2019. Enverus has eight fields related to the first treatment job (e.g., hydraulic fracturing) in its well table; start date, end date, qualifier, treatment type, vendor, stage count, total proppant, and total fluid. The analysis used the presence (i.e., not null) of two or more values in the eight treatment job fields to classify a well as hydraulic fractured. The Enverus first treatment information availability significantly increases after 2010, making this approach more appropriate for subsequent years. When comparing the developed estimation approach with the annual hydraulically fractured well estimates determined by Gallegos et al. (2015) for 2011, 2012, and 2013, the observed approximate average difference in well counts was 2%. There was a strong correlation between the Enverus estimated and FF total annual hydraulically fractured well counts between 2015 and 2019, which provided further evidence that the approach was reasonable. Not all treatment date fields in the Enverus dataset are populated; therefore, the best available date was used as the hydraulic fracturing date in the presented analysis based on the following priorities: end treatment date, start treatment date, completion date, or spud date.

FF has preserved operator reported disclosure form information, including data quality issues and limitations, as the reporting framework has matured over time. For example, although Portable Document Format (PDF) forms are available for all FF wells, the machine-readable

format (i.e., CSV) data for FF 1.0 is limited to the well header (e.g., API14, well name) information without chemical data. There have been significant improvements in data quality during the evolution of FF into its current state (3.0); however, human error has contributed to data quality issues requiring attention and care during quantitative analyses. To address these quality issues, the data before examination was process using the steps pioneered by previous researchers (Allison, 2021; Konschnik and Dayalu, 2016; Trickey et al., 2020; U.S. Envrionmental Protection Agency, 2016a) and applied data quality criteria where appropriate (See Section 3.2.2.3 Uncertainty and Data Quality).

First, the FF system, duplicate, and withheld rows were flagged. A row is classified as a system row if it contains no relevant chemical information and the Chemical Abstract Service (CAS) number or ingredient name fields contains the text strings "listed" or "system." As discussed above, O&G companies report additives and chemicals separately when using the system disclosure approach to improve chemical transparency and simultaneously protect trade secrets. This protocol results in data rows containing no chemical-level information and only additive-level information, which was removed from the dataset to calculate withholding metrics. In addition, only the first occurrence of duplicate form rows was kept for the analysis. Duplicate form rows were identified as containing all the same values for ingredient name, CAS number, percent of hydraulic fracturing fluid mass, and percent of the additive mass. FF withheld chemical rows were flagged if the CAS number field contained a "trade secret" synonym or variation (including misspellings).

A list of ninety-nine "trade secret" synonyms or variations was manually curated by reviewing unique FF CAS number values, and the full list of synonyms has been provided in the Appendix A. For reference, Trickey et al. (2020) and Konschnik and Dayalu (2016) used eighty-

two and seventy-nine "trade secret" synonyms or variations, respectively. A critical difference between the research presented in this Chapter and previous approaches, from a withholding classification perspective, is the presented analysis did not consider invalid and not available CAS numbers as withheld because these categories of data could be related to quality issues or other circumstances, not necessarily transparency driven.

Duplicate forms were recognized as having identical API14 numbers, job end dates, base water volumes, total ingredient masses, and percent hydraulic fracturing mass sums. A form or well was classified as withheld if it had one or more withheld chemical rows. The same approach for identifying system forms, using system rows identified above, and an additional criterion of the Supplier column contained the text string "Listed Above," which indicates a separation of additive and chemical information. The annual frequencies of estimated hydraulically fractured wells, FF wells, and FF withheld wells are in Figure 11. Withheld and system classifications and frequencies were limited to forms and wells with machine-readable chemical information (i.e., FF 2.0 and 3.0). Therefore, well withholding frequencies before 2014 are under reported in Figure 11. The FF job end date was used as the hydraulic fracturing date in the analysis.

Figure 11. Annual well count plot with estimated hydraulic fractured (HF) wells, FracFocus (FF) wells, FracFocus withheld (WH) wells, and FracFocus wells with quality filters (QF).

Two metrics commonly used in previous evaluations and research to measure hydraulic fracturing chemical transparency are the form withholding rate and ingredient withholding rate (Allison, 2020; Konschnik and Dayalu, 2016; Trickey et al., 2020; U.S. EPA, 2016a; Waxman et al., 2011). The form withholding rate categorizes a form as withheld if it contains one or more withheld chemicals. This metric was calculated by dividing the total number of withheld forms by the total number of disclosure forms (with machine-readable chemical information) for a given period. Although the form withholding rate is useful, it stops short of measuring broader system-level transparency changes for all fractured wells, which provides important context for stakeholders. Specifically, the scope of this metric is limited to disclosed wells and does not capture proportional changes relative to the total number of all fractured wells. The ingredient withholding rate is a more granular indicator that reports the proportion of ingredients classified as withheld relative to the total number of ingredients disclosed for a given period. This perspective relies on the binary chemical withholding classification and does not measure changes in withheld ingredients' mass proportions. In some cases, multiple chemicals can be grouped into a single FF withheld entry or row, causing inaccuracies in the chemical withholding rate. Alternative measures were investigated for assessing hydraulic fracturing transparency trends because the existing metrics did not exhibit movement relative to significant policy changes or appear to capture the full perspective.

This study defined and utilized two additional metrics in response to form and ingredient withholding rates limitations: well disclosure rate and average form percent mass withholding rate. The well disclosure rate divides the total number of wells (defined by unique API14 numbers) disclosed in FF, regardless of withholding classification, by the total estimated hydraulic fractured wells for a given period. It is necessary to calculate this metric at the well

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level because form-level frequencies are not available for fractured wells not disclosed. The average form percent mass withholding rate was calculated by summing the mass percent of withheld chemicals at a form level and averaging those values over a given year. The total percent mass of a treatment job was chosen as the preferred metric over only the additive chemical percent mass because the withholding of base fluid and proppant components is a feasible circumstance.

The transparency metrics described above were used to investigate general hydraulic fracturing disclosure annual trends between 2010 and 2019 without regard to the disclosure form approach. These performance indicators were critical for assessing if the system disclosure approach contributed to improvements in chemical information availability. This analysis provides descriptive statistics and associated plots for comparison purposes and compare means with two-sided t-tests for statistical inferences. Although some of the statistics exhibit non-normal distribution characteristics, t-testing is appropriate because of the large sample sizes.

3.2.2.3. Uncertainty and Data Quality

Uncertainties in these analyses arise from data quality, human error, biases, and estimations. Regarding the well disclosure rate, the method used for estimating the total frequency of hydraulically fractured wells relies on the best available data. The number of wells disclosed in the FF dataset does not include disclosures made outside of FF directly to the state agency per state regulations. Uncertainty from the Enverus, FF, and Gallegos et al. (2015)'s data sources is inherited. Enverus has significant resources and a vested commercial interest in maintaining a high degree of quality in its proprietary data. Gallegos et al. (2015) is a peer-reviewed source from a federal agency that implies quality information. FF has proven valuable for its regulatory intent. However, from a research perspective, it has known data quality

limitations that require attention. The data quality criteria used to mitigate these FF issues in previous research were adopted to reduce uncertainty in this study (Allison, 2021; Konschnik and Dayalu, 2016; Trickey et al., 2020; U.S. Envrionmental Protection Agency, 2016a).

FF data quality criteria and related processing do not imply regulatory compliance issues or an inability for FF to meet its currently intended regulatory purpose. The FF data used in form withholding rates, average ingredient withholding rates, and average mass percent withholding rates did not include system rows, duplicate rows, duplicate forms, multiple forms, or forms containing chemicals with null or zero percent mass values. Before calculating these performance indicators, forms with job end dates not between 2011 and 2019, total percent mass outside a 95% to 105% tolerance, and a total mass greater than the 95% high confidence interval from the FF total data population were removed. The application of the data quality criteria filters resulted in an approximate 49.7% reduction of the available FF forms for analysis, reducing the form count from 175,354 to 88,260 between 2011 and 2019. Figure 11 provides a graphical comparison of annual FF well frequencies before and after data quality filtering (QF). It was confirmed that the remaining high-quality sample data set was representative of the full FF data set by comparing approach proportions, withholding proportions, water base fluid volume means, and total ingredient mass means. Appendix A provides additional details regarding these comparisons.

3.3. Results and Discussion

3.3.1. General Hydraulic Fracturing Perspective

In general, information availability is critical for all risk assessment and decision-making processes. Although a clear definition for risk assessment data quantity and quality requirements does not typically exist, experienced risk evaluators use uncertainty to communicate how

evidence limitations impact their assessments and characterization of risk (Yokota and Thompson, 2004). A lack of information can lead to a perception of elevated risk; however, the absence of data and knowledge, or its presence, is not necessarily indicative of true risk levels. For example, the pursuit of more sustainable and "greener" chemicals (Harry et al., 2020; Shen and Somasundaran, 2019; Zimmerman et al., 2020) may lead companies to protect related research and development investments with confidentiality or trade secret claims. Regardless, real and perceived risks have led to hydraulic fracturing chemical disclosure receiving substantial attention recently (Adgate et al., 2014; Annevelink et al., 2016; Guo et al., 2020; Hill et al., 2019; Kaden and Rose, 2016; King, 2012; Ma et al., 2018; Maloney et al., 2017; McKenzie et al., 2012; NAS, 2018; Saunders et al., 2018; Torres et al., 2018, 2016; U.S. EPA, 2016a; Vengosh et al., 2014; Vidic et al., 2013).

Hydraulic fracturing has occurred in the U.S. since 1947. The technology reached broad commercialization in the 21st century, and public concerns quickly followed, reaching a tipping point in 2009. At this point, Congress investigated the process (Waxman et al., 2011) and urged the U.S. EPA to study its relationship with drinking water resources more comprehensively (U.S. EPA, 2016a). State regulators and associated national organizations (i.e., GWPC and IOGCC) charged with protecting human health and the environment while efficiently developing O&G resources embraced and led the challenge to improve O&G chemical transparency. Between 2011 and 2015, all major oil and gas-producing states adopted hydraulic fracturing chemical disclosure regulations, and, currently, 28 states have disclosure regulations in place (GWPC, 2021; Konschnik and Dayalu, 2016). Federal regulatory, public, special interest, and industry stakeholders have encouraged and influenced chemical visibility along the way, which has led to variations between states. For example, the timing of reporting (i.e., before or after work) and

type of reporting permitted (i.e., traditional, system, or both) vary on state jurisdiction.

Similarities in current regulations include requiring O&G operators to disclose fracturing job

information: company, well identifiers, well location, job dates, and ingredient (e.g., name,

supplier, purpose, identifiers) information. Other researchers have provided comprehensive

comparisons regarding the similarities, difference, and timing of state regulations (Fisk and

Good, 2019; Konschnik and Dayalu, 2016).

Struggles between state and federal regulatory primacy on chemical disclosure during

hydraulic fracturing applications have appropriately settled under state jurisdiction (BLM, 2020).

At the root of state and federal primacy discussion is the Energy Policy Act of 2005, which

excludes "the underground injection of fluids or propping agents (other than diesel fuels)

pursuant to hydraulic fracturing operations related to oil, gas, or geothermal production

activities" from the Safe Drinking Water Act (U.S. Congress, 2005). However, federal regulators

fittingly govern all chemicals in commerce, including hydraulic fracturing chemicals, and

associated decisions made appropriately at the beginning of the chemical's life cycle (*Federal

Insecticide, Fungicide, and Rodenticide Act*, 1996; U.S. EPA, 2020b). Some stakeholders have

petitioned to increase the scope of federal regulations and scrutiny over oil and gas chemicals

(Earthjustice, 2011), but no significant changes have resulted from these lobbying efforts. At the

state level, lobbying for regulatory improvements have revolved around five key issues:

disclosure repository (i.e., FF, state repository, or both), timing of disclosure (i.e., before or after

job), increased reporting to state agencies, substantiation of proprietary claims, and public

opportunity for challenging claims. California and Wyoming have been referenced as have the

most comprehensive and stringent hydraulic fracturing disclosure requirements, which can be

considered indicative of successful state advocacy efforts. However, Konschnik and Dayalu

(2016) did not observe significant variations in chemical withholding rates between states despite differences in regulations.

In 2010, it took a Congressional investigation to gather hydraulic fracturing chemical information by requesting it directly from O&G service companies (Waxman et al., 2011). It is worth noting that companies exercised their rights to withhold information from Congress based on trade secret and confidential business claims when responding to this inquiry. Congress reported that service companies used more than 2,500 additives containing approximately 750 unique chemicals between 2005 and 2009. Around 279 additives included proprietary or "trade secret" components. Between 2011 and 2016, the U.S. EPA used a portion of its multi-million dollar drinking water study budget to identify 1,039 unique hydraulic fracturing chemicals with an 11% chemical withholding rate (U.S. EPA, 2016a).

Using data obtained privately from GWPC for June through December of 2013, the Department of Energy (DOE) reported form and ingredient withholding rates of 84% and 16.7%, respectively (U.S. DOE, 2014). Konschnik and Dayalu (2016), following a similar approach for data acquisition, identified 983 unique chemical substances in the process of calculating form and ingredient withholding rates of 92.3% and 16.5%, respectively, for FF disclosures submitted through April 13, 2015. Trickey et al. (2020) analyzed 152,476 disclosure forms and 4,159,917 rows of data acquired from the FF website with treatment dates between January 1, 2011, and December 31, 2018. After discovering an 18% chemical ingredient withholding rate and similar withholding rates between traditional and system disclosure approaches (85% and 88%, respectively, for Q4 2018), Trickey et al. (2020) claimed that the FF register and system disclosure approach are ineffective at increasing chemical transparency.

FF 1.0 opened in April 2011, and enhancements to FF 2.0 occurred in 2013. This conversion provided the public access to chemical ingredients beyond the Material Safety Data Sheet (MSDS) and the inclusion of data quality control protocols. In 2016, FF transitioned to version 3.0, incorporating additional data quality controls, embracing a default system approach, and improving the user interface. FF moved beyond only providing access to PDF formatted data and started releasing Structured Query Language (SQL) and CVS formats in 2015 and 2017, respectively (GWPC, 2021).

In 2020, a stakeholder with access to a smartphone or computer connected to the internet has access to over 175,000 hydraulic fracturing chemical disclosures and almost 5 million rows of chemical data that can be download for analysis. In addition, open-source Python code is available and continually refined to make the processing and analysis of this FF information more accessible and consumable to stakeholders (Allison, 2021). FF is continuously under development with the intent of further improving public transparency in the 25 states that either require or allow disclosures in the register (GWPC, 2021).

As shown in Figure 12a, there has been a clear downward trend in the average number of total and withheld hydraulic fracturing ingredients since 2014. Figure 12b provides trends for the annual well disclosure rate, form withholding rate, and average form ingredient withholding rate. The well disclosure rate rapidly climbs from 0% to approximately 91.7% between 2010 and 2013. The metric levels off to approximately 95.5% in 2018 and 2019. Note that the method used for estimating the total frequency of hydraulic fractured wells is imperfect, and the number of wells disclosed in the FF dataset does not include disclosures made outside of FF directly to the state agency per state regulations. The well disclosure rate is helpful in mapping transparency

over time. It appears valuable in real-time during transitional policy years because it provides immediate, measurable feedback for transparency policy decisions and actions.

Between 2011 and 2019, the form withholding rate averaged 80.0%, with a range of approximately 69.9% and 85.7%. Minimal changes in the form ingredient withholding rate occurred between 2011 and 2019. The rate averaged 15.25% across this period, with a range of 10.5% and 17.0%. The average disclosure form withholding rate and ingredient withholding rates are comparable to previously reported values ranging from 84% to 92.3% and 11% to 18.5%, respectively (Konschnik and Dayalu, 2016; Trickey et al., 2020; U.S. DOE, 2014; U.S. EPA, 2016a). Disclosure form and ingredient withholding rates before 2013 are likely less reliable (under-reported) because the practice at the time was to report only MSDS information.
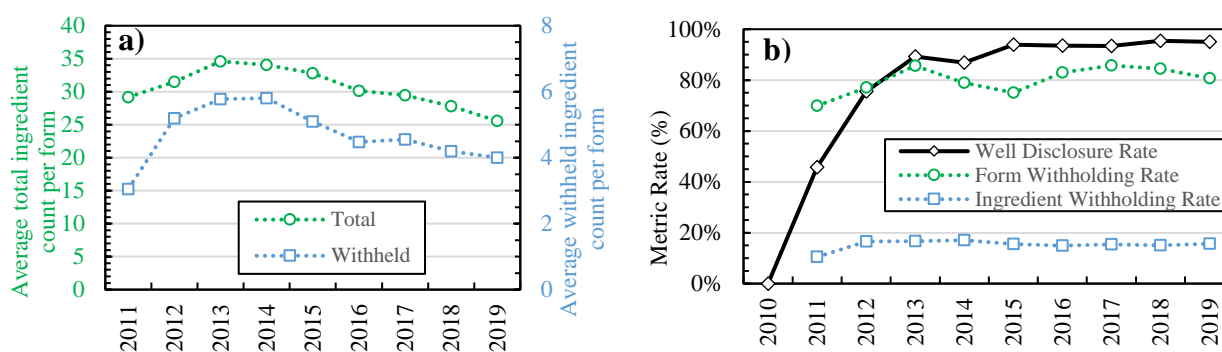
Figure 12. Annual hydraulic fracturing a) average total and withheld ingredient frequencies and b) well disclosure, form withholding, and ingredient withholding rates.

Figure 13 provides the average annual hydraulic fracturing disclosure form ingredient percent mass withholding rate with a 95% confidence interval between 2013 and 2019. The average form percent mass withholding rate trend was limited to data generated after 2013 because it required FF 2.0 or later data with machine-readable chemical data. The analysis observed a general downward trend for this metric's mean with an approximate reduction of 47.1% (0.142% to 0.075%) over the period. A linear regression of the average annual form

percent mass withholding rate yields a declining slope of 0.0082% withheld mass per year with a coefficient of determination (R^2) of approximately 0.76. Assuming this rate is sustained, one could presume that the mass withholding rate would continue approaching zero within the next decade. State specific annual ingredient percent mass withholding rates are provided in Appendix A. A comprehensive investigation of the relatively higher standard deviation seen in 2016 and 2017 was not conducted; however, it is hypothesized that the potential causes of this increase in variability are the FF 3.0 conversion in 2016 and volatile market conditions within this timeframe. The impact of market conditions on hydraulic fracturing activity is apparent with an approximate 67.1% drop in hydraulic fractured well frequency between 2014 and 2016 caused by lower commodity prices.
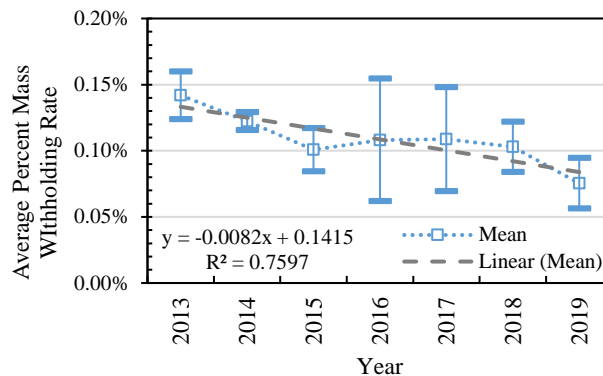
Figure 13. Annual hydraulic fracturing average percent mass withholding rate with 95% confidence intervals and a linear trend.

3.3.2. Disclosure Approach Perspective

The default FF disclosure approach was transitioned to the system approach in 2016 after encouragement from the U.S. DOE with an expectation that it would increase chemical transparency (U.S. DOE, 2014). Therefore, this study focused its evaluation on the differences between the traditional and system approaches from 2016 to 2019. The system approach became the dominant disclosure approach in 2017 and has maintained its majority to date, with

approximately 64.3% of all disclosure forms in 2019 (Figure 14a). The application of quality

criteria reduced the available traditional and system form data for analysis by 22.3% and 25.2%,

respectively. The similarities between the two approaches was confirmed using the 2019 mean

total base water volume as a non-withholding test statistic (p-value of 0.738).
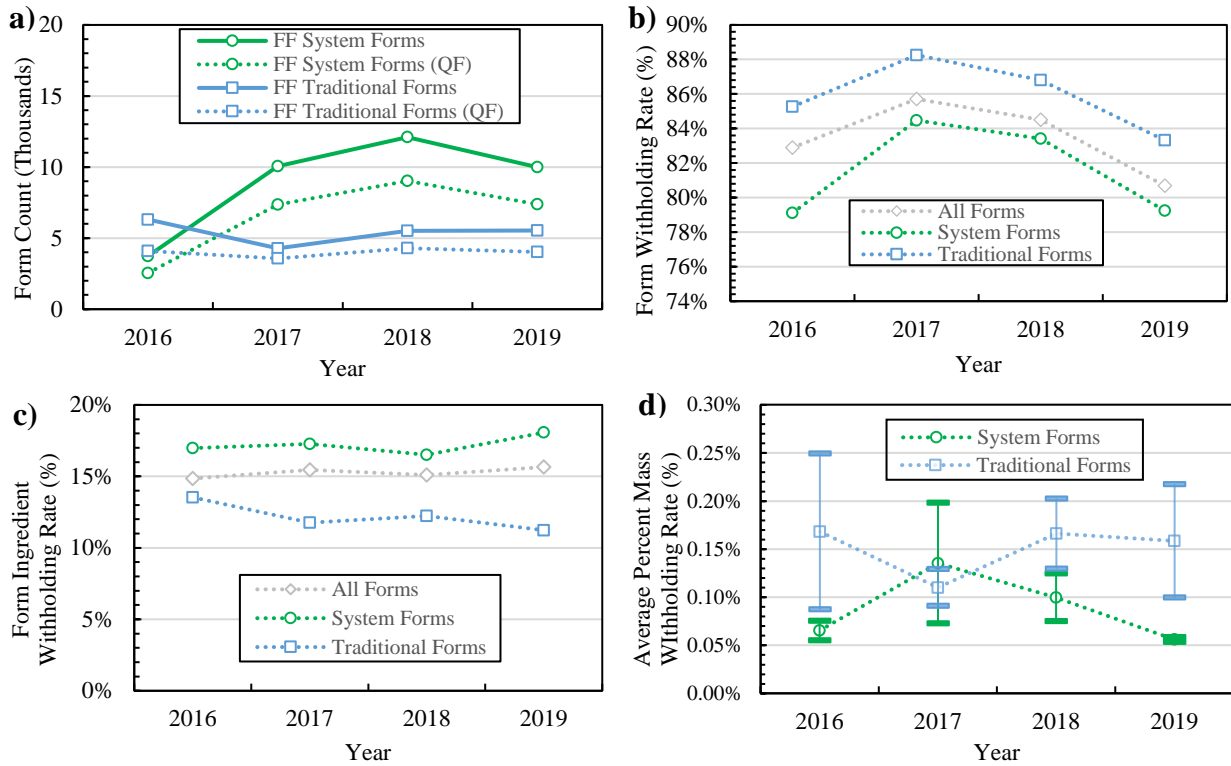
Figure 14. Annual hydraulic fracturing transparency trends between 2016 and 2019 by disclosure approach. a) Total FracFocus (FF) and quality filtered (QF) form frequencies, b) Form withholding rates, c) Form ingredient withholding rates, and d) Average form percent mass withholding rate with 95% confidence interval.

There is a 2.2% decrease in the overall form withholding rate when comparing 2016 and

2019. Although a clear trend does not appear to exist for this metric, the system approach annual

form withholding rate is consistently lower than the traditional approach rate, indicating an

apparent reducing impact on the overall rate (Figure 14b). The ingredient withholding rates for

both approaches have minimal variability over the evaluation period. The system approach

annual ingredient withholding rate is consistently more than the traditional approach and,

therefore, has an increasing impact on the overall rate (Figure 14c). The system approach improves the form withholding rate and worsens the ingredient withholding rate, which are conflicting chemical transparency signals. This situation helps illustrate the limitation and challenges associated with only using these two existing metrics and the need for additional perspectives.

The form percent mass withholding rate above helps stakeholders understand general trends in hydraulic fracturing chemical transparency. Figure 14d illustrates the application of this metric to the system and traditional disclosure approaches. Between 2016 and 2019, the system and traditional approach percent mass withholding rates averaged 0.078% (95%CI: 0.060% - 0.095%) and 0.130% (95%CI: 0.105% - 0.156%) with medians of 0.022% and 0.023%, respectively. A p-value of 0.0008 was calculated when comparing mean values, indicating a significant difference (p-value < 0.01) in mean values. This difference is even more substantial in 2019 where the system and traditional approach have means of 0.044% (95%CI: 0.042% - 0.047%) and 0.132% (95%CI: 0.078% - 0.186%), respectively. The system approach percent mass withheld is 66.3% less than the traditional approach in 2019, and a p-value of 1.74×10^{-5} validates the significance of the difference in mean values. In 2017, an anomaly was observed where the system disclosure mean (0.114%) was greater than the traditional disclosure mean value (0.097%). A comparison of these means yielded a p-value of 0.68, indicating no significant difference between the approaches in 2017. It is hypothesized that the cause of this anomaly was change management challenges during the simultaneous adoption FF 3.0 and ramp-up of O&G activity levels within this timeframe.

Two out of three transparency indicators lead stakeholders to believe that embracing the system approach increased chemical transparency between 2016 and 2019. The ingredient

withholding rate signals a chemical withholding rate increase for system disclosures. However, there is a potential for chemical grouping during reporting and subsequent errors in the ingredient withholding rate calculation. For this reason, it is believed that the percent mass withholding rate is a preferred metric for assessing trends in transparency after appropriate data quality criteria are applied. The grouping of chemicals should not significantly impact the percent mass withholding rate leading to more reliable reporting and communications. Also, it is worth acknowledging that O&G companies have a choice between approach options for each disclosure. This study did not investigate this scenario or situation; however, a company trying to protect its trade secrets and maximize transparency would likely choose the system approach when using proprietary chemicals. Furthermore, that same company may choose to use the traditional approach when not using proprietary chemicals. The impact of this choice on transparency metrics merits acknowledgment and consideration during policy discourse.

3.3.3. Holistic Perspective

From a holistic chemical perspective, there are over 350,000 chemicals and mixtures worldwide in chemical inventories, and approximately 50,000 and 70,000 of these chemicals are classified as confidential or ambiguously described, respectively (Wang et al., 2020). As of June 2020, the Toxic Substance Control Act (TSCA) Chemical Substance Inventory contains over 86,000 chemicals; approximately 41,500 are active (or reported in commerce), of which 8,140 are classified as confidential business information and withheld from the public (U.S. Envrionmental Protection Agency, 2021). In 2018, the TRI National Analysis indicated that 32.1 billion pounds of toxic production-related waste was managed, and 3.8 billion pounds was disposed or released at over 21,500 covered facilities across the United States (U.S. EPA, 2020c). Federal "right to know" reporting regulations are limited in terms of chemical and

facility scope. For example, there are only 788 chemicals on the TRI and facilities not within specific industries (e.g., manufacturing, mining, electric power generation), having ten or more full-time equivalent employees, or managing TRI covered chemicals above an annual threshold are not included in reporting. Despite these limitations, the TRI Program, founded on transparency, is claimed to be an "accidental success story" and has outperformed all other U.S. EPA command-and-control environmental regulations (Fung and O'Rourke, 2000).

Although hydraulic fracturing has been utilized for over half a century, recent changes in the process, frequency, and proximity to populated areas have motivated public, regulatory, academic, and industry stakeholders to increase efforts to understand and mitigate associated environmental and human health risks (State Review of Oil & Natural Gas Environmental Regulations, 2019; Torres et al., 2016; U.S. EPA, 2020b; Waxman et al., 2011) Chemical transparency and characterization are significant aspects of these risk mitigation campaigns (National Research Council, 1996), and valuable context arises from comparing the amount and proportion of hydraulic fracturing chemical confidential claims with those found globally across all industries. Figure 15 synthesizes and summarizes approximate chemical and withholding rates worldwide, in the TSCA inventory, or associated with hydraulic fracturing. The 2019 hydraulic fracturing chemical withholding rate of 15.7% determined in this analysis is comparable to the worldwide confidentiality claim rate (14.2%) and 2020 TSCA active chemical confidential business information claim rate (19.7%). Therefore, current hydraulic fracturing chemical withholding rates do not appear significantly different from those found across all industries in the U.S. or worldwide.

~14.2% of Chemicals Worldwide Claimed Confidential (All Industries)

350,000 Chemicals Registered Worldwide

70,000 Ambiguously Described

50,000 Claimed Confidential

~19.7% of TSCA Active Chemicals Claimed CBI (All Industries)

41,500 Active TSCA Chemicals

8,140 Confidential TSCA Chemicals

650 TRI chemicals reported annually at covered facilities

~15.7% of HF Chemicals are Withheld per Form

1,076 HF unique chemicals reported

169 Estimated HF unique chemicals withheld (2019)

Figure 15. An approximate number of unique chemicals and withholding rates from worldwide, TSCA, and U.S. hydraulic fracturing perspectives. Bubble sizes are representative of chemical frequencies. (U.S. EPA, 2021; Wang et al., 2020; Yost et al., 2016a)

3.4. Policy and Practice Implications, and Summary

Transparency is the starting point for risk-based decision making. Control structures can adapt quickly to accommodate changes in stakeholder expectations, as was seen over the past decade in the O&G industry. A significant amount of public, research, and regulatory activity focusing on hydraulic fracturing chemical disclosures and risks erupted after over 60 years of utilizing the technology. Transparency performance indicators and associated rationale were not clearly defined before significant policy changes began to address stakeholder concerns. All parties were left anchored to a few metrics that do not provide the full picture or context. Significant improvements in hydraulic fracturing disclosure rules and data availability have presented the opportunity to study and develop additional value accretive performance indicators and conduct retrospective policy analyses. Regarding the primary research questions, the analysis presented above indicates that the availability of hydraulic fracturing data has

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significantly increased, and current hydraulic withholding rates are comparable to broader

chemical withholding rates in the U.S. and worldwide across all industries. The performance

indicators developed and used in this study fill a gap in measuring hydraulic fracturing chemical

disclosure policy performance and show that the system disclosure approach has contributed to

improvements in transparency.

"Transparency systems always begin as imperfect compromises and must be adapted to

keep pace with changing markets, technology, and political priorities" (Fung et al., 2007). This

study suggests that quick and iterative state regulatory and data management policies laid the

foundation for continuous transparency advancements. All stakeholders (i.e., public, state,

federal, academic, special interest, researchers, and industry) contributed to this rapid increase in

hydraulic fracturing chemical transparency. There should be steady improvements in chemical

visibility, relying primarily on existing state O&G policies and FF information technology

infrastructure. Shifting away from this foundation has the potential to slow or halt progress. State

regulators and FF should consider incorporating performance indicators in stakeholder

communication tools and reports. The raw data is useful, but the summary system-level

indicators would enhance the overall understanding of industry trends in chemical transparency.

FF could also adopt additional data validation protocols based on the data quality steps used in

research to reduce data processing requirements. Public and regulatory stakeholders would

benefit from defining policy transparency performance indicators in advance of rulemaking and

applying these metrics for cross-industry comparisons. This study did not identify another

chemical disclosure framework across any industry that provided timely and convenient

application-specific chemical information comparable to FF.

From a practice perspective, O&G operators and service companies should consider incorporating system-level metrics into corporate public reporting (GRI Global Sustainability Standards Board, 2020; International Petroleum Industry Environmental Conservation Association et al., 2020) and continuously striving for improvements in chemical transparency. These entities should consider applying hydraulic fracturing chemical disclosure knowledge to other aspects of their operations. Early data engineering, science, analytics, and reporting investments can lead to effective performance management tools and prove valuable in changing political environments. These recommendations are not limited to the oil and gas industry and should be evaluated across all applicable industries when appropriate.

All humans on this earth have a vested interest in prudent chemical management and associated human health and environmental risk-based decisions. The desire for increases in information quantity and quality to assist risk managers and decision-makers is a common and admirable goal. It is important that data limitations are not used as excuses when critical, system, and innovative thinking can open novel perspectives and analysis techniques that help us meet immediate decision-making objectives and achieve progress (National Research Council, 1996; U.S. DOE, 2020).

4. TEMPORAL AND COMPARATIVE ANALYSES OF HYDRAULIC FRACTURING CHEMICALS WITH THE POTENTIAL TO IMPACT DRINKING WATER RESOURCES [3]

4.1. Introduction

The world has 442.1 billion tons of unconventional crude oil and 227 trillion cubic meters of unconventional natural gas reserves (Wang et al., 2016). Without HF technology and chemicals, most of these natural energy resources would be inaccessible and the associated economic implications could not be realized. However, the benefits associated with HF technology must be evaluated holistically in the context of risks, including known hazards to drinking water resources (U.S. EPA, 2016a; Vengosh et al., 2013). The U.S. was the first country to see broad commercialization and use of this disruptive technology, which triggered public concerns and government action. The U.S. HF experience offers learnings for other nations, which is why it was selected for this case study's scope.

The U.S. Congress identified shortcomings in available HF additive information in 2010 and subsequently conducted a preliminary investigation to identify chemicals used in the process (Waxman et al., 2011). An immediate flurry of valuable HF chemical research and regulatory efforts followed this preliminary government inquiry, but there is a need to reexamine the system's current state and dynamics to understand trends in systemic environmental and public health risks (as discussed in Chapter 3). In addition, this area of study provides a unique

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[3] The material in this chapter was co-authored by Christopher Hill, Dr. Om Yadav, and Dr. Eakalak Khan. Christopher Hill had primary responsibility for data collection and analysis. Christopher Hill was the primary developer of the conclusions that are advanced here. Christopher also drafted and revised all versions of this chapter. Dr. Om Yadav and Dr. Eakalak Khan served as advisors and proofreaders for the work conducted by Christopher Hill.

opportunity to further analyze the power of transparency as a system or regulatory control tool (Jobe, 1999; U.S. EPA, 1997).

In 2016, based on urging from Congress, the U.S. EPA released its valuable and extensive study regarding the potential impacts of HF on drinking water resources (U.S. EPA, 2016a). A key aspect of this study was determining the identity, frequency, scope, and information availability of chemicals intentionally added to HF fluids for onshore unconventional oil and gas well stimulation. The EPA identified 1,084 unique chemicals used in hydraulic fracturing fluids by analyzing information and references available, including disclosures from FF 1.0 for over 38,000 production wells hydraulically fractured between January 2011 and February 2013. EPA's valuable study, along with list of unique HF chemicals, has been and continues to be leveraged by many researchers (Chen et al., 2021; Elliott et al., 2017; Xu et al., 2019) and remains the primary source of chemicals associated HF in EPA's CompTox database. Therefore, EPA's study and list of chemicals as a reference point throughout this study. Konschnik and Dayalu (2016) expanded EPA's list with 263 additional chemicals, and Wetherbee et al. (2020) built a web-based tool specifically for identifying HF chemical that targets certain hormonal pathways. However, an updated and accessible list of unique HF chemicals does not exist, and systemic trends in chemical variety and selection have not been conducted. Advancements in FF (i.e., HF disclosure data), data science tools, contextual chemical research/inventories, and chemical information availability provided an opportunity and efficient means to address this research gap. In doing so, the accessibility of systemic HF chemical information and context for stakeholders are improved and progress toward increased transparency and safer chemical selection is fostered.

In general, broad U.S. regulatory requirements limiting the use of specific chemicals or associated chemical characteristics for HF in key hydrocarbon producing states do not exist, beyond those imposed by existing federal chemicals laws (e.g., TSCA). Disclosure has been the primary regulatory focus of State O&G Agencies, with primacy over OUOGD (Fisk and Good, 2019; Ralston and Kalmbach, 2018; State Review of Oil & Natural Gas Environmental Regulations, 2019). Industry and academic tools have been developed to assess the sustainability or hazard level of HF chemicals, additives, and fluid mixtures (Hu et al., 2019, 2018; Hurley et al., 2016; Shen and Somasundaran, 2019; Xu et al., 2019; Yost et al., 2017). The use of these voluntary tools is perceived to help the OUOGD systems reach a lower level of chemical risk to public health and the environment. However, a systemic evaluation of the hazard levels has been impeded by HF chemical information availability and quality. This study takes the first steps to remove these actual and perceived data-related research barriers and open the door for valuable exploration in the area of systemic risk to drinking water resources.

Building on the work presented in Chapter 3 which focused on measuring and trending HF chemical transparency, the primary research objectives for this study are to identify HF chemicals currently (as of 2020) in use and disclosed in the U.S. to determine how they have changed over time (since 2014). Secondary, the study investigates the impact of production type (i.e., oil and gas) and state jurisdiction on HF chemical variety. Lastly, HF chemicals identified are compared with chemical lists from other researchers (including EPA's 2016 HF study), EPA's Safer Chemical Ingredient List (SCIL), and substances suspected in contact with (unrelated to HF) drinking water, food, and cosmetics published by other researchers and domestic and international environmental agencies. Addressing these objectives required significant effort to clean and process over 5 million rows of U.S. FF data and synthesize other

diverse data sources (e.g., public chemical databases, industry proprietary databases). This work

provides a repeatable FF data processing approach that synthesizes and improves FF data

processing best practices used in research to date. In addition, for those less interested in data

processing, the deliverables spare stakeholders these laborious efforts and provide useable

resources to investigate impacts to drinking water resources potential caused by HF or pursue

other research ventures related to HF chemicals.

4.2. Material and Methods

4.2.1. Data Sources

This study utilizes and synthesizes several diverse data sets from regulatory, industry, and

academic sources. The primary source of information used is the U.S. FF database (GWPC,

2021), which is the main U.S. HF disclosure platform developed by the GWPC and IOGCC with

funding from the U.S. DOE. Oil and gas companies submit disclosure forms containing HF job

information, like company, well identifiers, well location, job dates, additives, and chemical

ingredients, to the FF database. As discussed in Chapter 3, this information is accessible to the

public in CSV, SQL, and PDF. The dataset used in this study was accessed April 4th, 2021 and

limited to HF jobs ending between 2014 and 2020. The temporal constraints used were

influenced by EPA's previous research, which captured 2013 activity and the FF 2.0 transition in

2013. In addition, the 2014 boundary offers more comparable, consistent, and quality data.

The FF information was enriched by merging it with proprietary Enverus data (Enverus,

2021). Specifically, the API number was used as a unique identifier to associate a production

type (i.e., oil or gas), validated state names, and hydrocarbon play/basin to each disclosure in FF.

In addition, an available open-source FF python project developed by others (Allison, 2021) was

used as a quality verification for the developed cleansing process outputs.

The EPA's 2016 HF study chemical inventory (U.S. EPA, 2016a), TSCA Chemical Inventory (U.S. EPA, 2021), European Chemical Agency (ECHA) Chemical Inventory (ECHA, 2021), and PubChem database (National Library of Medicine, 2021) were used to match valid Chemical Abstract Service numbers (CASN) and chemical names to HF ingredients found in FF. This work utilized EPA's CompTox Chemical Database to gather available HF chemical information, cross-reference identified HF chemical list with previously reported HF chemicals, and compared identified HF chemicals with known or suspected drinking water, food, and cosmetic additives and contaminants. Table 1 is a catalog of CompTox lists used with corresponding descriptions, number of chemicals, and the date last updated.

Table 1. CompTox lists with descriptions, chemical counts, and upload dates.
(U.S. EPA, 2020)

Identifier	Descriptions	Chemicals Count	Updated
EPAHFR	Chemicals associated with hydraulic fracturing, including found in produced water, from 2005-2013, as reported in EPA's HF Study. (U.S. EPA, 2016a)	1640	2018-01-29
EPAHFRTABLE2	Chemicals found in EPA's HF Study Table H-2, which included chemicals reported to be used in hydraulic fracturing fluids from 2005-2013. (U.S. EPA, 2016a)	1082	2018-11-16
FRACFOCUS	Chemicals associated to the FracFocus chemical registry in CompTox.	40	2019-11-16
SCILFULL	EPA's Safer Chemical Ingredients List (SCIL) 2019	965	2019-11-16
CCL 4	The Contaminant Candidate List (CCL) is a list of contaminants that are known or anticipated to occur in public water systems and are not currently subject to EPA drinking water regulations. (U.S. EPA, 2016b)	96	2017-12-28
EXTRACTPIPES	Chemicals from the article 'Characterization of Leachable Chemical Substances from Common Drinking Water Piping Materials' (Pizzurro et al., 2018)	151	2019-11-16
FDAFOODSUBS	Substances Added to Food inventory previously known as Everything Added to Foods in the United States.	3116	2020-10-28
FOODCONTACTSDB	A chemical database created by the Food Packaging Forum Foundation providing an overview of intentionally used food contact chemicals. (Groh et al., 2020)	9368	2021-03-22
EUCOSMETICS	A combined inventory of ingredients in cosmetic products (2000, SCCNFP/0389/00 Final) and revised inventory (2006, Decision 2006/257/EC), prepared for NORMAN by P. von der Ohe (UBA) and R. Aalizadeh (Uni. Athens).	2878	2017-07-14

4.2.2. Data Analysis Tools

In addition to Microsoft Excel (365 v 2103 32 bit), the following data science tools were utilized in the analysis; Anaconda Navigator (v 1.9.12), Spyder (v 4.0.1) and Python (v 3.7.6) along with Numpy (v 1.18.1), Pandas (v 1.0.1), FuzzyWuzzy (v 0.18.0), and python-Levenshtein (v 0.12.2) packages. Numpy and Pandas packages were used for data navigation and analysis. The FuzzyWuzzy and python-Levenshtein packages relying on simple ratio Levenshtein linguistics distance calculations were used to match FF CASN and ingredient names strings with valid CASN found in the EPA's HF study, TSCA, or EC chemical inventories.

4.2.3. Data Processing and Analysis Workflow

FF data used in the analysis was filtered to disclosures between 2014 and 2020 and cleansed by removing duplicate rows, system rows, and duplicate forms. The cleansing, withheld row flagging, and Enverus merging steps are defined in detail in Chapter 3. The FF "CAS Number" and "Ingredient Name" fields were concatenated and used this new field as a unique identifier. For each unique "CAS Number" and "Ingredient Name" combination, a cleansed "CAS Number" (spaces and special characters removed) was first compared with EPA's 2016 HF chemical list CASNs using the FuzzyWuzzy extractOne method. If an EPA HF chemical match was not identified, the FF "Ingredient Name" was compared with the EPA's HF chemical ingredient names and FF "CAS Number" with a combined list of TSCA and EC inventory CASN. A simple ratio match score of 95 (out of 100) was the threshold for defining an automated resolved CASN match. All automated "best match" CASN results were manually reviewed and curated where appropriate.

Each unique "CAS Number" and "Ingredient Name" combination was classified as "Unresolved" (i.e., CASN unidentifiable), "Withheld" (i.e., proprietary and intentionally

withheld), or "Resolved" (i.e., "best match" CASN identifiable). FF-open (Allison, 2021) "best guess" CASN were associated with the correct FF rows using the concatenated "CAS Number" and "Ingredient Name" fields. Enverus well production type, state, and play/basin were merged to FF data using the API number as the unique identifier. The resolved CASN was used to query EPA's CompTox database for chemical information and compare HF and reference drinking water, food, and cosmetic chemical lists. Figure 16 summarizes the data processing and analysis workflow.
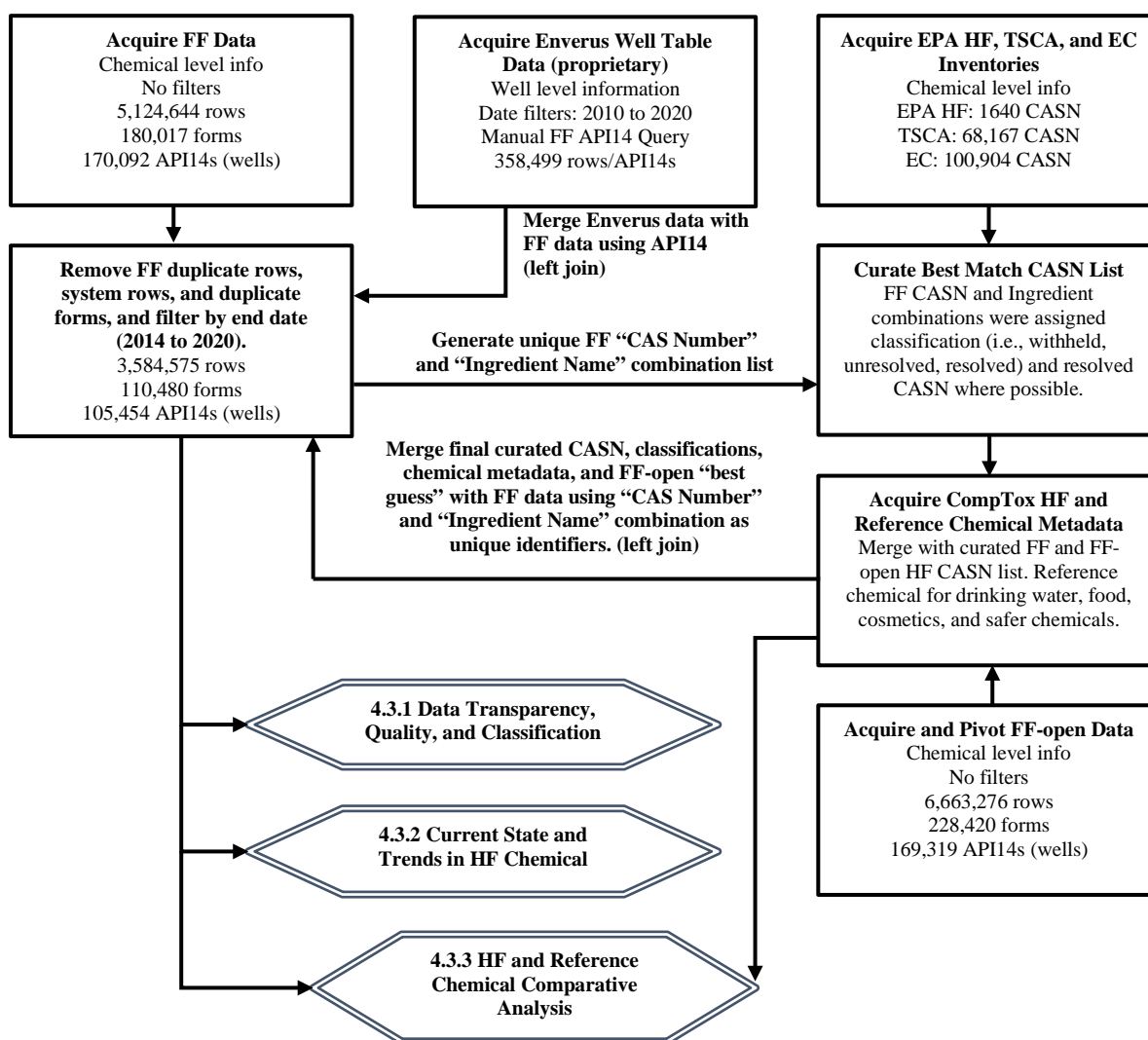
Figure 16. Data processing and analysis workflow.

4.2.4. Uncertainty and Data Quality

As is common in all research, data quality, human error, biases, and estimations approaches have undoubtedly generated uncertainties in the analyses provided. Uncertainty and data quality was inherited from all data sources used; primarily FF, Enverus, and EPA CompTox. However, care was taken to utilize high-quality, peer-reviewed governmental and proprietary datasets as described above. Throughout this study, independent research is used to ensure the presented analysis is comparable to previous work and critical assumptions and uncertainties are provided.

4.3. Results and Discussion

4.3.1. Data Transparency, Quality, and Classification

The primary focus of this section is to provide an overview of data transparency, quality, and classification from a FF chemical row perspective. Figure 17 summarizes the percent of total and "Resolved" processed FF rows classified (i.e., "Resolved," "Withheld," and "Unresolved) and subclassified (i.e., "HF CASN Match," "HF Name Match," "Inventory CASN Match," "Curated Match," or "Curated Match – Override"), respectively. The term "curated" implies a manual process. A manual "override" of automated matching occurred in 0.17% of the FF rows. A majority (83.52%) of the FF ingredient rows were "Resolved" with validated CASNs. The automated matching of the FF "CAS Number" field with an EPA's HF or TSCA/EC inventory chemical CASN was effective in determining the "best match" for 96.6% of the processed FF rows. Manual curation, including some overrides of automated matching, encompassed 1.14% of the matched rows. The analysis compared the FF CASN "best match" with the FF-open project "best guess" and found 99.6% similarity in CASN for overlapping non-withheld FF rows.
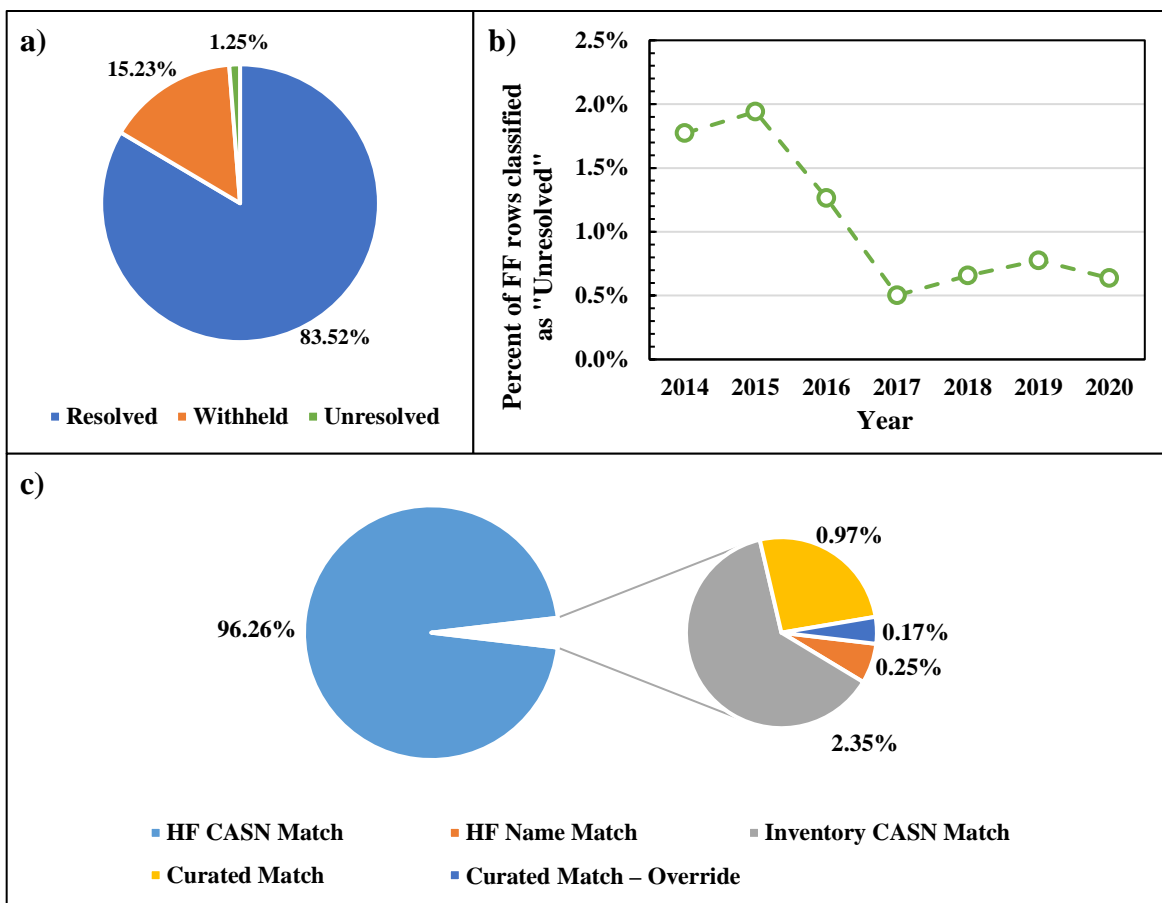
Figure 17. a) Total percent of processed FF rows classified as "Unresolved," "Withheld," or "Resolved," b) annual percent of processed FF rows classified as "Unresolved," and c) total percent of "Resolved" FF rows subclassified as "HF CASN Match," "HF Name Match," "Inventory CASN Match," "Curated Match," or "Curated Match – Override."

Approximately 15.23% of the processed FF rows were classified as "Withheld" between 2014 and 2020, with an annual range of 14.13% to 16.12%. These results are comparable with average disclosure ingredient withholding rates previously reported values ranging from 11% to 18.5%, including Chapter 3 (Hill et al., 2021b; Konschnik and Dayalu, 2016; Trickey et al., 2020; US Department of Energy, 2014; U.S. EPA, 2016a). In addition, the HF chemical withholding rates are similar to TSCA (19.7%) and global (14.2%) confidential claim rates across all industries (U.S. EPA, 2016a; Wang et al., 2020). The analysis presented in Chapter 3

observed the average percent of HF fluid mass withheld on chemical disclosure forms decreased ~46.8% between 2013 and 2019.

"Unresolved" and "Withheld" chemical rows contribute to uncertainty in research and present limitations for all stakeholders in their pursuit of systemic research. The percent of "Unresolved" FF rows is an indicator of data quality. Between 2014 and 2020, approximately 1.25% of the processed FF rows were classified as "Unresolved." However, a significant reduction in this metric from a high of 1.94% in 2015 to 0.64% in 2020 was observed. Reflecting on the step-change in data quality in 2016 and 2017, this study investigated FF system historical events to determine potential causes for this improvement. Since FF opened in April 2011, there have been two significant enhancements to the platform. In 2013 and 2016, data accessibility and quality advancements were incorporated into the register. Figure 17b clearly shows that the 2016 upgrades positively impacted the stakeholder's ability to extract usable CASN and chemicals names from the system.

The overall quality of valid CASN matching to FF ingredient rows is comparable with other research and adequate for systemic analysis of HF chemical trends. The research methodology and supporting materials provided enhance data accessibility for stakeholders and researchers, addressing claims that more HF chemical data is needed to better understand risks to drinking water resources caused by HF (Avidan et al., 2019; Shrestha et al., 2017). However, there remains an opportunity to improve and automate processing steps and conduct additional research to increase CASN source quality, matching, and enrich accuracy. It is believed that the best solution to enhance data quality would be for oil and gas operators and service companies to ensure accurate information on disclosure forms and FF to incorporate additional data validation steps into the register. Increased transparency and quality would positively impact policy

decision-making, and further enhancement in stakeholder's ability to analyze the wealth of existing data can contribute to their participating in policy decision-making processes.

4.3.2. Unique HF Chemical Trends

With the "resolved" CASN FF rows discussed above, the current state and trends in unique HF chemicals disclosure are explored. The selection of HF chemicals used in OUOGD is a product of complex, multi-variable decision-making. This study takes the first step necessary to understand the variety and changes in HF chemicals impacting system risk and behavior. The unique HF chemicals identified are compared with those chemicals reported in EPA's 2016 study. In this section, the analysis contrasts the HF chemicals with EPA's SCIL to determine if there are indications that the OUOGD system is trending toward fewer and safer chemicals. It is acknowledged that the EPA SCIL comparison is preliminary, limited, and inconclusive. However, the approach is a helpful initial scoping step toward more sophisticated, comprehensive, and conclusive research.

Based on the analysis summarized in Figure 18, a total of 1,244 unique HF chemicals were identified and disclosed between 2014 and 2020. Including all chemicals reported in EPA's 2016 study, the total count of disclosed unique HF chemicals rises to 1,325. Approximately 62.4% (776) of the 1,244 HF chemicals identified in this study were reported by the EPA; approximately 37.6% (468) were not. However, when evaluated on an annual average basis, approximately 75.7% of the unique HF chemicals identified in this study were included in EPA's 2016 HF chemical list. Seventy-two (of the 1,244) chemicals were consistently observed in 10% or more of the U.S. FF disclosure forms, which is greater than the 35 (of 1084) chemicals identified by EPA for this criterion. The range of chemical differences could be associated with various targeted product types or plays (or basins) targeted (See sections 4.3.2.1. Production

Type Analysis and 4.3.2.2. State Analysis) for each study period. For reference, early modern U.S. OUOGD focused on natural gas. However, oil has recently become the predominant hydrocarbon targeted in development (Yergin, 2020).
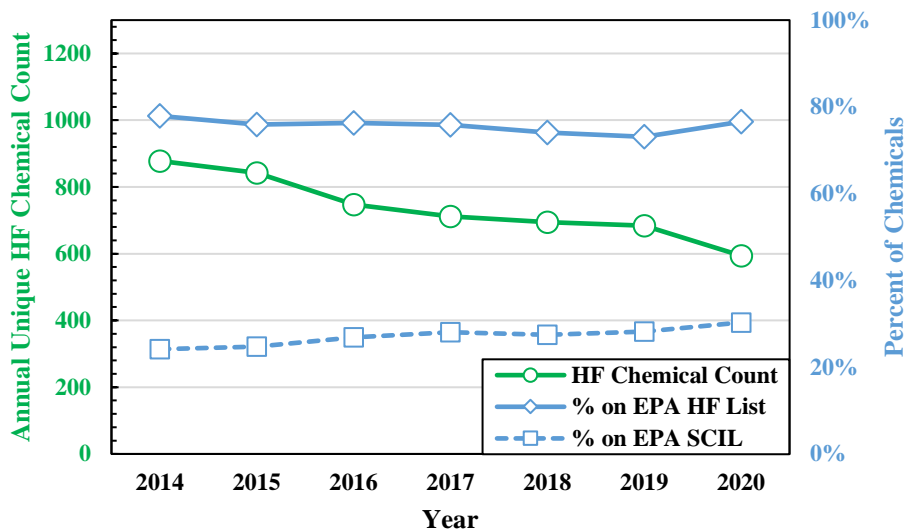
Figure 18. Annual unique HF chemical count trends with percent previously reported as HF chemicals in EPA's 2016 HF study and percent classified as Safer Chemical Ingredients (i.e., green circle, green half-circle, or yellow triangle) by the EPA.

A 32.3% (878 to 594) reduction in the number of unique HF chemicals was observed between 2014 and 2020. The root cause of this significant reduction in HF chemical variety is unknown and requires additional investigation. It is hypothesized that knowledge, economics, and social pressure (regarding risk and sustainability) have been influencing factors. An examination of the effect of production type, regulatory jurisdiction, and play/basin variety on HF chemicals is provided in section 4.3.2.1 Production Type Analysis and 4.3.2.2 State Analysis below.

EPA's Safer Chemical Ingredients List is a valuable resource for all industries and businesses striving to select safer products for the environment and public health. The EPA categorizes chemicals as "verified to be of low concern based on experimental and modeled

data" (green circle), "expected to be of low concern based on experimental and modeled data" (green half-circle), "best-in-class chemical and among the safest available for a particular function" (yellow triangle), and "not be acceptable for use in products that are candidates for the Safer Choice label" (grey square). The unique HF chemicals identified between 2014 and 2020 contained no chemicals labeled "grey square." Figure 18 illustrates the percentage of HF chemicals in the "green circle," "green half-circle," or "yellow triangle" groups. Approximately 21.6% (269) of the 1,244 HF chemicals are within these favorable SCIL categories. There is a slightly increasing trend from 24.1% in 2014 to 30.3% in 2020, indicating a potential transition toward safer chemicals or away from more hazardous chemicals, which is an opportunity for further investigation.

4.3.2.1. Production Type Analysis

To determine if macro industry and economic trends significantly influenced the observed reduction in annual unique HF chemicals between 2014 and 2020, the data from a production type (i.e., oil or gas) perspective was analyzed. Production type metadata is not included in FF. However, recall the FF chemical data was merged with Enverus proprietary information using API numbers, which allowed the association of production type with chemical level information. Some FF disclosures and chemicals were not included in the following analysis because FF and Enverus API numbers did not match or API number was associated with an Enverus production type that was not oil or gas.

The production type analysis is summarized in Figure 19. Most of the chemicals identified were used in both oil and gas wells. However, specific ingredients are unique to each product type. Oil wells consistently use more unique chemicals for well stimulation than gas wells. This finding is expected because oil hydrocarbon molecules are more complex relative to

natural gas. Fracturing tight oil formations requires adding chemicals to address potential

production and integrity issues (e.g., paraffin) specific to this production type.
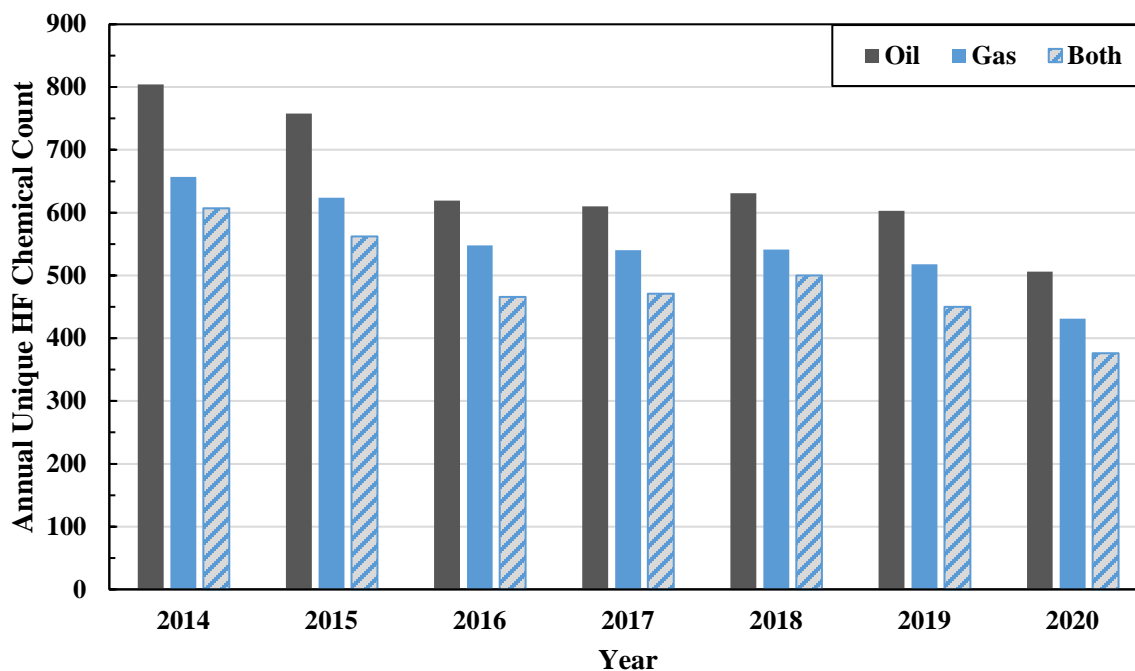
Figure 19. Unique HF chemical count annual trends by production type.

Both production types have seen a reduction in HF chemical variety between 2014 and

2020. Oil-related chemicals dropped approximately 37.1% (804 to 506). Gas-related chemicals

were reduced by 34.4% (657 to 431) over the same period. Based on this analysis, the system

factors (e.g., knowledge, economics, social pressure) influencing the range of HF chemicals in

use appears to be impacting both oil and gas product type wells similarly, and macro business

and economic dynamics associated with targeted well production types are not the root cause of

the reduction in chemicals.

4.3.2.2. State Analysis

Differences in regulatory jurisdiction can influence system behavior. Since states have

primacy over most OUOGD activities, the current condition and trends in HF chemical diversity

among states was explored. The eight states with the most FF HF chemical disclosure activity between 2014 and 2020 were selected as representative for this analysis; Texas (TX), Oklahoma (OK), Colorado (CO), North Dakota (ND), New Mexico (NM), Pennsylvania (PA), Wyoming (WY), and Ohio (OH). It was found that the inclusion of all states artificially suppressed descriptive statistics (e.g., mean, median) because some less active states had limited HF activity and data points. Figure 20 illustrates the annual state unique HF chemical count trends.
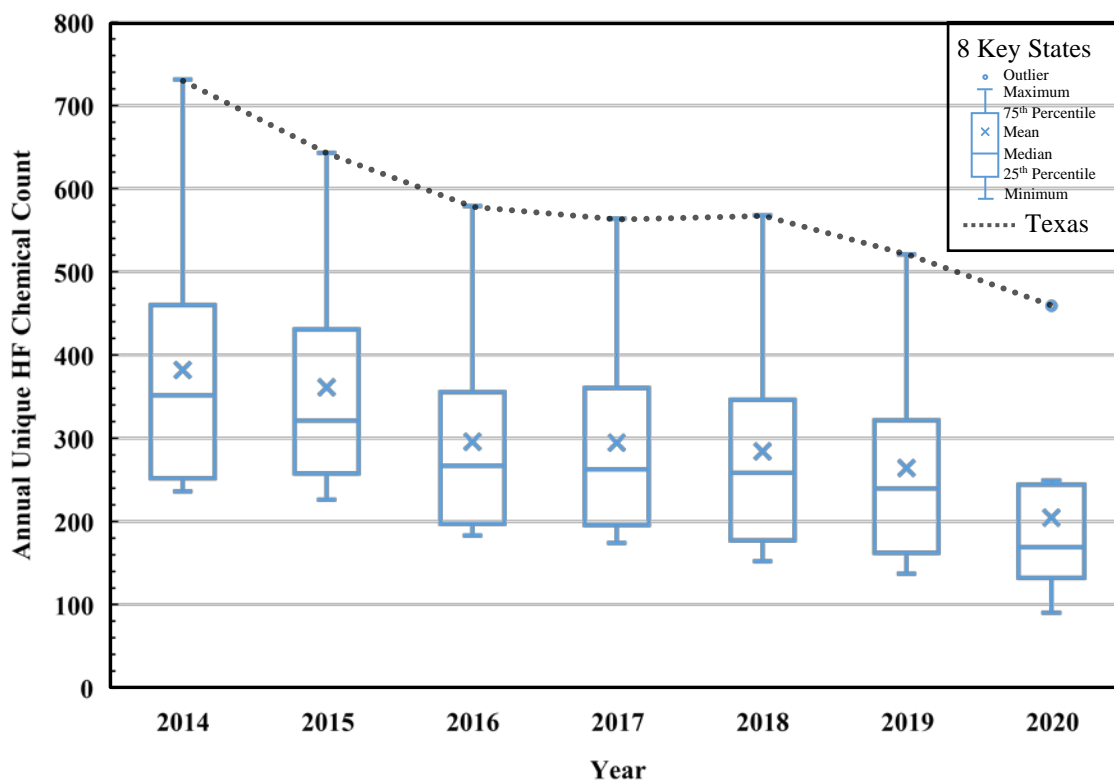
Figure 20. Unique HF chemical count annual trends by state. Key states (TX, OK, CO, ND, NM, PA, WY, OH) values captured in the boxplot and Texas only values defining upper bound are reported in the line graph.

In general, states realized a reduction in HF chemical diversity between 2014 and 2020. The average annual number of unique chemicals used within the eight key states dropped approximately 46.6% (382 to 204). Based on this analysis, the system factors (e.g., knowledge, economics, social pressure) influencing the range of HF chemicals disclosed appear to be

impacting all states similarly. However, the general analysis of the eight representative states highlighted the relatively higher level of chemicals used in the State of Texas, which defined the upper statistical boundary in Figure 20. This observation led us to investigate the correlation of play/basin activity with HF chemical variety, as shown in Figure 21.
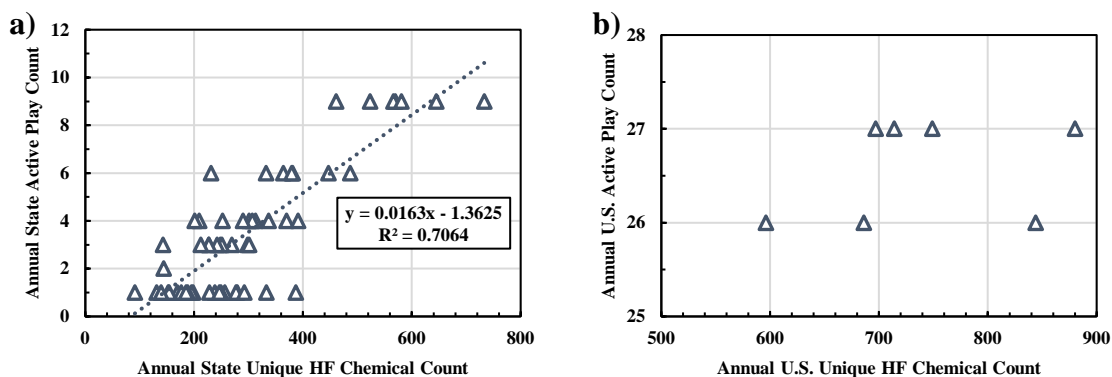
Figure 21. Annual a) state and b) U.S. unique HF chemical count correlated with annual active play count between 2014 and 2020 for the 8 key states (TX, OK, CO, ND, NM, PA, WY, OH).

The annual state active play/basin and unique HF chemical count correlation were fitted ($R^2 = 0.7064$) with linear regression, as shown in Figure 21a. A relatively strong relationship between variables at the state level indicates the number of active plays/basins influences the variety of chemicals used and disclosed. This finding is important because it supports that the oil and gas industry selects HF chemicals based on reservoir properties. The same analysis was attempted for all annual development activities across the U.S. to determine if the number of basins targeted in a given year was the cause of the trend in reduced HF chemicals between 2014 and 2020, shown in Figure 21b. This analysis illustrates an active play/basin count between 26 and 27 has been maintained at a national level over the period of interest, and a correlation between the variables is not apparent. Therefore, the diversity in basin activity impacts the annual quantity of unique HF chemicals used within a state, but it does not describe the national trend toward fewer chemicals.

4.3.2.3. HF and Reference Chemical List Comparative Analysis

Establishing context is an initial and critical step in risk management (ISO, 2018). There has been a significant amount of valuable research regarding the environmental and public health risks associated with HF chemicals (U.S. EPA, 2016a; Yost et al., 2017, 2016a, 2016b). However, this study could not identify peer-reviewed comparisons between reference chemicals with more direct environmental and public exposure pathways and HF chemicals. For a preliminary comparison, 12,354 readily available reference chemicals categorized as known or suspected to be in contact (unrelated to HF) with drinking water, food, or cosmetics (See Table 1 for list details) were selected using EPA's CompTox database. This section describes, and Figure 22 illustrates, the highlights from comparing the 12,354 reference and 1,244 HF chemicals. This analysis reinforces the usefulness and importance of EPA's CompTox, ECHA's register, and other chemical database investments.

HF Chemicals (1,244)	Parameter	Reference Chemicals (12,354)
70.0% (867/1,244)	Dataset Similarity	7.0% (867/12,354)
92.4% (1,150/1,244)	ToxVal (toxicological)	90.3% (11,161/12,354)
5.4% (67/1,244)	IRIS (toxicological)	1.8% (220/12,354)
30.2% (375/1,244) 0.0215 +/- 0.0022 mol/kg	TEST Rat Oral LD50 (toxicological)	44.4% (5,479/12,354) 0.0193 +/- 0.0005 mol/kg
38.6% (480/1,244) 2.77 +/- 0.47 mol/L	OPERA Water Solubility (chemical property)	63.4% (7,828/12,354) 0.698 +/- 0.055 mol/L

Figure 22. HF and reference chemical preliminary comparison. Representation of occurrence, toxicological, and physicochemical data availability for risk assessment.
"Data similarity" captures the number of chemicals found in both lists (867) and the total percent of said chemicals in a given list. Toxicity Estimation Software Tool (TEST) rat oral LD50 and Open Structure Activity Relations App (OPERA) water solubility 95% confidence intervals are reported.

Drinking water resources are not intentionally subjected to HF chemicals. However, the risk of drinking water contamination caused by accidental surface spills, subsurface migration, or well blowouts exists. Prudent operators and service companies utilize robust operating management systems, standard operating procedures, engineering designs, and best management practices to reduces the risk of accidental breaches in primary (e.g., pipe, tank) and secondary (e.g., lined berms around the tank) containments (American Petroleum Institute, 2012b; OGP and IPIECA, 2014). State and federal regulations are in place to ensure compliance with minimum risk management standards related to chemical release mitigation, reduction, containment, and remediation (State Review of Oil & Natural Gas Environmental Regulations, 2019). In contrast, known water, food, and other consumer product chemical additives and contaminants, like those found in the reference chemical list, are more certain to reach environmental and human

receptors. In these cases, researchers and regulators focus on understanding exposure levels (dose) and associated risk of adverse outcomes (response) (National Research Council, 2009).

The hypothesis was that when compared with HF chemicals, reference chemicals would have:

- a low level of chemical similarity,

- more available toxicity, fate, and transport information, and

- lower toxicity and mobility in the environment

However, from a chemical or dataset similarity perspective, it was found that HF chemicals made up approximately 7.0% of the reference chemicals, and 70.0% of the HF chemicals were in the reference chemical list (Figure 23). The relatively high similarity in chemicals was not expected given the risk perception surrounding HF chemicals (Chittick and Srebotnjak, 2017; Elliott et al., 2017; Stringfellow et al., 2017a) and more direct human health exposure pathways of the reference chemicals. Other researchers have thoroughly identified and investigated water, food, and cosmetic chemical hazards separately (Groh et al., 2020; Li and Suh, 2019; Pizzurro et al., 2018), and readers are directed to these references for further discussion regarding these topics. Stringfellow et al. (Stringfellow et al., 2017b) compared chemical-use between hydraulic fracturing and other oil and gas operations, but did not explore how these chemicals differed from known water, food, and cosmetic additives and contaminants.

HF Chemicals
(1,244)

Reference Chemicals
(12,354)

70.0% Similarity (867 out of 1,244)
- Food-Related (68.6%, 854 out of 1,244)
- Cosmetic-Related (15.0%, 187 out of 1,244)
- Water-Related (3.7%, 46 out of 1,244)
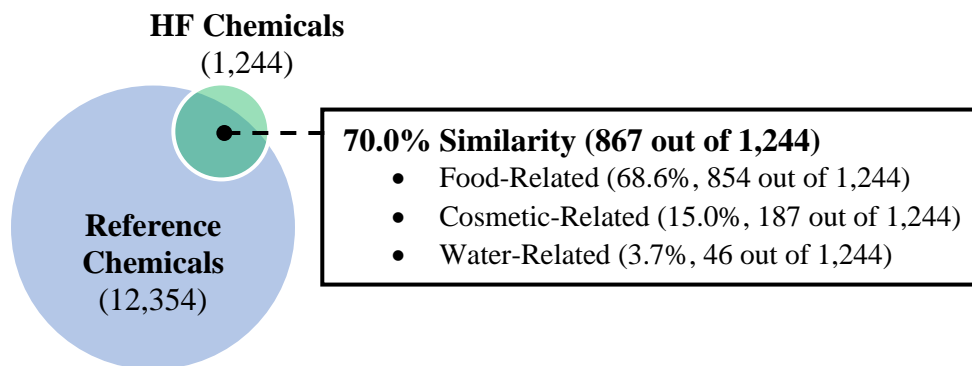
Figure 23. HF and reference chemical similarity.
Depicted similarities are based on the percent of HF chemicals identified between 2014 and 2020. Some reference chemicals are related to more than one category (i.e., food, cosmetic, water); therefore, the sum of related percentages is greater than the total similarity.

In Table 2, reference and recently (2014 to 2020) disclosed HF chemicals were compared with those HF chemicals previously identified by EPA for having high oral slope factors (OSF) (Yost et al., 2016a). Six of the ten high OSF chemicals determined by the EPA were reported in HF fluids between 2014 and 2020. Chromium(VI) was the only high OSF chemical not specified in the reference chemical list, and all nine of the overlapping chemicals were associated with food contact (Groh et al., 2020). Quinoline and 1,3-butadiene were also associated with cosmetics and drinking water pipes, respectively (Pizzurro et al., 2018; U.S. EPA, 2020). It is crucial to note that association does not conclusively indicate human exposure or health risk, which is valid for reference and HF chemicals. However, these findings do highlight research opportunities regarding holistic chemical risk information availability, knowledge, perception, and decision making.

Table 2. EPA's 2016 study chemicals with the highest OSF used in HF fluids compared with reference chemicals and HF chemicals.
(Yost et al., 2016a)

CASN	Chemical Name	OSF (per mg/ kg-day)	EPA OSF Source	Reference Chemical	HF Chemical[1]
91-22-5	Quinoline	3	IRIS[2]	Y	Y
302-01-2	Hydrazine	3	IRIS	Y	
7440-38-2	Arsenic	1.5	IRIS	Y	Y
111-44-4	Bis(2-chloroethyl) ether	1.1	IRIS	Y	
106-99-0	1,3-Butadiene	0.6	CalEPA[3]	Y	
79-06-1	Acrylamide	0.5	IRIS	Y	Y
18540-29-9	Chromium(VI)	0.5	CalEPA		
75-21-8	Ethylene oxide	0.31	CalEPA	Y	Y
75-56-9	1,2-Propylene oxide	0.24	IRIS	Y	Y
100-44-7	Benzyl chloride	0.17	IRIS	Y	Y

[1] Identified from U.S. FF register between 2014 and 2020. [2] IRIS = Integrated Risk Information System. [3] CalEPA = California Environmental Protection Agency.

Limitation in available HF chemical toxicological information has been claimed by many researchers (Stringfellow et al., 2017a; Trickey et al., 2020; U.S. Envrionmental Protection Agency, 2016a; Waxman et al., 2011; Yost et al., 2016a, 2016b). Based on the original research presented in this dissertation, there are gaps in HF chemical toxicological data. However, this study sought to understand if these limitations were unique to HF chemical or a more general systemic issue. The ToxVal database aggregates toxicity values from 18 separate public databases and, as of August 2018, contained "772,721 toxicity values from 29 sources of data, 21,507 sub-sources, 4,585 journals, and 69,833 literature citations" (U.S. EPA, 2020). The EPA's Integrated Risk Information System (IRIS) is included in the ToxVal database, but IRIS is governed by a more rigorous process than other ToxVal resources and, therefore, IRIS values are independently reported as well. The ToxVal and IRIS databases consist of many different toxicity dose measures captured at study or chemical levels, including measures such as EPA

Regional screening levels, reference dose (RfD), reference concentrations, slope factors, point of departure, lowest observed adverse effect levels, no observed adverse effect levels, no effect levels, low effect levels, cancer-related quantities (e.g., cancer slope factors, inhalation unit risk), and other derived quantities. Both ToxVal and IRIS-specific metadata have been incorporated into the EPA's CompTox system, making CompTox an efficient and effective resource for conducting a preliminary comparative analysis of different chemical lists.

When exporting a list of chemicals from EPA's CompTox system, the ToxVal and IRIS fields register a "Y" with a hyperlink to the values when toxicity data is available. These binary CompTox features were used to determine the percent of chemicals with ToxVal and IRIS toxicological information. Approximately 92.4% and 90.3% of the HF and reference chemicals, respectively, were indicated as having ToxVal values in CompTox. Regarding IRIS values, it was found that approximately 5.4% and 1.8% of the HF and reference chemicals, respectively, were reported in CompTox.

The ToxVal and IRIS comparisons suggest that there was no significant difference in the availability of toxicological information between HF and reference chemicals. Therefore, HF toxicological data limitations are potentially a product of a systemic issue and not unique to the oil and gas industry. This specific hypothesis requires additional investigation. However, other shortcomings in toxicological information across all sectors have been acknowledged by others (Silbergeld et al., 2015; Wang et al., 2020, 2019). In addition, researchers and regulatory agencies worldwide are investing heavily to continuously improve chemical information systems and content (Evans et al., 2019; National Academies of Sciences, Engineering, 2017; Westphal et al., 2017; Williams et al., 2017). Chemical Quantitative Structure Activity Relations (QSAR)

modeling is one technology accelerating the availability of chemical property information that can be used in risk assessments and decision making (Lowe and Williams, 2021).

QSAR embodies various chemical property and activity prediction techniques based on their structural similarity to chemicals with established activities and properties. Based on QSAR technology, EPA has developed the Toxicity Estimation Software Tool (TEST) and Open Structure Activity Relations App (OPERA). TEST's primary purpose is predicting toxicological values. OPERA focuses on calculating expected physicochemical properties and environmental fate. Both TEST and OPERA estimated values have been incorporated into the CompTox Dashboard. It is worth noting that there are uncertainties and limitations of these estimation tools. For example, they cannot estimate properties for the inorganic chemicals or mixtures.

The TEST rat oral lethal dose (LD50) and OPERA water solubility parameters were selected to conduct a preliminary comparison of the availability of QSAR toxicological and environmental fate property values for HF and reference chemicals. The TEST rat oral LD50 toxicity parameter forecasts the amount of a chemical per body mass (mol/kg) that will cause death in 50% of an animal test group. The humane aspect of QSAR is clearly another benefit of developing and using this technology. The OPERA water solubility physicochemical property value calculates the maximum chemical quantity that can dissolve in water (mol/L).

Reference chemicals were found to have a higher percentage of TEST rat oral LD50 and OPERA water solubility values in CompTox. A contributing factor to these results is the proportion of inorganic chemicals and chemical mixture in the HF chemical list. However, the research findings are clear; reference chemicals have a higher percentage of available QSAR toxicity and physicochemical property information. An investigation of the TEST rat oral LD50 and OPERA water solubility value statistics provided additional insights worth noting. For

example, assuming a normal distribution and using a 95% confidence interval, there does not appear to be a significant difference between HF and reference chemical TEST rat oral LD50 values at 0.0215 +/- 0.0022 mol/kg and 0.0193 +/- 0.0005 mol/kg, respectively. A significant difference in OPERA water solubility values was observed, as shown in Figure 22.

The U.S. EPA generated QSAR predicted oral toxicity values for 44% (515 / 1,173) of HF, flowback, and produced chemicals that they identified and investigated (Yost et al., 2016b), which is comparable and slightly above the proportions found in the analysis present here. However, peer-reviewed research that contrasted the availability of HF chemical information with a list of non-HF reference chemicals for reference was unable to be identified. Existing research has focused primarily on the availability and characteristics of HF chemicals without the more holistic reference chemical perspective. This study shows that there is value in expanding the scope of chemical evaluations to provide systemic context to stakeholders and understand sources of potential chemical contamination and exposures to drinking water resources.

4.4. Summary

Risks to drinking water resources caused by OUOGD are controlled by a complex and dynamic sociotechnical system comprised of interconnected functions. It is critical that researchers, policymakers, and industry leaders investigate system dynamics to understand functional behaviors, including current risk levels and trends. The research presented in this chapter explores the evolution of HF chemicals between 2014 and 2020, providing a temporal analysis of additives used and disclosed in FF during OUOGD in the U.S. The provided updated list of hydraulic fracturing chemicals, evaluation of influencing factors, information availability assessment, and comparison with known or suspected water, food, or cosmetic contaminants or

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ingredients have critical implications on future research. The foundational research presented in this chapter indicates past progress and future opportunities for improvement related to hydraulic fracturing chemical stewardship. It serves as a building block and a catalyst for increased momentum toward safer chemicals and transparency across all industries in the future.

5. SYSTEMIC HYDRAULIC FRACTURING CHEMICAL RISK INDICATORS FOR ASSESSING RELATIVE HAZARD LEVELS TO DRINKING WATER RESOURCES

5.1. Introduction

There is a global trend towards and demand for more sustainable business practices and associated performance measures. Greenhouse gas reporting has seen the most use and interest, but chemical stewardship is an intriguing topic in this realm with significant opportunities for further research and application. As discussed previously, OUOGD and hydraulic fracturing are targeted industrial activities for public objection related to the potential for adverse environmental and public health impacts. The risk to drinking water resources from hazardous hydraulic fracturing chemicals is a specific concern that has received considerable public attention. Although there has been a significant amount of research on this topic, the following research questions have not been answered:

1. How should systemic hydraulic fracturing chemical hazard levels be measured?

2. Has the systemic hydraulic fracturing chemical hazard level increased or decreased?

The study described in this chapter directly explores these questions and presents a novel approach to measure relative changes in systemic risk indicators that can be applied to hydraulic fracturing chemical or other industrial activities for policy-level decision making or performance monitoring.

This chapter aims to weave sustainability, systemic risk analysis, and hydraulic fracturing chemical hazard indicatorconcepts together in the development of an original method for measuring and monitoring chemical risk and stewardship during OUOGD using hydraulic fracturing. Sustainability indicators have gained popularity and proven successful in reporting

progress and fostering accountability within organizations and society. Systemic risk assessments and indicators are valuable tools that are maturing quickly and gaining traction in practice. It is a short intellectual jump to connect and notice the similarities in sustainability and systemic risk indicators; moreover, how these ideas can be combined with hydraulic fracturing chemical hazard and "green" indicators and assessment tools to inform policy decisions and increase stakeholder awareness. However, this jump has yet to be made in peer-reviewed literature.

The environment and public health are at risk from the potential exposure to more than 350,000 chemicals in commerce (Wang et al., 2020). Regulatory frameworks worldwide are improving quickly; however, they are perceived as inadequate for managing chemical risks and not a holistic solution to the problem. There is a need to develop novel and simple chemical risk mental models and indicators that can be used to measure and foster continuous improvement in chemical stewardship and risk reduction. These types of tools can be used by many system control functions (e.g., regulators, industry, non-government organizations). Hydraulic fracturing chemicals are an ideal breeding ground for exploring and developing this topic due to the importance to stakeholders and the current availability of information through mandatory disclosure regulations. In addition, this subject opens the opportunity to investigate the recent influence of transparency on voluntary risk reduction by industry stakeholders.

To address the questions stated above, the following research objectives were utilized to guide the contents of this chapter:

1. Critically review existing chemical hazard indicators and assessment concepts
2. Develop an original approach for measuring systemic hazard levels to drinking water resources from hydraulic fracturing chemical

Through these objectives, the study intends to foster increased momentum toward safer chemicals and transparency across all industries in the future.

5.2. Background

5.2.1. Hydraulic Fracturing Chemical Hazard Indicators and Tools

General pressure within the OUOGD control structure defined in Chapter 2 and a desire by industry stakeholders to be good corporate citizens have resulted in "green" progression related to HF chemicals. Table 3 summarizes the general HF chemical categories, purposes, and associated "green" progression reported by Harry et al. (2020). Thomas et al. (2019) provided additional context regarding efforts toward more sustainable hydraulic fracturing fluids.

Performance, cost, and environmental and health risk/impact are the primary factors affecting industry decision-making regarding hydraulic fracturing chemical selection. There are trade-offs between and within these criteria. For example, considering only environmental and health risk/impact, an operator may choose to utilize produced water, which is high in natural salts and impurities, to conserve fresh water. Doing so may require the use of additional or more hazardous chemicals. Narrowing in on chemical hazards, several assessment systems have been developed to which have helped drive the discussion and action toward more sustainable products. Hu et al. (2019) bifurcated these tools into hazard screening and indexing classifications. Both types are qualitative and primarily based on toxicity, persistence, and fate/transport. Hazard screening is defined as labeling a chemical with a valid hazard designation or severity level. Outputs are easy to communicate, but they are challenging to use in comparing multiple chemicals. Hazard indexing digests risk information into a single measure or metric using rules and aggregation formulas. Although helpful in comparing chemicals and decision-making, inappropriate aggregation can lead to improper hazard characterization. Integrated

approaches combining these two types of systems have been proposed to address limitations.

Table 4 provides a representative list of hydraulic fracturing chemical hazard assessment tools

found in peer-review research. Chemical decision analysis framework is a term synonymous

with hazard assessment systems (Mitchell et al., 2013; Yost et al., 2017).

Table 3. Summary of green progression in hydraulic fracturing chemicals
(Harry et al., 2020)

Chemical Category	Purpose	Green progression
Friction reducers	Minimize surface treating pressures	Development of dry-powdered materials with no oil phase and required the use of surfactants, reduced volume, less volatility, and hazardous characteristics. The use of hydrotreated (no benzene, toluene, ethylbenzene, and xylene or BTEX) mineral oil, EPA Design for Environment (DFE)-listed and drinking water approved polymers.
Guar Slurries	Proppant suspension and delivery into fractures	Guars are non-toxic and biodegradable. Cross-linkers have from antimony and chromium to boron, aluminum, titanium, and zirconium.
Breakers	Remove friction reducers and viscosifying agents	Development of enzymatic breakers, like hemicellulose for polysaccharide-based systems. Acrylamide systems require oxidizing breakers, like persulfate or peroxides.
Solvents	Carrier fluid for other chemical additives	Transition away from diesel and light distillates without detectable BTEX and extremely low aromatic content. Utilization of seed oils.
Biocides	Control bacteria and microorganisms to prevent corrosion.	Use of ultraviolet light and mechanical methods. Use of sustainability chemical scores, like Offshore Chemical Notification Scheme (OCNS). Evaluation of phage and enzymes bio-control.
Scale inhibitors	Prevent the formation of precipitates and associated equipment failures.	Development of dry products with reduced volumes requirements, less volatility, and EPA-DFE listed. Replacing synthetic polymers with biobased polymers, like polyaspartic acid.
Acid additives	Corrosion inhibitors and iron-reducing agents to prevent integrity issues caused by acid.	Transition to chemicals with comparably "greener," like propoxylated propargyl alcohol and mercaptans.
Chelating agent	Bind dissolved ions in water that could negatively impact gelling agent	Replacement of ethylenediaminetretraacetic acid and nitrilotrisacetic acid with citric acid, carboxylic acids, and iminodisuccinic acid.
pH adjusting agents	Optimize fracture fluid pH for other additive performance	Relatively unchanged and uses hydrochloric acid, acetic acid, sodium hydroxide, sodium carbonate, and sodium bicarbonate.
Clay stabilizers	Prevent swelling and migration of clays	Transition from potassium chloride to lower volume synthetic polymers, and subsequently from synthetic polymers to choline chloride and salts of biodegradable simple amines.

Table 4. A representative list of hydraulic fracturing chemical hazard assessment tools.

Tool / System Name	Category	Reference
Quantitative Ranking Measure of Oil Field Chemical Environmental Impacts	Hazard Indexing	Jordan et al. (2010)
Chemical Hazard Rating System	Hazard Indexing	Hepburn (2012)
Chemical Scoring Index	Hazard Indexing	Verslycke et al. (2014)
Hydraulic Fracturing Fluid Greenness Assessment System (HyFFGAS)	Hazard Indexing	Hurley et al. (2016)
Intrinsik Screening-level Assessment System	Hazard Screening	Intrinsik (2013)
GreenScreen®	Hazard Screening	CPA (2016)
Integrated Chemical Hazard Screening and Indexing System	Hazard Screening and Indexing (Integrated)	Hu et al. (2019)

The application of the hydraulic fracturing chemical hazard assessment tools has been limited to the chemical, additive, and combine fracturing fluid levels. Peer-reviewed research regarding the measurement of system or system functions (e.g., operators, service companies, regulators) hydraulic fracturing chemical hazard level performance could not be identified. A review of sustainability chemical indicators found in corporate responsibility and sustainability reports guidance documents was conducted to determine if these types of system-level risk metrics exist in practice (GRI Global Sustainability Standards Board, 2020; IPIECA et al., 2020; Sustainability Accounting Standards Board, 2018). Although spills, occupational safety, and other health and environmental metrics were covered within these documents, systemic measurement of risk associated with the chemical selection for use in operations was directly not captured.

5.2.2. Systems-Theoretic Accident Model and Processes

As discussed in Chapter 2, STAMP is a compelling theory for conceptualizing and communicated accident causation, and STPA is the associated hazard assessment technique. STPA is not a chemical hazard or risk assessment technique; however, it is valuable for characterizing the importance of system feedback loops, performance indicators, and communication related to systemic chemical risk.

In STPA, two types of loss scenarios can lead to risk or an accident; an unsafe control action occurs or a safe control action is improperly or not executed. Focusing on the occurrence of hazardous control actions, a key contributor is an inadequate controller process model informed by incorrect feedback/information or not informed at all (no feedback). Regarding hydraulic fracturing chemicals, there is significant information available within the oil and gas industry (e.g., operators and service companies) and publically. However, this information is challenging to consume beyond individual fracture jobs at higher system functional levels, as discussed in Chapter 4. The applications of existing chemical hazard assessment tools at chemical, additive, and fracture fluid levels do not capture system behaviors and emergent properties. Risk and sustainability indicators for monitoring systemic hazard levels are lacking. Developing methods and metrics that can be operated within higher system functions is necessary to prevent unsafe conditions and foster improved chemical stewardship.

5.3. Methodology

The methodology presented below is specific for calculating annual system risk indicators associate with U.S. onshore unconventional oil and gas development. The scope of these metrics can be adapted for varying system levels/functions or time horizons. Both weighted (from average percent mass) and unweighted risk indicators are provided for reference but

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utilizing the weighted metrics is recommended because they are more representative of system dynamics.

5.3.1. Data Sources

This study utilizes the U.S. FF database (GWPC, 2021) and EPA's CompTox Chemical Database, similar to Chapter 4. The FF dataset used was accessed on April 4th, 2021 and limited to HF jobs ending between 2014 and 2020. The proprietary Enverus data (Enverus, 2021) was not necessary to conduct the presented analysis. HF chemical information was gathered from EPA's CompTox Chemical Database. Specific CompTox chemical parameters of interest were QSAR predicted values for toxicity (i.e., rat oral lethal dose with 50% mortality) (mol/kg), water solubility (mol/L), biodegradation half-life (days), Henry's constant (atm.m^3/mol), soil adsorption coefficient (K_{oc}, L/kg), and octanol/water partition coefficient (K_{ow}, dimensionless). These parameters were selected because they are representative of critical factors (toxicity, persistence, and mobility) found in existing chemical hazard assessment systems and relevant to drinking water resource risk. QSAR is not currently applicable to inorganic chemicals, chemical mixtures, or CASN representing multiple chemicals; therefore, risk parameter data for CASN associated with these categories were not available from CompTox or included in specific risk indicator calculations.

5.3.2. Data Analysis Tools

Similar to Chapters 3 and 4, Microsoft Excel (365 v 2103 32 bit), Anaconda Navigator (v 1.9.12), Spyder (v 4.0.1) and Python (v 3.7.6) along with Numpy (v 1.18.1) and Pandas (v 1.0.1) were used for data navigation and analysis.

5.3.3. Data Processing and Analysis Workflow

FF data used in the analysis was filtered (2014 to 2020), cleansed, and processed by removing duplicate rows, system rows, duplicate forms, and assigning CASN or appropriate designation to ingredient rows. Most cleansing and processing steps are defined in detail in Chapter 3, Chapter 4, and Appendix A. General composition results are based on the entire data set after data quality filters were applied. Risk indicator results are calculated from a subset of the data with available QSAR parameters of interest on EPA's CompTox dashboard (Appendix B). The steps below summarize the data processing and analysis workflow beyond what has been previously described in this dissertation.

Estimated normalized form average annual mass percent of key constituents:

1. Categorize each CASN.

   o Water: 7732-18-5

   o Sand: 14808-60-7, 7631-86-9, 112926-00-8, 60676-86-0, 112945-52-5, 69012-64-2

   o Other Ingredients:

     ▪ Chloride salts: 7647-01-0, 7647-14-5, 7447-14-5, 7447-40-7, 10043-52-4

     ▪ Guar gum: 9000-30-0

     ▪ Carbon dioxide: 124-38-9

     ▪ All other CASNs

2. Calculated the average form annual mass percentage for constituent categories by summing the mass percentages for each constituent across all disclosure forms and dividing this sum by the number of disclosure forms in a given year.

3. Sum the average annual mass percentage for all constituent categories to produce a total mass percent for a given year. *Results in this step ranged from 100.43% to 100.69%.*

4. Divide each average annual mass percentage by the total mass percent to obtain a normalized annual mass percent for each key constituent.

Toxicity, persistence, and fate/transport mass percent weighted risk indicators:

1. Calculated the form average annual mass percentage for each CASN by summing the mass percentages for that chemical across all disclosure forms and dividing that sum by the number of disclosure forms within a given year.

2. Remove water, sand, guar gum, chloride salts, and carbon dioxide from the dataset, and filter chemicals to those with available risk parameters (e.g., water solubility, toxicity) of interest. *Ideally, all chemicals would have available risk parameter data and this step would not be necessary.*

3. Sum the chemical average annual mass percentages to produce a total mass percent in a given year for the remaining chemicals with risk parameter data.

4. Divide each chemical average annual mass percentage by the total mass percent to obtain a normalized annual mass percent for all chemicals with available risk parameters.

5. Multiply the normalized chemical average annual mass percentage by its associated variable of interest and sum these values for a given year. The results of this step are the annual percent mass-weighted risk indicator values.

Toxicity, persistence, and fate/transport mass percent unweighted risk indicators:

1. Filter chemicals to those with available risk parameters (e.g., water solubility, toxicity) of interest. *Ideally, all chemicals would have available risk parameter data, and this step would not be necessary.*

2. Average the risk parameter of interest for all chemicals disclosed in a given year to calculate the annual unweighted risk indicator.

Aggregated relative risk indicator:

1. Select and calculate risk indicators (r_{ij}) of interest for a given timeframe to be aggregated (i = indicator, j = time period). The following annual metrics were selected for the analysis provided:

   o Annual well count (unique FracFocus API14 count)

   o Estimated normalized other ingredient mass percent value (defined above)

   o Toxicity, persistence, and fate/transport mass percent weighted risk indicators; rat oral LD50, water solubility, biodegradation half-life, Henry's constant, soil adsorption coefficient, and octanol/water partition coefficient.

2. Assign a weight for the risk indicators (w_i) to be aggregated and selected in step 1. An equal weighting was used for the analysis provided (8 risk indicators, 12.5% weighting each).

3. Determine if a high or low risk indicator value is associated with higher risk. For the purposes of this analysis:

   o Well count – Higher value, higher risk

   o Other ingredient mass percent – Higher value, higher risk

   o Rat oral LD50 – Lower value, higher risk

- Water solubility - Higher value, higher risk

- Biodegradation half-life - Higher value, higher risk

- Henry's constant - Lower value, higher risk

- Soil adsorption coefficient - Lower value, higher risk

- Octanol/water partition coefficient - Lower value, higher risk

4. Normalize risk indicators (R_{ij}) on a scale of 0 (lower risk) to 100 (higher risk). For the analysis provided, annual values between 2014 and 2020 were used.

- For higher value-higher risk indicators, divide all annual values by the maximum annual value for the risk indicator ($r_{i,max}$).

$$R_{ij} = \frac{r_{ij}}{r_{i,max}} \times 100$$

- For low value-higher risk indicators, calculate the reciprocal of dividing the annual values by the minimum annual value for the risk indicator ($r_{i,min}$).

$$R_{ij} = \left(\frac{r_{ij}}{r_{i,min}}\right)^{-1} \times 100$$

5. Calculate the aggregated risk indicator (A_j) by summing the products of multiplying the assigned risk indicator weight (step 2, w_i) and normalized risk indicator value (step 4, R_{ij}).

$$A_j = \sum R_{ij} \times w_i$$

5.3.4. Data Uncertainty and Research Limitations

Data uncertainty and research limitation discussed in Chapters 3 and 4 apply to this Chapter as well. A significant limit that must be acknowledged for this Chapter is related to the

scope of inputs for the reported risk indicators. Since the data used to calculate these metrics is based only on a subset of chemicals with available QSAR parameters of interest, they should not be used to extrapolate system behavior or property claims. This study is intended to demonstrate an approach for calculating system chemical hazard risk indicators. However, additional information and analysis are necessary to fully understand system dynamics and make associated claims. In addition, it is acknowledged that QSAR has associated uncertainty that should be considered when reviewing the following analysis.

5.4. Results and Discussion

5.4.1. Well Count and Transparency

As discussed in Chapter 3, OUOGD activity levels and chemical transparency are indicative of risk levels. Figure 11 (Chapter 3) depicts a significant drop in hydraulically fractured annual well counts between 2014 and 2020, signaling a reduction in systemic risk to drinking water resources. Transparency can be considered an indirect measure of hazard levels. Previous research has shown a strong correlation between chemical stewardship and disclosure (Jobe, 1999), making transparency potentially an ideal leading performance metric for understanding hazard levels and chemical stewardship culture within a system function. Chapter 3, and specifically Figure 12b and 13, provide evidence that HF chemical transparency has drastically increased over the last decade. However, further research is necessary to support the claim that there is a relationship between transparency and HF chemical risk levels.

5.4.2. Chemical Variety and General Composition

As shown in Figure 24, water and sand are the major components of hydraulic fracturing fluid. Other ingredients and chemicals make up the remainder of the stimulation fluid. Between 2014 and 2020, the estimated total annual percent mass of water remained relatively constant

(84.9% to 86.8%) and averaged 85.9%. Sand has seen a steady increase in mass percent over the same period, 11.7% in 2014 to 13.3% in 2020. Other ingredients (not water or sand) have seen a drastic reduction in the estimated total annual percent mass, 3.4% in 2014 to 0.8% in 2020. If carbon dioxide, guar gum and popular chloride salts (hydrogen chloride, potassium chloride, sodium chloride, calcium chloride) are removed, the other ingredient's annual mass percent dropped from 1.98% to 0.67%. In some cases, chloride salts are reported as water mixtures in FF and the water mass is contributed by chloride salts. The chemical identification process developed in Chapter 4 and used in this chapter would report the total mass of water and salts in these cases as salts. Removing these chloride salt constituents and benign guar gum slurry provides greater certainty that the estimated total mass percent reduction of chemicals observed is not associated with reporting inconsistencies in these components.
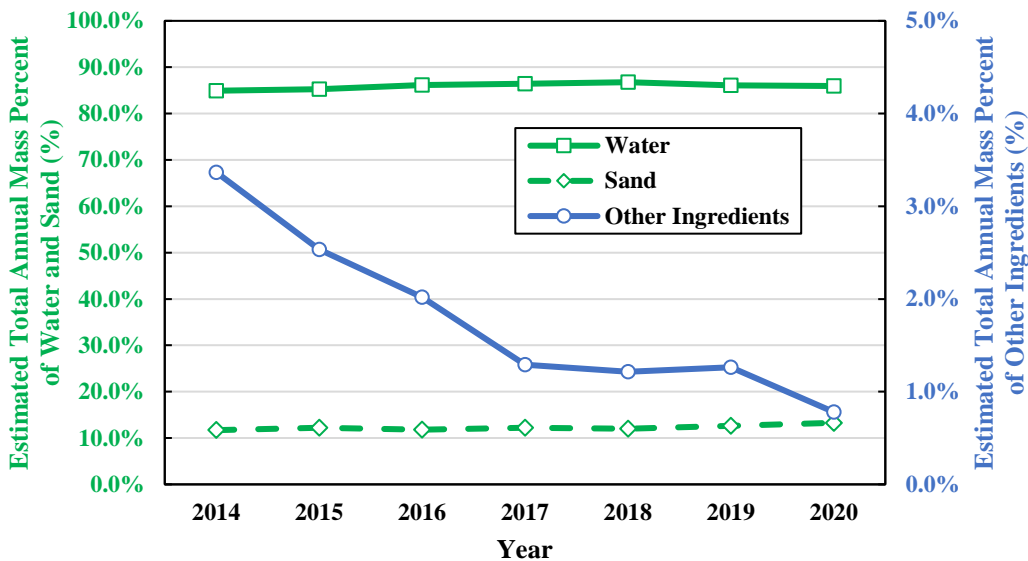
Figure 24. General hydraulic fracturing composition estimated total annual mass percent of key constituents.

5.4.3. Toxicity

Rat oral lethal dose with 50% mortality (LD50) is a valuable parameter for assessing the toxicity of a chemical or mixture. Expressed in mol/kg, the lower the value, the more significant

the toxicity risk. Other factors (e.g., RfD, OSF) are more appropriate for directly assessing oral toxicity risk to humans caused by drinking water contamination (U.S. Envrionmental Protection Agency, 2016a; Yost et al., 2016a, 2016b). However, the rat oral LD50 parameter is a readily available QSAR parameter within the CompTox dashboard and has more experimental data. The normalized annual mass percent of chemicals used to calculate the toxicity risk indicators has declined, similar to all non-water and sand additives between 2014 and 2020, as shown in Figure 25. The unweighted average annual rat oral LD50 exhibited little variability (0.0212 to 0.0240 mol/kg) between 2014 and 2020, with a slightly increasing trend. The weighted indicator increased between 2014 and 2015, but it declined to 0.283 mol/kg by 2019. Based on a subset of chemicals, these initial results indicate hydraulic fracturing toxicity levels have not significantly changed over the study period.
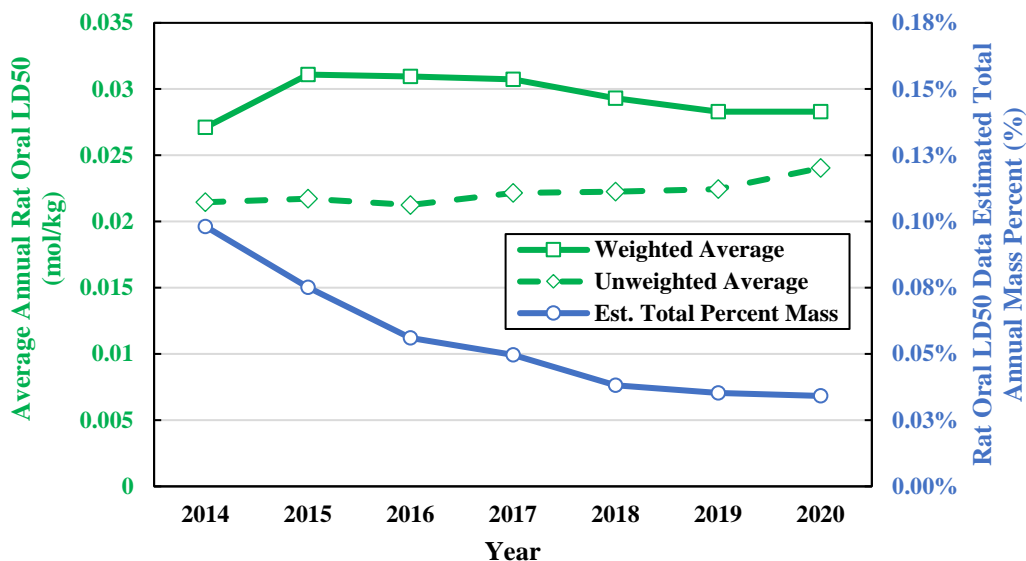
Figure 25. Annual rat oral LD50 risk indicator and mass percent for the associated dataset.

5.4.4. Mobility

Octanol/water partition coefficients (K_{ow}), soil adsorption coefficients (K_{oc}), and water solubility are important parameters for understanding chemical or mixture mobility in aqueous

solutions (Yost et al., 2017). K_{ow} and K_{oc} are expressed dimensionless (log) and L/kg, respectively, with higher values indicating lower mobility and less risk because the chemicals have a greater tendency to leave aqueous solutions. Water solubility is measured as mol/L, and higher values correlate to higher risk levels because they signify a chemical's ability to move quickly into and through aqueous solutions. All three of these parameters are available within the CompTox dashboard's predicted values (U.S. EPA, 2021). The normalized annual mass percentages of chemicals used to calculate the mobility risk indicators have declined, similar to all non-water and sand additives between 2014 and 2020, as shown in Figures 26, 27, and 28.

Figure 26 illustrates that the unweighted average annual K_{ow} was variable (0.715 to 1.213) between 2014 and 2020, but did not present a discernable trend. The weighted indicator increased significantly from -0.068 to 1.481 over the same period, suggesting a lower risk level. The differences between unweighted and weighted K_{ow} risk indicator trends suggest that the proportion of chemicals with a lower mobility (higher K_{ow}) have increased although the average of the chemicals has remained constant. Tetradecane (629-59-4) appears to have the most significant impact on the increase in K_{ow} for the subset of chemicals with QSAR data.
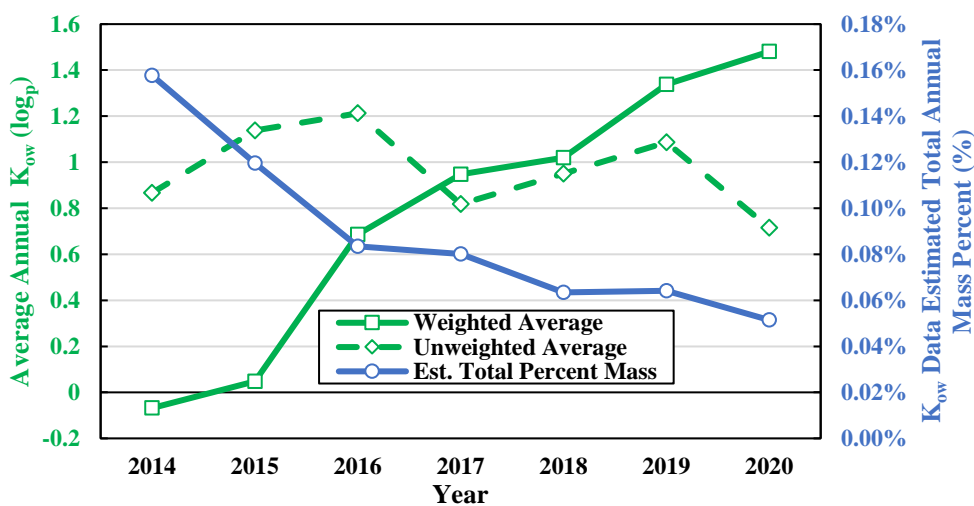
Figure 26. Annual octanol/water partition risk indicator and mass percent for the associated dataset.

Figure 27 illustrates the unweighted average annual K_{oc} was variable (1731.8 to 8237.4 L/kg) and declined between 2014 and 2020. Although difficult to observe in the figure, the weighted indicator increased by approximately 381% (255.25 to 974.74 L/kg) over the same period, implying a trend toward lower drinking water risk level. Tetradecane (629-59-4) and sorbitan, mono-(9Z)-9-octadecenoate (1338-43-8) appear to have the most significant impact on the increase in soil adsorption properties for the subset of chemicals with QSAR data.
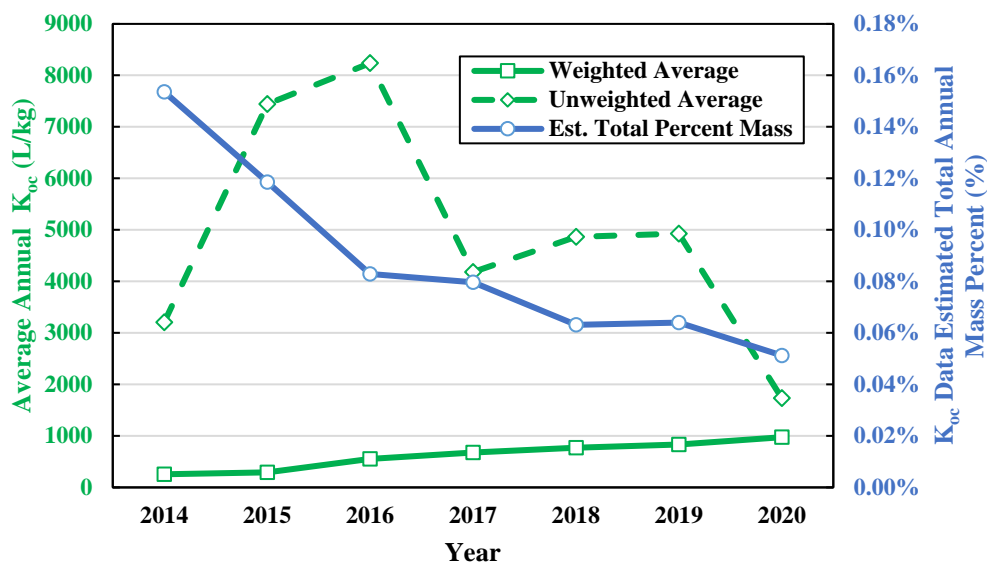
Figure 27. Annual soil adsorption risk indicator and mass percent for the associated dataset.

As shown in Figure 28, the unweighted average annual water solubility was relatively flat between 2014 and 2020. The weighted indicator average 9.87 mol/L over the same period with no apparent trend, which suggests no changes in risk level associated with this metric. Methanol (67-56-1) appears to have the most significant impact on water solubility for the subset of chemicals with QSAR data.
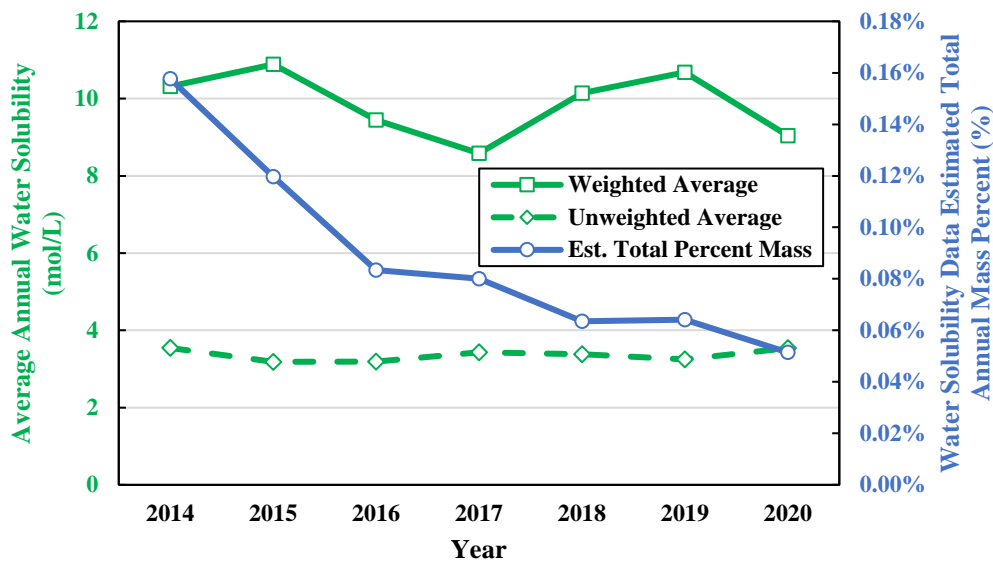
Figure 28. Annual water solubility risk indicator and mass percent for the associated dataset.

5.4.5. Volatility

Henry's constant ($atm.m^3/mol$) is a helpful parameter for assessing the volatility of a chemical. If a chemical is volatile, it is more likely to leave an aqueous solution and not reach a drinking water resource if spilled. A lower Henry's constant represents lower volatility and a higher risk to drinking water sources (Faber et al., 2017). As shown in Figure 29, the normalized annual mass percentages of chemicals used to calculate the volatility risk indicators have declined, similar to all non-water and sand additives between 2014 and 2020.

The unweighted average annual Henry's constant risk indicator exhibits a drastic drop (0.227 to 0.012 $atm.m^3/mol$) between 2019 and 2020. This drop was caused by the fact decamethylcyclopentasiloxane (541-02-6) was not observed in 2020 hydraulic disclosure forms but was present in all other years. The weighted indicator decreased slightly between 2014 and 2020 from 0.0343 and 0.0296 $atm.m^3/mol$, but there is not an identifiable trend associated with this metric. The weighted results, based on a subset of chemicals, suggest risk levels related to this parameter have not significantly changed over the study period. In addition, the extreme

sensitivity of the unweighted metric highlights the increase in reliability of and preference for the weighted metric.
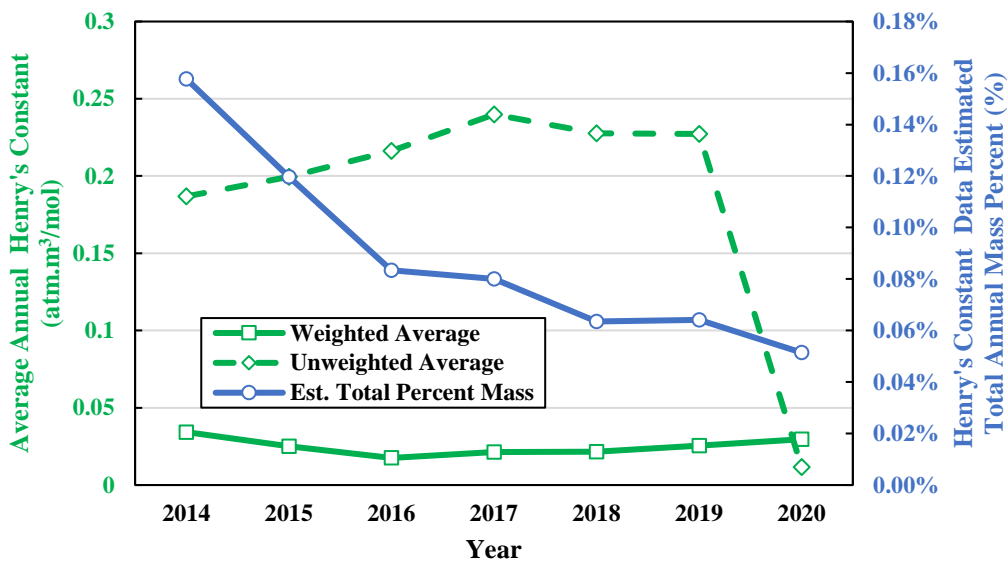
Figure 29. Annual volatility risk indicator and mass percent for the associated dataset.

5.4.6. Persistence

Biodegradation half-life (days) is a helpful parameter for assessing the longevity and persistence of a chemical in the environment. An easily and quickly biodegradable chemical is less likely to reach a receptor of concern before it is naturally remediated by microorganisms. A lower biodegradation half-life is indicative of lower risk to drinking water sources (Rogers et al., 2015). The unweighted average annual biodegradation half-life risk indicator presents a surge centered in 2018 at a level of 13.9 days; however, the difference in value between 2014 and 2020 is minimal. This drop was caused by the fact decamethylcyclopentasiloxane (124-38-9) was not observed in 2020 hydraulic disclosure forms but was disclosed in all other study years. The weighted indicator has remained relatively unchanged between 2014 and 2020, averaging 8.13 days. These initial results based on a subset of chemicals suggest risk levels related to this parameter have not significantly changed over the study period.

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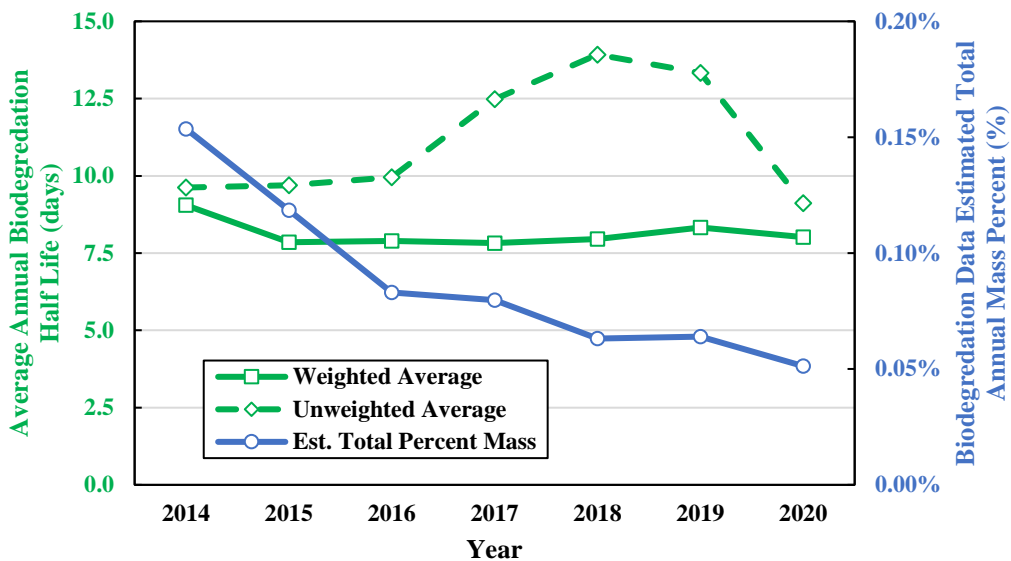
Figure 30. Annual biodegradation half-life risk indicator and mass percent for the associated dataset.

5.4.7. Aggregated Relative Risk Indicator

Figure 31 illustrates the annual aggregated relative risk indicator with contributing parameters of interest. There is a 42.6% reduction in the aggregated metric between 2014 and 2020. Well count, chemical concentration, soil adsorption, and octanol/water partition have the most significant impact on the combined indicator's decreasing trend over this period. The well count and chemical concentration inputs are based on the full FracFocus data set. However, as discussed above, the other contributing parameters are calculated from a subset of chemicals with available QSAR values.
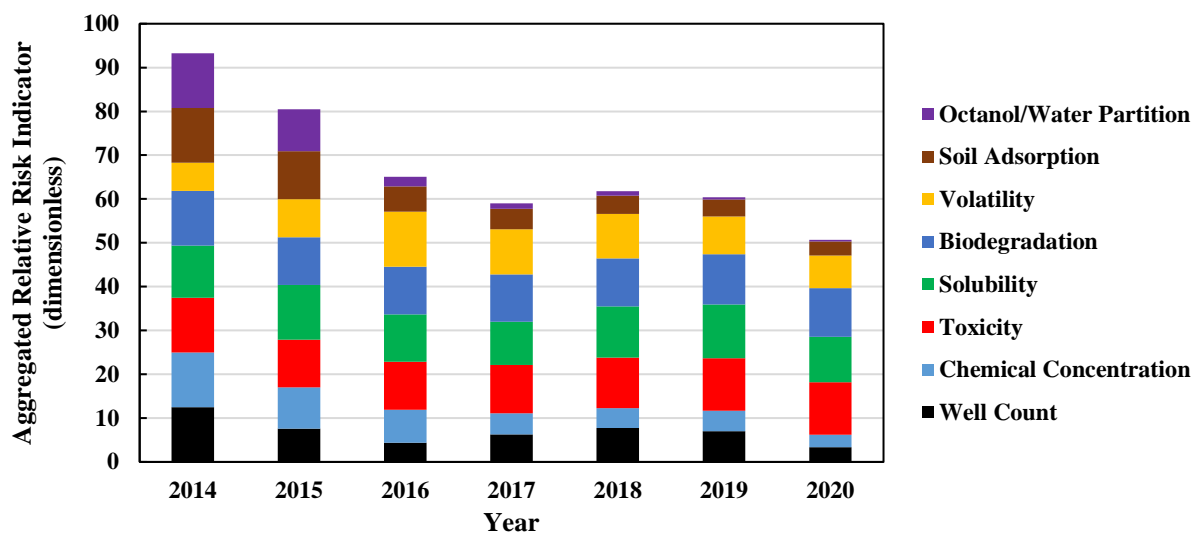
Figure 31. Aggregated relative risk indicator trend.

Referencing Table 4, the aggregated relative risk indicator presented in this section should be grouped with indexing hydraulic fracturing chemical hazard assessment tools (Hu et al., 2019). However, this new approach is unique because it captures systemic risk levels and moves beyond the chemical, additive, and fracturing fluid paradigms (Hurley et al., 2016). In addition, this methodology can be easily adapted to capture different time periods, systems/functional boundaries, and risks (e.g., changing input parameters). The aggregated relative risk indicator is limited to monitoring comparative system changes in chemical risk to drinking water resources. In its current state, the technique does not offer a means to clearly define and screen specific hazard levels. However, with the objective of monitoring and driving continuous improvement, stakeholders will find significant value in this metric.

5.5. Summary

A repeatable approach for processing U.S. FF hydraulic fracturing chemical disclosure information and CompTox chemical information into insightful systemic risk indicators was presented in this chapter. There appears to be a clear and definitive change in hydraulic fracturing activity levels and the annual form average mass percentages for non-water and sand

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additives. However, other calculated mass percent weighted risk indicators, based on a subset of chemicals, suggest that there has been little change in hydraulic fracturing chemical toxicity and persistence hazard levels to drinking water. Chemical mobility risk levels appear to have decreased. Further research applying the approach and risk indicators discussed in this Chapter to a more significant subset of hydraulic fracturing chemicals, and potentially experimental data, is necessary to make claims related to system toxicity, persistence, and fate/transport risk levels and dynamics.

6. CONCLUSIONS AND FUTURE WORK RECOMMENDATIONS

6.1. Conclusions

Hazards associated with HF chemicals are a primary public concern. Novel systemic risk analysis methods have recently been developed to help society address "wicked problems." However, in general, these systemic risk assessment techniques have not been applied to OUOGD or specifically for determining HF chemical hazards. In addition, approaches used to holistically assess HF chemical transparency, variety, and hazard levels either did not exist or had seen limited innovation over the past decade.

In this dissertation, the development and application of systemic risk and sustainability indicators to HF chemicals were successfully demonstrated. The effectiveness of a system paradigm proved effective and insightful to understand historical trends and the current state of HF chemical transparency, variety, and risk factors. Therefore, it addressed limitations in past research approaches and associated knowledge gaps.

In Chapter 2, systemic causation models were reviewed and applied to OUOGD. Comprehensive OUOGD process and control structure models were developed, which aligns with objective 1. This work fills a significant research opportunity with the first critical review and feasibility study of applying systemic causation models to assess environmental and public health risks associated with OUOGD and provides a catalyst for future research. After examining popular linear and systemic risk assessment methods, benefits, and limitations, a critical assessment of systemic techniques in OUOGD was provided. A three-level OUOGD process model (field development, pad-well, and well-phase) was synthesized from incomplete models found in the literature. The STAMP was applied to elucidate a general risk control structure from diverse and multi-disciplinary references. Further, this general control structure was used to

highlight the importance of leveraging systemic analysis approaches for environmental and public health risk management in OUOGD. The increasing significance of these methods given the adoption of new digital technology (e.g., drones, robotics, big data analytics, artificial intelligence, internet of things) to decision-making is evident.

The exploration and development of HF disclosure metrics and trends are provided in Chapter 3, achieving objective 2. Investigating chemical transparency is an essential step in the research process because information availability is critical to performing risk assessments. In Chapter 3, two new policy-level performance indicators were developed and presented for measuring HF chemical transparency to address the limitations of existing metrics and provide additional perspectives to stakeholders, which is an important contribution to this field of study. Based on the new indicators, state-level policy changes and the FF register have increased HF chemical transparency over the past decade and continue to drive measurable improvements. The percent of wells with publicly disclosed ingredients increased from ~0% to 95% (2010-2019), and the average percent of HF fluid mass withheld on chemical disclosure forms decreased ~46.8% (2013-2019). The percent ingredient mass withholding was used to compare the two current regulatory chemical disclosure form approaches (system and traditional). In 2019, the average percent of HF fluid mass withheld on system approach chemical disclosure forms (0.044%) was 66.3% less than the traditional forms (0.132%). This research presented in Chapter 3 improves stakeholder capabilities to understand, evaluate, and communicate the effect of chemical transparency policy decisions and corporate practices.

Chapter 4, relating to objective 3, presented a novel method for processing publicly and proprietary HF chemical information to examine chemical variety over time and influencing factors. In addition, it provided valuable and new risk context in the form of a comparative

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analysis between hydraulic fracturing and non-hydraulic fracturing reference chemical list, including reported food, cosmetics, and water-related additives and contaminants. The quantity and quality of disclosed HF chemical information are significant barriers for stakeholders attempting to perform systemic environmental and public health research. Critical field contributions from the work provided in this chapter include the development of a repeatable approach for processing HF chemical disclosure data, filling a gap in peer-review literature by examining HF chemical trends between 2014 and 2020, and comparing HF chemicals with a list of reference chemicals known or suspected to be in contact (unrelated to HF) with drinking water, food, or cosmetics. In total, 1,244 unique HF chemicals were identified. Compared with EPA's 2016 HF chemical disclosure research, 480 new chemicals were identified, and 318 previously reported chemicals were not observed. The annual unique chemical counts were found to have dropped from 878 to 594 (32.3%) over the 6-year period, while data quality and transparency have increased. Approximately 69.7% of the identified HF ingredients were found in a list of reference chemicals known or suspected to be in contact (unrelated to HF) with drinking water, food, or cosmetics. Chemical differences between production types (gas and oil) and states were also reviewed. The finding revealed that the sociotechnical system surrounding HF is dynamic and moving toward fewer and, in general, safer chemicals.

The repeatable approach for reporting systemic hydraulic fracturing chemical risk factors developed and documented in Chapter 5, achieving objective 4, is an essential step forward in this field of study. The method produced for generating an annual composite HF well is unique and foundational for future research because it provides the estimated average mass percent for each HF chemical disclosed in the U.S. for a given year. The methodology can be easily adapted for varying spatial and temporal boundaries. Analyzing the estimated total annual mass percent

of water, sand, and other ingredient indicated a significant decrease (3.4% to 0.8%) in chemical additives (i.e., non-water and sand) between 2014 and 2020. Another important contribution of this work is developing an original technique for calculating percent mass-weighted average risk indicators associated with variables of interest. Toxicity (i.e., rat oral LD50), mobility (i.e., octanol/water partition coefficient), volatility (i.e., Henry's constant), and persistence (i.e.,) risk factors were selected for examination. Readily available *in silico* data, generated using QSAR, from EPA's CompTox databases was used to illustrate the percent mass-weighted average calculations and provide insights into systemic HF chemical risk factor trends. Hydraulic fracturing activity levels and the annual form average mass percentages for non-water and sand additives indicate a lower level of systemic chemical risk to drinking water. Chemical mobility risk levels, based on K_{ow} and K_{oc} metrics, appear to have decreased. However, the calculated mass percent weighted risk indicators, based on a subset of chemicals, suggest that there has been little change in hydraulic fracturing chemical toxicity and persistence system hazard levels. An aggregated relative risk metric was developed and applied to unveil 42.6% risk reduction between 2014 and 2020. Well count, chemical concentration, soil adsorption, and octanol/water partition have the most significant impact on the combined indicator's decreasing trend over this period. These risk indicators can be used as value feedback between system functions throughout the OUOGD control structure to prevent drift toward a more hazardous system state or promote a safer system state.

OUOGD and HF remain current global energy policy issues, and understanding associated environmental and public health risks is an essential aspect of these topics. The research presented in this dissertation provides immediate value to diverse stakeholder groups

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(public, researchers, policymakers, industry) regarding HF chemical transparency, variety, and hazard levels. In addition, it lays a solid foundation for future research.

6.2. Future Work Recommendations

This dissertation highlights the value and opportunities for new and updated systemic studies regarding HF chemical hazard dynamics and associated risk to the environment and public health. Recent lessons learned from the oil and gas industry should be used to study broader chemical transparency policies, information systems, and communication strategies. The content throughout this document captured some research implications and proposed future perspectives. In this section, specific implications and recommendations for researchers and practitioners are provided. In general, researchers and practitioners (i.e., companies and regulators) should thoughtfully embrace system thinking in their work to enhance the associated body of knowledge for understanding and preventing OUOGD accidents with potential impacts on public health and the environment.

6.2.1. Systemic Risk Assessments

For researchers, the opportunities to advance the topic of systemic risk assessments in OUOGD appear limitless. A first step would be to apply systemic hazard analysis to previous OUOGD environmental and public health risk assessment case studies that relied on linear causation concepts and models. In addition, comparing the two thought processes and results would be worthy of academic contributions. The development of case- and risk-specific control structures required for this research would be valuable to business, regulatory, and public stakeholders. Focusing on threats to water sources (quality and quantity) and air quality is recommended because these media have received most of the attention in policy discussion and peer-review research to date. Researchers should leverage and help improve the FF and Risk

Based Data Management System developed by GWPC (Groundwater Protection Council, 2021, 2020) with sponsorship by the U.S. Department of Energy, as well as EPA's CompTox dashboard, NIH's PubChem, and other existing chemical databases. Society will benefit from the continuous enhancement of systemic risk monitoring capabilities and information system usability. These are noble research objectives that will undoubtedly help ensure the safe development of unconventional hydrocarbon resources.

Other researchers have identified current safety and risk management research momentum in the areas of inherently safer design, risk quantification, dynamic risk assessments, and incorporation of human factors (Khan et al., 2015). There are no reasons to deviate from these general risk areas, and applying systemic hazard analysis approaches to OUOGD can contribute to these valuable research areas. In addition, there are opportunities to study why systemic frameworks, techniques, and tools are challenging to develop, employ, and adopt.

For practitioners (e.g., operators, service companies, regulators), change can be simultaneously challenging and fruitful; all benefits come with costs and risks. Partnering with universities and consulting companies that have experience with systemic hazard assessment techniques in addition to linear causation-related capabilities is recommended. Invest in applying these methods and seek related training for leaders, risk managers, and engineers. Researchers should supplement existing hazard and risk assessment activities in the development process and accident investigations with systemic hazard and accident analysis tools. Followed activities should include comparing results with traditional approaches and communicating learnings with stakeholders to foster a shared mental model. Practitioners will find the methods discussed in this dissertation (Chapter 2) critical during risk-based decision-making processes related to complex OUOGD system(s) composed of human, digital, and physical elements.

6.2.2. Transparency

The significant amount of hydraulic fracturing chemical information (Groundwater Protection Council, 2021) and open-source data science tools (Allison, 2021) made available over the past decade opens up vast research opportunities, with relatively low entry barriers, for understanding related chemical transparency and risk trends. Research leveraging these resources to develop novel analytical methods for tracking specific chemicals or chemical types withheld over time would benefit stakeholders by showing the evolution and duration of hydraulic fracturing chemical trade secret claims. In addition, investigating the relationship between chemical disclosure, hazard levels, and innovation would be valuable because innovation is central to trade secrets and confidentiality claims. Likewise, studying public decisions and actions informed by the currently available information could help stakeholders understand if additional information is necessary. Industry, state, federal, special interest, and academic stakeholders appear to use FF data; however, the public use and perception of the available information have not been sufficiently studied. Chemical transparency metrics should be developed and standardized across all industries to allow for objective cross-industry comparisons to help shape and prioritize holistic policy changes when and where appropriate.

6.2.3. Chemical Variety and Hazard Levels

With an updated list of chemicals and a repeatable process for cleaning public HF chemical disclosure information, the opportunity to investigate potential adverse environmental and public health impacts, including drinking water resource contamination, caused by HF is enhanced. It is recommended that researchers seize this opportunity. In addition, there is significance in performing and updating risk assessments, fate and transport, and toxicological studies related to hydraulic fracturing chemicals that may have been conducted on stale

information and comparing these results with reference chemicals. There appear to be research opportunities associated with addressing risk-risk and risk-benefit trade-offs systemic analysis methods. For example, the purpose of some toxic HF chemicals is to protect wellbore mechanical integrity (e.g., barriers to drinking water resources), which means they are both hazards and risk controls. Research integrating additional chemical information into the defined risk metrics found in Chapter 5 will allow for system behavior claims.

Supporting "greener" chemical product development and related decision support tools should be a priority. In addition, maturing and fostering the use of environmental, social, and governance key performance indicators related to industrial chemicals would be beneficial. An improved understanding of chemical risk metrics and related research could lead to valuable and novel knowledge of system behaviors, risk-benefit decisions, management practices, and risk perception. The foundational research presented in this dissertation indicates past progress and future opportunities for improvement related to hydraulic fracturing chemical stewardship. Future research, practice, and policies that can increase momentum toward safer chemicals and transparency across all industries in the future are anticipated.

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APPENDIX A. DISCLOSURE AND TRANSPARENCY METRICS AND TRENDS

SUPPORTING INFORMATION

A.1. Literature Review Search Terms

'chemical risk*,' 'chemical disclosur*,' 'chemical transparen*,' 'chemical withhold*,' 'withheld chemical*, 'hydraulic fracturing,' 'oil and gas,' 'unconventional oil,' 'unconventional gas,' 'petroleum,' 'hydrocarbon resources,' 'shale oil,' and 'shale gas.'

A.2. FracFocus Column Names

'UploadKey', 'JobStartDate', 'JobEndDate', 'APINumber', 'StateNumber', 'CountyNumber', 'OperatorName', 'WellName', 'Latitude', 'Longitude', 'Projection', 'TVD', 'TotalBaseWaterVolume', 'TotalBaseNonWaterVolume', 'StateName', 'CountyName', 'FFVersion', 'FederalWell', 'IndianWell', 'Source', 'DTMOD', 'PurposeKey', 'TradeName', 'Supplier', 'Purpose', 'SystemApproach', 'IsWater', 'PurposePercentHFJob', 'PurposeIngredientMSDS', 'IngredientKey', 'IngredientName', 'CASNumber', 'PercentHighAdditive', 'PercentHFJob', 'IngredientComment', 'IngredientMSDS', 'MassIngredient', 'ClaimantCompany', 'DisclosureKey'

A.3. FracFocus Quality Filter Summary

1. Removed duplicate rows

2. Removed system rows

3. Removed duplicate forms

4. Removed forms not between 2011 and 2019

5. Removed forms containing non-system rows with percent mass values null or equal to 0

6. Removed forms with total percent mass not between 95% and 105%

7. Removed forms with total mass not less than the high 95% confidence interval of the unfiltered dataset (430,235,008 pounds)

A.4. FracFocus Withholding Synonyms

' Proprietar', ' Proprietary', '3rd Party Proprietar', '3rd party proprietar', '7732-18-5/ propr', '7732-18-5proprietary', 'Business Confidental', 'CBI', 'CONFIDENTIAL', 'CONFIDENTIAL BUSINES', 'COnfidential', 'Coinfidential', 'Condidential', 'Conf Bus Info', 'Confdential', 'Confid. Bus. Info', 'Confidenial', 'Confidentail', 'Confidental', 'Confidentia1', 'Confidential', 'Confidential ', 'Confidential Busines', 'Confidential Info', 'Confidnetial', 'Confindential', 'Confinential', 'P', 'PRIOPRIETARY', 'PROP', 'PROPRIERARY', 'PROPRIERTARY', 'PROPRIETARY', 'PROPRIETARY ', 'PROPRIETARY 0.10', 'PROPRITARY', 'PRORIETARY', 'Porprietary', 'Priprietary', 'Prop', 'Prop.', 'Properitary', 'Propietary', 'Propietary ', 'Propreitary', 'Propreitory', 'Propriatary', 'Proprieatary', 'Proprietar', 'Proprietart', 'Proprietarty', 'Proprietary', 'Proprietary ', 'Proprietary ', 'Proprietary ', 'Proprietary Blend', 'Proprietaryl', 'Proprietatry', 'Proprietery', 'Proprietory', 'Propriety', 'Propritary', 'Proptietary', 'TRADE SECERET', 'TRADE SECRET', 'TRADE SECRETS', 'TS', 'Third Party', 'Trad Secret', 'Trade', 'Trade Name', 'Trade SEcret', 'Trade Seceret', 'Trade Secert', 'Trade Secrer', 'Trade Secret', 'Trade Secret ', 'Trade Secret , disc.', 'Trade Secret, disc.', 'Trade Secrte', 'Trade secret', 'Trade secret.', 'TradeSecret', 'confidential', 'p', 'prop', 'propietary', 'propriatary', 'proprietarty', 'proprietary', 'proprietory', 'proprietry', 'propriety', 'trace secret', 'trade Secret', 'trade seccret', 'trade secret', 'trade secret ', 'ts'

A.5. Annual Well Frequencies

Table A1. Annual well frequencies.

Year	Gallegos et al., 2015	Estimated HF Wells	FF Wells*	FF Wells Withheld*	FF Wells After Quality Filters*
2010	25,569	25,569			
2011	29,650	29,650	13,921	143	28
2012	31,073	31,073	24,155	1,223	384
2013	29,114	29,114	26,686	16,730	9,042
2014		30,935	27,401	21,425	14,335
2015		17,436	16,613	12,656	8,247
2016		10,168	9,640	7,871	5,006
2017		14,633	13,797	11,626	8,755
2018		17,662	16,942	14,396	10,687
2019		15,767	14,999	12,373	9,209

*FracFocus wells were filtered for date range (2011 to 2019)

A.6. Annual Form Frequencies

Table A2. Annual form frequencies.

Year	FF Forms*	FF Forms Withheld*	FF Forms After Quality Filters	FF System Forms*	FF System Forms After Quality Filters*
2011	14,303	152	93	2	1
2012	24,921	1,301	850	44	37
2013	27,958	17,915	13,605	970	709
2014	28,796	22,659	20,190	1,814	1,631
2015	17,350	13,325	11,213	1,463	1,306
2016	10,053	8,257	6,655	3,740	2,551
2017	14,353	12,151	10,923	10,070	7,355
2018	17,626	15,007	13,314	12,103	9,023
2019	15,530	12,747	11,417	9,989	7,383

*FracFocus wells were filtered for date range (2011 to 2019)

A.7. Annual Average Chemical Frequencies (After Quality Filters)

Table A3. Annual average chemical frequencies (after quality filters).

Year	Total Chemicals	Withheld Chemicals	System Form Total Chemicals	System Form Withheld Chemicals	Traditional Form Total Chemicals	Traditional Form Withheld Chemicals
2011	29.15	3.05				
2012	31.48	5.19				
2013	34.60	5.77				
2014	34.08	5.81				
2015	32.82	5.10				
2016	30.15	4.48	30.16	5.12	30.14	4.08
2017	29.44	4.55	29.29	5.06	29.76	3.50
2018	27.81	4.20	27.39	4.52	28.71	3.51
2019	25.57	4.00	25.55	4.62	25.59	2.87

A.8. Annual System Approach Disclosure Form Proportions

Percent of hydraulic fracturing disclosure forms classified as using the system approach before and after applying data quality criteria.

Table A4. Annual system approach disclosure form proportions.

Year	FF System Forms*	FF System Forms After Quality Filters
2011	0.0%	1.1%
2012	0.2%	4.4%
2013	3.5%	5.2%
2014	6.3%	8.1%
2015	8.4%	11.6%
2016	37.2%	38.3%
2017	70.2%	67.3%
2018	68.7%	67.8%
2019	64.3%	64.7%

*FracFocus wells were filtered for date range (2011-2019)

A.9. Annual Well Withheld Disclosure Proportions

Percent of hydraulic fracturing disclosure forms classified as "withheld" before and after applying data quality criteria.

Table A5. Annual well withheld disclosure proportions.

Year	FF Form Withholding Rate*	FF Form Withholding Rate After Quality Filters*
2011	1.1%	69.9%
2012	5.2%	77.1%
2013	64.1%	85.6%
2014	78.7%	78.9%
2015	76.8%	75.0%
2016	82.1%	82.9%
2017	84.7%	85.7%
2018	85.1%	84.5%
2019	82.1%	80.7%

*FracFocus wells were filtered for date range (2011-2019)

A.10. Base Water Volume Descriptive Statistics

Table A6. Base water volume descriptive statistics (all values are in gallons, except counts).

Statistic	FF Forms (2011-2019) *	FF Forms After Quality Filters (2011-2019)	FF System Forms After Quality Filters (2019)	FF Traditional Forms After Quality Filters (2019)
count	140,915	88,260	26,312	15,997
sum	908,394,818,002	596,673,585,380	278,950,035,179	155,775,885,286
max	592,516,724	71,598,798	63,899,934	40,778,556
99ci_h	6,496,238	6,821,713	10,726,789	9,901,161
95ci_h	6,484,321	6,807,053	10,696,860	9,862,101
mean	6,446,403	6,760,408	10,601,628	9,737,819
std	7,262,283	7,070,268	7,881,374	8,019,953
95ci_l	6,408,484	6,713,762	10,506,396	9,613,537
99ci_l	6,396,567	6,699,102	10,476,466	9,574,476
min	0	0	0	0
95pctl	20,571,508	21,127,928	24,624,843	24,087,699
75pctl	9,637,770	10,457,062	15,543,192	15,727,730
median	4,322,954	4,752,573	9,736,385	8,852,718
25pctl	983,275	785,392	4,754,836	2,194,080
05pctl	34,268	32,172	56,376	34,915

A.11. Total Ingredient Mass Descriptive Statistics

Table A7. Total ingredient mass descriptive statistics (all values are in pounds, except counts).

Statistic	FF Forms (2011-2019) *	FF Forms After Quality Filters (2011-2019)	FF System Forms After Quality Filters (2019)	FF Traditional Forms After Quality Filters (2019)
count	170,890	88,260	7,383	4,034
sum	40,611,881,768,285	4,761,844,848,302	725,466,699,442	415,543,764,642
max	10,852,153,305,775	424,677,580	424,677,580	399,504,919
99ci_h	501,775,875	54,531,952	100,801,450	106,364,578
95ci_h	438,615,162	54,393,380	100,194,137	105,562,481
mean	237,649,258	53,952,468	98,261,777	103,010,353
std	42,386,214,756	66,830,925	84,712,682	82,701,661
95ci_l	36,683,355	53,511,557	96,329,417	100,458,226
99ci_l	-26,477,358	53,372,984	95,722,104	99,656,129
min	0	0	0	0
95pctl	176,034,747	194,902,998	243,176,278	239,983,800
75pctl	53,316,208	88,353,648	160,012,741	169,605,824
median	797,369	23,758,742	90,309,914	95,488,528
25pctl	0	719,615	10,445,521	18,147,349
05pctl	0	0	0	0

A.12. Average Percent Mass Withholding Rate Descriptive Statistics

Table A8. Average percent mass withholding rate descriptive statistics (all values are in percent mass, except counts).

Statistic	FF Forms (2013-2019)*	FF Forms After Quality Filters (2013-2019)	FF System Forms After Quality Filters (2019)	FF Traditional Forms After Quality Filters (2019)
count	102,061	87,317	7,383	4,034
max	475.0000%	96.5368%	2.9325%	89.5431%
99ci_h	0.2694%	0.1214%	0.0474%	0.2026%
95ci_h	0.2640%	0.1188%	0.0467%	0.1857%
mean	0.2469%	0.1107%	0.0444%	0.1319%
std	2.7890%	1.2236%	0.0999%	1.7438%
95ci_l	0.2298%	0.1026%	0.0422%	0.0781%
99ci_l	0.2244%	0.1000%	0.0414%	0.0612%
min	0.0000%	0.0000%	0.0000%	0.0000%
95pctl	0.4015%	0.3047%	0.1647%	0.1375%
75pctl	0.0967%	0.0830%	0.0542%	0.0445%
median	0.0403%	0.0305%	0.0183%	0.0180%
25pctl	0.0091%	0.0017%	0.0003%	0.0013%
05pctl	0.0001%	0.0000%	0.0000%	0.0000%

* Removed System and duplicate rows.

A.13. Annual Average Percent Mass Withholding Rates by Disclosure Approach

Table A9. Annual average percent mass withholding rates by disclosure approach.

Year	System Form Percent Mass Withholding Rate Mean*	Traditional Form Percent Mass Withholding Rate Mean*	System Form Percent Mass Withholding Rate Std*	Traditional Form Percent Mass Withholding Rate Std*
2016	0.052%	0.143%	0.235%	2.445%
2017	0.114%	0.097%	2.525%	0.549%
2018	0.083%	0.144%	1.101%	1.135%
2019	0.044%	0.132%	0.100%	1.744%

*After quality filters

A.14. Annual Well Disclosure, Form Withholding, and Ingredient Withholding Rates

Table A10. Annual well disclosure, form withholding, and ingredient withholding rates.

Year	Well Disclosure Rate	Form Withholding Rate*	Ingredient Withholding Rate*	Average Percent Mass Withholding Rate*
2010	0.00%			
2011	46.95%	69.89%	10.48%	
2012	77.74%	77.06%	16.50%	
2013	91.66%	85.56%	16.69%	0.142%
2014	88.58%	78.94%	17.04%	0.122%
2015	95.28%	74.98%	15.53%	0.101%
2016	94.81%	82.90%	14.85%	0.108%
2017	94.29%	85.71%	15.45%	0.109%
2018	95.92%	84.51%	15.09%	0.103%
2019	95.13%	80.69%	15.65%	0.075%

*After quality filters

A.15. Annual Form Withholding and Ingredient Withholding Rates by Disclosure

Approach

Table A11. Annual form withholding and ingredient withholding rates by disclosure approach.

Year	System Form Withholding Rate*	Traditional Form Withholding Rate*	System Ingredient Withholding Rate*	Traditional Ingredient Withholding Rate*
2016	79.11%	85.26%	16.97%	13.53%
2017	84.47%	88.26%	17.27%	11.77%
2018	83.41%	86.81%	16.51%	12.24%
2019	79.25%	83.32%	18.07%	11.24%

*After quality filters

A.16. Traditional Hydraulic Fracturing Chemical Disclosure Approach Form

Hydraulic Fracturing Fluid Product Component Information Disclosure

Job Start Date:	6/7/2019
Job End Date:	6/20/2019
State:	Texas
County:	Martin
API Number:	42-317-41902-00-00
Operator Name:	Diamondback E&P LLC
Well Name and Number:	Shortes 40 Unit 2LS
Latitude:	32.47391500
Longitude:	-101.72338300
Datum:	NAD27
Federal Well:	NO
Indian Well:	NO
True Vertical Depth:	8,168
Total Base Water Volume (gal):	18,483,528
Total Base Non Water Volume:	0

Frac Focus Chemical Disclosure Registry

GROUNDWATER PROTECTION COUNCIL

INTERSTATE Oil & Gas COMPACT COMMISSION

Hydraulic Fracturing Fluid Composition:

Trade Name	Supplier	Purpose	Ingredients	Chemical Abstract Service Number (CAS #)	Maximum Ingredient Concentration in Additive (% by mass)**	Maximum Ingredient Concentration in HF Fluid (% by mass)**	Comments
Water	Operator	Carrier/Base Fluid					
			Water	7732-18-5	100.00000	89.65107	None
Sand	Santrol	Proppant					
			Silica	14808-60-7	100.00000	9.72581	None
HA04-10-15% HCL	Reagent Chemical	Acidizing					
			Water	7732-18-5	85.00000	0.39649	None
			Hydrogen Chloride	7647-01-0	15.00000	0.06997	None
CNS-127L	PFP Industries	Anionic Friction Reducer					
			Polyacrylamide	9003-05-8	80.00000	0.05675	None
			Nonylphenol Ethoxylate	9016-45-9	50.00000	0.03547	None
BX 1919 FracGlass	BEXCO	Diverter					
			Synthetic Polymer	Proprietary	82.50000	0.04524	None
CS 14R	BEXCO	Clay Stabilizing Agent					
			Clay Stabilizer	67-48-1	22.50000	0.00574	None
IC5-Iron Control	Solnexus	Iron Control					
			Water	7732-18-5	60.00000	0.00134	None
			Acetic Acid	64-19-7	60.00000	0.00134	None
			Citric Acid	77-92-9	30.00000	0.00067	None
LG1W4	BEXCO	Guar Slurry					
			Trade Secret	64742-47-8	55.00000	0.00116	None
CI200-Corrosion Inhibitor	Economy Polymers	Corrosion Inhibitor					
			Methanol	67-56-1	60.00000	0.00040	None
NE116-Plexbreak 116	Chemplex	N/E Surfactant					
			Methanol	67-56-1	50.00000	0.00017	None
			Alkyl Quarternary Ammonium Chlorides	7173-51-5	25.00000	0.00009	None
			Isopropanol	67-63-0	5.00000	0.00002	None
			Diethanolamide	111-42-2	2.00000	0.00001	None

Ingredients shown above are subject to 29 CFR 1910.1200(i) and appear on Material Safety Data Sheets (MSDS). Ingredients shown below are Non-MSDS.

* Total Water Volume sources may include fresh water, produced water, and/or recycled water
** Information is based on the maximum potential for concentration and thus the total may be over 100%

Note: For Field Development Products (products that begin with FDP), MSDS level only information has been provided.
Ingredient information for chemicals subject to 29 CFR 1910.1200(i) and Appendix D are obtained from suppliers Material Safety Data Sheets (MSDS)

Figure A1. Traditional hydraulic fracturing chemical disclosure approach form.

A.17. System Hydraulic Fracturing Chemical Disclosure Approach Form with Research

Data Processing Steps

Figure A2. System hydraulic fracturing chemical disclosure approach form with research data processing steps.

APPENDIX B. CHEMICALS USED IN HF DRINKING WATER TOXICITY, PERSISTENCE, AND FATE/TRANSPORT RISK INDICATOR CALCULATIONS

PREFERRED_NAME	ORAL RAT_LD50 (MOL/KG)	BIODEG HALF-LIFE_ (DAYS)	HENRY'S LAW CONSTANT (ATM-M³/MOLE)	SOIL ADSORP. COEFF $K_{OC\_}$ (L/KG)	OCTANOL WATER_ PARTITION K_{OC} (LOG)	WATER SOLUBILITY (MOL/L)
Methanol	-	7.57468	4.55795E-06	2.75443	-0.768744	32.6434
Ethylene glycol	0.0107895	7.56532	5.99948E-08	5.59292	-1.35982	14.3907
Choline chloride	-	4.13405	1.80848E-05	12.1051	-2.03656	4.64483
Isopropanol	0.0537032	7.53284	8.08862E-06	3.4364	0.0519477	9.00523
Methenamine	0.00756833	34.0792	1.52861E-07	132.233	-0.164859	0.243402
Potassium carbonate	-	7.57763	3.7792E-09	3.85959	-0.991871	0.0170393
Isobutane	0.00877001	10.2271	0.452597	17.8833	2.75772	0.00127184
Ethanol	0.0171396	4.59705	5.01351E-06	1.59008	-0.309717	18.103
Citric acid	0.0167109	4.09194	1.54655E-10	119.011	-1.64024	4.90398
Acetic acid	0.0576766	4.59912	1.00453E-07	1.00727	-0.170189	13.4017
Glutaraldehyde	0.00660693	3.6748	1.64442E-07	21.9208	-0.138385	1.66425
Tetrakis(hydroxymethyl)phosphonium sulfate	-	-	9.97106E-09	-	0.658086	0.56913
Propargyl alcohol	0.00190546	4.70932	5.61983E-06	6.04601	-0.379439	17.8018
Dazomet	0.00166725	4.35852	2.67833E-10	10.0245	0.630444	0.0154425
Propylene pentamer	-	3.7118	0.000407166	1495.74	4.30804	1.68005E-05
Undecane	0.0476431	7.02874	0.147228	715.928	6.53656	2.77518E-08
Ammonium acetate	0.0486407	4.59912	1.00453E-07	1.00727	-0.754198	13.4017
Butane	0.0963829	7.39001	0.471425	22.8012	2.88914	0.00108058
2-Butoxyethanol	0.0110408	4.43924	1.59344E-06	67.3685	0.828046	1.07776
Sodium bicarbonate	-	7.57763	3.7792E-09	3.85959	-0.698834	0.0170393
Formic acid, potassium salt	-	6.10776	1.67961E-07	5.39642	-0.954526	10.578
Glycerol	0.113763	5.37604	1.72905E-08	3.57275	-1.86013	11.9579
Triethanolamine	0.0340408	3.6689	5.8416E-11	18.9028	-1.00059	6.70355
Tetramethylammonium chloride	-	14.793	0.207737	16.1593	-2.63956	1.74124
N,N'-Bis[2-[bis(2-hydroxyethyl)methylammonio]ethyl]-N,N'-bis(2-hydroxyethyl)-N,N'-dimethyl-1,2-ethanediaminium tetrachloride	-	212.58	1.12707E-10	3560.95	0.448417	0.163925
Dodecane	0.0343558	10.0083	0.144964	1557.81	6.09948	2.16933E-08
2,2-Dibromo-3-nitrilopropionamide	-	6.48935	2.24037E-09	5.31943	0.819694	0.0622964
Acetic anhydride	0.0151705	7.55998	1.18288E-06	16.0933	0.228498	1.1766
Tridecane	0.0246604	12.0308	0.144541	1897.74	6.20222	2.54754E-08
Tetradecane	0.0238232	22.8926	0.018499	3056.69	7.59851	1.33518E-08
Furfuryl alcohol	0.00247742	4.44606	1.76634E-07	12.1871	0.279294	10.1981

PREFERRED_NAME	ORAL RAT_LD50 (MOL/KG)	BIODEG HALF-LIFE_ (DAYS)	HENRY'S LAW CONSTANT (ATM-M³/MOLE)	SOIL ADSORP. COEFF $K_{OC\_}$ (L/KG)	OCTANOL WATER_ PARTITION K_{OC} (LOG)	WATER SOLUBILITY (MOL/L)
2-Mercaptoethanol	0.00487529	4.10964	9.71333E-07	9.63243	-0.390373	12.737
2-(Hydroxymethyl)-2-nitro-1,3-propanediol	0.0144544	6.7308	4.3762E-08	10.4463	-1.71689	9.80476
Ethylbenzene	0.0269153	7.97895	0.00784744	170.406	3.1503	0.00164047
1,2-Propylene glycol	0.0534564	4.268	6.05478E-08	2.3048	-0.918877	13.1545
Formic acid	0.0416869	6.10776	1.67961E-07	5.39642	-0.540235	10.578
Sorbitan, mono-(9Z)-9-octadecenoate	0.0659174	4.47877	1.13064E-08	14096.1	4.76345	5.98702E-06
Glycolic acid sodium salt	0.0122462	4.71857	5.37489E-09	7.3753	-1.87726	3.04018
Didecyldimethylammonium chloride	0.000677641	37.3309	1.5708E-06	14558.7	2.68311	1.33946E-08
Triethylene glycol	0.0803526	7.57623	4.62289E-09	34.4384	-1.74729	6.65589
Fumaric acid	0.00959401	5.33546	6.77597E-09	8.6883	-0.480755	0.0613067
1-Butoxy-2-propanol	0.0134896	4.62946	1.55302E-06	28.6002	1.01577	0.914376
Propane	0.0147571	7.51578	0.392059	8.6207	2.36022	0.00143983
Ethanolamine	0.0371535	4.71522	5.96167E-08	4.35443	-1.31189	16.3514
Naphthalene	0.0109648	3.02366	0.000439338	913.843	3.29634	0.000245181
D-Glucitol	0.0912011	6.65126	9.16758E-11	61.7277	-2.38029	3.30821
Sucrose	0.05188	4.65877	2.22077E-11	41.4259	-3.69895	6.10813
Sodium carbonate	-	7.57763	3.7792E-09	3.85959	-0.698834	0.0170393
Ethylenediaminetetraacetic acid tetrasodium salt	0.00479733	4.96007	2.27935E-11	37.8169	-1.51285	0.00342189
Calcium carbonate	-	7.57763	3.7792E-09	3.85959	-0.999448	0.0170393
2-(2-Butoxyethoxy)ethanol	0.0380189	3.67678	7.19083E-09	36.5981	0.56022	6.15347
2-Ethyl-1-hexanol	0.0130918	4.34434	3.02603E-05	61.7104	2.89345	0.00703873
Diethanolamine	0.0203236	3.67054	2.96888E-09	3.98126	-1.43017	9.50892
2-(2-Ethoxyethoxy)ethyl acetate	0.0528445	4.13542	4.57787E-05	22.6365	0.454846	5.51152
D-Limonene	0.0368129	2.93262	0.022543	2297	4.51408	9.09154E-05
Benzyltrimethylammonium chloride	-	12.2353	0.0377046	6816.13	-2.17068	8.53595E-05
4,4-Dimethyl oxazolidine	0.0103514	5.40291	7.1898E-07	11.7892	0.757919	4.15061
Sodium erythorbate	0.0885116	3.53988	8.44548E-10	151.535	-2.16424	2.07263
Tributyltetradecylphosphonium chloride	-	-	9.28405E-07	-	6.06921	1.11831E-08
Phosphonic acid, [[(phosphonomethyl)imino]bis[2,1-ethanediylnitrilobis(methylene)]]tetrakis-	0.0101391	4.07594	2.69398E-11	58.8288	-3.47319	0.367533
Pentane	0.091622	5.025	1.24351	34.1828	3.38778	0.000591003
2-Methylbutane	0.0338844	6.05292	0.60086	56.7424	3.00337	0.000666351
1,2,4-Trimethylbenzene	0.0282488	4.01399	0.00620397	846.864	3.62962	0.000473872
Benzyl chloride	0.0153462	4.86936	0.00291872	75.1454	2.30213	0.00484108
1-Propanol	0.00990832	4.43043	7.41659E-06	3.03193	0.248727	10.4512

PREFERRED_NAME	ORAL RAT_LD50 (MOL/KG)	BIODEG HALF-LIFE_ (DAYS)	HENRY'S LAW CONSTANT (ATM-M³/MOLE)	SOIL ADSORP. COEFF $K_{OC\_}$ (L/KG)	OCTANOL WATER_ PARTITION K_{OC} (LOG)	WATER SOLUBILITY (MOL/L)
Acetone	0.0626614	7.56577	3.53224E-05	3.6548	-0.23752	17.0631
1,3-Dimethylbutylamine	0.00687068	5.18818	0.000031071	29.8408	1.50612	1.38766
Lactic acid	0.0494311	5.43152	8.92977E-09	10.1804	-0.720713	3.22296
2-Hydroxy-N~1~,N~1~,N~1~,N~3~,N~3~,N~3~-hexamethylpropane-1,3-bis(aminium) dichloride	-	7.20618	4.52862E-05	263.147	-2.24101	0.230261
2-Methyl-1-propanol	0.0128825	3.67057	9.7678E-06	12.0246	0.761386	1.11957
Urea	0.0363915	7.5801	5.43991E-09	1.41784	-1.88328	9.18616
Benzoic acid	0.0103276	6.6407	2.66769E-07	31.66	1.87054	0.331734
Aminotrimethylene phosphonic acid	0.0161436	4.58428	1.57001E-11	70.8421	-3.5292	3.34074
N,N-Dimethylformamide	0.0474242	7.57424	7.35845E-08	15.761	-1.01029	13.691
tert-Butyl hydroperoxide	-	7.56503	4.89813E-06	14.4244	1.23147	6.69313
Trimethyl borate	-	7.60384	9.79077E-05	18.6762	0.772815	3.28289
Propylene carbonate	0.0288403	4.12751	1.50428E-08	22.7124	-0.409571	1.71502
Methyl salicylate	0.0153815	3.54314	7.70245E-08	55.7648	2.54681	0.0149092
4-Nonylphenol	0.0116681	3.73484	1.05562E-05	6913.46	5.75732	3.02827E-05
Choline bicarbonate	-	4.13405	1.80848E-05	12.1051	1.37797	4.64483
Sodium acetate	0.0486407	4.59912	1.00453E-07	1.00727	-1.21999	13.4017
Dibromoacetonitrile	0.000961612	5.7488	4.27371E-06	81.0326	2.01986	0.236931
Acetyltriethyl citrate	0.0141906	3.81664	2.00823E-09	259.148	1.63803	0.00768279
Diethylenetriamine	0.03155	3.67146	2.96485E-09	4.03999	-0.82862	9.63793
Lactose	0.0572796	4.83929	2.15008E-11	41.3923	-3.26167	0.58306
1,3,5-Trimethylbenzene	0.0272898	3.00739	0.00867811	658.527	3.50232	0.000408968
1,2,3-Trimethylbenzene	0.0433511	4.01295	0.00444257	631.602	3.62541	0.000619463
2-Hydroxy-N,N-bis(2-hydroxyethyl)-N-methylethanaminium chloride	-	4.12505	5.99178E-11	30.1914	-0.693208	11.2941
1-Butanol	0.0105439	4.43732	8.83859E-06	3.22078	0.879541	0.950064
Diethylene glycol	0.0382825	6.13275	2.96077E-09	4.08583	-1.09389	9.41761
Formaldehyde	-	8.20857	3.49471E-07	2.72646	0.349206	14.6625
Tetraethylenepentamine	0.0126474	4.24899	7.9165E-11	10.5872	-0.262153	34.4327
(9Z)-N,N-Bis(2-hydroxyethyl)octadec-9-enamide	0.0246037	5.81727	1.04058E-10	14008.7	4.33785	0.000110722
3-Phenylprop-2-enal	0.0179061	4.81723	6.57199E-05	66.9829	1.89921	0.0107571
Glycine, N,N-bis(carboxymethyl)-, trisodium salt	0.00665273	3.67571	2.83042E-10	63.6266	-1.60361	0.309304
Tetrasodium etidronate	0.0348337	3.67827	2.40378E-09	47.4887	-0.901835	3.34461
Bronopol	0.000629506	4.84982	2.6965E-07	10.3771	-0.413783	1.25417
Glyoxal	0.0218776	7.57643	3.38633E-09	7.17319	-0.0751466	17.1861

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Butyl glycidyl ether	0.0137721	3.8151	0.000128299	50.55	0.630557	0.155178
Hexanedioic acid	0.0288403	7.44342	2.51431E-09	22.1542	0.0798162	0.152466
Ammonium thioglycolate	0.00133968	3.66942	3.02695E-09	9.35874	0.119592	10.8351
L-Glutamic acid	0.0215278	3.55378	4.97703E-10	21.5301	-3.68797	0.689195
N-Methyl-2-pyrrolidone	0.0186209	4.60985	3.23426E-09	56.0104	-0.458463	10.0212
Glycolic acid	0.00466659	4.71857	5.37489E-09	7.3753	-1.11093	3.04018
1-Propanol, zirconium(4+) salt	-	4.43043	7.41659E-06	3.03193	-2.36755	10.4512
1-Benzylquinolinium chloride	0.00205116	22.8953	4.55311E-06	9858.6	0.438377	7.2266E-07
Toluene	0.0169824	2.0148	0.00662645	117.115	2.72879	0.00591811
3-Hydroxybutyraldehyde	0.0146893	4.2732	2.47856E-07	10.633	-0.329657	11.2015
2-Aminoethanol hydrochloride	0.0283139	4.71522	5.96167E-08	4.35443	-1.42368	16.3514
2-Methyl-2-nitro-1,3-propanediol	0.00456037	4.09344	6.86542E-08	13.7329	-1.91447	5.91256
Nitromethane	0.0512861	7.57229	2.86351E-05	5.50312	-0.30094	1.76391
Potassium bicarbonate	-	7.57763	3.7792E-09	3.85959	-0.991871	0.0170393
Ethanol, 2-[2-[2-(tridecyloxy)ethoxy]ethoxy]-, hydrogen sulfate, sodium salt	-	4.22759	3.3617E-07	14028.7	3.1703	0.00260198
Mirataine BET-E 40	0.00152405	8.40028	3.58148E-08	10081.3	5.58082	7.01433E-07
1-Dodecyl-2-pyrrolidinone	0.0214289	5.83066	1.24462E-07	1584.2	4.20336	0.000858845
Diallyldimethylammonium chloride	-	4.93604	0.114147	1309.78	-3.18631	0.793828
4-Methyl-2-pentanone	0.0233346	4.11302	5.68153E-05	40.9047	1.31136	0.137342
1-Decanol	0.017378	5.6663	3.18976E-05	388.688	4.56753	0.000180499
Docusate sodium	0.00872971	4.73629	6.59987E-09	15063.1	2.21148	0.000443227
Sodium hydroxy methanesulfonate	0.00286418	4.11925	3.41368E-08	2.90877	-2.38343	3.35249
Triazinetriethanol	0.00654636	4.936	9.59642E-09	133.215	-1.46495	0.6514
Sodium ditridecylsulfosuccinate	-	13.0948	3.19631E-08	20521	6.91963	2.66327E-05
Thioglycolic acid	0.00218776	3.66942	3.02695E-09	9.35874	0.0901028	10.8351
Triethyl phosphate	0.000899498	4.90451	3.61967E-08	60.5996	0.800133	2.69531
Triisopropanolamine	0.0313329	5.85958	7.77335E-11	29.7281	0.177277	4.33089
N,N-Dimethyldecylamine oxide	-	5.66612	0.000414686	1699.04	4.53582	3.37607E-05
Sodium L-lactate	-	5.43152	8.92977E-09	10.1804	-1.10237	3.22296
1-Decanamine, N-decyl-N-methyl-, N-oxide	0.000638263	-	3.8088E-07	-	6.71266	5.91844E-06
Ammonium acrylate	0.00126474	4.71683	1.98681E-07	7.90304	-0.320317	13.8505
1-Octanol	0.0354813	4.93871	2.46425E-05	36.3607	2.99985	0.0041301
Sodium octyl sulfate	0.0063387	4.29273	1.51406E-08	193.227	0.242003	0.0898742
Sodium decyl sulfate	0.00574116	4.22734	3.48686E-09	328.063	0.555646	0.0148353

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5-Chloro-2-methyl-3(2H)-isothiazolone	-	4.76066	2.28704E-07	52.9944	-0.0499906	0.299525
2-Butoxy-1-propanol	0.00986279	4.63011	1.52926E-06	41.9962	1.02344	0.73471
Peracetic acid	-	3.68107	2.13465E-06	7.92939	-0.874968	13.1724
Butyl lactate	0.0287078	4.64165	2.44103E-07	17.7316	1.67196	0.273588
Nitrilotriacetic acid trisodium monohydrate	0.00665273	3.67571	2.83042E-10	63.6266	-1.60451	0.309304
Phenol	0.00461318	4.59014	3.36246E-07	27.0339	1.46171	0.91429
Carbonic acid disodium salt, compd. with hydrogen peroxide (H2O2) (2:3)	-	7.57763	3.7792E-09	3.85959	-1.62226	0.0170393
Formamide	-	6.11645	9.73585E-08	3.21896	-1.50846	22.2407
(((2-[(2-Hydroxyethyl)(phosphonomethyl)amino)ethyl)imino]bis(methylene))bisphosphonic acid, compd. with 2-aminoethanol	0.00977237	3.67988	1.5238E-11	49.9084	0.956388	0.860654
3,4,4-Trimethyloxazolidine	0.00877001	4.97745	2.16092E-05	68.6099	0.519011	1.32799
Sodium DL-lactate	0.0494311	5.43152	8.92977E-09	10.1804	-1.10237	3.22296
Butanedioic acid, sulfo-, 1,4-bis(1,3-dimethylbutyl) ester, sodium salt	0.0111944	4.26523	4.18861E-10	909.956	0.415289	0.00157052
Sodium thiocyanate	-	7.56289	9.15947E-07	26.8532	-0.318999	13.8593
Bisphenol A	0.0179887	15.145	1.25155E-07	1436.23	3.32044	0.000745153
Triethanolammonium glycolate	0.0280543	3.6689	5.8416E-11	18.9028	0.837594	6.70355
Acrylamide	0.00153109	5.16781	2.48431E-08	49.5928	-0.670491	8.98889
N,N-Dimethyl-methanamine-N-oxide	-	7.5873	9.81242E-05	5.52839	-0.213527	2.00128
Hydroxy acetic acid ammonium salt	0.0122462	4.71857	5.37489E-09	7.3753	-1.35971	3.04018
Sodium ethasulfate	0.00776247	3.65214	2.84972E-08	26.832	0.242942	0.132377
[[(Phosphonomethyl)imino]bis[6,1-hexanediylnitrilobis(methylene)]]tetrakis-phosphonic acid	0.00909913	4.07601	2.57776E-11	52.8591	-1.53483	0.420111
Sodium formate	-	6.10776	1.67961E-07	5.39642	-1.2513	10.578
2-Acrylamido-2-methyl-1-propanesulfonic acid	0.00516416	4.63792	1.33899E-09	18.0865	1.80328	0.310958
1-Methoxy-2-propanol	0.0488652	4.27926	9.14241E-07	10.447	-0.315774	11.0975
Ammonium lactate	0.0494311	5.43152	8.92977E-09	10.1804	-0.863157	3.22296
Di(2-ethylhexyl) phthalate	0.0796159	4.81176	2.60504E-07	86757	7.52479	1.75353E-07
FD&C Yellow 5	-	5.69224	3.09763E-11	45.2121	0.385801	0.0021599
Pentasodium nitrilotris(methylenephosphonate)	0.0161436	4.58428	1.57001E-11	70.8421	-2.5812	3.34074
2-Methyl-3(2H)-isothiazolone	-	4.29098	2.30284E-08	54.9187	-0.0974589	0.317768
Isopropylamine	0.00375837	6.44876	1.49076E-05	3.43404	0.260811	16.8762

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Ethyl acetate	0.06223	4.12611	0.0001348	18.1744	0.731494	0.91182
2-Phosphono-1,2,4-butanetricarboxylic acid	0.0357273	3.5491	1.35168E-11	29.2094	-0.00256852	1.12088
Cobalt(II) acetate	-	4.59912	1.00453E-07	1.00727	-1.53495	13.4017
3-Methoxypropylamine	0.0339625	4.28	5.08078E-07	12.3856	-0.0590897	11.9312
Tetradecyldimethylbenzyla mmonium chloride	0.0022856	13.8033	3.7294E-07	14485	1.76626	1.29383E-08
2-N-Dibutylaminoethanol	0.011324	5.68951	1.26839E-05	274.848	2.64867	0.0230322
Phthalic anhydride	0.0101391	3.73557	1.6929E-09	36.3099	1.59708	0.0412953
.beta.-Alanine, N-(2-carboxyethyl)-N-(2-ethylhexyl)-, sodium salt (1:1)	-	5.19438	3.41538E-10	90.6198	1.1938	0.0250431
Dodecene-1-sulfonic acid, sodium salt	-	4.801	2.53573E-08	1687.43	1.46571	0.00418267
4,4'-Diphenylmethane diisocyanate	0.0453942	5.2566	1.88443E-06	1167.83	2.86046	3.18876E-05
Acetaldehyde	0.018197	7.56818	6.60901E-05	2.57283	-0.33813	16.0518
1-(Nitromethyl)cyclobutan-1-ol	-	4.09829	1.42793E-06	27.3021	-2.44787	2.89721
Sulfuric acid, monohexyl ester, sodium salt	0.00580764	4.29392	2.74314E-08	28.2743	-1.00026	0.867651
Ethylenediaminetetraacetic acid, disodium salt	0.00479733	4.96007	2.27935E-11	37.8169	-1.51285	0.00342189
Trisodium ethylenediaminetetraacetate	0.00479733	4.96007	2.27935E-11	37.8169	-1.51285	0.00342189
1,3-Propanediol	0.0753356	4.57655	6.07289E-08	9.0968	-1.039	9.1862
Isoascorbic acid	0.0826038	3.53988	8.44548E-10	151.535	-1.85074	2.07263
Tetrapropylammonium bromide	-	6.92966	0.0671819	1220.99	-3.02625	0.00159064
(S)-2-Hydroxypropionic acid	0.0494311	5.43152	8.92977E-09	10.1804	-0.720713	3.22296
2-Amino-2-methylpropan-1-ol	0.00899498	7.05103	5.93383E-08	9.07417	-0.91689	11.2062
(E)-Crotonaldehyde	0.00688652	3.67349	1.47885E-05	10.6536	0.68219	2.07517
2-Hydroxyethyl acrylate	0.00322107	4.45354	1.38152E-07	9.46777	-0.208695	8.57631
Ampicillin	0.0148594	34.8852	1.52158E-11	86.8972	1.34848	0.028782
Citronellol	0.0208449	3.53679	5.06981E-06	130.266	3.90856	0.00211118
Geraniol	0.0206063	4.46853	5.60618E-07	96.8741	3.55828	0.00150491
(2Z)-3,7-Dimethylocta-2,6-dien-1-ol	0.02208	4.46853	5.60618E-07	96.8741	3.55828	0.00150491
Phthalic acid	0.0311172	5.35753	1.63008E-09	11.7825	0.749604	0.101808
Dapsone	0.00469894	17.9875	3.52669E-11	108.154	0.971703	0.000996638
Triethylenetetramine	0.0187932	3.6823	3.83167E-11	33.6474	-0.369429	32.5101
Pentaethylenehexamine	0.0121899	4.68903	8.97729E-11	83.1163	0.220101	5.75262
Triethanolamine hydrochloride	0.0280543	3.6689	5.8416E-11	18.9028	-1.27201	6.70355
Potassium oleate	0.0498884	5.3554	6.05302E-08	2355.33	0.927166	4.34358E-08
1-(1-Naphthylmethyl)quino linium chloride	0.00243781	39.8348	7.34004E-07	137155	0.768137	2.46635E-08

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Amaranth	0.0177419	15.4397	6.4421E-11	38.8541	2.04363	0.236366
Oleic acid	0.0391742	5.3554	6.05302E-08	2355.33	7.6389	4.34358E-08
Ethylenediamine	0.0389045	8.42387	1.74196E-09	4.24117	-2.03814	16.6177
1-Hexadecene	0.0414954	5.98358	0.00129154	3015.26	7.92899	3.39893E-09
C.I. Pigment Red 5	-	11.5926	2.81221E-09	145649	5.83292	3.09343E-08
Ethylene oxide	0.00427563	7.57226	0.000147922	3.07646	-0.299668	22.6296
(2,3-dihydroxypropyl)trimethyl ammonium chloride	-	4.13131	1.02516E-07	12.1575	-0.0837767	7.65492
1,4-Dioxane	0.0335738	9.35852	4.89581E-06	16.9364	-0.269108	11.4104
Glycine, N-(carboxymethyl)-N-(2-((carboxymethyl)amino)ethyl)-, trisodium salt	0.00552077	4.50099	2.25195E-11	11.1533	-1.44292	0.420506
beta-Alanine, N-(2-carboxyethyl)-N-dodecyl-, monosodium salt	0.0102565	5.79429	1.67174E-08	3300.77	1.51401	0.00315721
Disodium ethylenediaminediacetate	0.0274789	4.4881	4.63629E-10	107.861	-0.985797	0.392901
2-Bromo-3-nitrilopropionamide	0.00511682	4.09538	1.61977E-09	2.16797	-0.915593	0.704963
1-Propoxy-2-propanol	0.0354813	4.6124	9.58475E-07	19.9057	0.589335	8.38015
Ethylenediaminetetraacetic acid, diammonium copper salt	0.00479733	4.96007	2.27935E-11	37.8169	-1.88738	0.00342189
Potassium acetate	0.0486407	4.59912	1.00453E-07	1.00727	-1.62995	13.4017
Benzene	0.0295801	6.02896	0.00552001	56.1326	2.13105	0.0226306
2,2-Dibromopropanediamide	-	15.1433	4.19085E-10	4.70637	-0.773652	0.0220169
1-Octadecene	0.0308319	10.0705	3.32225E-05	3992.65	9.08477	6.69328E-09
Cetylethylmorpholinium ethosulfate	0.000843335	13.6446	3.59592E-07	14049.3	0.677614	6.32153E-07
L-Glutamine	0.0334965	3.54478	4.68522E-10	59.6249	-3.64014	0.282563
Nitrilotriacetic acid	0.00785236	3.67571	2.83042E-10	63.6266	-1.61719	0.309304
Thiocyanic acid, ammonium salt	-	7.56289	9.15947E-07	26.8532	0.595575	13.8593
Methoxyacetic acid	0.00539511	3.67302	6.37221E-08	10.4367	-0.637892	11.0679
Aniline	0.00399945	5.59717	2.01854E-06	39.8649	0.901937	0.385699
Isoquinoline	0.00533335	13.5778	8.66549E-06	643.812	2.0809	0.0348838
Dolomite	-	7.57763	3.7792E-09	3.85959	-0.821277	0.0170393
(3-Aminopropyl)silanetriol	-	4.13542	1.21952E-08	63.2517	-0.204847	1.57979
Benzyldimethyldodecylammonium chloride	0.00222844	15.1888	1.97178E-06	6767.13	1.78357	4.88464E-09
Sodium diacetate	-	4.59912	1.00453E-07	1.00727	-1.62463	13.4017
(3-Chloro-2-hydroxypropyl)trimethylammonium chloride	-	3.97023	1.27299E-05	268.161	-2.04306	2.07663
Amino tris(methylene phosphonic acid), potassium salt (1:x)	0.0161436	4.58428	1.57001E-11	70.8421	-2.61298	3.34074

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Quinaldine	0.00578096	4.56354	4.47694E-05	1061.13	2.59009	0.00431882
Acetophenone	0.0125893	5.38902	1.04081E-05	63.0544	1.5825	0.0515866
1,2-Benzisothiazolin-3-one	0.00609537	3.74206	1.64844E-08	73.142	0.803321	3.36109E-06
3-{[3-(Aziridin-1-yl)propanoyl]oxy}-2-({[3-(aziridin-1-yl)propanoyl]oxy}methyl)-2-(hydroxymethyl)propyl 3-(aziridin-1-yl)propanoate	0.00161808	4.22762	1.18744E-11	251.401	-0.69838	0.0283269
5-Bromo-2-nitrobenzotrifluoride	0.00889201	3.55622	0.000189861	785.318	2.85754	0.00212914
Decyldimethylamine	0.00394457	3.90164	0.00153376	683.517	3.40555	0.000412133
Trimethylamine hydrochloride	0.0129718	9.06601	0.000104207	16.4664	-2.63553	14.9947
Imidodicarbonic diamide	-	6.31046	2.59917E-09	10.8016	-1.04434	0.0698406
alpha-Lactose monohydrate	-	4.83929	2.15008E-11	41.3923	-2.72663	0.58306
Sodium benzoate	0.0134896	6.6407	2.66769E-07	31.66	-1.55843	0.331734
Potassium (E,E)-hexa-2,4-dienoate	0.03155	3.55957	6.64839E-07	21.2556	-1.78679	0.0197647
Trimethylamine	0.0168267	9.06601	0.000104207	16.4664	0.160553	14.9947
Copper phthalocyanine	-	152.698	1.03291E-09	60564.8	2.22523	3.64948E-06
Isobutene trimer	0.0457088	8.26998	0.112846	1962.83	5.01597	1.26866E-06
N-[3-(Trimethoxysilyl)propyl]ethane-1,2-diamine	0.0234963	3.81668	2.80284E-08	34.5002	0.92854	0.503996
C.I. Direct Red 81 disodium salt	-	3.36372	5.22569E-11	140265	2.85105	0.000757281
Diisobutyl ketone	0.0288403	4.08896	0.000189641	213.676	3.27043	0.0182284
2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester	0.00514044	4.1294	2.08757E-08	28.4971	-0.297809	4.17725
Magnesium stearate	-	18.9526	6.64788E-08	3946.22	5.60253	2.08416E-06
Sodium chloroacetate	0.000993116	7.12262	9.31406E-09	4.56291	-1.03573	8.66995
Epichlorohydrin	0.00408319	4.11432	6.91706E-05	9.99986	0.451574	0.71112
Carbon	-	18.9477	0.0627508	3.18035	1.0888	0.0063108
Quinoline	0.00465586	13.7434	8.66445E-06	1254.8	2.03132	0.0479786
1-Undecanol	0.0317687	5.67177	0.000019189	673.105	4.42381	0.00017251
1-Dodecene	0.0504661	6.8265	0.0663635	1085.02	5.84468	9.30703E-08
Acrylic acid	0.00157761	4.71683	1.98681E-07	7.90304	0.350125	13.8505
Thiourea	0.00539511	12.6258	3.57263E-09	7.08091	-1.04933	1.86779
N,N'-Dibutylthiourea	0.00271019	4.82995	6.00275E-08	302.445	2.74855	0.043122
(2-Hydroxyethyl)ammonium mercaptoacetate	0.00133968	3.66942	3.02695E-09	9.35874	1.39704	10.8351
Methylenediurea	0.00704693	4.44154	1.77117E-10	46.4175	-0.583006	0.221682
4-Ethyloct-1-yn-3-ol	0.00648634	3.55427	2.42546E-05	71.1611	3.32413	0.00400455
Diammonium dihydrogen ethylenediaminetetraacetate	0.00479733	4.96007	2.27935E-11	37.8169	-1.51687	0.00342189
Cumene	0.020893	14.9574	0.0113666	521.484	3.66274	0.000521787

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Trimethylolpropane tris(2-methyl-1-aziridinepropionate)	0.0092045	5.67084	4.11328E-08	192.084	3.36143	0.00226062
C.I. Acid Red 1	0.0157398	4.27326	3.80026E-11	40.4981	1.56587	0.296667
C.I. Acid Violet 12, disodium salt	0.0170216	4.90373	3.86397E-11	40.5994	1.34442	0.295035
Dimethyl succinate	0.0559758	4.13297	1.16226E-05	25.7163	0.350452	0.17275
Dimethyl glutarate	0.0336512	4.13236	1.14037E-05	19.9057	0.62167	0.370035
Dimethyl adipate	0.0430527	3.67709	2.19931E-06	13.5698	1.03007	0.0354182
Octamethylcyclotetra siloxane	0.00368978	214.816	11.9941	3064.9	6.74116	1.69853E-08
Diammonium citrate	0.0142561	4.09194	1.54655E-10	119.011	-1.72236	4.90398
Dodecamethylcyclohexa siloxane	-	214.792	9.56995	25167.8	9.05882	1.15175E-08
Decamethylcyclopenta siloxane	-	214.797	32.9313	8156.49	8.02976	4.58211E-08
Benzylhexadecyldimethyla mmonium chloride	0.00229615	14.2908	8.38606E-07	10110.9	2.26088	1.56095E-08
1-Dodecanol	0.0368129	6.28062	2.21925E-05	3305.33	5.12883	1.78881E-05
4,6-Dimethyl-2-heptanone	0.0183654	4.69532	0.000188622	214.082	3.15196	0.00446181
3-Aminopropyltriethoxy silane	0.0134276	4.22752	2.80671E-06	282.955	2.89427	0.033744
FD&C Yellow 6	-	8.32091	1.27777E-09	51.8547	1.7788	0.0258827
FD&C Blue No. 1	-	15.6358	8.54445E-10	137262	4.53818	0.000110113
Acrylonitrile	0.000787046	3.6819	0.000136709	4.11662	0.249091	1.41385
Acetic acid, 2,2'-oxybis-, disodium salt	0.00922571	3.67433	5.27069E-10	25.734	-0.59514	3.09497
Diethylene glycol monomethyl ether	0.0374111	3.67822	3.15215E-09	11.1487	-0.505186	8.33529
Dodecylbenzene	0.0196336	5.39627	7.21858E-06	3649.08	8.64603	1.04463E-08
2-(Dimethylamino)ethyl acrylate methochloride	-	3.81461	0.000467134	43.8271	-1.69239	0.487322
1,3-Propanediol, 2-amino-2-methyl-	0.0760326	4.83432	1.25748E-08	5.49093	-1.29273	9.50761
Rhodamine B	-	-	2.74762E-08	-	1.94937	0.000166771
[(Carboxymethyl)amino] acetate	-	4.45569	5.20756E-10	33.2644	-2.01503	0.755434
N-(3-Chloroallyl)hexaminium chloride	-	41.5402	3.30181E-06	141.202	0.582586	0.572174
Benzaldehyde	0.0120226	5.92924	2.67377E-05	32.5093	1.47434	0.062603
1,2-Propylene oxide	0.00959401	4.10863	0.000137481	2.9335	0.0288776	1.6203
4-Methoxyphenol	0.012106	5.34773	2.20524E-07	136.151	1.57887	0.299991
Sodium 2-propenoate	0.00126474	4.71683	1.98681E-07	7.90304	-0.965074	13.8505
1-Tetradecene	0.0363915	6.47817	0.0110015	1968.49	6.86646	1.08471E-08
1-Eicosene	0.0178238	21.1742	5.38179E-06	4740.45	9.22942	5.98375E-09
Magnesium carbonate (1:1)	-	7.57763	3.7792E-09	3.85959	-0.732008	0.0170393
2-Methoxy-1-propanol	0.0423643	4.12535	7.03413E-07	10.522	-0.313305	10.6544

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Trisodium (2-hydroxyethyl)ethylenediaminetriacetate	0.00924698	5.16224	2.232E-11	49.3872	-1.52153	0.0602701
Chloromethane	0.00570164	13.7954	0.00883123	12.5443	1.0801	0.113079
[[(Phosphonomethyl)imino]bis[2,1-ethanediylnitrilobis(methylene)]]tetrakis-phosphonic acid, ammonium salt (1:x)	0.0101391	4.07594	2.69398E-11	58.8288	-3.4549	0.367533
2,3,4,5-Tetrafluorobenzoic acid	0.00469894	4.09531	1.10379E-06	49.4537	2.73927	0.0136556
2-Chloro-4-fluorobenzoic acid	0.0223872	3.55604	2.1256E-09	41.9319	2.29652	0.0019436
2,5-Difluorobenzoic acid	0.0105682	3.56318	2.69905E-07	28.5739	1.72954	0.014321
2,6-Difluorobenzoic acid	0.0107399	4.07783	2.66827E-07	28.2332	1.59166	0.0194721
Benzoic acid, 2-fluoro-	0.00677642	4.09642	1.73644E-08	41.988	1.77152	0.0506968
4-Chloro-2-fluorobenzoic acid	0.00736207	3.55675	2.12337E-09	41.9594	2.26806	0.00232541
4-Fluoro-3-(trifluoromethyl)benzoic acid	0.00845279	3.55372	3.32325E-10	123.176	2.78182	0.00572753
4-Fluoro-2-(trifluoromethyl)benzoic acid	0.00629506	3.55264	2.62459E-08	64.8807	2.81762	0.00590103
2,4-Difluorobenzoic acid	0.0135831	3.56332	5.85385E-09	52.2285	1.89535	0.0145653
2-(Trifluoromethyl)benzoic acid	0.00756833	3.56268	2.70239E-07	26.3529	2.83856	0.025
2,4,5-Trifluorobenzoic acid	0.00749894	3.56334	1.50939E-08	63.0822	1.8621	0.0109414
3-(Trifluoromethyl)benzoic acid	0.0111686	3.5592	3.42629E-09	69.2449	2.94988	0.000785332
Benzoic acid, 4-(trifluoromethyl)-	0.01	4.07571	2.73575E-07	93.8732	3.09663	0.00501409
Benzoic acid, 3,5-difluoro-	0.011246	4.07749	2.66119E-07	28.8215	1.80268	0.0131429
Benzoic acid, 4-fluoro-	0.011995	4.09587	2.12178E-09	44.9419	2.06898	0.00857428
2,3,4-Trifluorobenzoic acid	0.00599791	3.56334	1.51458E-08	64.1144	2.27272	0.0109976
alpha-Methylstyrene	0.0353183	8.2292	0.00401085	344.119	3.4795	0.000978084
7,4'-Dihydroxyisoflavone	0.00154882	19.0435	1.26455E-09	809.77	3.24262	0.000255351
Thiamine hydrochloride	0.00161808	4.3795	9.36084E-10	199.11	-0.787819	0.00602862
2-Hydroxyethylammonium acetate	0.0283139	4.71522	5.96167E-08	4.35443	1.34048	16.3514
Vinyl acetate	0.0155597	4.12439	0.000165762	23.6504	0.730749	0.234782
2-Methyl-2,4-pentanediol	0.0169824	5.3513	1.04874E-07	15.2204	1.00685	8.36254
Tedizolid phosphate disodium salt	-	5.66879	1.02768E-11	38.8702	2.07161	0.000021156
Acrolein	0.00115878	3.67504	0.000120843	4.07989	-0.00921304	3.75427
1,6-Hexanediamine dihydrochloride	0.00635331	6.29598	1.60704E-07	27.3584	-1.55936	3.91401
4,4'-Diaminobiphenyl methane	0.00291072	19.8298	1.06746E-07	98.0993	1.58894	0.00499465
1,2,3-Propanetricarboxylic acid, 2-hydroxy-, hydrate (1:1)	0.0142561	4.09194	1.54655E-10	119.011	-1.72129	4.90398

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N,N-Bis(2-hydroxyethyl)dodecanamide	0.0284446	5.79822	1.05789E-09	1347.03	3.60417	0.0514058
N-Oleyldiethanolamide	0.0379315	5.8242	1.65183E-09	14320.6	6.74328	9.59034E-05
Trimethoxy[3-(oxiran-2-ylmethoxy)propyl]silane	0.0656145	4.29228	5.85357E-07	266.308	1.33922	0.192134
1,3-Dichloropropene	0.00398107	5.37147	0.0023686	46.2635	2.03987	0.0179152
3-[(3-Butoxy-2-hydroxypropyl)(dimethyl)azaniumyl]-2-hydroxy-1-propanesulfonate	-	4.90628	1.62777E-09	173.9	-0.577257	0.0340966
Phosphonic acid, [1,6-hexanediylbis[nitrilobis(methylene)]]tetrakis-	0.00763836	3.68031	2.59482E-11	58.1112	-4.42906	0.0305259
Dodecyl(2-hydroxy-3-sulphonatopropyl)dimethylammonium	-	8.78551	3.98914E-08	6435.66	3.51333	0.000877512
Hexadecane	0.044157	17.0605	0.0013041	2928.85	8.07999	3.97668E-09
1-tert-Butoxy-2-propanol	0.0323594	4.12152	1.44634E-06	20.8659	1.2256	0.951784
Phosphoric acid, 2-ethylhexyl ester, compd. with 2,2'-iminobis[ethanol]	-	3.67944	1.16227E-07	14.5626	0.599163	0.142081
Morpholine	0.0186209	7.24522	6.82819E-07	8.97993	-0.858237	11.4713
2-Phenoxyethanol	0.0128529	5.47167	2.87663E-07	67.6996	1.16071	0.195134
Benzenesulfonic acid	0.0156315	16.1593	1.33959E-08	32.9401	1.20016	0.92371
1-(2-Aminoethyl)piperazine	0.0094189	4.07384	2.96775E-09	33.6814	-0.70018	10.3961
n-Hexane	0.0630957	8.96342	0.492255	165.951	3.90054	0.000126707
Decane	0.0517607	8.99194	0.153501	454.45	5.01367	3.66611E-07
Isooctadecanoic acid, ester with 1,2,3-propanetriol	0.0438531	5.77399	6.7691E-08	2419.23	0.594892	1.36513E-06
Dichloromethane	0.008531	15.2515	0.00326427	27.5998	1.25139	0.176432
Tris(hydroxymethyl)phosphine oxide	0.0291743	15.0681	1.67653E-08	21.0408	-0.98031	1.85376
Trisodium citrate	0.0142561	4.09194	1.54655E-10	119.011	-2.24515	4.90398
4-Aminobenzoic acid	0.0214289	3.11477	4.52077E-10	312.524	0.824077	0.0677224
Heptane	0.0891251	7.01128	0.395392	321.749	4.65904	3.24633E-05
1,1,2,2,3,3,4,5,6,7-Decafluoro-2,3-dihydro-1H-indene	0.000105196	5.34448	0.00415745	15558.5	4.67998	0.00101336
Perfluoromethylcyclopentane	0.0017338	5.43594	0.0127703	939.844	4.68483	9.89867E-05
Perfluoro-1,2-dimethylcyclobutane	-	4.5902	0.0128146	955.279	4.8353	9.92975E-05
Perflunafene	0.00040738	8.05501	0.0153705	24388.6	8.35262	0.000010686
Perfluoro-1,2-dimethylcyclohexane	0.000479733	5.24444	0.0120096	30960.2	6.58854	1.16359E-05
Perfluoroethylcyclohexane	0.000606736	7.59065	0.0119919	31950.4	6.66679	1.15921E-05
Perfluoro-1,3-dimethylcyclohexane	0.000544503	5.75719	0.0120067	30657.5	6.58882	1.16702E-05
Perfluoro-2-methyl-3-ethylpentane	-	4.59192	0.0122996	795480	4.71744	2.14514E-06
Perfluoromethylcyclohexane	0.000785236	8.39688	0.0122081	21668.4	5.5266	3.75814E-05

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Perfluoroisohexane	0.000860994	5.4357	0.0132926	4597.02	3.79894	3.47264E-05
Undecafluoro(heptafluoro-propyl)cyclohexane	0.000451856	7.59282	0.0156783	24165.8	8.70868	9.57555E-06
Perfluoro-1,3,5-trimethylcyclohexane	0.000377572	6.82939	0.0159281	26202.1	8.42115	2.51429E-06
1,1,2,2,3,4,4,5,5,6-Decafluoro-3,6-bis(trifluoromethyl)cyclohexane	0.00061235	6.80703	0.0120046	31968.1	6.58974	1.18686E-05
Undecafluoro(1,1,1,2,3,3,3-heptafluoropropan-2-yl)cyclohexane	0.000416869	5.25406	0.015847	24308.5	8.70862	2.46583E-06
Perfluoro dimethylethylpentane	0.000240436	6.75239	0.0159576	142916	4.92706	1.56367E-06
2-[2-(2-Butoxyethoxy)ethoxy]ethanol	0.0257632	3.67873	8.02138E-09	201.715	0.821761	4.83609
1,3-Dimethylol-5,5-dimethylhydantoin	0.0241546	4.63873	2.80244E-09	22.1186	-0.688627	0.160012
Heptasodium diethylenetriaminepentamethylenephosphonate	0.0101391	4.07594	2.69398E-11	58.8288	-3.43471	0.367533
Solketal	0.0296483	4.12307	5.44921E-07	38.2167	-0.171616	4.96438
5,5-Dimethylhydantoin	0.00767362	4.4523	3.3301E-08	20.3438	-0.479162	0.276764
m-Xylene	0.0175792	9.98709	0.00713593	178.277	3.19855	0.00151975
Ethylenediaminetetraacetic acid	0.00479733	4.96007	2.27935E-11	37.8169	-1.52846	0.00342189
Triacetin	0.0220293	4.135	2.10571E-08	16.1262	0.250519	0.257786
2-(Bromomethyl)-1,3-dinitrobenzene	-	4.61246	3.7943E-07	657.836	2.26038	0.00100995
Sodium D-gluconate	0.11749	3.55732	1.83519E-10	126.513	-2.39369	2.0848
Dazomet	0.00166725	4.35852	2.67833E-10	10.0245	0.630444	0.0154425
2-Ethoxyethanol	0.0285102	4.12295	4.72999E-07	12.0957	-0.319912	11.0976
Phosphonic acid (dimethylamino(methylene))	0.0222844	3.67956	2.38109E-09	39.7541	-0.822655	0.41483
Butylated hydroxytoluene	0.00647143	14.7955	8.00138E-06	4489.84	5.09929	2.75616E-06
Sodium 1-octanesulfonate	0.0074817	3.90478	1.34052E-08	262.656	0.209638	0.09673
Tetrasodium ethylenediaminetetraacetate dihydrate	0.00479733	4.96007	2.27935E-11	37.8169	-1.51402	0.00342189
Oleic acid isopropanolamide	-	4.61886	3.41195E-08	13656.8	6.29045	0.000152466
D-Lactic acid	0.0494311	5.43152	8.92977E-09	10.1804	-0.720713	3.22296
Perfluoro-2,3-dimethylbutane	0.000271019	7.56788	0.0134104	4640.19	3.92422	3.48677E-05
Allura Red C.I.16035	0.0190985	7.82333	1.23543E-09	94.7202	1.07134	0.000131896
1-Amino-2-propanol	0.0256448	4.07554	5.70892E-08	5.21152	-0.963546	13.2976
Pentanedioic acid, 2-methyl-1,5-dimethyl ester	-	4.28687	1.27253E-05	17.6228	1.04747	0.139293
Biphenyl	0.0184927	30.8193	0.000307534	1868.86	4.0099	4.57866E-05
Ferric ammonium citrate	0.0142561	4.09194	1.54655E-10	119.011	-2.42289	4.90398
Zirconium(4+) tetrakis(1-carboxyethan-1-olate)	-	5.43152	8.92977E-09	10.1804	-2.37375	3.22296

PREFERRED_NAME	ORAL RAT_LD50 (MOL/KG)	BIODEG HALF-LIFE_ (DAYS)	HENRY'S LAW CONSTANT (ATM-M³/MOLE)	SOIL ADSORP. COEFF $K_{OC\_}$ (L/KG)	OCTANOL WATER_ PARTITION K_{OC} (LOG)	WATER SOLUBILITY (MOL/L)
Dimethyldioctadecylammonium chloride	-	212.793	8.31648E-07	20474.8	7.52824	6.88859E-09
1-Propanaminium, 3-[(2-ethylhexyl)oxy]-2-hydroxy-N-(2-hydroxy-3-sulfopropyl)-N,N-dimethyl-, inner salt	-	7.23635	1.46134E-09	1110.47	0.615925	0.0131096
2-Hydroxyethyl disulfide	0.00379315	57.4794	9.42773E-08	219.644	0.897509	1.48789
Sodium dodecyl sulfate	0.00709578	4.68114	2.32822E-07	1234.14	1.59845	0.00589587
Acetic acid, 2-hydroxy-2-phosphono-	0.0372392	4.46577	2.48533E-09	18.9108	-1.62981	0.855352
Nitrilotriacetamide	0.00508159	4.45241	1.3869E-11	60.8155	-2.07435	0.000731683
Sodium 4-methylbenzenesulfonate	0.0156315	4.97523	1.34127E-08	73.5089	-2.53909	3.59185
Cyclohexane	0.063387	49.8446	0.1506	96.5031	3.44041	0.000721446
1,6-Hexanediamine	0.00827942	6.29598	1.60704E-07	27.3584	0.121053	3.91401
1,2-Dibromo-2,4-dicyanobutane	0.00169824	3.55097	1.03948E-05	336.71	1.88958	0.0864626
Tributyl phosphate	0.0151705	3.67991	1.12246E-06	264.326	3.99711	0.00105481
N,N'-Ethylene distearylamide	0.0224388	201.254	2.71852E-08	20521	9.16007	3.00901E-08
(2-Hydroxy-3-(tridecyloxy)propyl)trimethy lammonium chloride	0.00356451	5.67447	1.86422E-07	8631.38	0.546403	4.77154E-05
Platinum(2+) potassium chloride--ethene--water (1/1/3/1/1)	-	9.92301	0.227707	3.22692	-0.887361	0.0142435
Limonene	0.0354813	2.93262	0.022543	2297	4.51408	9.09154E-05
Ethaneperoxoic acid, sodium salt (1:1)	-	3.68107	2.13465E-06	7.92939	-1.03262	13.1724
Bromodifluoromethyl diethylphosphonate	-	4.13774	5.32467E-08	49.4867	1.65018	0.0426144
9-Decenamide, N,N-dimethyl-	-	5.14418	8.00992E-06	539.879	2.86066	0.0124811
Ethanone, 2-chloro-1-(4-hydroxyphenyl)-	0.0092045	3.55491	2.01716E-09	154.57	1.82491	0.0642623
Diphenyl phosphite	-	4.58512	1.30357E-06	320.852	3.52074	0.000260533
Laureth-7 carboxylic acid	0.0151356	4.95472	8.50192E-09	2430.32	5.55928	0.00324916
C.I. Pigment Red 48, calcium salt (1:1)	-	3.35278	1.57041E-10	138.592	-0.28472	3.38431E-05
2-(Dimethylamino)ethyl acrylate	0.00781628	4.28823	2.56074E-05	25.9737	0.0188148	0.931105
Glycine, N-(2-((carboxymethyl)amino)ethy l)-N-(2-hydroxyethyl)-, disodium salt	0.0103039	4.6592	2.33343E-10	31.107	-1.2783	0.26956
2,7-Naphthalenedisulfonic acid, disodium salt	0.0336512	11.0612	3.93473E-07	669.468	-0.765864	0.257869
Methyl acetate	0.0599791	3.68137	0.000115429	7.88083	0.179503	3.03682
Andrographolide	8.45279E-05	86.5748	5.50898E-10	432.635	2.2003	2.41656E-05
Naphthalene-1,3,5-trisulfonic acid	-	11.0748	7.74903E-12	88.3056	1.32472	0.663269
Naltrexone methobromide	-	158.181	1.30095E-10	73498.2	-2.51122	0.00374149
1-Hexene	0.0701455	5.74462	0.229891	176.196	3.39013	0.000591295

PREFERRED_NAME	ORAL RAT_LD50 (MOL/KG)	BIODEG HALF-LIFE_ (DAYS)	HENRY'S LAW CONSTANT (ATM-M³/MOLE)	SOIL ADSORP. COEFF K_{OC}_ (L/KG)	OCTANOL WATER_ PARTITION K_{OC} (LOG)	WATER SOLUBILITY (MOL/L)
Dimethylaminoethanol	0.0160694	4.12703	4.87827E-07	44.8862	-0.136558	11.2137
3-(Dimethylamino) propylamine	0.011298	4.28762	1.05748E-05	46.284	0.0359374	9.77971
Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	0.0156315	15.2986	3.27441E-08	29918	10.1874	9.38521E-07
Octadecanoic acid, calcium salt	-	18.9526	6.64788E-08	3946.22	0.810892	2.08416E-06
1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-	-	237.067	9.68466E-11	134215	8.85439	7.19338E-06
Tris(2,4-di-tert-butylphenyl) phosphite	-	144.955	1.44087E-06	139181	4.79068	2.17134E-06
Aluminate (Al(OH)63-), (OC-6-11)-, magnesium carbonate hydroxide (2:6:1:4)	-	7.57763	3.7792E-09	3.85959	-0.680731	0.0170393
Cyanox CY 1790	-	89.215	9.00353E-08	87243.2	5.95019	3.95856E-05
Calcium lactate	-	5.43152	8.92977E-09	10.1804	-1.51452	3.22296
Basic Blue 54	-	4.24216	4.72854E-06	2049.14	0.550289	5.49363E-06
Tetramethylolphosphonium chloride	-	-	9.97106E-09	-	-2.79661	0.56913
2-(2-Methoxypropoxy)propanol	0.0289068	4.28504	3.67038E-09	20.8725	0.417909	3.36736
4,4'-(Propane-2,2-diyl)diphenol--2-methyloxirane (1/1)	-	15.145	1.25155E-07	1436.23	1.44656	0.000745153
1,3-Dibromo-5-fluorobenzene	0.00557186	5.78939	6.66237E-05	616.57	3.78735	0.0010107
1-Bromo-3-chloro-2-fluorobenzene	0.00339625	5.06127	0.00010176	1388.42	3.76514	0.00330923
Benzene, 1,3-dibromo-5-methyl-	-	11.8866	0.00148789	1472.19	3.7221	2.23092E-05
1-Bromo-2,3,4-trifluorobenzene	0.00586138	7.09961	0.00713841	847.259	3.53739	0.0097495
Benzene, 1-bromo-3,5-dichloro-	0.00632412	5.80995	0.00148375	3111.52	3.82871	8.64413E-05
2-Bromo-1-chloro-4-fluorobenzene	0.00860994	4.81938	5.37354E-05	805.726	3.89959	0.00330556
Benzene, 1-iodo-3,5-dimethyl-	-	8.65105	0.000474782	537.896	3.80849	0.000013072
1,4-Dibromo-2,5-difluorobenzene	0.00485288	5.91499	0.0137629	1333.36	3.87541	0.00099187
Naphthalene, 2-bromo-	-	29.7229	0.000455225	723.245	4.48302	0.000039719
Benzene, 1,2-dibromo-4-methyl-	-	10.8611	0.000256525	1710.2	4.16326	2.22924E-05
1,3,5-Tribromobenzene	-	26.4075	0.00117347	2018.79	4.50915	3.17318E-06
2-(Acetyloxy)-3-[(15-carboxypentadecyl)oxy]propyl 2-(trimethylazaniumyl)ethyl phosphate	-	4.22719	3.43267E-08	20964.6	5.02946	0.000474449
o-Xylene	0.0218776	6.00171	0.00525141	178.668	3.11985	0.00164364
2-Acrylamido-2-methylpropanesulphonate sodium salt	0.00528445	4.63792	1.33899E-09	18.0865	-1.95509	0.310958

| PREFERRED_NAME	ORAL RAT_LD50 (MOL/KG)	BIODEG HALF-LIFE_ (DAYS)	HENRY'S LAW CONSTANT (ATM-M^3/MOLE)	SOIL ADSORP. COEFF K$_{OC\_}$ (L/KG)	OCTANOL WATER_ PARTITION K$_{OC}$ (LOG)	WATER SOLUBILITY (MOL/L)
C.I. Pigment Orange 5	0.00378443	10.0673	6.43367E-08	1056.09	3.4885	3.07494E-05
Pigment Red 2	0.00374111	44.0633	1.85587E-09	73108.2	5.88832	9.11589E-06
Benzenesulfonic acid, 4-(phenylamino)-, monosodium salt	0.0101391	9.93773	3.45236E-11	379.777	-1.14738	0.00670478
Glycine, N,N-bis(carboxymethyl)-, ammonium salt (1:3)	-	3.67571	2.83042E-10	63.6266	-1.6068	0.309304
Glycine, N,N-bis(carboxymethyl)-, ammonium salt (1:2)	-	3.67571	2.83042E-10	63.6266	-1.6068	0.309304
Benzenesulfonic acid, 4-dodecyl-, compd. with 2-aminoethanol (1:1)	0.00397192	9.0719	1.64678E-07	3494.65	1.09145	3.31634E-05
Tetraethylene glycol monoethyl ether	0.0526017	4.90902	6.33816E-09	206.865	-0.119202	5.28272
4-Methylbenzenesulfonic acid	0.0149279	4.97523	1.34127E-08	73.5089	1.21514	3.59185
2-[2-(2-Ethoxyethoxy)ethoxy]ethanol	0.0579429	4.58733	1.06029E-08	25.2137	0.0319662	5.61702
Methanesulfonic acid	0.00174181	5.12339	2.21363E-08	4.36562	-0.394912	10.3696
Trisodium citrate dihydrate	0.0142561	4.09194	1.54655E-10	119.011	-2.70034	4.90398
3,7-Dimethyl-2,6-octadienal	0.0142561	4.51242	5.53111E-05	91.635	2.99753	0.0086826
methyl 9-decenoate	0.0116413	5.14833	0.000178809	655.433	4.13289	0.000176434
2-(2-Ethoxyethoxy)ethanol	0.0635331	3.6803	3.47571E-09	27.6439	-0.537154	7.45304
9-Dodecenoic acid, methyl ester	-	5.71213	0.000150315	1436.97	4.95088	1.32028E-05
4-Amino-1-naphthalenesulfonic acid	0.0409261	13.0831	3.67599E-11	324.764	-0.688951	0.0102984
1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, inner salt	0.00215774	5.68498	2.75345E-07	13416.5	4.86354	1.03453E-06
3,6-Dimethyl-2,5-dioxo-1,4-dioxane	0.0630957	3.67498	1.84707E-09	66.8132	-0.743018	0.523223

APPENDIX C. SUMMARY FIGURES
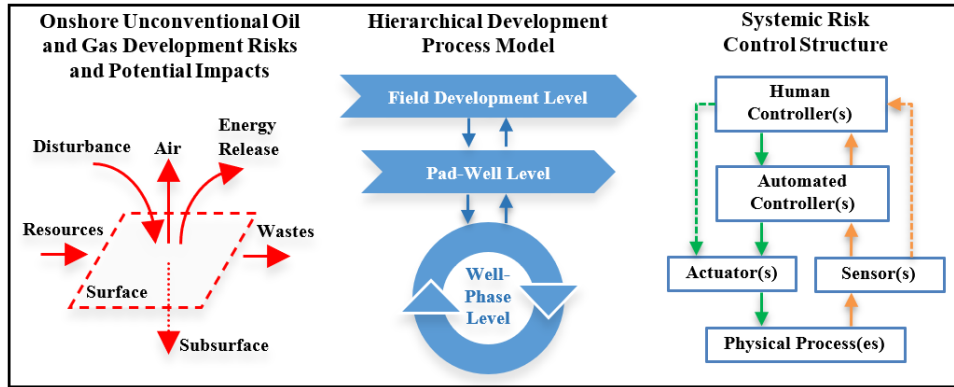
Figure C1. Graphical summary of Chapter 2 (systemic risk analyses in OUOGD).
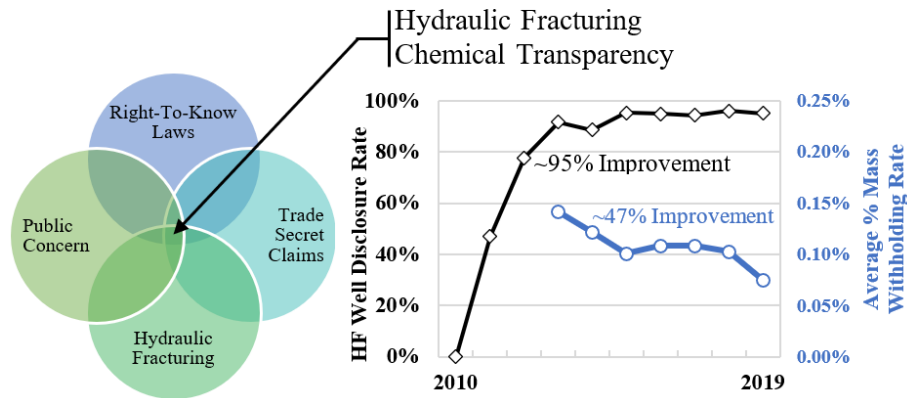

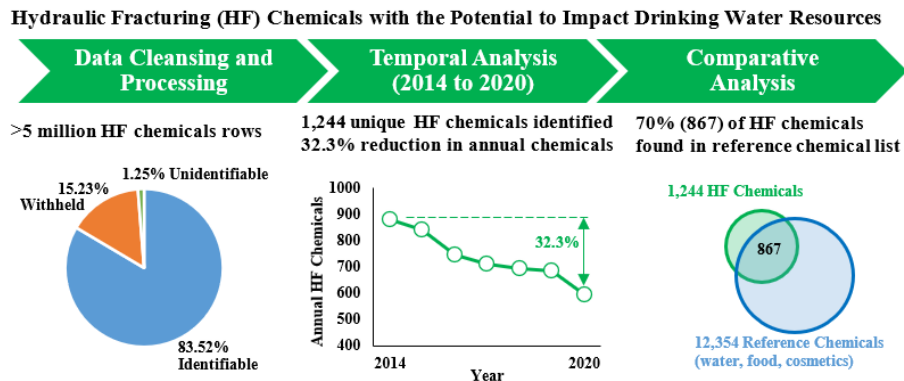Figure C2. Graphical summary of Chapter 3 (chemical transparency).

Figure C3. Graphical summary of Chapter 4 (HF chemicals and context).

Systemic Hydraulic Fracturing Chemical Risk to Drinking Water

⬇ **Well Count**   ▬ **Biodegradation**

⬇ **Chemical Concentration**   ▬ **Volatility**

▬ **Toxicity**   ⬇ **Soil Adsorption**

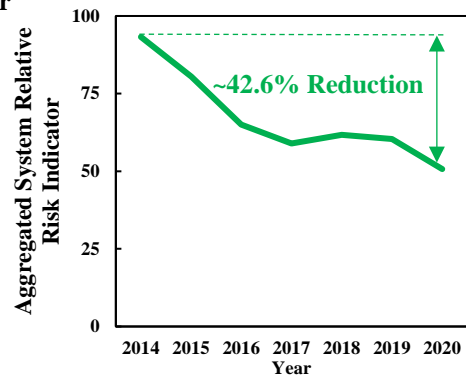▬ **Solubility**   ⬇ **Octanol/Water Partition**

Figure C4. Graphical summary of Chapter 5 (HF chemical risk indicators).