Introducing an Ontology Based Framework for Dynamic Hazard Identification

by

©Abdul Aziz

A Thesis
submitted to the School of Graduate Studies
in partial fulfillment of the requirements for the degree of

Master of Engineering

Faculty of Engineering and Applied Science

Memorial University of Newfoundland

October 2017

St. John's Newfoundland

Abstract

An automated hazard identification technique can substantially contribute to risk assessment efficiency. This work presents an effort to introduce a dynamic hazard identification technique, which can translate the event propagation scenario into a graphical representation with probabilistic interpretation of hazards. Expert knowledge based database structure and probabilistic data driven dynamics were implemented on an ontology-based intelligent platform. A simple demonstration utilizing semantic web-based Web Ontology Language (OWL) was transformed into the Probabilistic-OWL (PR-OWL) based Multi Entity Bayesian Network (MEBN), which was incorporated with prior probabilities, to produce Situation Specific Bayesian Networks (SSBN) referring to hazard probabilities. A generalized and detailed dynamic hazard scenario model was then developed based on this same framework following the proposed methodology. Two open-source software, `Protégé` and `UnBBayes`, were used to develop the models. Case studies with different operational and environmental scenarios were presented to demonstrate the applicability of the generic model. To verify the application, the ontology based hazard scenario model was implemented on 45 individual accidents (from the CSB Database) with different operational aspects. This model was further used for causality studies and hazard mitigation measures.

Acknowledgments

I would like to take the opportunity to thank Dr. Salim Ahmed and Dr. Faisal I. Khan for their generous help, support and valuable suggestions. Since the first day, they have been crucial guides on this difficult voyage. Especially, I am grateful for the generous support, guidance and suggestions from Dr. Salim Ahmed during my research work. In times of frustration , they encouraged me and provided directions and flexibility to work.

Throughout my time at Memorial University, I was lucky to have Professors Dr. Faisal I. Khan and Dr. Salim Ahmed as my mentors in the field of safety and risk engineering. Dr. Leonard Lye and Dr. Aziz Rahman, my course teachers, helped me to improve my analytical skill and enhanced my knowledge of experimental methods and natural gas engineering. The encouragement and support I received from my fellow researchers Mohammad Aminul Islam Khan, Jannatul Naeema, Tanjin Amin, Pewei Xin, Javad Hashemi and Seikh M. Fahim is also greatly appreciated. My gratitude also goes to all my previous institutions for helping me recognize the importance of process safety in an industrial perspective and choose this field for my graduate study.

I would like to express the highest gratitude to my parents who always encouraged me to prioritize knowledge over everything and to head to higher studies.

No matter what, my beloved wife was always beside me, supporting my academic voyage. Without her sacrifice and enormous support to my graduate studies, it would be impossible.

Finally, the financial support provided by the Natural Sciences and Engineering Research Council of Canada, School Graduate Studies, Memorial University of Newfoundland was essential to complete the work. I want to thank the Faculty of Engineering & Applied Sciences at Memorial University of Newfoundland for giving me the opportunity in this program and the Centre for Risk Integrity and Safety Engineering (C-RISE) for letting me join the team with full support.

Table of Contents

List of Tables

List of Figures

List of Abbreviations

AI	Artificial Intelligence
BLEVE	Boiling Liquid Vapour Explosion
BMIR	Biomedical Informatics Research
BN	Bayesian Network
CSB	Chemical Safety Board of United States of America
DRA	Dynamic Risk Assessment
EPA	Environmental Protection Agency
FCA	Formal Concept Analysis
FMEA	Failure Mode and Effect Analysis
FTA	Fault Tree Analysis
GUI	Graphic User Interface
HAZID	Hazard Identification
HAZOP	Hazard and Operability Study
HIRA	Hazard Identification and Ranking
LPD	Local Probability Distributions
MEBN	Multi-Entity Bayesian Network
MFrag	MEBN Fragment
MTheory	MEBN Theory
NFPA	National Fire Protection Agency

OSHA	Occupational Health and Safety Association
OWL	Web Ontology Language
PHA	Process Hazard Analysis
PR-OWL	Probabilistic Web Ontology Language
PSM	Process Safety Management
QRA	Quantitative Risk Assessment
RDF	Resource Description Framework
RV	Resident Variables
SCADA	Supervisory Control and Data Acquisition
SSBN	Situation Specific Bayesian Network
UML	Universal Markup Language
VCE	Vapor Cloud Explosion
W3C	World Wide Web (WWW) Consortium
XML	Extensive Mark-up Language

Chapter 1

Introduction

1.1 Overview

Prevention and mitigation of hazards are fundamental contributing factors of risk management in process industries. Hence, identifying the domains which pose greater risks and the hazards that can threaten potential loss is the primary step. Once the hazards and domains are identified, risk assessment and mitigation measures can be implemented for the better safety of any system.

Although hazard identification can sound simple, this is the most rudimentary and crucial part of the process. It demands a decent amount of time and the participation of experts from the field of interest. As newer technologies are being implemented over time to cope with safety requirements and production demands, various hazards and vulnerable points are getting newer perspectives. To deal with such constraints of time, value and risk factors, numerous efforts have introduced different Hazard Identification techniques. Some examples of the common methods can be found in later sections. But these are mostly case oriented, qualitative and lack dynamic behaviour. However, some recent works have been done to overcome these constraints.

This work introduces a dynamic hazard identification methodology which is more versatile, can quantify hazard probabilities, and provides an ontology based platform to facilitate a wide range of applications and scope of future developments. The proposed dynamic hazard identification methodology based on scenario modeling, utilizing an ontology based data structure to generate a first order Bayesian Logic based network for a generic hazard identification scenario. Scenario based hazard identification has been proposed earlier but the use of ontology based framework has been the unique feature which is useful to develop a quick and reusable platform for automatic updates.

1.2 Previous Works

Dynamic hazard identification is an established concept that captures system variations and offers mechanisms to use updated process knowledge and information [Paltrinier et al., 2015]. Methodologies for dynamic hazard identification includes the Dynamic Procedure for Atypical Scenarios Identification (DyPASI) [Paltrinier et al., 2013], dynamic risk assessment [Kalantarnia et al., 2009] and risk barometer [Knegtering and Pasman, 2013]. Applications of these approaches have been documented in the literature, e.g. [Wilday et al., 2011], [Paltrinieri et al., 2014] and [Villa et al., 2016]. Some other methods with the goal to improve hazard identification procedures by making those dynamic in nature have been proposed recently[Batres et al., 2014, Wu et al., 2013]. However the most recent work of Dynamic Hazard Identification [Xin et al., 2017] is based on the Bayesian graphical network which provides a better sense of dynamic behaviour by updating the occurrence probabilities based on historical data in a known hazard scenario. However, these approaches are and mostly case specific and requires extensive modeling.

1.3 Motivations & Challenges

As dynamic hazard identification is a process-oriented and expertise-intense process, a knowledge modeling based methodology can be adopted to capture the process knowledge. When the process knowledge can be represented in an efficient and accessible framework, it can easily be adapted to in various process risk management applications (*e.g.* automated hazard identification, expert systems). The adaptive dynamic method can be used to overcome the limitations of current techniques.

The challenges of this research can be called as barriers in the development of this work. The most common challenges identified, are listed below.

- Process knowledge is the core of knowledge-based model for hazard scenario development. In the current approach, an ontology can provide knowledge based database structure, which might require a major amount of time. However, once developed, the model is reusable. Therefore, the end users can utilize the model with a general understanding of the process.

- There are thousands of processes and each one is different. Developing an individual model for each industrial setting is a very challenging task. However, a generalized model can reduce the effort. As ontology provides reusability and ease of updates, a generalized model should have the versatility to be implemented in most of the similar cases with minimal changes.

- Historical data has never been easy-to-obtain information. Therefore, the model can be based on expert opinion, experience and common understanding of hazard scenarios. However, the dynamic behaviour introduces the ease of utilizing historical data. The probability declaration values can be saved and updated over time.

- Ontology is a qualitative database platform for Artificial Intelligence (AI). Therefore, a *Java* based comprehensive tool could be developed for automatic import and quantitative reasoning utilizing the universal framework. However, available tools can be used for demonstration purpose and a specialized expert system can be recommended as future work.

1.4 Problem Statement & Objective

Dynamic hazard identification is a quantitative assessment technique, which requires qualitative knowledge along with historical data for probabilistic assessment. A hazard identification should be able to provide the assessment of hazards along with hazard propagation scenario. The dynamic model should provide the versatility of updating the model over time for greater suitability.

The primary goals of this research work can be listed as followings:

- Firstly, to propose a unique dynamic hazard identification methodology which should have the following characteristics-

  1. can incorporate process knowledge and history based information in an explicit model,
  2. has the ability to visualize and share hazard propagation scenario,
  3. utilize available statistical tools (*e.g.* Bayesian Network) for quantitative reasoning,

4. can provide probabilistic assessment of hazards based on available evidence and
5. features accessibility for dynamic update of historical information.

- Secondly, to capture process knowledge of targeted domain in a well-established knowledge modeling platform. The framework should provide the ability to design, store, share and reuse qualitative information required for hazard scenario modeling. Once developed the model should provide the preliminary knowledge base for further modeling.

- Thirdly, to demonstrate the proposed methodology a versatile and generic hazard scenario model applicable for most process facilities is to be developed. The model should be working in order to provide a probabilistic assessment of fire-explosion-toxicity hazards.

- Finally, to test the validity and efficiency, this generic model should be implemented on different hazard scenarios with known outcomes. Implementing the model in previous accidents can indicate the prospects of the model.

This work adopts an ontology based framework to implement the proposed hazard scenario methodology. The ontology based platform can provide the necessary data structure for automation and World Wide Web Consortium(W3C) based web storage provides versatility and updating capabilities. Moreover, utilizing the First Order Bayesian Logic based probabilistic network provides the dynamic behaviour to quantify hazards with the ability to update the probabilities from historical data. The developed model has been applied in different accident scenarios to validate the versatility and efficacy.

1.5 Thesis Organization

This thesis is a compilation of the research and work done with the goal to implement an ontology based framework for dynamic hazard identification of process industries. The following chapters contain detailed study and outcomes related to the research.

Chapter 2 contains a relevant detailed literature survey. Details concerning ontology, applications and scope with examples of previous works are compiled accordingly. A brief background of risk assessment, hazard identification are included. The tools and software are also introduced briefly.

Chapter 3 mostly focuses on a new dynamic hazard identification technique, adopting an ontology framework. Based on the methodology, a hazard scenario model has been developed and validated with case studies. An ontology based modeling approach is demonstrated with a simple model.

Chapter 4 describes the model predictions for 45 different accident scenarios from CSB database. This chapter also includes further application of the model in causality analysis and hazard mitigation approaches.

Chapter 5 discusses about the results obtained from the study.

Chapter 6 consists of the concluding remarks and future scopes of the work.

Appendices document the supporting information and detailed results.

Chapter 2

Literature Review

2.1 Ontology

The concept of ontology is rooted in Greek Philosophy and later was introduced to computer science with a slightly different description. Starting from Aristotle's metaphysics, it is now a widely used platform of knowledge representation and artificial intelligence. This section briefly describes philosophical ontology and its adoption and development in computer science and current applications related to the work.

Aristotle, one of the world's greatest philosophers, in his writings on *Metaphysics* searched for the primary constitutive element the *"Essence"* of being, asked *"What is being?"*, and concluded that all beings in the world must have some *"thing"*, some characteristic, which give the property of *"being"* to the objects. He distinguished between first principle and essence. Principle is the "source point of something" while essence is the "intrinsic reason of existence of being"[Aristotle, 1994, Sánchez et al., 2007, cited in]. In fact, Aristotle never used the term *"Ontology"*, or *"Metaphysics"*. It was Andronicus of Rhodes, another Greek philosopher, who introduced metaphysics from the writings of Aristotle. In the late seventeenth century *"Metaphysics"* was divided into two streams: *"metaphysica generalis"* (General Metaphysics) and *“metaphysica specialis”*(Special Metaphysics). Special metaphysics is deal with philosophical theology, psychology and cosmology. General metaphysics, also called *"ontologia"* or "Ontology" deals with a general concept of beings and their relations, searching the intrinsic reason to name any *'thing'* as a *'being'* or as a hierarchical classification of beings based on common characteristics. [Sánchez et al., 2007]

During the late 1980s, computer scientists looked to ontology as a basis of knowledge engineering with numerous interpretations to develop artificial intelligence . All the interpretations summarize *"Ontology"* as a formal/informal specification of concepts of the knowledge base or logical theories with the purpose of expressing specific domain knowledge. The concise definition: *"Ontology is an explicit specification of conceptualization and it's a systematic account of existence"* [Gruber, 1993]. While Aristotle's 'essence of beings' investigates nature as classes and their determination or attributes (also known as-*Epistemology*[1]) , in knowledge engineering formal ontology can virtually deal with any 'thing' for both knowledge representation and acquisition. *"In practice, formal ontology can be intended as theory of distinctions, which can be applied independently , i.e. :*

- *among the entities of the world (Physical objects, events regions, quantities of matter...);*
- *among the meta-level categories used to model the world(concept, property, quality, state, role, part...)" [Giaretta and Guarino, 1995]*

According to its use in AI, ontology is an "engineering artifact", consisting of specific

[1] A branch of philosophy, which is study of knowledge. Epistemology studies the nature of knowledge, justification, and the rationality of belief.

"vocabulary" to describe reality, plus a set of explicit assumptions referring to the intended interpretation of the vocabulary. *"In the simplest case, an ontology describes a hierarchy of concepts related by subsumption relationships; in more sophisticated cases, suitable axioms are added in order to express other relationships between concepts and to constrain their intended interpretation."* [Guarino, 1998]

In general description, formal representation of the knowledge of a domain requires a set of objects that exist and an accessible way of representing the relations. An ontological framework provides the structure of a knowledge based domain. A set of representational vocabulary that defines the entities exists and describes the relationships amongst them (*e.g.*classes, relations, functions etc.). A formal *Ontology* comprises an understandable text to reproduce the domain knowledge.

2.1.1 Ontology Development & Knowledge Modeling

An ontology describes the acquired knowledge of a domain in a machine interpretable form. From plant taxonomies to website listings, it has long been used as a platform. But the specific purposes of ontology development are discrete. These are listed below. [Noy et al., 2001]

- To share common understanding of the structure of information among people or software agents
- To enable reuse of domain knowledge
- To make domain assumptions explicit
- To separate domain knowledge from operational knowledge
- To analyze domain knowledge

Thus, developing an ontology is more related to defining a set of data and the structure to be used as a framework. *Problem solving methods, domain independent applications, and software agents use ontologies and knowledge bases built from ontological data* [Noy et al., 2001]. The knowledge base utilizing ontology does not follow a strict methodology. The acquisition of a domain idea and its representation totally depend on the purpose and usability of information. Thus, the iterative modeling process effectively reflects the expertise and the concept of an individual. However, it consists of some vital steps including following.

- Identifying the domain-range and scope of ontology
- Definition of classes and subclasses of the taxonomic hierarchy
- Defining relations and attributes with relevant descriptions
- Introducing values or instances according to the class description.

When identifying the domain and scope of ontology, the concept and specific purpose should be clear. The *What*, *Why* , *How* or *Who* kind of questions, also called competency questions, should be answered to circumscribe the limits and usability of the ontology. Thus a concept of class hierarchy and property definitions can be achieved for the modeling. Generally a formal ontology consists of Classes, Rules or relations (Properties), Attributes (Datatypes) and Individuals (Instances).

Classes defines the primary entities in the system. Each class represents a group of entities or subclasses with some common relations or attributes. A subclass is an entity of a class, and the class it belongs to is called a superclass. A class hierarchy is the classification based on proper taxonomy, which is the backbone of an ontology for a knowledge model.

Rules or Relations describes the relations between classes. They are the properties through which the classes are related. These rules can also have functional, transitive, reflexive or symmetric properties.

Attributes are also called *Datatypes*, as they define the value type, range/limits and cardinality [2]. Attribute types can be String, Number, Boolean, Category, Instances etc. These add data restrictions and limit to the framework.

Individuals or Instances are the values in the knowledge base. Each class contains a set of individuals to complete the knowledge base.

Class Description describes the relationship within the domain. Each *Class* contains a set of *Instances*, described with *Rules* or *Properties* and defined/restricted by *Attributes*.

2.1.2 Web Ontology Language or OWL

To Incorporate an Ontology based framework in AI development and knowledge modeling, computer scientists created a universal language named "Web Ontology Language (OWL)", which is developed and maintained by the World Wide Web Consortium (W3C). OWL is designed to be used by applications for machine interpretability of information instead of human interpretation[McGuinness et al., 2004]. The OWL describes web content using the Extensive Markup Language(XML) and Resource Description Framework (RDF) along with formal semantics. Therefore, ontologies based on OWL have become a versatile base for development of Artificial Intelligence, with

[2] Cardinality defines how many values a slot can have which allows single or multiple values in one slot.

greater extent of interpretability both humans and machines. This method of conceptualization had been adopted in biological science and information systems for decades. Nowadays, with the development of OWL, this versatile network has been being adopted to different engineering applications. The later sections further describe the application and development of formal ontology based frameworks and OWL.

2.1.3 Probabilistic Ontology and Multi Entity Bayesian Network(MEBN) in Artificial Intelligence

Ontologies based on the Web Ontology Language (OWL) can be used for information management and presentations, but OWL some constraints. OWL based ontology cannot deal with quantitative reasoning or uncertainty, which means it has limitations when processing partial information. However, most of the systems in the universe have to deal with uncertainty. Extension of the language with added uncertainty using Bayesian statistics helped to restore the problem, called the Probabilistic Web Ontology Language (PR-OWL)[Da Costa et al., 2008]. *Probabilistic Ontology is an explicit, formal knowledge representation that expresses knowledge about a domain of application which includes (i) types of entities of the concept in the domain, (ii) properties of the entities, (iii) relationships among entities, (iv) Processes and events that occurs with the entities, (v) statistical regularities that characterize the domain, (vi) inconclusive, incomplete, unreliable, dissonant knowledge related to the domain, (vii) uncertainty about all forms of knowledge* [Costa et al., 2005].

PR-OWL has been developed and implemented on the platform of the Multi Entity Bayesian Network (MEBN) and has been used effectively in various applications having uncertainty [Costa et al., 2006]. Subsequently, a newer version of PR-OWL has been being used, named PR-OWL 2. Application of this knowledge based information management system has been proposed for complex systems with diverse sources of data to improve the efficacy of the intelligent models [Laskey et al., 2010].

The Multi-Entity Bayesian Network (MEBN) is an extension of the Bayesian Network (BN) based on first-order Bayesian logic and probability theory. Like Bayesian Networks, MEBN theories use directed graphs to specify joint probability distributions for a collection of related random variables [Laskey, 2008]. MEBN theories represent knowledge as a collection of MEBN Fragments (MFrags), and each MFrag contains uncertainty information about the part of the domain having dependencies using different variables. The fragment graph can contain context,input and resident random variables compiled with the uncertainty hypothesis and logical dependencies. The fragment models (MFrags) are interrelated with other MFrags within the domain through context and input variables. A collection of MFrags with consistency together defines the joint probability distribution for instances of each random variable [Carvalho et al., 2009]. Among many efforts to introduce uncertainty logic in formal ontology and support artificial intelligence using the Bayesian Network[Fenz et al., 2009] and MEBN based probabilistic ontology [Carvalho et al., 2007] , are of note. Ultimately, among all these methods UnBBayes has the most applications in the field of artificial intelligence for fraud detection [Carvalho et al., 2010a] and maritime domain applications [Laskey et al., 2011][Carvalho, 2011]. Based on a similar platform an intelligent simulation module for Predictive Situational Awareness with Probabilistic Ontologies (PROGNOS)[Carvalho et al., 2010b] has been in development.

2.1.4 Ontology: Applications & Scopes

Starting from philosophical Epistemology, an ontological framework has been adopted in knowledge engineering and artificial intelligence(AI). Primarily, the application started with medical informatics, phylogenetic analysis and plant taxonomy in biological sciences, data science and artificial intelligence in computer science. Ontology attracted building the data structure of expert systems, when human expertise worth sharing as knowledge base is required along with the data. Biomedical informatics and AI development scientists have been using ontology based framework for decades.

However, Ontology Engineering has been introduced by researchers as a useful tool for knowledge management in the field of process design [Brandt et al., 2008]. *ONTO-CAPE* provides deep insight of various types of ontology for chemical process systems [Wiesner et al., 2008]. An ontological framework has been introduced for implementation in process safety analysis [Daramola et al., 2011], HAZOP study [Zhao et al., 2009] and operational risk management [Lykourentzou et al., 2011]. The work has introduced smart, automated safety and risk analysis tools based on ontological framework Fault Tree Analysis(FTA) and HAZOP are a established tool for root-cause analysis for any process incidents to understand the most probable process incidents from any fault induced. However, Formal Concept Analysis (FCA) is a data mining tool for data analysis and knowledge discovery. We will use HAZOP and FTA to build up the knowledge base and develop the incident based domain using FCA, which can produce a binary matrix to facilitate computing systems. FCA consists of *Formal Objects & Formal Attributes*, which together produce a binary relation to build formal context. The formal context can be demonstrated by cross table and a lattice structure is used to visualize the relations[Batres et al., 2009]. The FCA table can be used to prepare the binary matrices for each fault scenario. Each fault propagation domain will be nested in the primary ontology structure as as incident/event based warning domains. Semantic Web database can be used for more efficient process monitoring to identify the major incidents [Elhdad et al., 2013]. Additionally, using the fault diagnosis tool based on ontological anomaly detection, can improve security of any automated process in case of cyber intrusions in the SCADA system [Jeffrey Hieb, 2009].

An ontological framework has been introduced in the fault diagnosis of electrical networks through alarm ontology [Bernaras et al., 1996]. An ontology based framework had been used in electrical engineering [Zhou et al., 2015] [Pradeep et al., 2012] with great efficacy. Recently, this idea has been adapted for failure mode effect analysis studies [Ebrahimipour et al., 2010] and process control systems [Melik-Merkumians et al., 2010]. A detailed method of fault diagnosis based on FMEA has been proposed by the researchers based on a case study of a pneumatic valve [Ebrahimipour and Yacout, 2015]. The same group of researchers proposed a detailed study of the application of the ontological framework in fault diagnosis and physical asset integrity management [Vahid Ebrahimipour, 2015]. Fuzzy Logic is another type of reasoning, introduced as FuzzyOWL2 [Bobillo and Straccia, 2011] used for Artificial Intelligence.

2.2 Softwares & Tools

2.2.1 Protégé

`Protégé` [Musen and Team, 2015] is a Java[3] based open source ontology development platform, developed by the Stanford Center for Biomedical Informatics Research (BMIR) at Stanford University. Since the 1980s, *Protége* has been the skeletal platform for *Knowledge Acquisition* to support expert systems (AI) in medical informatics. *Protége is neither an expert system itself nor program that builds an expert system directly; instead Protége is a tool that helps users to build other tools that are custom-tailored to assist with knowledge acquisition for expert systems in specific application areas.*"[Musen, 1989]

Different versions of this software have been developed to assist knowledge based models, *Protége -2000* was published with an open-source license for the accessibility of developers and used plug-in based architecture to provide versatility. This was a revolutionary step for knowledge engineering, as this new tool mostly focused on "domain experts" instead of knowledge engineers, plug-in architecture and the re-usability of the model in different platforms. Thus, the introduction of the *Semantic Web* to store all the ontological information in a single online platform came into practice [Gennari et al., 2003]. However, in later years, by the introduction of *Web Ontology Language (OWL)* as a plug-in editor named *Protégé OWL Plug-in* [Knublauch et al., 2004] provided this software with a universal platform to be a user interface based ontology editor.

As *Protége* is open source, many Java based Application Programming Interfaces

[3]Java is a class-based, object oriented general purpose programming language which can perform on different platforms without repetitive compilation.

(API) are available with the core software. `Protége 4.1`[4] is used in this work and has following functionality [Yu, 2011] :

- Can create ontologies using OWL/OWL2.
- Edits and visualizes ontology as classes , properties and relations.
- Defines logical Characteristics in OWL expressions.
- Edits OWL instances for semantic markup.
- Can use reasoners(e.g. FaCT++, HermiT) as plug-in extensions.
- Is reusable and can be imported or exported as OWL/RDF/XML files.
- Can be extended through industry standard *Java OSGi* based plug-in architecture.

However, among several other different ontology editor tools (e.g. *Ontolingua, WebOnto, OntoSaurus, ODE, KADS22*), *Protége* offers ease of learning with a reasonable degree of application [Duineveld et al., 2000].

2.2.2 UnBBayes

`UnBBayes`,[5] is the Graphical User Interface (GUI) tool to develop and edit probabilistic OWL ontology in PR-OWL environment to generate MEBN [Section 2.1.3]. The UnBBayes project was created because of necessity of introducing uncertainty in ontology or knowledge representation. *Uncertainity is ubiquitous. Any representation scheme intended to model real-world action and processes must be able to cope with*

[4] Protégé (4.1), Stanford Center for Biomedical Informatics Research (BMIR) at Stanford University School of Medicine CA USA, 2011 *http://protege.stanford.edu*(Latest Version: 5.0, 2016)

[5] UnBBayes (4.21.18) GNU General Public License, Version 3, 2007, *https://sourceforge.net/projects/unbbayes/*

effects of uncertain phonomena. [Costa et al., 2005]" This tool was developed based on the *Java* application by the Artificial Intelligence Group(GIA) of the computer science department at the *Universidade de Brasília*[6].

Based on the *Bayesian Network's* graphical and theoretical structure, *UnBBayes* provides a framework for building probabilistic graphical models and performing reasoning. Its open source license and plug-in support provide the ultimate versatility and adaptability to different platforms. The driving factors of *UnBBayes* design and development consist:

- *Being an operative platform for dissemination of concepts and usefulness of probabilistic reasoning.*
- *Being an easy-to-use and configurable visual tool.*
- *Being an achieving extensibility and variability.* [Matsumoto et al., 2011]

However, this tool not only implements probabilistic graphical formalism,but also offers a wide range of plug-ins for the Bayesian Network(BN), Influence Diagram(ID), Multiple-Sectioned Bayesian Network (MSBN), Hybrid-Bayesian Network(HBN), Object-Oriented Bayesian Network (OOBN), Probabilistic Relational Model(PRM), Multi-Entity Bayesian Network (MEBN), Probabilistic-Web Ontology Language (PR-OWL), parameter learning, structure learning, incremental learning of BN, statistical data sampling, classification performance evaluation, data mining and several other algorithms for Bayesian inference.

Although there are other tools available for graphical Bayesian Network generation, this tool provides the unique feature of importing OWL based ontology and effectively

[6] University of Brazil, website: http://www.unb.br/.

utilizes the class-relation-attributes-instances structure in a graphical model, which can produce a Bayesian Network incorporating the logical uncertainty information.

2.3 Hazard Identification and Process Safety

'Hazard' can be defined as the possible situations or scenarios, which might cause potential damage loss or injury; while 'risk' is the chance or probability of any loss, damage or illness as a result of being exposed to the hazard. Risk estimation process lies within three basic questions - *"What can go wrong?"*, *"How bad could it be?"* and *"How often it might happen?"*; which answers about hazards, consequences and occurrence probabilities respectively [CCPS, 2010]. Therefore, in any system or cases, the preliminary step of isolating the hazards according to the nature of potential threats can be called as hazard identification. However, in complex chemical processes hazardous events are results of set of unfavorable conditions or causes, which may be called as hazard scenario. Any kind of hazard appears as a complimentary outcome of a hazard scenario.

In chemical process industries, common process hazards can be categorized into- chemical, thermodynamic, electrical/ electromagnetic, mechanical and health hazards. Any incident or hazardous event might consist of one or more of these hazard types and this preliminary idea of the potential hazards might be obtained from basic knowledge of engineering with help of process flow diagrams, material properties etc. This idea of deducing potential hazards is called preliminary process hazard analysis (PPHA or PHA), which a basic technique of hazard identification. [Wells, 1996]

Different hazard identification techniques such as the Checklist review, Safety Review, What-If-Analysis, Hazard and Operability Study (HAZOP),Failure Mode and Effects analysis (FMEA) and many others are already established in industrial practice. What-if-analysis and Checklist Review is a list of questionnaire or items to improve process safety and hazard analysis. HAZOP lists the hazardous outcomes of possible process deviations. Any of the above methods can be adopted in safety review. FMEA focuses on equipment/system failure types and consequences, based o the functionality. Further details in these processes can be found in literature [Mannan, 2004] [CCPS, 2010]. However, these methods are quite time consuming and slow in nature, as these require a team of experts and intense brainstorming. Moreover, sometimes the outcome cannot be quantified because of its qualitative nature, depending on the process. Therefore, development of a smart and effective identification technique has been considered as a prospective area or research in this topic.

Automatic and expert systems for hazard identification has been proposed in previous studies. Hazard Identification and Ranking (HIRA)[Khan and Abbasi, 1998] has been developed and applied for fire, explosion and toxic release scenarios. A knowledge-based intelligent system named HAZOPExpert[Venkatasubramanian and Vaidhyanathan, 1994] has been proposed for chemical process systems and developed. The computer aided software tool HAZID[McCoy et al., 1999] had been proposed for automatic hazard identification. Blended Hazard Identification (BL-HAZID)[Seligmann et al., 2012] is another automated technique which combines a function-goal-relationship with FMEA and FTA for HAZID in process systems. All these methods have similar goals, improvement of the hazard identification technique for a more responsive and dynamic procedure.

2.4 Accident Database : Overview and Impact

The intrinsic property of "Hazard" can only be identified through previous experience or study of similar incidents. Study of historical accidents/incidents provides a good basis for identifying and eliminating possible hazards. Industrial accidents like the *Bhopal Disaster(1984)*[7] were important lessons of accident history. Reporting of accidents/incident in a database is mandatory in most industries.

A typical accident database requires the reporting of accident details such as the type of chemicals released along with the quantity released, the cause of the incident, the number of fatalities, number of injuries and degree and number of evacuations. The information is used to summarize the types of incidents, the different initiations or causes for incidents, common chemical releases and the severity of their consequences.[Prem et al., 2010]

The accident database can be used for statistical purposes, further learning or modeling. However, *many accident reports, for both minor and major accidents, fail to identify all the lessons that can be learned from them.*[Kletz, 2009] Therefore, more detailed investigation is required whenever necessary. Accident modeling of disasters like the *BP Texas Refinery Explosion (2005)* can reveal the risk of catastrophic events using mathematical prediction models and lead to safe practices[Khan and Amyotte, 2007].

Independent organizations like the *United States Chemical Safety Board(CSB)*[8] provide through investigations and recommendations to improve regulatory standards. Since the formation of this Board in 1998, CSB has conducted more than 60 through investigations with detailed recommendations. CSB proposed the modernization of

[7] One of the most devastating Industrial Disasters : Release of lethal gas from Union Carbide's MIC storage tank killed thousands of people on December 1984, in Bhopal, India.

[8] website:http://www.csb.gov/

"Combustible Dust Standard", "Process Safety Management Regulations", "Emergency Response Planning" and "Preventive Maintenance" . The Occupational Health & Safety Association (OSHA), National Fire Protection Agency (NFPA), Environmental Protection Agency (EPA) and other regulatory bodies have adopted their recommendations to update safety standards and operating procedures.

Although compliance with safety standard regulations minimizes the risk of accidents, 40% of the incidents in CSB database occurred in processes covered by the Occupational Safety and Health Administration's (OSHA's) process safety management (PSM) regulations. Insights from the accident database identified process design, safeguards, operation and maintenance, abnormal/non-routine operations, process hazard analysis failures, human and organizational factors, process changes, proximity, emergency response, etc. as the contributors to most of the incidents. Findings suggest that process hazard analysis(PHA) studies are only performed when required by regulations, but failed to identify the hazards [Baybutt, 2016]. Therefore, the CSB database is a valuable resource to improve PHA and HAZOP performance as part of Inherent Safety[Amyotte et al., 2011].

For chemical industries, the major hazards are fire, explosion and toxic release. Although fire is the most common, explosion is more significant in terms of its damage potential (e.g. fatality or property damage). Toxic release has the highest potential of fatalities, toxicity or contamination in the areas of proximity [Khan and Abbasi, 1999]. Additionally, fire-explosion and toxicity can occur simultaneously or consequently depending on the propagation of an event.

Chapter 3

Ontology Based Framework in Dynamic Hazard Identification

Hazard Identification is the principal inception of risk assessment and management. Therefore, the objective is to seek for an easily accessible and efficient method to identify and quantify the associated hazards in certain industrial scenarios. This chapter introduces an effective methodology to model probabilistic assessment of hazards in a dynamic model. The methodology then utilizes an ontological framework to model the hazard scenario and probabilistic reasoning to estimate the probable hazards in common industrial environments. The purpose of using an ontological framework is to introduce semantic-web based knowledge management which can be a vital framework to introduce automation and artificial intelligence (AI) in hazard identification techniques. In the following section, a methodology is proposed to develop a dynamic hazard identification model based on scenario modeling. Then an ontology based probabilistic modeling approach is described with a simple demonstration. Finally, a complete and generalized hazard scenario model has been developed with the insight of the proposed dynamic modeling methodology, adopting an ontology based Bayesian reasoning approach. The versatile model was tested with multiple case studies, described later in this chapter.

3.1 Dynamic Hazard Identification Methodology

Dynamic risk assessment(DRA) is a continuous procedure which can be updated over time. Like the preliminary step of DRA, the hazard identification and assessment process must be updated over time. Therefore, approaches suggesting dynamic hazard identification have been proposed. Some other recent works introduce the bow-tie method in process hazard identification [Saud et al., , Nakayama et al., 2016]. The goal of this section is to present a scenario based dynamic hazard identification which combines both process faults and event propagation as scenarios. Mapping of scenarios has been adopted in the literature using the Bayesian Network with quantitative assessment[Xin et al., 2017]. Although proposed methodology utilize the scenario based modeling, the proposal is different in procedure and aims to develop an expert system based on knowledge-modeling.

In chemical process industries, common hazard identification methods are developed for the same purpose but with different approaches. While Preliminary Hazard Analysis(PHA) looks for generalized overall hazards and events, the Hazard and Operability Study(HAZOP) focuses on the process parameters and Failure Mode Effects Analysis (FMEA) is mostly equipment oriented. However, to develop a realistic model, a scenario based modeling approach is required to completely capture information of an accident scenario, either from experience or visualization [Khan, 2001]. Therefore, an event based hazard progression scenario can be considered, to outline the model, using the process parameters contributing to the initiating event or causation followed by a set of events or leading to final hazard. Hazards might be of many types; however, for chemical industries, fire, explosion and toxicity pose most potential risks [Khan and Abbasi, 1999]. To develop a Hazard scenario for process industries, scenarios leading to fire, explosion or toxicity are considered. A knowledge based model for identifying the important hazards, causes and parameters involved might provide enough information to develop the generalized model. A probabilistic interpretation utilizing expert systems can be deduced to introduce quantitative assessment. A step-by-step methodology (Figure:3.1) illustrates the proposed idea of dynamic hazard modeling.

The preliminary step of the hazard identification technique is to outline the applicable domain, *i.e.*, limit the boundaries of a process or unit to model the hazard scenario. A hazard scenario consists of conditions, propagating events and hazards. A process hazard scenario can be conceptualized and visualized from prior accidents and events or from the PHA/HAZOP/FMEA studies. Therefore, to share the idea of a scenario, a generalized hazard scenario checklist can be developed where the operational aspects, conditions and progression of events are classified as classes and sub-classes, which we can call a knowledge model. A progression of events with the contributing parameters can lead to the final hazard. In the following section, a model has been developed as a classification which represents the integral information required to determine the most probable hazards.

When a knowledge based hazard scenario model has been developed, it can be utilized to develop the probabilistic data model for the quantitative assessment. Any statistical modeling tool which can incorporate uncertainty for probabilistic reasoning and which can be updated over time will complete the dynamic hazard identification model. The parameters or factors identified above are constant; however, the values or attributes are supposed to change over time. Therefore, a reusable probabilistic

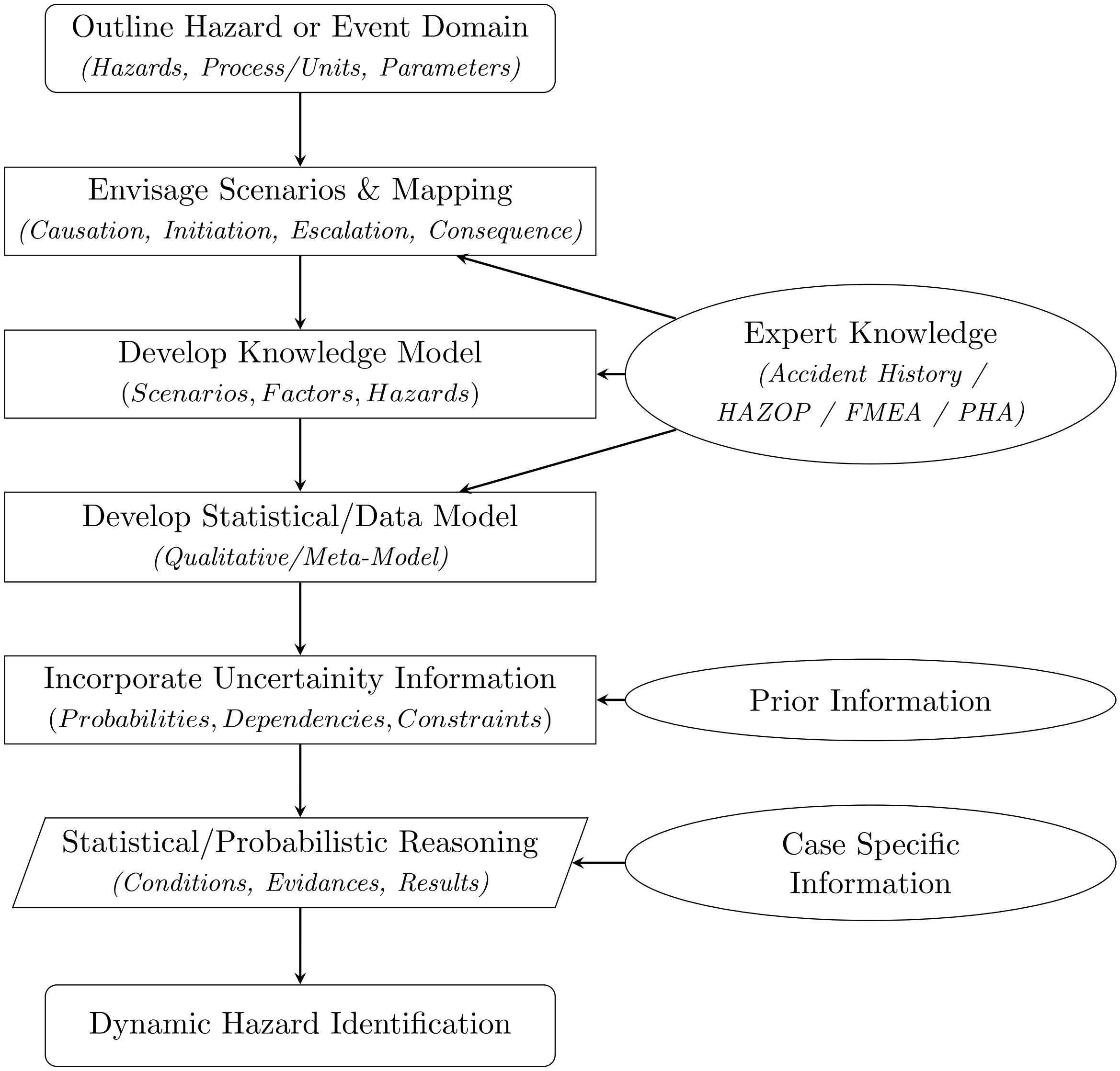


Figure 3.1: Dynamic Hazard Identification modeling Methodology

network is necessary to introduce the dynamics to this system. This work employs the ontology based framework for the knowledge based data model and the Probabilistic Web Ontology Language (PR-OWL) has been taken into account to aid the probabilistic assessment. Detailed methods with examples are discussed in later sections.

3.2 Probabilistic Modeling & Ontology Framework: A Simple Demonstration

The ontology based framework can be a versatile tool for knowledge modeling of a specific unit/domain to represent a formal concept in Probabilistic Web Ontology Language (PR-OWL) and execute probabilistic reasoning using Bayesian statistics. Before implementing the dynamic hazard identification methodology (Section 3.1), this section describes a generalized approach for ontology based probabilistic modeling with a simple demonstration. The methodology is partially adopted from the `UnBBayes` developer's team, and was initially developed for fraud detection [Carvalho et al., 2010a], medical diagnosis, vehicle and marine vessel's identification[Laskey et al., 2011, Carvalho, 2011, Carvalho et al., 2010b]. The methodology comprises of the few principal steps as of Figure 3.2. A step by step demonstration is provided with a simple example.

The first step of this approach is to accumulate detailed knowledge and domain specific ideas for the overall process. The goal is to deliver complete knowledge of the domain scenario with entities, relations and instances which will be the frame of the formal ontology. To demonstrate the methodology, a simple case of a predictive hazard identification model can be considered, which can deal with any abnormal events matching them with the known types of events and predict the most probable hazards from predefined probability values. The simple fire hazard scenario consists of four predefined *eventtypes*- *overpressure*, *leakage*, *rupture* and $overflow$ and can predict four states of hazards- $Fire$, $Explosion$, $MaterialLoss$ & $NoHazard$. This model describes the conditions- presence of the $flammablematerial$ and *ignition* in the event. A UML diagram (Figure:3.3) illustrates the relations and entities in the

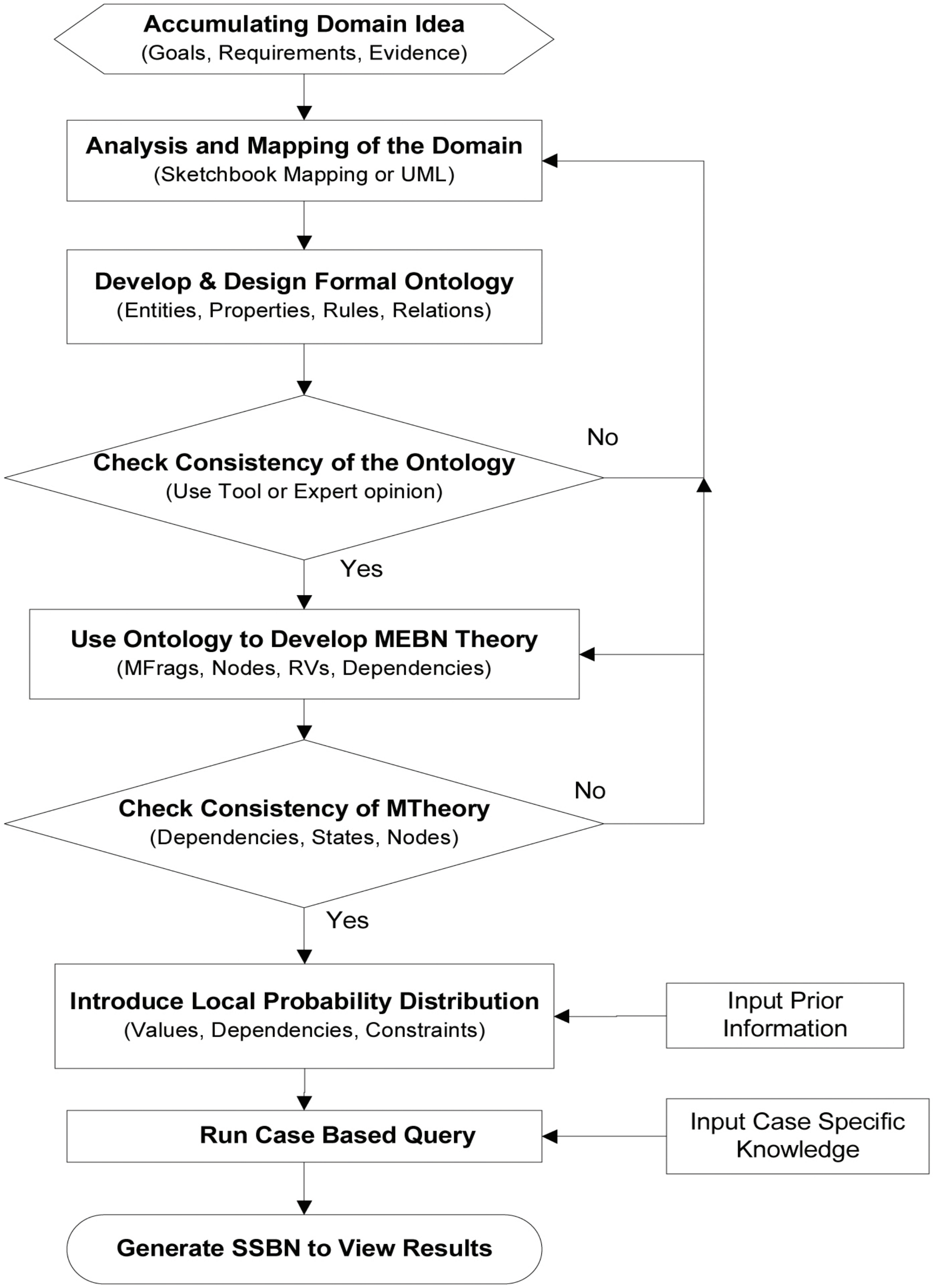


Figure 3.2: Ontology Based Bayesian Reasoning Methodology (Adapted and modified from[Carvalho, 2011])

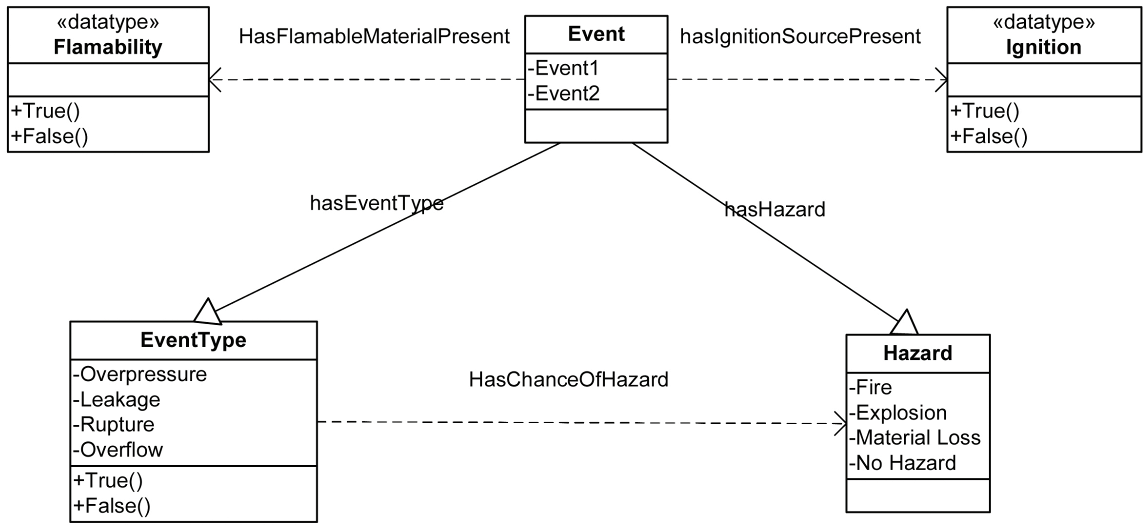


Figure 3.3: Basic Fire Hazard Scenario UML Modeling

lightweight hazard model. This simple model is considered for easy understanding and to avoid complexities in MEBN modeling.

The second step consists of the development of the formal ontology, which is one of the most versatile ways to represent a knowledge model or domain concept. This framework provides both machine and human accessibility and can be reused for different purposes. This process can be aided by the Web Ontology Language (OWL)which has been discussed in the literature survey (chapter 2). Open source software- `Protége` [1] can be used for the ontology development. The definition of classes, properties and relations has to be specified in this step. The UML diagram in Figure 3.3 is a guide to model the ontology. There are only three classes- *Event, Eventtype*, and *Hazard*. There are two object-properties *hasHazard, hasEventtype*. Object-property *hasHazard* has *Event* as domain and *Hazard* as range. Similarly *hasEventtype* has the domain and ranges of *Event* and *Eventtype* respectively. To keep the ontology

[1] Protégé (4.1), Stanford Center for Biomedical Informatics Research (BMIR) at Stanford University School of Medicine CA USA, 2011 *http://protege.stanford.edu*

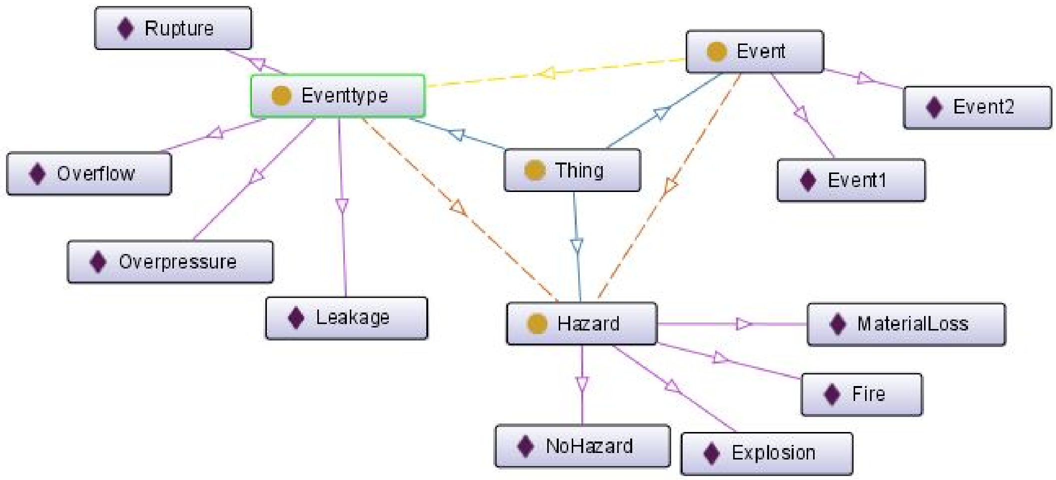


Figure 3.4: Lightweight Hazard Ontology

simple, three boolean datatypes- *hasChanceofHazard, hasFlammableMaterialPresent, hasIgnitionSourcePresent* can be added. The data-types have *Event* & *Eventtype* as their domains and boolean data-type as ranges. As the final step of the ontology development, the individuals or instances must be added in corresponding classes. The final ontology relations with the instances is demonstrated in Figure 3.4. The different colors of the arrow defines different relations amongst the entities.

In the next step, the Multi Entity Bayesian Network (MEBN) can be used to introduce probabilistic reasoning to the existing ontology. More details about MEBN can be found in Chapter 2. This step is similar to Bayesian Network (BN) mapping, not as the whole network, but as fragments called 'MEBN Fragments' (MFrags), which altogether construct 'MEBN Theory' (MTheory). Random variables (RVs) and resident nodes should be linked with the previously developed ontology. The OWL ontology developed based on the lightweight hazard model can be imported in the `UnBBayes` [2] environment to modify and save OWL ontology files with probabilistic information. In the demonstration model, there are only three Mfrags: $EventtypeMF, HasChanceOfHazardMF$ and $HazardMF$. To keep the linkage with the ontology, all variables (random, context, ordinary) should be introduced from previously developed OWL ontology properties. The datatypes and states can introduced from the individuals added in the ontology or new states can be introduced through plug-ins. The complete MEBN model is demonstrated in Figure 3.5. At this point, the MEBN model should be ready to incorporate probabilistic information in the next step.

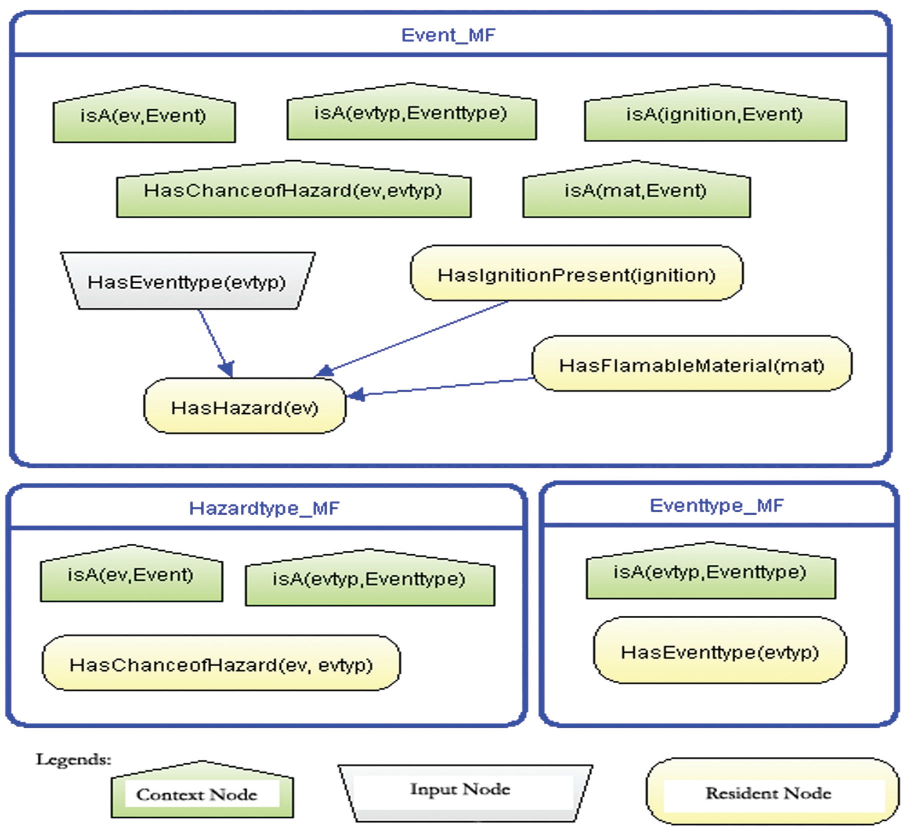


Figure 3.5: MEBN Theory for simple Hazard Model

[2]UnBBayes (4.21.18) GNU General Public License, Version 3, 2007, *https://sourceforge.net/projects/unbbayes/*

In the next step of the methodology, probabilistic information should be added in the MEBN model to incorporate probabilistic reasoning. In the `UnBBayes` environment, Local Probability Distributions (LPD) for all resident nodes have to be provided as prior knowledge. In addition, conditional dependencies and constraints with default values are included in this step. The default values for the *haseventtype* resident node-states are: Leakage(5 %), Overflow (7 %), Rupture (3%) and Overpressure (85%). In all cases of $hasChanceofHazard$, and $hasIgnitionSourcePresent$ node, the default values to be true are considered as 10%. The default LPD of $hasFlammableMaterialPresent$ is 70% true. The decision node $hasHazard$ has conditional probabilities which had been described in logical expressions. Part of the logical expression can be seen in Figure 3.6. The LPD definitions should be saved and compiled for a consistent output while executing the query.

The `UnBBayes` query tool can generate a situation specific Bayesian network (SSBN) that only shows the values for a specific case for a certain node and its contributing nodes. Case specific information can be saved and stored as the knowledge base and can be reused. In the demonstration, the resident node $hasHazard$ had conditional probability, so a query for the $Event1$ to be *true* for leakage could be run, without adding any other knowledge base. In this case the model should use the default values to calculate the probabilities. The Bayesian belief bar shows acceptable values(Fire=27.76%, Explosion=28.31 %, Mat.Loss=26.07%, NoHazard=17.86%) derived from the default LPD distribution (Figure 3.7). If the $hasIgnitionPresent$ node is changed to be true(100%) and *hasEventtype*= leakage (100%) from the be-

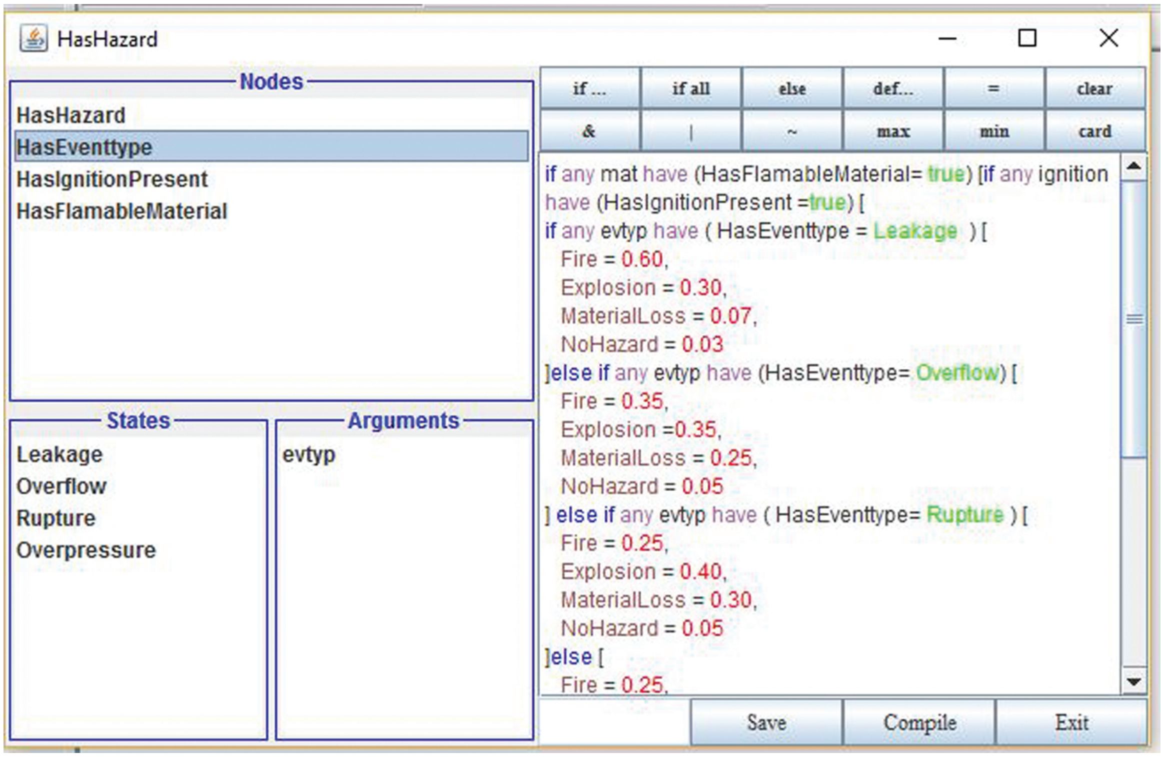


Figure 3.6: LPD definition for simple Hazard Model

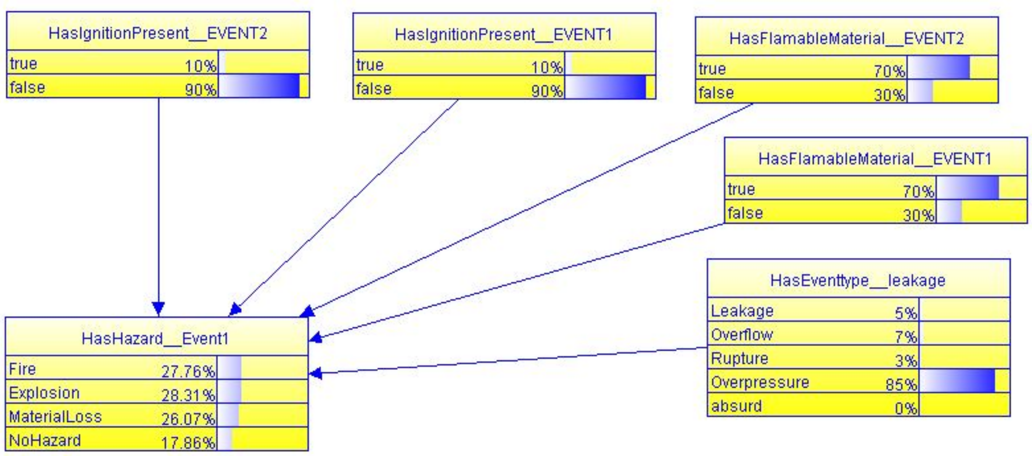


Figure 3.7: Testing the MEBN simple hazard model(Belief Bar shows default LPDs)

lief bar to propagate the evidence, the result shows an acceptable hazard scenario (Fire=55.5%, Explosion=28.2%, Mat.Loss=9.07%, NoHazard= 7.23%) in Figure 3.8. The tests confirm that the model can provide probabilistic assessment of a hazard scenario.

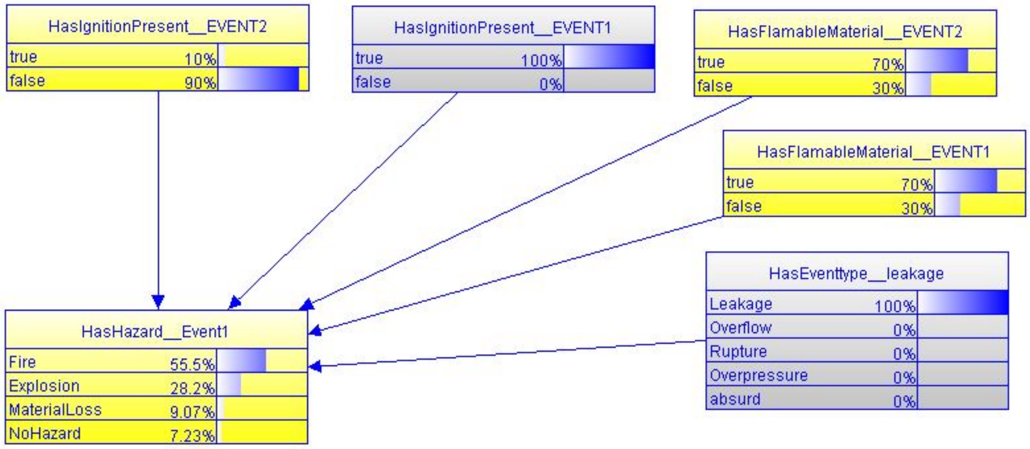


Figure 3.8: Testing the MEBN simple hazard model(Belief Bar shows propagation of events for leakage and ignition)

The SSBN generation completes the probabilistic reasoning based on the ontology based framework. The complete model has features of reasoning and updates prior information, adding individuals and save them for reuse, which make this tool easy to use, adaptive and versatile.

3.3 Ontology-based Dynamic Hazard Identification Model

The proposed approach in this section comprises knowledge modeling of dynamic hazard scenario based on the methodology in Section 3.1 and conceptualizes the domain in Probabilistic Web Ontology Language (PR-OWL) to execute the probabilistic reasoning as demonstrated in Section 3.2. The innovative approach of this article is to implement the proposed dynamic hazard identification methodology (Figure 3.1) for process operations, which requires an assortment of ideas, and both knowledge based and data driven uncertainty. Therefore, an application of the ontology based framework with a Bayesian reasoning approach (Figure 3.1) can contribute greatly to expert systems in hazard identification. Following the steps of general methodology in (Section-3.1), efforts have been concentrated on development of an ontology based hazard scenario model applicable in most process industries.

3.3.1 Outlining Domain & Envisaging Hazard Scenario

First, the hazard scenario domain and relevant factors leading to major hazards have to be outlined. It is most important to identify involved process parameters and anomalous situations for hazards and to collect evidence to support the hazard scenario. Then the parameters, conditions and events are characterized to integrate the scenario. As there is no unique way to design a knowledge-based model, this part requires repetitive procedure and rigorous brainstorming to focus on the goal of scenario modeling. To complete a hazard scenario, operating parameters, external conditions and additional features with the progression of events are involved. As the goal of this work is to develop a generic dynamic hazard scenario model, a hazard

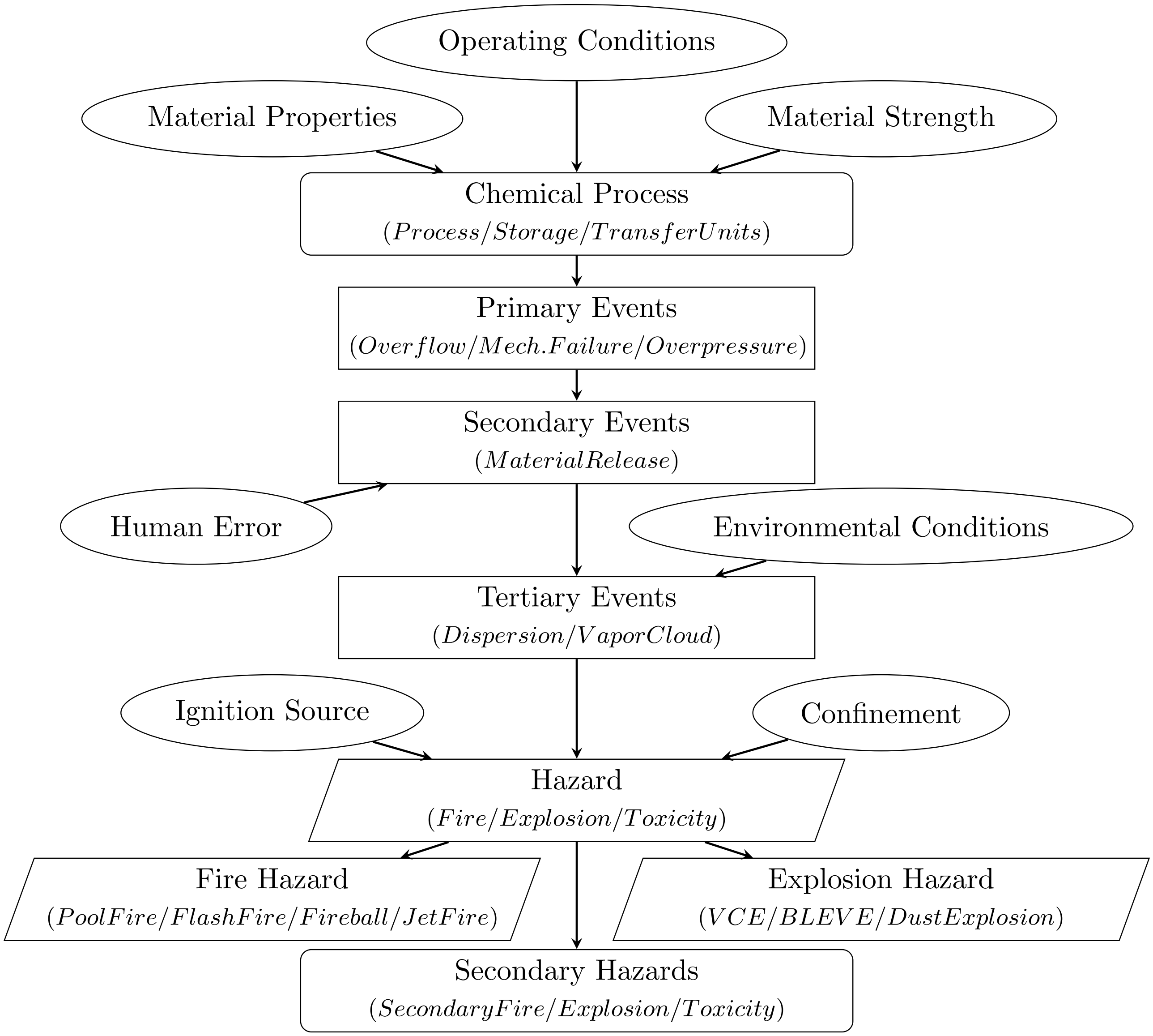


Figure 3.9: Hazard scenario map for common process hazards.

scenario classification is adapted as the domain to accommodate process parameters, relations, sequential events and hazards; this will be the skeleton of the dynamic or knowledge model. This classification captures the general idea of a process industry, involving operational aspects, external factors, causation and propagation of hazards. This scenario is illustrated in figure 3.9.

Hazard Scenario : Knowledge-Based Model

1. Conditions
   (a) Operational Aspects
      i. Operating Conditions
         A. Temperature
         B. Pressure
         C. Flow rate
         D. Unit capacity
         E. Source of ignition
         F. Confinement
         G. Heat Flow
      ii. Material properties
         A. Combustibility
         B. Physical State
         C. Toxicity
         D. Vapour pressure
      iii. Strength of Materials
      iv. Process Type (Reaction)
   (b) Environmental Conditions
      i. Atmospheric Conditions
      ii. Location
2. Human Factor
3. Primary events
   (a) Overflow
   (b) Mechanical failure
   (c) Reaction Runaway
4. Secondary Events
   (a) Material release
5. Tertiary Events
   (a) Dispersion
   (b) Vapour Cloud Formation
   (c) Dust Cloud Formation
6. Hazards
   (a) Fire Hazard
      i. Pool fire
      ii. Flash fire
      iii. Jet fire
      iv. Fireball
   (b) Explosion Hazard
      i. Dust explosion
      ii. VCE
      iii. BLEVE
   (c) Toxic Hazard
7. Secondary Hazards
   (a) Secondary Fire
   (b) Secondary Explosion
   (c) Toxic Exposure

3.3.2 Development of an Ontology-Based Hazard Scenario

To complete the knowledge-based model for hazard identification, statistical and data modeling incorporates uncertainty information are essential. This work utilizes ontology based data structure to develop the basic framework. Developing the ontology is related to defining a set of data and the structure to be used as a support framework for the knowledge base [Noy et al., 2001]. When identifying the domain and scope of ontology, the concept and specific purpose should clear. *What How* or *Whom* kind of questions, also called competency questions, should be answered to circumscribe the limits and usability of the ontology. *Operational Aspects, Scenario* and *Hazard* are the classes for the hazard scenario ontology. Similarly, Operating Parameters such as *Pressure, Temperature* and *Flow-Rate* are the subclasses of their Superclass *OperatingConditions*. The hazard scenario classification can be called class-hierarchy. Hazard Ontology has Functional Properties (*e.g.*, *haspressure* defines the relation of the scenario to the operating conditions). And *Operating Conditions ,Primary Events, Secondary Events, Tertiary Events* and *Hazards* are sequentially dependent. *hasIgnitionSourcePresent* has a *Boolean* data-type, which involves only a *True/False* answer. *Individuals* or Instances are the values in the knowledge base. Each class contains a set of individuals to complete the knowledge base. In the Hazard ontology each operating parameter has *high, Low* or *Normal* value, which were added as instances. These individuals provide the states to construct probabilistic ontology. `Protégé` is used to develop the Hazard Identification Ontology, illustrated in Figure 3.10. `Protégé`[Musen and Team, 2015] is a `Java`- based open source ontology development platform, which has been the skeletal platform for *Knowledge Acquisition* to assist expert systems (AI)[Musen, 1989] in medical informatics and other fields.

3.3.3 Incorporating Uncertainty Information: MEBN Model & LPD Data

The Multi Entity Bayesian Network (MEBN) can be used to introduce probabilistic reasoning to the hazard scenario ontology, utilizing PR-OWL. This step is similar to Bayesian Network (BN) mapping; however, not as the whole network, but as frag-

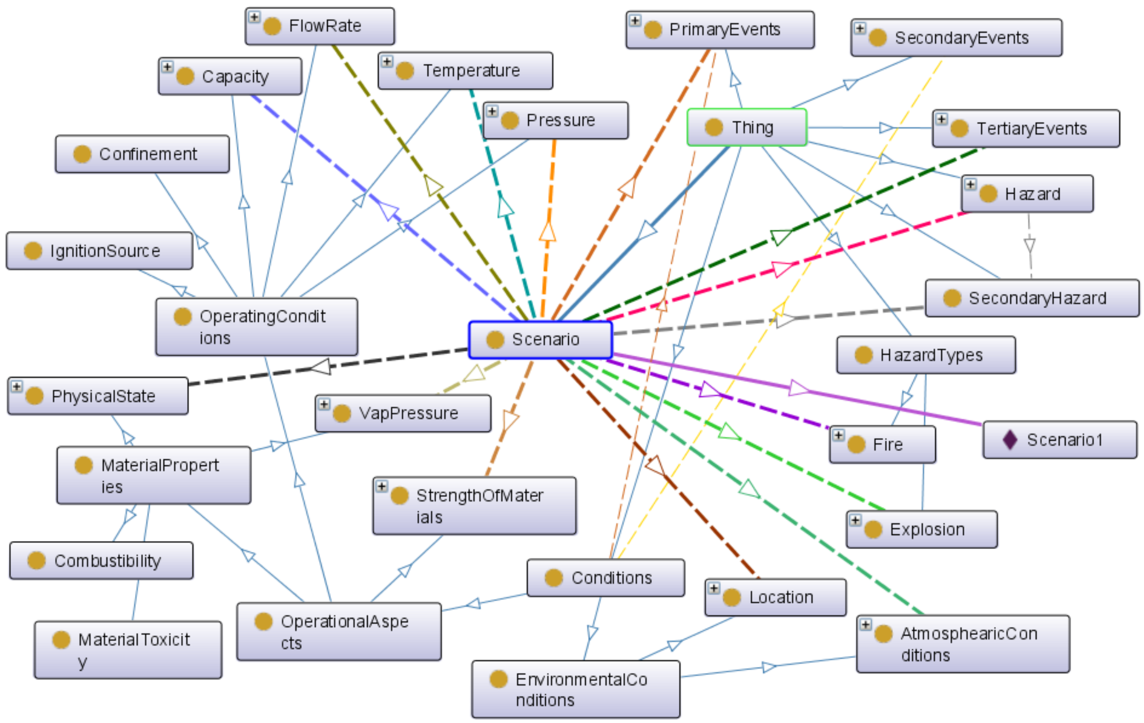


Figure 3.10: Detailed ontology model for hazard identification.

ments called *MEBN Fragments* (MFrags). There are five *MFrags* in the model, which represent each step of event propagation leading to any hazard. All the *MFrags* of a domain are combined to obtain *MEBN Theory* (MTheory). The `UnBBayes`- based MEBN Model of the detailed Hazard Scenario Model looks like Figure 3.11. These *MFrags* contain context, input and resident random variables compiled with the uncertainty hypothesis and logical dependencies. The *MTheory* altogether defines the whole domain through context and input variables. Each individual/instance of each class node has mutually exclusive, collectively exhaustive possible states. A proper linkage among the variables with dependencies and constraints will deliver a consistent MEBN model.

`UnBBayes` is a versatile and easy Graphical User Interface (GUI) tool to develop and edit probabilistic OWL ontology in the PR-OWL environment to generate MEBN

[Matsumoto et al., 2011], which was developed based on the *Java* application by Artificial Intelligence Group(GIA) of the computer science department at the *Universidade de Brasília*[3]. Based on *Bayesian Network's* graphical and theoretical structure, `UnBBayes` provides a framework for building probabilistic graphical models and performing reasoning.

Uncertainty is ubiquitous. Any representation scheme intended to model real-world

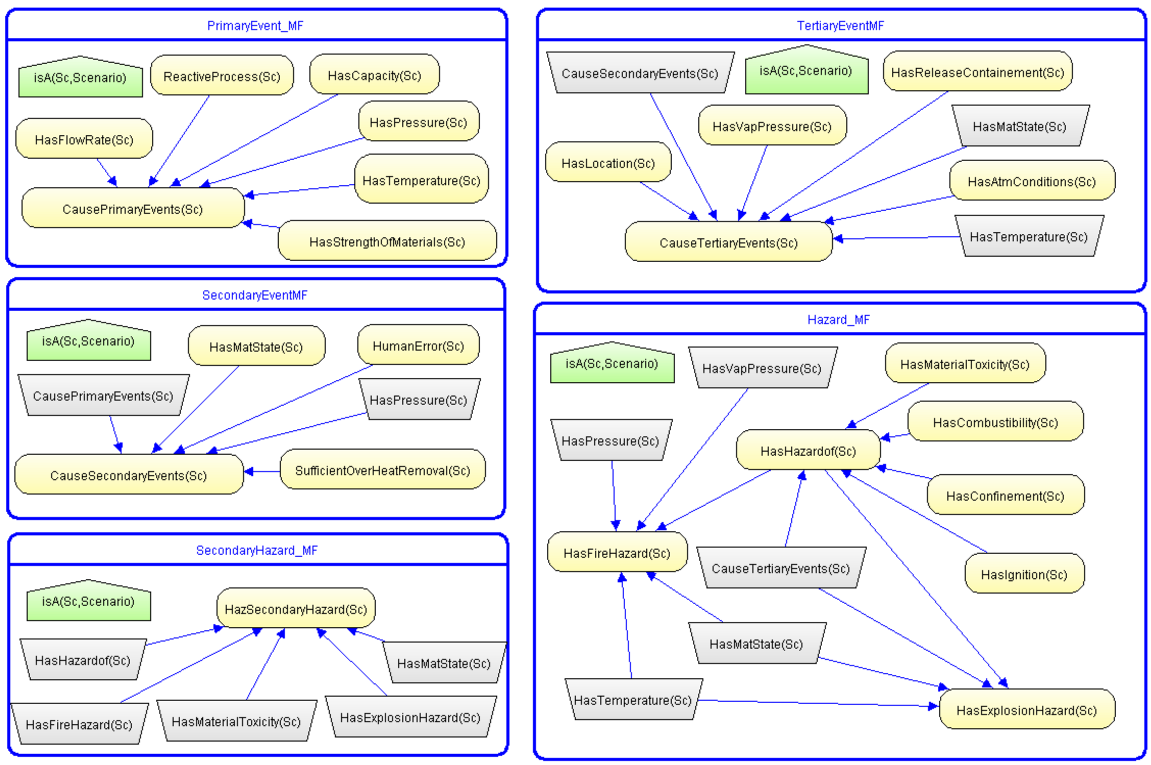


Figure 3.11: MEBN Fragments for the Detailed Hazard Scenario Model.

action and processes must be able to cope with effects of uncertain phenomena. [Costa et al., 2005] Thereby, uncertainty introduces the dynamics in the hazard scenario model. All random variables have conditional or unconditional probability distribution linked to the respective nodes in the PR-OWL environment. To build probabilistic hazard ontology in `UnBBayes`, the Local Probability Distributions (LPD) for all

[3]University of Brazil, website: http://www.unb.br/.

resident nodes have to be provided as prior knowledge. The default LPD values can be declared from prior information or a rational knowledge base.

LPD Declaration[4] Example: ***causePraimaryEvent*** Node

```
if any Sc have (ReactiveProcess = true & HasCapacity
= LowCapacity)[if any Sc have ( HasFlowRate = HighFlowRate )
         [Overflow = 0.15, MechanicalFailure = 0.05,
         NormalOperation = 0.05, ReactionRunaway = 0.75]
 else [Overflow = 0.05, MechanicalFailure = 0.10,
         NormalOperation = 0.60, ReactionRunaway = 0.25]
         ]
else if any Sc have(ReactiveProcess= false & HasCapacity
=LowCapacity)[if any Sc have (HasFlowRate= HighFlowRate )
         [Overflow = 0.85, MechanicalFailure = 0.05,
         NormalOperation = 0.05, ReactionRunaway = 0.05]
 else [Overflow = 0.15, MechanicalFailure = 0.10,
         NormalOperation = 0.60, ReactionRunaway = 0.15]
         ]
else if any Sc have( HasStrengthOfMaterials = LowStrength)
[if any Sc have (HasFlowRate= HighFlowRate )[if any Sc have
( HasPressure = HighPressure ) [ if any Sc have
 (HasTemperature  = HighTemperature )
         [Overflow = 0.05, MechanicalFailure = 0.8,
         NormalOperation = 0.13, ReactionRunaway = 0.02]
 else [Overflow = 0.10, MechanicalFailure = 0.37,
         NormalOperation = 0.50, ReactionRunaway = 0.03]
         ]
else [Overflow = 0.05, MechanicalFailure = 0.25,
         NormalOperation = 0.65, ReactionRunaway = 0.05]
         ]
else [Overflow = 0.05, MechanicalFailure = 0.20,
         NormalOperation = 0.70, ReactionRunaway = 0.05]
         ]
else [Overflow = 0.03, MechanicalFailure = 0.10,
         NormalOperation = 0.85, ReactionRunaway = 0.02]
```

As data is mostly case centric, and this a generic model, the knowledge-base was developed based on expert opinion and a basic understanding of hazard propagation behaviour. Each mutual conditional dependency, constraint with discreet probabilistic data is declared in this step as a simple logical statement. A sample is listed following this section. Successful compilation of the LPD values and conditions com-

[4] The LPD description for the rest of the model is listed in Appendix A

plete the modeling of dynamic hazard scenario model in the PR-OWL2 environment. This model can be used for situation specific queries and results can be viewed as Bayesian belief network. This step is the most significant part of dynamic modeling. As this step can introduce prior probabilities, this model can be updated using historical values for use over time. The extension of this work building an automatic import tool/plug-ins can improve the dynamics.

3.3.4 Probabilistic Reasoning: SSBN

To perform a query using the hazard scenario model, the information for the specific case is inserted in the model. The `UnBBayes` query tool generates a situation specific Bayesian network (SSBN) that shows the probabilistic values and contributing nodes for the scenario. Different scenarios can be saved and stored as the knowledge base and can be reused. The feature of adding individuals and different cases makes this tool easy to use, modify and reuse in different situations. Figure 3.12 illustrates the dynamic hazard identification Bayesian network with default values.

3.4 The Dynamic Hazard Identification Model: Case Studies

To test and validate the model, several previous accidents are used as case studies. This section describes four different scenarios that can be predicted using our model. The results are compared with the historical outcomes.

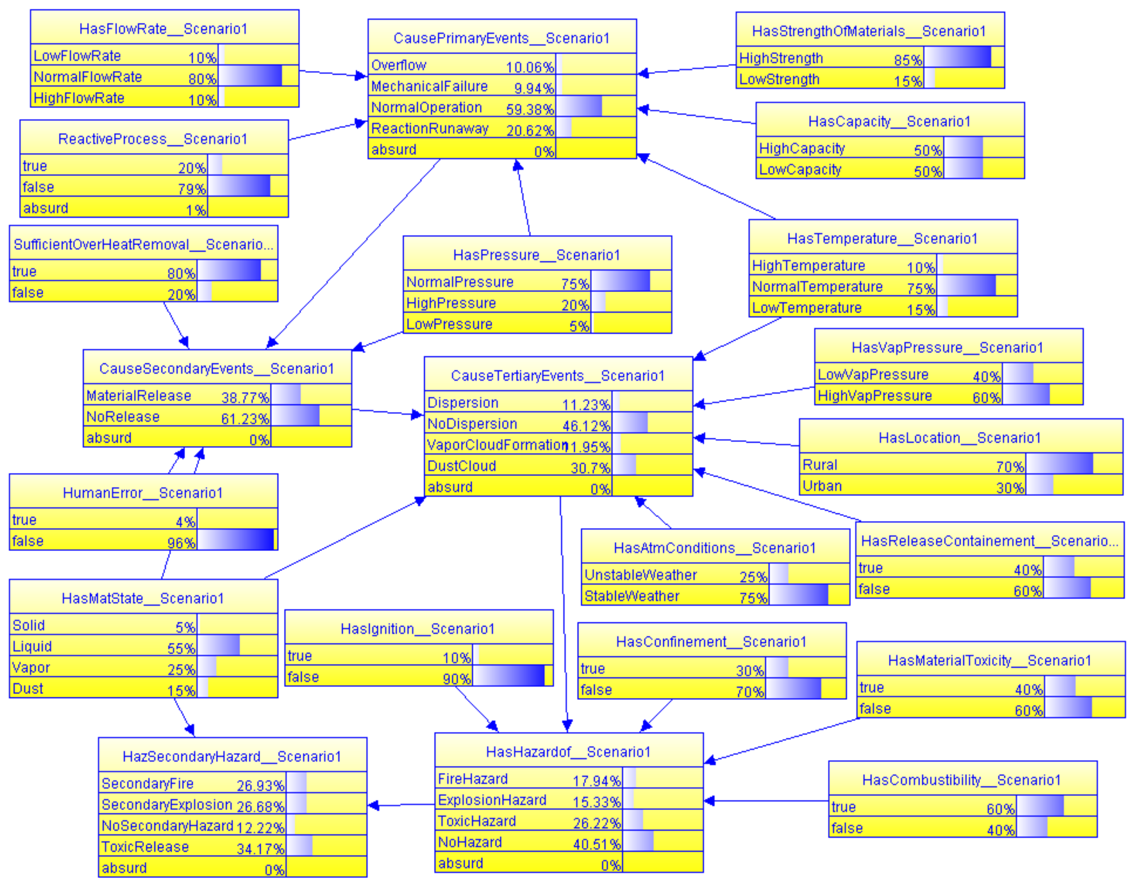


Figure 3.12: Basic SSBN for the Hazard Scenario Model.

3.4.1 Vapour Cloud Explosion in Danvers, 2006

A vapor cloud explosion occurred on November 22, 2006 in Danvers, Massachusetts. According to `CSB Report` [5], a tank of flammable liquid was heated due to an accidentally open steam valve on the heater coil, thus vaporized the liquid. Gradually released vapor formed a vapor-cloud, which was ignited and caused vapor cloud explosion in a congested area. This evidences wes used in the model and it predicted Explosion(51%) as the most credible hazard and Vapour Cloud Explosion (35.3%) as the most probable type. Figure 3.13 shows the result for this case study.

[5] CSB US Chemical Safety Board. CAI / Arnel Chemical Plant Explosion, *http://www.csb.gov/cai-/-arnel-chemical-plant-explosion/*

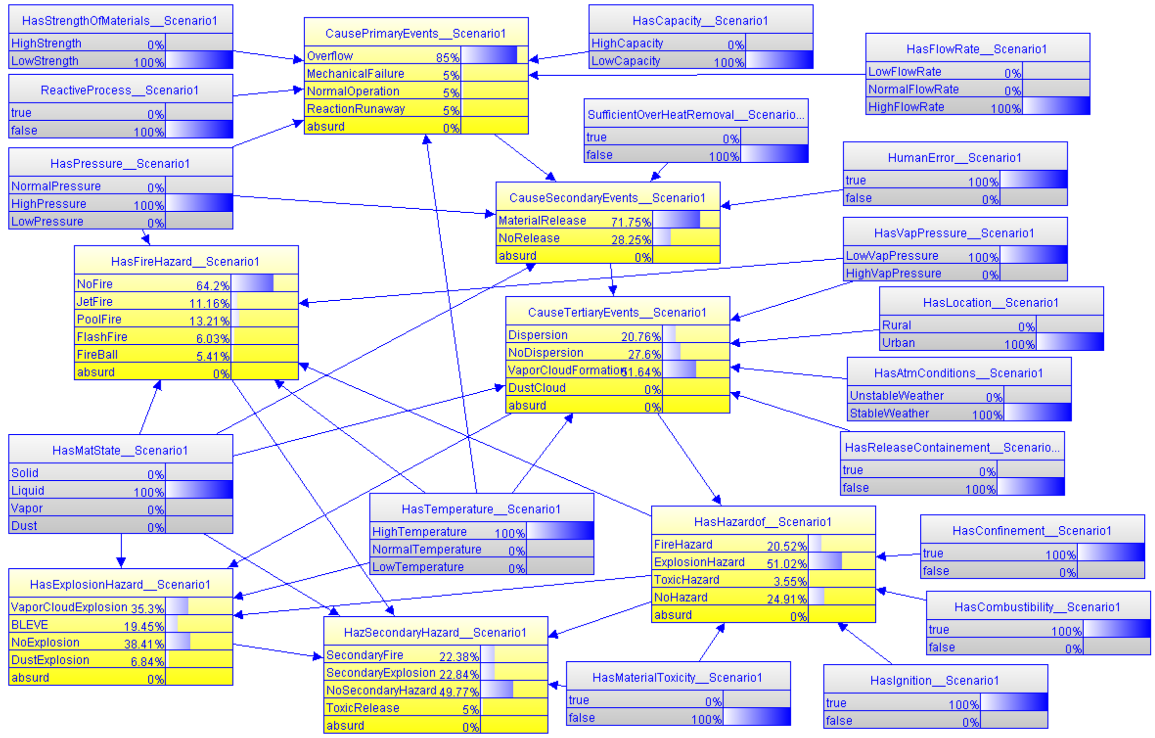


Figure 3.13: Results for the Vapour Cloud Explosion Danvers, Massachusetts on November 22, 2006.

3.4.2 Chevron Refinery Fire and Explosion in Richmond, 2012

On August 6, 2012, an explosion followed by fire caused destruction in the Chevron Refinery in Richmond, CA, USA. According to the CSB investigation[6], the accident caused due to failure of a low strength High-temperature Gas Oil Draw Pipe: the minor leakage in the low strength was increased by improper actions which agitated the line to fail completely, a high temperature fuel was released on the unit floor and a large vapour cloud was formed. The ignition was triggered from the source of

[6] US Chemical Safety Board (CSB) website: *http://www.csb.gov/chevron-refinery-fire/*

leakage as the liquid temperature was well above the flash point. A timely evacuation decision helped to avoid any death, but severe damage caused loss of production for more than a year. The model used these data as evidence to simulate the scenario (Low Strength Material, High Temperature, High Capacity, Low vapour Pressure Liquid, Stable Weather, Highly Combustible, Ignition Source Present). The final predicted result (Figure- 3.14) shows the chance of Explosion=36.07 % and type of explosion to be VCE = 30.63%.

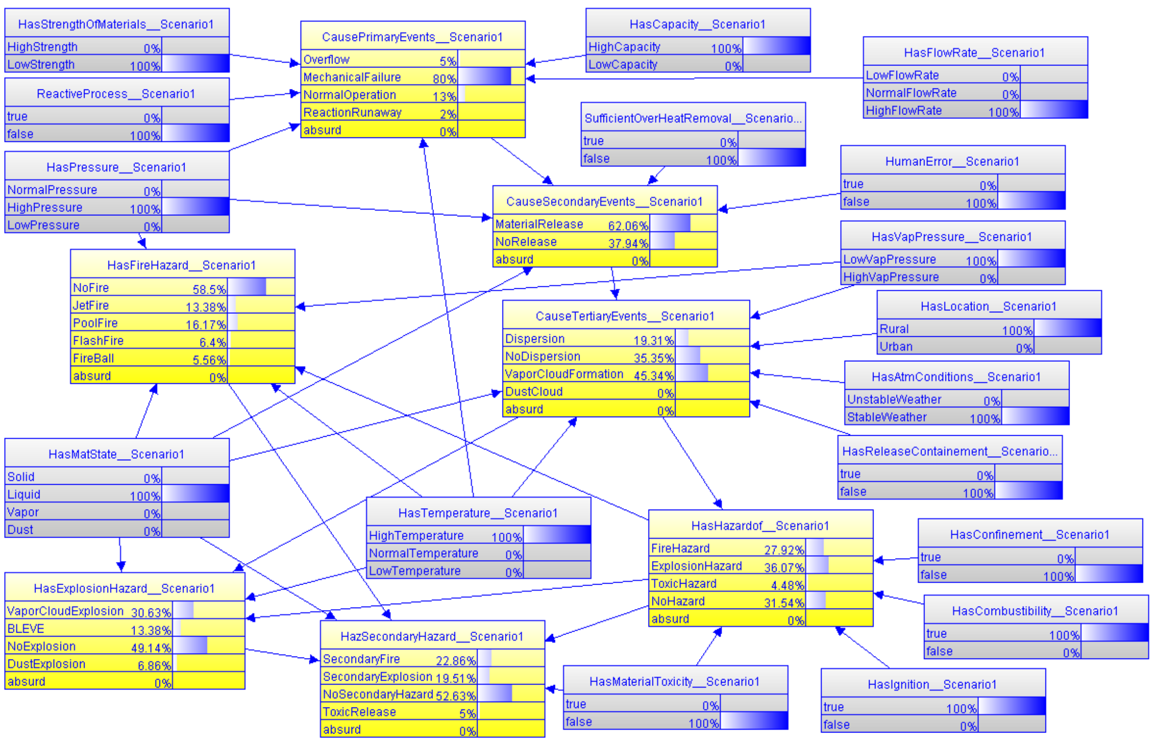


Figure 3.14: Results for the Vapour Cloud Explosion case study for Richmond Chevron.

3.4.3 Dupont Chemical Toxic Release, Texas, 2014

The Dupont Corporation Toxic Chemical Release in La Porte, TX on November 13, 2014 caused at least 4 deaths due to toxic exposure. According to CSB reports during a troublesome startup operation, a valve to vent header was left open during hot-water flushing to remove a pipeline blockage. As the running circulation pump was left unnoticed and the blockage was cleared, the vent header tank filled with toxic liquids. The operators intended to drain the liquid opened a valve and they drained inside a building. Highly volatile-liquid created toxic vapor, which caused toxic exposure to the operators and led to death. Our model counts the mistake as an event of material release and all other evidences to simulate the scenario. The model predicted Toxicity = 67 %(Figure: 3.15).

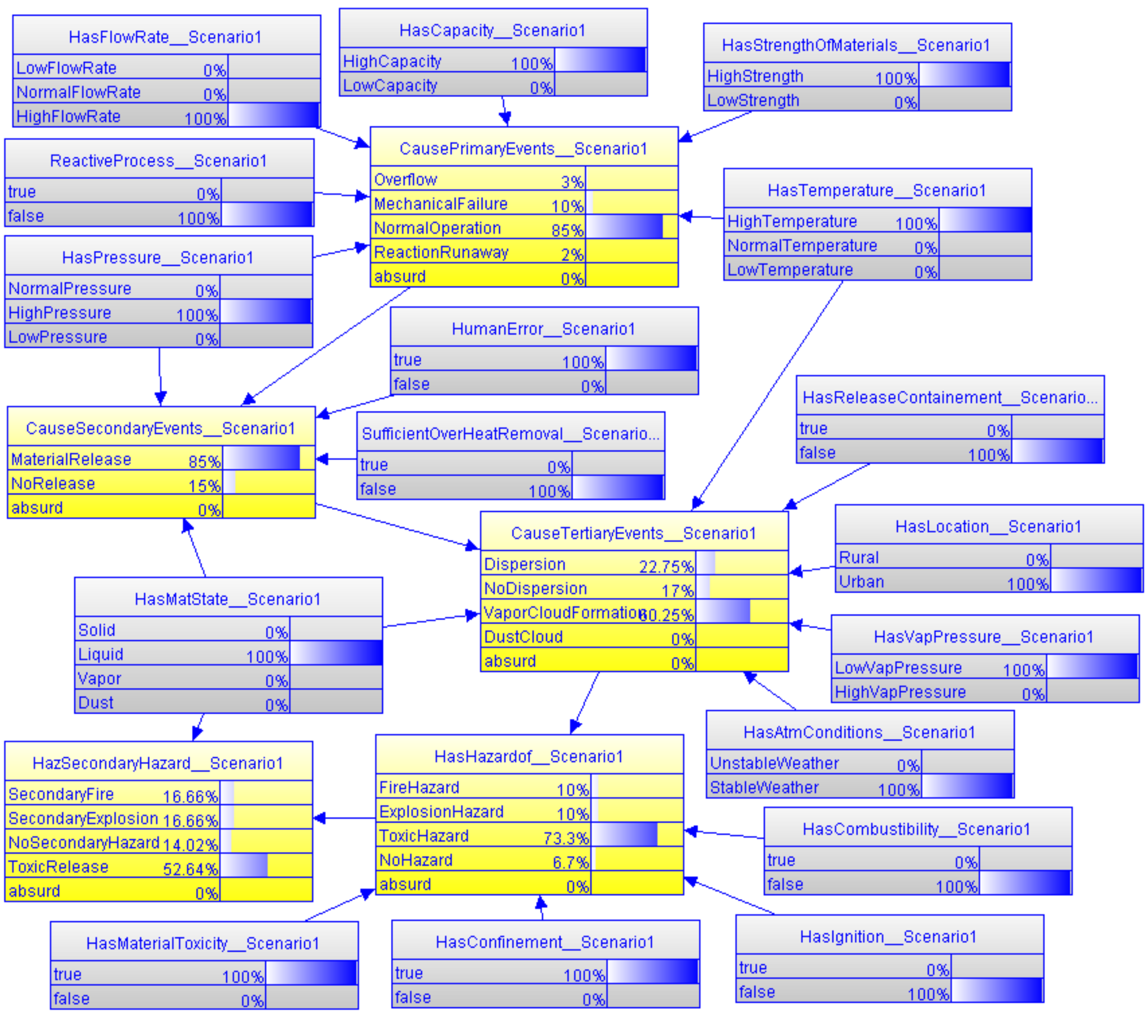


Figure 3.15: Results for the Dupont Toxic-Exposure case study.

3.4.4 Caribbean Petroleum Corporation Tank Explosion & Fire, 2009

On October 23, 2009, The Caribbean Petroleum Corporation (CAPECO) near San Juan, Puerto Rico, faced a fire and explosion accident due to tank overflow. During a gasoline reception pumping operation, an automated tank gauging system failed to show the correct tank level which caused a massive amount of gasoline overflow. The liquid pool inside the containment dike formed a layer of vapour cloud. Some of the liquid gasoline passed through drain reached wastewater treatment facility, where the cloud was ignited by electrical equipment. The ignition caused a large flash fire followed by a massive explosion. This accident was simulated in our model to determine the predictability. As input data, we considered the Low Capacity, High Flow Rate, Low Vapour Pressure Liquid, Combustibility and Ignition Source as principal evidences. The simulation result shows the chance of Fire = 39%, Explosion = 27 % and that the most probable type of fire is Flash Fire(30%). Figure: 3.16 shows the SSBN with results.

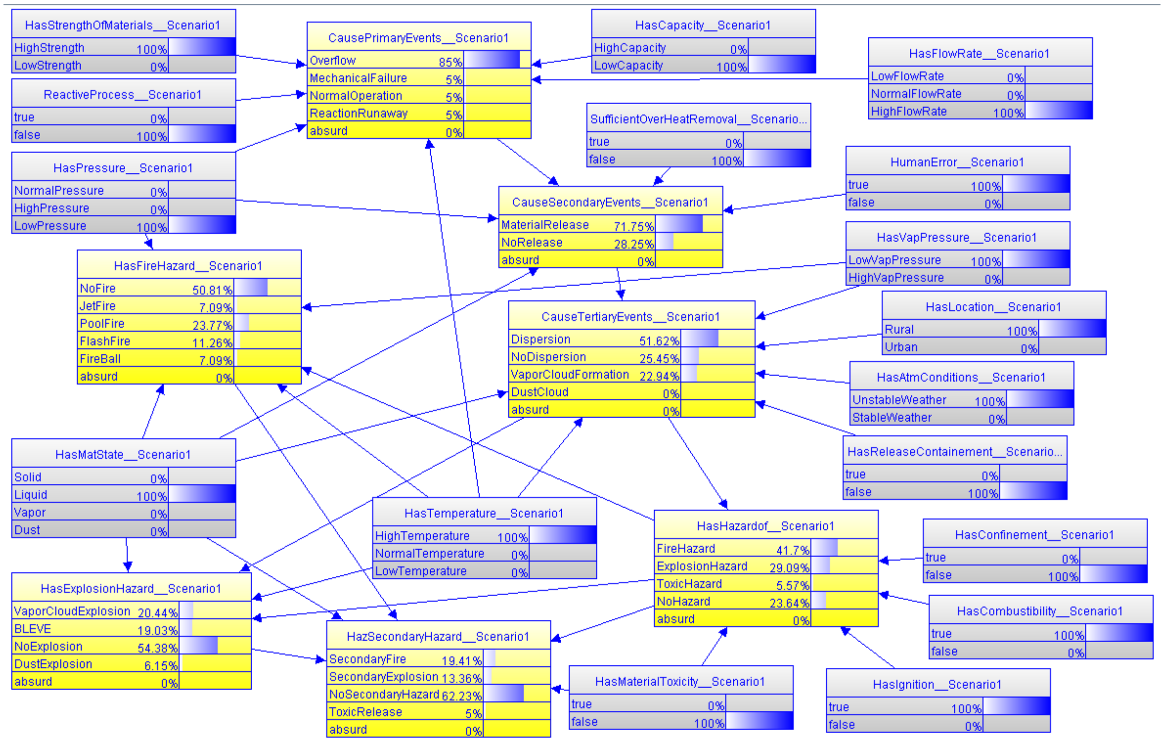


Figure 3.16: Results for CAPECO fire and explosion accident.

Chapter 4

Dynamic Hazard Identification Model: Application & Prospects

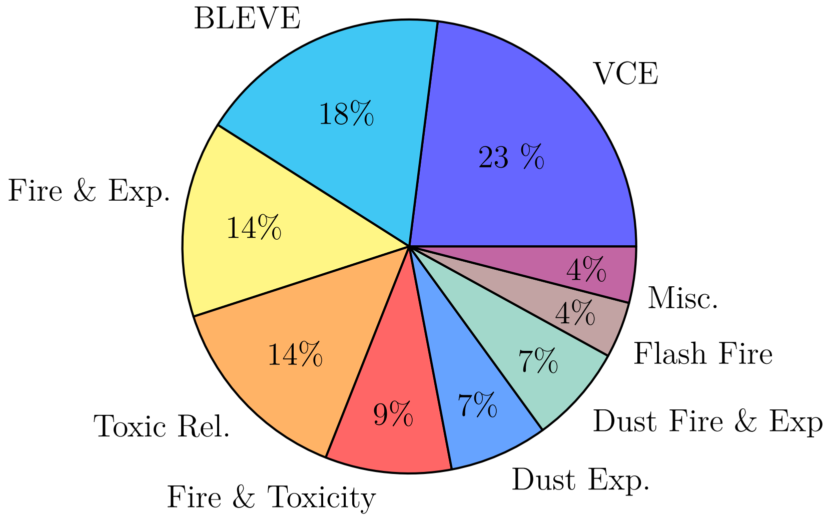
Investigation of previous accidents is the most effective way to enhance hazard scenario knowledge As part of the work, 45 previous accidents in US chemical industries were examined to contribute to the knowledge base. *The Hazard Scenario Model* was implemented both to predict hazards. The results were evaluated to check the validity of the model. Also, some the model was tested in reverse direction in some cases to identify the root causes of an accident. The first section describes the accidents; later sections include results, comparison and further tests of the model.

4.1 Industrial Fire, Explosion & Toxicity Accidents

The Hazard Scenario Model is a conceptual representation of a generalized Fire, Explosion or Toxicity hazard scenario. To validate the adaptability and precision of the model a total of 45 previous incidents from the *United States Chemical Safety Board(CSB)*[1] were considered for study. According the hazard types, there were Fire

[1]website:http://www.csb.gov/

Figure 4.1: Hazards according to types, from the accidents investigated



and Explosion (26) , Reactive Hazard (5), Dust Fire & Explosion (6) and Toxicity (8) Accidents. Table 4.1 briefly describes the accidents taken into account for model validation. Figure 4.1 represents a graphical representation of the actual hazards observed in the accidents.

Table 4.1: Description of Fire, Explosion and Toxicity Accidents Studied.

Serial No.	Accident	Short Description
1.	ConAgra Natural Gas Explosion and Ammonia Release, NC, 2009	During installation and commissioning of a new gas fired water heater, a new steel gas pipe was pressure tested with air. Air was being purged using natural gas and purged in a confined area. While trying to ignite the heater natural gas was purges in indoor plant area for an extended period. The natural gas was ignited from a electrical ignition source.
2.	Richmond Chevron Refinery Fire, 2012	A Distillation column collection pipe leaked due to low material strength at high temperature. The pipeline failed and spilled a high quantity of high-temperature Gas-Oil to form Vapour Cloud which subsequently ignited and caused a Vapour Cloud Explosion.
3.	BP Texas Refinery Explosion , 2005	During the Isomerization Unit start up , because of level transmitter failure, the distillation tower overflowed with temperature hydrocarbon to the blow-down drum. A vapour cloud of hydrocarbon was released into the atmosphere and then ignited causing an explosion.

4.	West Virginia Little General Store Propane Explosion, 2007	Propane leak from a tank during maintenance caused a massive amount of release. The gas entered the store through the ventilation duct and created a vapour cloud inside the store which later on ignited with blast of explosion. Human Error due to inexperience was the primary cause of release.
5.	Huston Marcus Oil and Chemical Explosion, 2004	A modified pressure vessel containing wax and hydrocarbons ruptured at high pressure due to fabrication flaws. This caused hydrocarbon release and fire. This then ignited the liquid inside the tank, which exploded. Most likely the Explosion was BLEVE.
6.	Puerto Rico Caribbean Petroleum Corporation (CAPECO) Fire & Explosion, 2009	A tank overflow during a pumping operation caused a large spill of gasoline. The Gasoline vapour dispersed and created a large vapour cloud. The cloud was ignited from electrical equipment and caused a Flash fire. The fire triggered a secondary explosion of the tank.
7.	West Fertilizer Fire & Explosion, Texas 2013	A Fertilizer storage facility caught fire. The stored nitrate fertilizer was heated, leading a fatal explosion due to explosive properties.

8.	Valero Refinery Propane Fire, Texas 2007	An elbow failed due to icing inside the line and led to a high pressure propane leak forming a vapour cloud. The vapour cloud ignited from the nearby boiler house and created a jet-fire.
9.	Veolia ES Technical Solutions Hazardous Waste Fire and Explosion, Ohio 2009	A flammable vapor of tetrahydrafuran (THF) was released from a waste recycling process, ignited, and violently exploded. Contact of THF with air may lead to a high pressure vent of the gas which might cause vapour cloud explosion as fireball.
10.	Herrig Brothers Farm Propane Tank Explosion, Iowa 1998	A Leakage in the propane tank due a broken pipeline caused a vapor fire in the propane storage tank. The fire heating the tank caused boiling of liquids inside the tank. After reaching a certain pressure, the tank exploded. The type of explosion was BLEVE.
11.	Silver Eagle Refinery Flash Fire and Explosion, Utah 2009	A 10" pipe below the distillate de-waxing unit failed due to corrosion and released hydrogen gas to the atmosphere. The gas created a vapour cloud and caused flash-fire sending workers to the hospital

12.	Carbide Industries Explosion, Louisville, Kentucky, 2011	A water leakage to an electric arch furnace with molten calcium carbide, caused overpressure of the furnace and released tons of debris and powdered gases. The high temperature furnace cover with water jacket having low material strength was suspected be exposed to high temperature "Boil-Up" spills and caused the leak in the furnace. Water in-touch with the molten metals created an extreme high pressure blow up and explosion.
13.	Williams Olefins Plant Explosion, Louisiana 2013	Amongst two water heated Re-boilers of a propylene fractionation tower, the 16 month standby re-boiler exploded due to high pressure. The stand-by re-boiler was suspected to be filled with high temperature process fluid and water was introduced to the reboiler as a part of unprecedented process diagnosis operation. The trapped propylene in the re-boiler overheated and exploded due to overpressure.

14.	EQ Hazardous Waste Fire and Explosion, Apex, NC, 2006	A flammable vapour release along causing chlorine from EQ hazardous waste facility caught fire with toxic smoke. The fire spread inside the facility and storage containers exploded subsequently causing numerous explosion fireballs. The toxic smoke led to evacuation of neighbourhood.
15.	Tosero Refinery Explosion, Washington 2010	A heat exchanger exploded due to high temperature and high pressure during commissioning after service. The low strength heat exchanger shell wall was weakened due to internal cracks caused by High Temp Hydrogen Attack (HTHA). The shell cracked due to high heat and pressure releasing hydrogen with hydrocarbon causing self ignition and fire.
16.	Hilton Hotel, San Diego, California, 2008	After Installation of new piping in the hotel under construction, gas was purged indoor and ignited causing explosion.
17.	Sterigenics International Ethylene Oxide Explosion, California, 2004	A sterilization chamber filled with explosive concentration of ethylene oxide found an ignition source in the ventilation oxidizer and exploded. The event was triggered by a human error of overriding the regular gas purge cycle.

18.	Kleen Energy Natural Gas Explosion, Middletown, CT, 2010	Natural gas was being used to clean new pipelines (aka Gas Blow) and purged in confined plant area. The high concentration of natural gas ignited and caused explosion.
19.	BLSR Fire, TEXAS, 2003	In an oilfield waste disposal facility, two personnels were disposing oilfield waste in an open pit. The waste contained volatile liquid which dispersed in air and caused the nearby truck to backfire. The bacfire ignited the vapor resulting in a flash fire.
20.	Partridge Raleigh Oilfield Explosion and Fire, Mississippi, 2006	An open pipe of nearby tank released flammable vapor during a hot-work. The flammable vapor was ignited and fire propagated to another connected tank containing crude oil and exploded.
21.	Formosa Plastics Corporation Explosion and Fire, Illiopolis, Illinois 2004	An operator opened a running vinyl-chloride reactor drain valve releasing high pressure-high temperature flammable materials. The building, filled with flammable vapour exploded within minutes.
22.	Formosa Plastics Corporation Fire, Point Comfort, Texas, 2005	A Propylene strainer drain valve broke when stuck by a forklift, causing large liquid leak. The liquid caused a vapour cloud and ignited causing fire.

23.	Praxair Propylene Cylinders Fire, St. Louis, Missouri 2005	Propylene cylinders overheated due to atmospheric high temperature in a storage facility and caused release of propylene. The released gas ignited from static charge and caused fire and accelerated series of explosions due to overheating of nearby cylinders.
24.	ASCO Acetylene Explosion, Perth Amboy, New Jersey 2005	A failed check valve caused acetylene flow back to a shed and accumulated through the open drain valve. The explosive mixture exploded, finding an ignition source.
25.	CITGO's Corpus Christi refinery, Texas 2009	A fire in the alkylation unit at CITGO's Corpus Christi refinery led to a release of hydrofluoric acid (HF). The alkylation unit makes high-octane blending components for gasoline. One worker was critically burned. Primary Fire & Secondary Toxicity (Chemical Burn)
26.	Horsehead Holding Company Explosion,Pennsylvania 2010	A buildup of superheated liquid zinc inside a ceramic zinc distillation column "explosively decompressed" and ignited.

27.	BP Ameco Polymers Plant Explosion, 2001	After a mechanical failure, a waste tank filled with molten plastic had a decomposition reaction causing high pressure. When the maintenance workers tried to open the tank lid for cleaning, the tank lid exploded, causing fatalities and damage to the unit.
28.	First Chemical Corp. Reactive Chemical Explosion, Mississipi 2002	An Out of Operation distillation tower partially filled with mono-nitro-toluene (MNT) was heated by leaky steam valve causing a runaway decomposition reaction with high temperature. The high temperature and pressure caused a massive explosion in the tower.
29.	Synthron Inc Explosion, Morganton, North Carolina 2006	A runaway reaction occurred in the batch reactor during an attempt to produce a larger sized batch. The overpressure ruptured reactor cap seal and released flammable vapour inside the building, which then exploded.
30.	Denvers Arnel Chemicals Vapor Cloud Explosion, 2006	Accidentally open steam valve overheated a tank and formed a vapour cloud leaking through the unsealed vent, causing a Vapour Cloud Explosion.
31.	T2 Laboratories Explosion, Jacksonville, Florida, 2007	Due to malfunctioning cooling system a runaway chemical reaction in MCMT reactor caused high temperature inside the reactor. As a result the vessel exploded with fire.

32.	Imperial Sugar Refinery Dust explosion, Georgia 2008	One of the largest Dust explosions, killing 14 people and injured many. Sugar dust was ignited inside a closed conveyor by contact with the high temperature bearings. The dust explosion caused several chain explosions and fireballs destroying the whole facility.
33.	AL Solutions Metal Recycling, West Virginia 2007	Metal combustible dust was ignited from a spark in the blender. The flashfire ignited and created a combustible vapour cloud leading to dust explosion.
34.	Hoeganaes facility Flash Fires, Tennessee 2011	The iron recycling facility had several fatal accidents with combustible dust flash fires. During a maintenance operation a combustible dust cloud was ignited from a metal spark and caused a flash fire alt least three times in the same year, causing total of 5 fatalities.
35.	West Pharmaceutical Explosion, North Carolina 2003	Accumulation of Polyethylene dust over the acoustic tile ceiling was agitated due to a small fire inside the facility, forming dust cloud. The dust cloud ignited from a source causing massive explosion inside the building.

36.	Hayes Lemars Plant, Indiana 2003	The factory prepared aluminum wheels. The aluminum dust from machining-grinding was collected through dust collector and fed to the furnace for remelting. A dust fire started inside the dust collector from metal spark or hot surface causing the flame-front to propagate back to the furnace area, releasing an airborne dust cloud, which exploded inside the confined plant area.
37.	CTA Acoustics, Kentucky, 2003	Polymer resin dust clouds from improper housekeeping operations dispersed inside the facility and found an ignition source from a open furnace door. The Dust cloud caused two small dust explosions. The consequence was dispersion of more accumulated dust and propagation of the explosions destroyed the whole production line.
38.	Dupont Chemical Toxic Release,Texas, 2014	An unnoticed valve left open during startup operation caused toxic liquid carryover to the blowout drum. The operators tried to purge the liquid and inhaled toxic gas resulting fatalities.
39.	DPC Enterprises Chlorine Release, Missouri 2002	A chlorine transfer hose ruptured during rail unloading, releasing a huge quantity of toxic gas.

40.	DuPont facility Toxic Exposure, West Virginia 2008	A toxic Phosgene gas hose was disconnected during cylinder replacement and created a toxic environment leading to fatalities.
41.	Bayer Crop Science, West Virginia	During a startup of the Methomyl unit, a runaway reaction occurred in the waste cooker and exploded, with flammable toxic material release and fire.
42.	MFG Chemical Inc. Toxic Gas Release, Dalton, Georgia, 2001	A chemical reactor overheated releasing toxic allyl alcohol vapour. The overheating caused overpressure and rupture of the tank seal.
43.	Millard Refrigerated Services Ammonia Release, AL, 2010	The refrigeration system was started after an unplanned shut-down without removing liquid from the circuit. As a result, a hydraulic shock was generated which led to rupture of the pipeline. Ammonia leaked to atmosphere and affected the community.
44.	Freedom Industries Chemical Release, WV, 2014	A leakage of hazardous materials led to toxic contamination of nearby river water, which resulted in contamination of water supply to the nearby community.
45.	Honeywell Plant Chlorione Release, LA, 2003	While unloading a railroad chlorine tanker, the transfer hose ruptured due to high pressure. The release lasted for 45 seconds before the operators responded by closing the shutoff valves. The exposure affected 11 workers.

4.2 Implementing The Hazard Scenario Model : Evidence and Results

The Hazard Scenario Model can predict different hazards from existing knowledge based data. The development of the primary hazard scenario was a knowledge-based model depending on th literature and investigations of the US Chemical Safety Board (CSB). However, to validate adaptability, the model was tested and trained with trials of accidents from previous database. For convenience the results are categorized based on the nature of scenario and listed in tabular form.

4.2.1 Fire & Explosion Scenarios

Chemical fire and explosion hazards are most commonly observed in process industries. For most of the cases material release due to *Mechanical Failure, Overflow, or Reaction Runaway*, and some cases were influenced by *Human Error* initiating the primary events. The propagation of event can lead to *Fire Hazard, Explosion Hazard or Toxicity* or all of these. Our results in Table 4.2 represents how the model predicts fire and explosion incidents based on the provided evidence.

Table 4.2: Explosion & Fire Accidents

Accident	**Important Evidence**[2] (*Scenario*)	**Results**
1. ConAgra Natural Gas Exp. and NH_3 Release, NC, 2009	Comb. Gas > Mat.Rel. > Conf. > Ig. > Exp.	Exp. = 51.60 % ; VCE = 43.24 %
2. Richmond Chevron Refinery Fire, 2012	Low St. > H T > H Cap. > LVP Liq. > Stable Weather > Mat.Rel. > VCFormation >Comb. >Ig. Source > VCE	Exp.=36.07 % ; Fire = 27.92%; VCE = 30.63%
3. BP Texas Refinery Exp. , 2005	Low Cap. > H Flow > HT > Overflow > Mat.Rel. > Vap.Cloud > Ig. >Comb. > No-Conf. > VCE	Exp. = 39.88 % ; Fire = 30.22 % ; VCE = 33.32 %
4. Little General Store Propane Exp., 2007	Hum.Err. > Mat.Rel. > Comb. gas > Dsp.> Conf.Space > Ig. >	Exp. = 42.6 %; VCE = 36.78%
5. Houston Marcus Oil and Chemical Exp., 2004	LowSt. > HP > HT > HCap. > Mat.Rel. > LVPLiq. > Dsp.> No Conf. > Comb. > Ig. > Fire > BLEVE	Exp. = 46.06 % ; VCE = 32.22% BLEVE = 18.79%
6. CAPECO Fire 2009 & Exp., 2009	Low Cap. > H Flow> LVP Liq. > Comb. > Ig. > Fire > Sec.Exp.	Fire =41.7%; FlashFire =20.65%
7. West Fertilizer Fire & Exp., Texas 2013	Solid Mat. > Mat.Rel. > Comb. > Ig. > Fire > Explosive Mat. > Sec. Exp.	Exp. =24.45%; D.Exp. = 17.64%

[2] Abbreviations Used; (*e.g.* Mat. Release= Mat. Rel , Temperature=T, Pressure=P, Vapor =V/Vap, High =H, Combustible=Comb. , Strength=St., Exp. =Explosion, Toxicity =Tox. , Capacity =Cap., Dispersion=Dsp., Vapor Cloud=VC)

8. Valero Refinery Fire, Texas 2007	LowSt. > H P > Mech. Fail > Mat.Rel. > LVPliq. > Ig. > Comb. > Fire	Fire = 42.82% ; JetFire=22.13% ; Sec.Exp.=38.69%
9. Veolia ES Tech. Sol. Fire and Exp., Ohio 2009	Mat.Rel. > Comb.Gas > Vap.Cloud > Ig. > VCE	Exp. = 34.66% ; Tox. = 46.94 %
10. Herrig Brothers Farm Propane Tank Exp., Iowa 1998	HP > Leakage > LowVPLiq. > Dsp.> Ig. Source >Fire > Liq. > Sec.BLEVE	Fire = 31.31 % ; JetFire=20.67%; Sec.Exp.=29.93%
11. Silver Eagle Refinery Flash Fire and Exp., Utah 2009	Gas>Low St.Mat.> HP > HFlow > HT > Mech.Fail > Mat.Rel. > Dsp.> VC > Comb. > Ig. > Fire	Fire = 38.8% ; Flashfire = 18.58%
12. Carbide Industries Exp., Kentucky, 2011	H T > Mech. Fail > Mat.Rel.> Non-Toxic & Non-Comb. Liq. > No. Ig.> Conf. Vessel > Exp. (BLEVE)	Mat. Rel.= 62.06 % (No Hazard)
13. Williams Olefins Exp., Louisiana 2013	Liq.> Mat. Rel.> H T > BLEVE	Exp. = 60.55 % ; VCE = 43.52 % ; BLEVE = 19.19%
14. EQ Hazardous Waste Fire and Exp., Apex, NC, 2006	Mat.Rel. > Comb. > Ig. > Toxic > Fire> Toxic Vap.	Fire = 34.66 % ; Tox. = 40.94 %

15. Tosero Refinery Exp., Washington 2010	Low St.(HTHA)> HT > HCap. > Gas > Mech.Fail >Mat. Rel.> VC >Comb.> Ig.> no Conf. > Fire	Fire =42.8%; FlashFire= 32.8%; SecExp. =38.6%
16. Hilton Hotel, San Diego, California, 2008	Comb. Gas > Mat.Rel. > Conf > Ig. > Exp.	Exp. = 48.34 % ; VCE = 39.93 %
17. Sterigenics Int. Ethylene Oxide Exp., California, 2004	Hum. Err. > Mat.Rel. > Conf. Vessel > Explosive Conc. > Exp.	Exp. = 49.67 % ; VCE = 37.74%
18. Kleen Energy Natural Gas Exp., Middletown, CT, 2010	Comb. Gas > Mat.Rel. > Conf.> Ig. > Exp.	Exp. = 49.09 % ; VCE = 39.6 %
19. BLSR Fire, TEXAS, 2003	Mat.Rel. > LVP Gas > Comb. > Ig. > Fire	Exp. = 32.79% ; Fire = 32.45 % ; VCE = 26.09 %
20. Partridge Raleigh Oilfield Exp. & Fire, Missisipi, 2006	Mat.Rel. > Ig. Source > Comb. Vap. > Fire > Conf. Tank > Exp.	Exp. = 49.43 % ; VCE = 41.67 %
21. Formosa Plastics Corporation Exp. & Fire, Illinois 2004	Hum. Err. > Mat.Rel. > H T Vap.> Conf. Space> Ig. > Exp.(VCE)	Exp. = 39 % ; VCE = 33.46 %
22. Formosa Plastics Corporation Fire, Texas, 2005	Hum. Err.> Low St. Mat.> Mech. Fail> Mat.Rel.> LVP Liq.> HT> VC> Ig. > VCE	Exp. = 37.17 % ; VCE = 31.58 %

23. Praxair Propylene Cylinders Fire, Missouri 2005	H T > H P Gas > Low St. Mat. > Insuff. Heat Rem.> Mech. Fail > Mat.Rel. > VC > Ig.(Static Charge) > VCE > Sec. Exp.	Fire = 30.73% ; Exp. = 36.75 % ; VCE = 33.34 %
24. ASCO Acetylene Exp., New Jersey 2005	Low St. Mat. > H Flow > Low Cap. > Mat.Rel. > Dsp.> Conf. space > Ig. > VCE > Sec. Fire	Exp. = 23.061 % ; VCE = 43.82 %
25. CITGO's Corpus Christi refinery, Texas 2009	Mat.Rel.> LVP Gas.> HT> VC> Ig. > Primary Fire & Sec. Tox. (Chemical Burn)	Fire = 34.02 % ; Tox. = 38.34 %
26. Horsehead Holding Company Exp.,Pennsylvania 2010	H P > H T > Liq. > Explosive > Conf. Space > Self Ig. > Exp.	Exp. = 41.87 % ; BLEVE = 18.74 %

4.2.2 Reactive Hazards

Reactive hazards are commonly known as Fire/Explosion/Toxicity Hazards posed by reactive chemical processes. A reactive hazard normally initiates by reaction run-away caused during any operating conditions. The Hazard model results for reactive hazard related industrial incidents are listed in Table-4.3.

Table 4.3: Accidents from Reactive Hazards

Accident	**Important Evidence**[3](*Scenario*)	**Results**
27. BP Ameco Polymers Plant Exp., 2001	Reac. Process > H Flow > Insuff. Heat Rem.> R. Runaway > Mat.Rel.> Exp. (BLEVE) > VCE	Exp. = 48.18 % ; BLEVE = 19.85 %
28. First Chem. Corp. Reactive Explosion, Mississippi 2002	Low St. Mat. > H P > Reac. Process> H Flow> R. Runaway > Insuff. Heat Rem.> Mat.Rel. > Exp.	Exp. = 56.67 % ; VCE = 28.3 %
29. Synthron Inc Exp., Morganton, North Carolina 2006	Reac. Process > Insuff. Heat Rem.> R. Runaway > Mat.Rel.>VC >Ig. > Exp.	Exp. = 53.02 % ; VCE = 44.2 % ; BLEVE = 9.86 %
30. Arnel Chemicals Vap. Cloud Exp., 2006	LowVP Liq. > H-T > H-P > Reac. process> Mat.Rel. > Conf.> Ig. > Exp.	Exp. =51%; VCE=35.3%
31. T2 Laboratories Explosions, Florida, 2007	Reac. Process > Conf.> Insuff. Heat Rem. > R. Runaway > HP > Mat. Rel.> BLEVE > Sec. Fire	Exp. = 61.01 % ; VCE = 43.82 %

[3] Similar abbreviations used as Table-4.2

4.2.3 Combustible Dust Fire And Explosions

Combustible dust in manufacturing industries is a potential hazard which needs proper attention. Most commonly, incombustible solids are ignored, but smaller size particles or dust can be dangerously combustible in certain concentration. Recent incidents in particulate-solid / combustible dust associated industries were examined. The model provides results (Table 4.4)which is in compliance with the real scenarios.

Table 4.4: Fire and Explosions due to Combustible Dust

Accident	**Important Evidence**[4](*Scenario*)	**Results**
32. Imperial Sugar Refinery Dust explosion, Georgia 2008	Dust > HCap. > >Mat. Rel.> Dsp> Conf. Space > Ig. Source> Flash Fire > Dust Exp.	Exp. = 49.95%; D. E.= 41.91%
33. AL Solutions Metal Recycling, West Virginia 2007	Dust> LowCap. > Hum. Err.>Mat. Rel.> Dsp> Conf. Space > Ig. > Flash Fire > Dust Exp.	Fire = 47 % ; Exp. = 19.64 %
34. Hoeganaes facility Flash Fires, Tennessee 2011	Dust > LessCap. > Hum. Err.>Mat. Rel.> Dsp> Conf. Space > Ig. Source > Flash Fire > Dust Exp.	Fire = 54.58 % ; DE = 33.15 % %
35. West Pharmaceutical Exp., North Carolina 2003	Dust> HCap. > Hum. Err.>Mat. Rel.> Dsp> Conf. Space > Ig. Source > Dust Exp.	Exp. = 49.95 % ; D E = 40.64 %
36. Hayes Lemars Plant, Indiana 2003	Dust > Low Cap. > Hum. Err.>Mat. Rel.> Dsp> Conf. Space > Ig. > Flash Fire > Dust Exp.	Exp. = 49.95 % ; D.E. = 41.29 %

[4]Similar abbreviations used as Table-4.2

37. CTA Acoustics, Kentucky, 2003	Dust> HCap. > Hum. Err.>Mat. Rel.> Dsp> Conf. Space > Ig. Source > Dust Exp.	Exp. = 56.58 % ; D. E. = 48.35 %

4.2.4 Toxic Exposure Accidents

Toxic Exposure is the hazard which is most dangerous for living beings. Toxicity incidents can be lethal or pose long term health effects to a widely exposed area. Table 4.5 list results of some of the accidents investigated.

Table 4.5: Toxicity Accident Results

Accidents	**Important Evidence** [5](*Scenario*)	**Results**
38. Dupont Chemical Toxic Release, 2014	Mat.Rel.> Low Vap P Liq. > H T > Dsp.> Conf. Space > No Ig. > Toxic Mat. > ToxicExposure	Tox. = 73.3%
39. DPC Enterprises Chlorine Release, Missouri 2002	Low St. Mat. > H flow Rate > H P > Tox. > No Ig. > Mat. Rel. > Toxic Exposure	Tox. = 69.83 %
40. DuPont facility Toxic Exposure, West Virginia 2008	Hum. Err. > Mech. Fail > Mat. release > Toxic Gas > No Ig. Source > Conf. > Toxic Exposure	Tox. =73.3 %
41. Bayer Crop Science, West Virginia	Hum. Err. > R. Runaway > Mech. Fail > Mat. Rel. > Comb. Tox. Gas >Ig. >No Conf. > Fire > Tox.	Fire= 45.14 % ; Tox. = 24.45 %

[5] Similar abbreviation used as Table-4.2

42. MFG Chemical Inc. Toxic Gas Release, Georgia, 2001	Reac. Process > Hum. Err. > R. Runaway > Mech. Fail > Mat. Rel.> Comb. Toxic Gas > Ig.> No Conf. > Fire > Tox.	Fire = 40.96%; Tox. = 30.72 %
43. Millard Refrigerated Services NH_3 Release, AL, 2010	H P(Hyd.Shock)> Low St. Mat. > Mat.Rel. > Tox. Gas > Dsp.> No Ig. > NotComb. > Tox.	Tox. = 72.83 %
44. Freedom Industries Chemical Release, WV, 2014	Low St. Mat. > H P > HVP Liq. > Mech. Fail > Mat.Rel. > Dsp.> Tox. Liq. > Toxic Exposure	Tox. = 67.46 %
45. Honeywell Plant Chlorine Release, LA, 2003	H P > Low St. Mat. > H Flow> Toxic Gas > Mat.Rel. > No Ig. > Tox.	Tox. = 69.28%

4.3 Analysis & Applications

4.3.1 Hazard Scenario Model For Risk Management

The Hazard Scenario Model included at least two mitigation factors (e.g. Sufficient Heat Removal, Release Containment) as controlling parameters in the scenario. Mostly "Human Error" was considered as the trigger for Dust related accidents. In this section the goal is to find out how much effect these mitigation factors have on the final hazard. To verify this, one or two selective nodes will have the opposite value of previous tests. The comparison of results for a few example cases are listed in Table: 4.6. The previous assumptions or significance of the selective nodes are as below.

Heat Removal: This node is represented in the model as '*hasSufficientHeatRemoval*' which is a controlling parameter of the reaction runaway. In most cases overheating due to reaction-runaway causing overpressure and material release, which might led to a hazardous situation.

Release containment: To prevent material release due to overflow or safety relief some process operations have containment facility (e.g. Flare, Dilution Tanks, Knockout-Drum) for safe discard of released material. Sometimes there are remotely operated isolation valves for mechanical failure which may minimize or stop any release situation. These options are considered in as a boolean value *hasReleaseContainment* node.

Human Error: Most hazards are direct and indirect result of human error. However, for dust explosion scenarios, human error has the most direct contribution. Poor Housekeeping, Material Agitation and Inadequate Maintenance can be considered to be in this criterion. For Particulate solid or Dust handling facilities "Human Error" is a vital controlling factor for potential hazards.

The comparison from Table 4.6 indicates that the controlling nodes have a significant effect on the final hazard. However, for reactive processes he overheat-protection impact is significant but cannot eliminate the potential final hazard. On the other hand, release containment or minimizing can reduce the risk of hazard most significantly . For Dust or solid handling facilities, Human Error creates most for potential Hazards.

Table 4.6: Hazard Scenario Model For Risk Management

Accident	**Actual Result**	**Controlling Parameter**	**Controlled Result**
Richmond Chevron Refinery Fire, 2012	Explosion=36.07 % ; Fire = 27.92%; VCE = 30.63%	Release Containment = True (Emergency Isolation)	Explosion= 13 % ; Fire = 13.5%; No Hazard = 68.5%
Valero Refinery Propane Fire, Texas 2007	Fire = 42.82 % Jet fire = 22.13 %	Release Containment = True (Remote Isolation)	Explosion= 13 % ; Fire = 13.5%; No Hazard = 68.5%
Little General Store Propane Explosion, WV, 2007	Explosion = 42.6 % VCE = 36.78%	Release Containment = True (Isolation valve or Stop ventilation)	Explosion= 17.5 % ; Fire = 9.5%; No Hazard = 68.4%
First Chemical Corp. Reactive Chemical Explosion, Mississippi 2002	Explosion = 56.67%; VCE = 28.3%	Sufficient Heat Removal = True (Overheat Control)	Explosion= 37.62 % ; Fire = 16.14%; No Hazard = 42.27%

Synthron Inc Explosion, Morganton, North Carolina 2006	Explosion = 53.02 % VCE = 44.02 %	Sufficient Heat Removal = True (OverHeat Removal)	Explosion = 3.92 % ; Fire = 15.08 % ; No Hazard = 46.92 %
T2 Laboratories Explosions, Jacksonville, Florida, 2007	Explosion = 56.84 % VCE = 41.11 %	Sufficient Heat Removal = True; (Overheat Protection)	Explosion = 37.62 % ; Fire = 16.14 % ; No Hazard = 42.27 %
Imperial Sugar Refinery Dust explosion, Georgia 2008	Explosion = 49.95 % % Dust Explosion = 41.91 %	Human Error = False; (Adequate Maintenance, Housekeeping)	Explosion = 16.01 % ; Fire = 9.23 % ; No Hazard = 70.12 %
AL Solutions Metal Recycling, West Virginia 2007	Fire = 47 % Dust Explosion = 19.64 %	Human Error = False (Better Housekeeping)	Explosion = 10.8 % ; Fire = 14.64 % ; No Hazard = 69.39 %
MFG Chemical Inc. Toxic Gas Release, Dalton, Georgia, 2001	Fire Hazard = 40.96% Toxicity = 30.72 %	Sufficient Heat Removal = True & Human Error = False	Fire Hazard = 29.04% Toxicity = 43.81 %

4.3.2 Hazard Scenario Model for Causality Analysis

A previous section describes Hazard Prediction from the evidence of any scenario. However, to check the contributions of the nodes, we ran the test for some predefined hazard and checked the results with limited evidences of the site and material properties. To run these tests we used three previous historical incidents to determine if the contributing factors could indicate the contribution of the event propagation in the incident.

PEPCON Disaster, Henderson, Nevada, 1988: A fire started in the Ammonium Perchlorate production and storage facility. The batch first caught fire in high temperature which spread because of dust and fiberglass building materials in the area. The fire caused two massive explosions consecutively. Heating of explosive materials due to fire caused the explosions.

Evidence: Secondary Explosion, Fire, High Temperature, Reactive Process, Combustible Material, Ignition, High Temperature.

Results: Flash Fire = 70.89 %

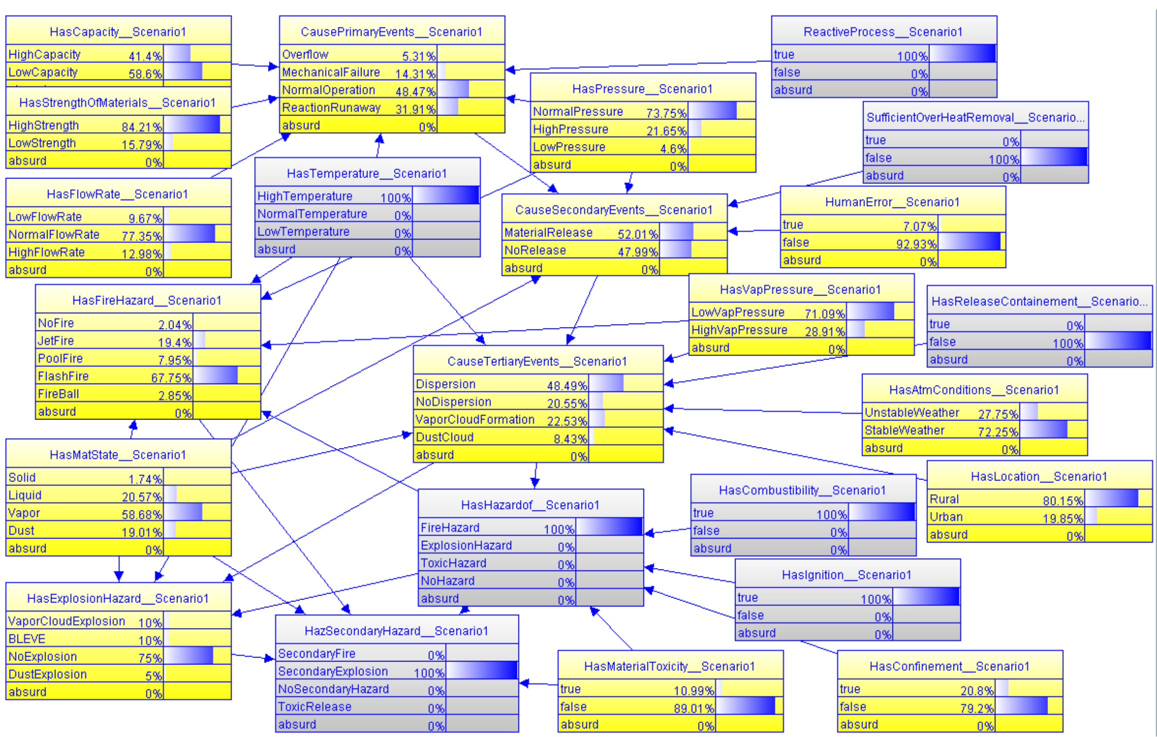


Figure 4.2: Results for the PEPCON Disaster diagnostic test.

Materials = 62.83% Vapor, 19.24% Dust, 16.53% Liquid

Dispersion = 49.33%

Material Release = 53.61%

Reaction Runaway = 32.85 %. [Details in Figure 4.2]

Union Carbide Disaster, Bhopal, India, 1986: Water carry-over into a Methyl iso-Cyanide (MIC) storage tank led to a runaway reaction which led to toxic gas release through a flare. Because the adsorption tower was inoperable, the toxic gas killed more than 3000 people around the plant.

Evidence: Toxic Vapor, Fire, Reaction Runaway, Reactive Process, Non-Combustible Material, Insufficient Heat Removal.

Results: Toxic Hazard = 73.11 %, Dispersion = 35.69% Vapor Cloud = 44.75%

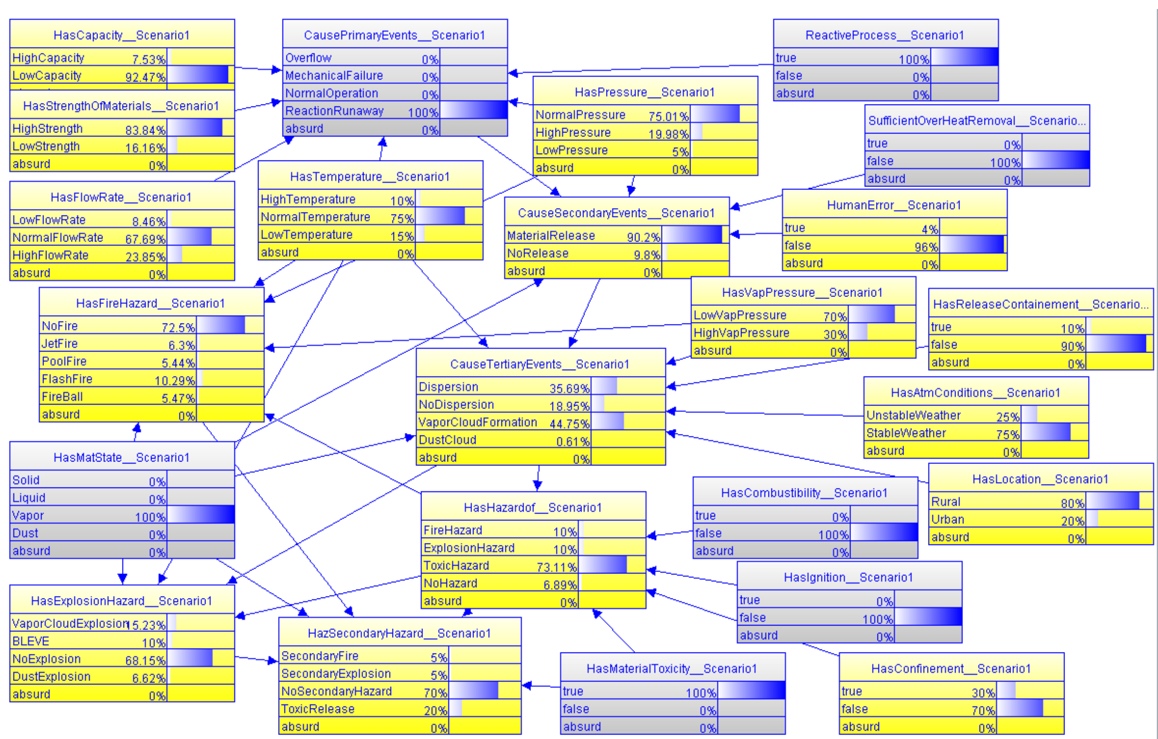


Figure 4.3: Results for the Bhopal Disaster diagnostic test.

Material Release = 90.2%. [Details in Figure 4.3]

Piper Alpha Disaster, North Sea, Off-shore Aberdeen, UK 1988: A series of explosion in the offshore oil rig and processing unit Piper Alpha caused the structure to collapse totally with 167 fatalities. The cause of the primary explosion is suspected to have been gas condensate leakage which led to the disaster.

Evidance: Explosion, High pressure, Non-Reactive Process, Combustible Material, Ignition, High Temperature, Low Vapour Pressure Liquid

Results: Vapour Cloud Explosion = 45.22 %,

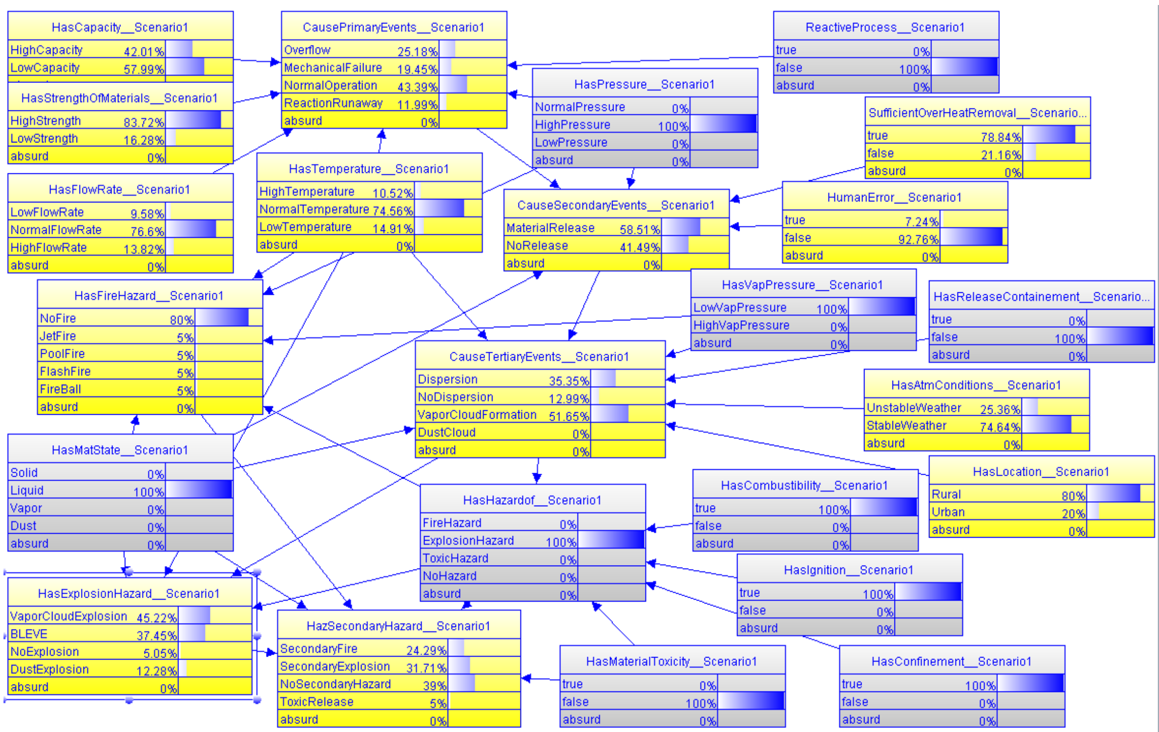


Figure 4.4: Results for the Piper-Alpha Disaster diagnostic test.

Dispersion = 35.35% Vapour Cloud Formation = 51.65%

Material Release = 58.51%

Overflow=25.18 % Mechanical Failure = 19.45 %. [Details in Figure 4.4]

Chapter 5

Results & Discussion

This chapter discusses the results obtained from implementation of the hazard scenario model in the historical accident database. The case specific results are listed in the previous chapter. The following mostly focuses on comparison of results and discussion.

5.1 Model Predictions & Actual Scenario

The goal of implementing the hazard scenario model was to evaluate and validate if the model behaviour was in agreement with the actual scenario. However, most of the results are in agreement with the actual scenario in Section 4.2. A statistical representation was prepared based on the results. Figure 5.1 illustrates the model results for the accidents discussed in an earlier section. From the tables in the earlier chapter, the columns show that the model mostly predicts the probable hazards correctly. However there are a very few exceptions lower accuracy for very few complex cases (*e.g.*Cases 7, 12 24).

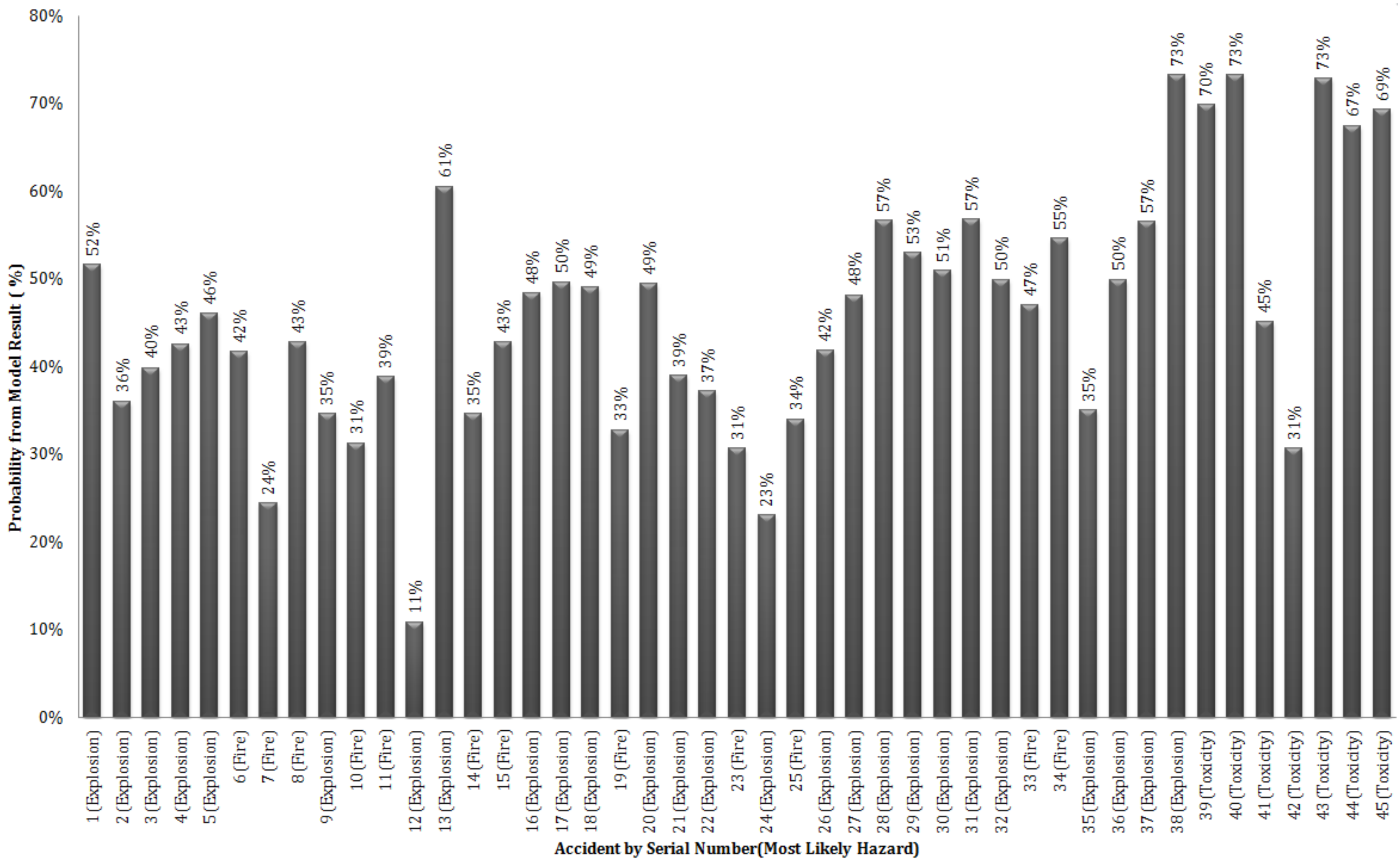


Figure 5.1: Hazard Scenario Model Results for the accidents taken into account for implementation

5.2 Discussion: Limitations & Scope

The hazard scenario modelwas developed based on the general ideal of hazard scenario using the proposed methodology for dynamic hazard identification. However, the primary target was to develop a versatile model for hazard identification, using the ontology based framework as a tool. Then the model was implemented to check whether or not the model could predict from actual evidence. From the results a set of limitations might be drawn which can help to upgrade the hazard identification model to produce an intelligent and quick hazard assessment tool. The results provide the following main factors to be taken into account as limitations of the dynamic hazard identification model.

Prior Probabilities Declaration(LPD): In the hazard scenario model, the default LPD values and conditions are described mostly based on expert knowledge and common logic. However, since quantification requires valid evidence and big datasets to derive probabilistic values, a generalized approach of assumptions was made to deduce the probabilistic values. Dependencies and LPD values were refined through theoretical targeted hazard scenarios to produce precise results. As the model is re-usable and there is scope to update the probabilistic information (LPD) and dependencies based on specific application, the results from this model are mostly the outcome of expert knowledge and understanding of the scenario. Probabilistic values from historical data could improve the precision of the result and introduce dynamic behavior of the model.

Human Error Consideration: Unwanted events due to human error are quite common in process industries. As the unique property of SSBN, any unwanted primary, secondary or tertiary events can be initiated in the model without providing primary evidence. However, to manually generate the scenario is not always effective. The model considers human error to trigger only secondary events. However, in some cases operating conditions were manipulated by human error (e.g. Arnel Chemicals industry explosion, Richmond Chevron Refinery Fire etc.) involving hazard propagation. Therefore, in some cases operating conditions represented human error rather then direct input of the human error node. Additionally, in the developed model, for dust explosion or fire scenario, $HumanError$ was considered as the vital factor to cause a solid material release, although in cases like the Imperial Sugar Refinery explosion, apparently the initiation was not likely from a single human error bur rather from the long term effects of poor housekeeping or design.

Type of Fire or Explosion: Classification of the type of fire or explosion is the major disadvantage of the model. From the results, the categories of Vapour cloud explosion, Dust-Explosion, Flash Fire and Jet Fire are quite adequate and easily interpretable. However, BLEVE, Fireball and Pool-fire are hazards that mostly occur as a result of a fire or explosion. Therefore, the model has limitations to predict these types of explosions *(e.g. Synthon Inc Explosion, Williams olefins Explosion, Huston Marcus Oil Explosion, Herrig Brothers Farm Propane Tank Explosion etc.)*.

Secondary Hazards: In this model secondary hazards were not considered in detail. However, most often secondary hazards were the major potential threat. In this model, fire was considered a secondary hazard of explosion and vise versa *(e.g. Tosero Refinery Explosion, Herrig Brothers Propane Tank Explosion)*. However, explaining secondary explosion is complicated; for example, the presence of combustible or explosive material nearby can cause consequent explosions (e.g. West Fertilizer Explosion). However, BLEVE is mostly a consequence of a primary fire or overheating. Based on evidence, the secondary hazards could be classified more clearly.

Type of Facility	Cases	Type of Accident			
		Fire & Explosion	Reactive Hazard	Dust Explosion	Toxicity
Hydrocarbon	9	8	1	0	0
Chemical Process	13	6	4	0	3
Manufacturing	6	0	0	6	0
Storage & Transfer	11	6	0	0	5
Others	6	5	0	0	0
Total	**45**	**26**	**5**	**6**	**8**

Figure 5.2: Accidents based on industry type and hazards.

Type of Facility: Table 5.2 provides a tabular representation combining both hazard type and industry type. The matrix indicates that Most of the accidents has been occurred in Chemical (31%)and Hydrocarbon (22%) related process industries, although seemingly less-threatening storage and transfer facilities (25%) had almost a similar number of accidents as the previous types. And almost all the dust-related incidents occurred in manufacturing industries. Thus type of hazards may vary depending on type industries. For example, operating an petroleum refining process can pose greater risk of fire and explosion than a chemical, pharmaceutical or storage facility. Similarly, chemical industries pose greater risk of toxic hazards than common petroleum refineries. Selection criteria of an facility and quantification of the the type in a Risk Index for different kind of facilities can be introduced for better impact *(e.g Richmond Chevron Refinery vs West Pharmaceutical vs. Dupont Facility)*.

Explosive or Self Ignition: Combustibility is not the only property of any material. In some cases materials can be explosive or pyrophoric, so do not require any external ignition source, rather than heat or oxygen (e.g. Horsehead Holding Company Explosion, West Fertilizer Explosion, Formosa Plastics Corporation Explosion). To simplify the model, only property of combustibility was taken into account. The prediction of this scenario of self ignition can also be described as a true/false statement. However, adding more states as material property can reduce the confusion but introduce more complexity to the description of dependencies.

Solid Material and Chemical Fire: The important limitation of this model is the prediction for solid material and chemical explosions. Explosions like *West Fertilizer* are caused by primary fire or overheating of material. The model prediction worked for the situation, but some other cases was not considered here, due to the explosive properties of solid materials.

Incombustible Liquid BLEVE Prediction: The significant exception for the model was the Carbide Industries Explosion, Louisville, Kentucky, 2011. A water leakage to an electric arch furnace with molten calcium carbide caused overpressure of the furnace and released tons of debris and powdered gases. The model could not predict BLEVE properly, as the material "water" was non-toxic and incombustible and there was lack of ignition, at the very high temperature. However the model could simulate Material Release as 62 %. This can be considered as an exception of this model's application.

Model Dynamics & Automated System: This work has been introduced as a framework for an automated hazard identification tool. However, all the steps here utilize different softwares and plug-ins to produce the MEBN model, which can refer to the most probable hazards as probabilistic values. Once the model has been prepared, modifications and input of LPDs as prior probabilities can take place with minimal effort. As all the tools used here are *Java* based open source software, a single and completely automated software tool can be a possible outcome as a future extension of the work, which can utilize the ontology based data structure to collect data, train and modify the model with ease of access.

As a Generic Hazard Identification Model, despite the limitations, this model can still predict the scenario effectively with a wide range of applications. A specific scenario based model could be improvised for more efficacious precision, which was not the primary goal. However, these case studies demonstrate that the goal to achieve a versatile model to quantify basic industrial hazards was accomplished.

Chapter 6

Conclusion

This work introduces an ontology based framework, to model and quantify the most probable hazard scenarios for different system properties as well as operational and environmental conditions. The aim is to reduce risk assessment and management efforts by using an automated procedure for hazard identification. The developed ontology-based model can be updated without extensive modifications and can be adapted for different systems.

The proposed methodology, based on scenario modeling, adopts the ontology based framework for the mapping and then converts to a Bayesian network for probabilistic assessment of hazards. The following features can be highlighted from the proposed dynamic hazard identification model.

- A dynamic hazard scenario development methodology has been proposed and adopted utilizing ontology based framework.
- A hazard scenario ontology is developed to illustrate the data structure and relations between elements.

- The Ontology has been implemented to develop a graphical representation based on the Bayesian Network.
- The generic model can be implemented for most fire/explosion/toxicity scenarios in the process industries.
- Hazards are identified as probabilities of occurrence.
- Probabilistic data are implemented based on expert knowledge, which can be replaced by historical data for any known domain.
- Declaration of prior probabilities introduce the dynamics of the model.
- Automatic data acquisition system and dynamic updates can be developed in future.

The dynamic hazard identification model was implemented for previous accidents to verify the effectiveness and prediction capability of the model. Although this is a generic model from knowledge based data, in almost all the cases the model predicted the most probable hazards successfully. Some additional applications for risk management and causality analysis were verified in different circumstances. The application results indicate the model to be effective in most cases. Although this model has limitations, a situation based application can be accomplished using historical data to upgrade the efficacy and adaptability of the model.

6.1 Future Scopes

Current work was motivated for dynamic hazard identification, adapting the ontology based framework to model the process hazard scenario. However, this modeling approach, along with the framework can be adapted to different risk management application. The future scopes can be described as below.

- Ontology based knowledge modeling approach can provide an explicit, accessible and reusable knowledge model to capture the process knowledge from background study. This model will be ready to be utilized for different applications which require process knowledge as a data-structure along with quantitative reasoning.

- Current work utilizes available OWL based ontology development software `Protégé` and PR-OWL based Bayesian reasoning software `UnBBayes`, which are open source and use similar `Java` based platform. However, this shared platform opens a possible extension leading to a unique hazard identification interface.

- The dynamics of the hazard scenario model is dependent on the LPD declarations, which can be updated over time. As the model was based on machine interpretable framework, an automatic data acquisition system can be designed to build the interlink between the model and database.

- Although this report explores the application of an ontology based framework in dynamic hazard identification, several other applications are in consideration. Knowledge based process monitoring focusing on event based alarm annunciation, probabilistic risk assessment through process fault scenario generation are the notable applications. Moreover, ontology modeling can be adopted in different risk modeling approaches which require qualitative information as evidence. An automatic expert system might overcome the challenges of developing an intelligent risk management tool in future.

Bibliography

[Amyotte et al., 2011] Amyotte, P. R., MacDonald, D. K., and Khan, F. I. (2011). An analysis of csb investigation reports concerning the hierarchy of controls. *Process Safety Progress*, 30(3):261–265.

[Aristotle, 1994] Aristotle (1994). *Metaphysics*. Oxford university Press, Oxford.

[Batres et al., 2014] Batres, R., Fujihara, S., Shimada, Y., and Fuchino, T. (2014). The use of ontologies for enhancing the use of accident information. *Process Safety and Environmental Protection*, 92(2):119–130.

[Batres et al., 2009] Batres, R., Shimada, Y., and Fuchino, T. (2009). A semantic approach for incident database development. In *IChemE Symp. Series*, volume 155, pages 477–484.

[Baybutt, 2016] Baybutt, P. (2016). Insights into process safety incidents from an analysis of csb investigations. *Journal of Loss Prevention in the Process Industries*, 43:537 – 548.

[Bernaras et al., 1996] Bernaras, A., Laresgoiti, I., Bartolome, N., and Corera, J. (1996). An ontology for fault diagnosis in electrical networks. In *Intelligent Systems Applications to Power Systems, 1996. Proceedings, ISAP'96., International Conference on*, pages 199–203. IEEE.

[Bobillo and Straccia, 2011] Bobillo, F. and Straccia, U. (2011). Fuzzy ontology representation using owl 2. *International Journal of Approximate Reasoning*, 52(7):1073–1094.

[Brandt et al., 2008] Brandt, S. C., Morbach, J., Miatidis, M., Theißen, M., Jarke, M., and Marquardt, W. (2008). An ontology-based approach to knowledge management in design processes. *Computers and Chemical Engineering*, 32(1–2):320 – 342. Process Systems Engineering: Contributions on the State-of-the-ArtSelected extended Papers from ESCAPE '16/PSE 2006.

[Carvalho et al., 2010a] Carvalho, R., Laskey, K., Santos, L., Ladeira, M., Costa, P., and Matsumoto, S. (2010a). *UnBBayes: modeling uncertainty for plausible reasoning in the semantic web*. Citeseer.

[Carvalho, 2011] Carvalho, R. N. (2011). *Representation and Modeling Methodology*. PhD thesis, George Mason University.

[Carvalho et al., 2010b] Carvalho, R. N., Costa, P. C. G., Laskey, K. B., and Chang, K.-C. (2010b). Prognos: predictive situational awareness with probabilistic ontologies. In *2010 13th Conference on Information Fusion (FUSION)*, pages 1–8. IEEE.

[Carvalho et al., 2009] Carvalho, R. N., Ladeira, M., Santos, L. L., Matsumoto, S., and Costa, P. C. G. (2009). A gui tool for plausible reasoning in the semantic web using mebn. In *Innovative Applications in Data Mining*, pages 17–45. Springer.

[Carvalho et al., 2007] Carvalho, R. N., Santos, L. L., Ladeira, M., and Costa, P. C. G. (2007). A gui tool for plausible reasoning in the semantic web using mebn. In *Seventh International Conference on Intelligent Systems Design and Applications (ISDA 2007)*, pages 381–386.

[CCPS, 2010] CCPS, editor (2010). *Guidelines for Chemical Process Quantitative Risk Analysis*. Center for Chemical Process Safety Guidelines series. Wiley.

[Costa et al., 2006] Costa, P. C., Laskey, K. B., and AlGhamdi, G. (2006). Bayesian ontologies in ai systems. In *Twenty Second Conference on Uncertainty in Artificial Intelligence (UAI 2006), Cambridge, MA, USA)*.

[Costa et al., 2005] Costa, P. C., Laskey, K. B., and Laskey, K. J. (2005). Pr-owl: A bayesian framework for the semantic web.

[Da Costa et al., 2008] Da Costa, P. C. G., Laskey, K. B., and Laskey, K. J. (2008). Pr-owl: A bayesian ontology language for the semantic web. In *Uncertainty Reasoning for the Semantic Web I*, pages 88–107. Springer.

[Daramola et al., 2011] Daramola, O., Stålhane, T., Moser, T., and Biffl, S. (2011). A conceptual framework for semantic case-based safety analysis. In *Emerging Technologies Factory Automation (ETFA), 2011 IEEE 16th Conference on*, pages 1–8.

[Duineveld et al., 2000] Duineveld, A., Stoter, R., Weiden, M., Kenepa, B., and Benjamins, V. (2000). Wondertools? a comparative study of ontological engineering tools. *International Journal of Human-Computer Studies*, 52(6):1111–1133.

[Ebrahimipour et al., 2010] Ebrahimipour, V., Rezaie, K., and Shokravi, S. (2010). An ontology approach to support fmea studies. *Expert Systems with Applications*, 37(1):671 – 677.

[Ebrahimipour and Yacout, 2015] Ebrahimipour, V. and Yacout, S. (2015). Ontology-based schema to support maintenance knowledge representation with a case study of a pneumatic valve. *Systems, Man, and Cybernetics: Systems, IEEE Transactions on*, 45(4):702–712.

[Elhdad et al., 2013] Elhdad, R., Chilamkurti, N., and Torabi, T. (2013). An ontology-based framework for process monitoring and maintenance in petroleum plant. *Journal of Loss Prevention in the Process Industries*, 26(1):104 – 116.

[Fenz et al., 2009] Fenz, S., Tjoa, A. M., and Hudec, M. (2009). Ontology-based generation of bayesian networks. In *International Conference on Complex, Intelligent and Software Intensive Systems*.

[Gennari et al., 2003] Gennari, J. H., Musen, M. A., Fergerson, R. W., Grosso, W. E., Crubézy, M., Eriksson, H., Noy, N. F., and Tu, S. W. (2003). The evolution of protégé: an environment for knowledge-based systems development. *International Journal of Human-computer studies*, 58(1):89–123.

[Giaretta and Guarino, 1995] Giaretta, P. and Guarino, N. (1995). Ontologies and knowledge bases towards a terminological clarification. *Towards very large knowledge bases: knowledge building & knowledge sharing*, 25:32.

[Gruber, 1993] Gruber, T. R. (1993). A translation approach to portable ontology specifications. *Knowledge Acquisition*, 5(2):199 – 220.

[Guarino, 1998] Guarino, N. (1998). Formal ontology and information systems. In *Proceedings of FOIS*, volume 98, pages 81–97.

[Jeffrey Hieb, 2009] Jeffrey Hieb, James Graham, J. G. (2009). An ontology for identifying cyber intrusion induced faults in process control systems. In Sujeet Shenoi, C. P., editor, *Critical Infrastructure Protection III*, volume 311 of *IFIP Advances in Information and Communication Technology*. Springer Berlin Heidelberg.

[Kalantarnia et al., 2009] Kalantarnia, M., Khan, F., and Hawboldt, K. (2009). Dynamic risk assessment using failure assessment and bayesian theory. *Journal of Loss Prevention in the Process Industries*, 22:600–606.

[Khan, 2001] Khan, F. I. (2001). Use maximum-credible accident scenarios for realistic and reliable risk assessment. *Chemical Engineering Progress*, 97(11):56–64.

[Khan and Abbasi, 1999] Khan, F. I. and Abbasi, S. (1999). Major accidents in process industries and an analysis of causes and consequences. *Journal of Loss Prevention in the process Industries*, 12(5):361–378.

[Khan and Abbasi, 1998] Khan, F. I. and Abbasi, S. A. (1998). Multivariate hazard identification and ranking system. *Process Safety Progress*, 17(3):157–170.

[Khan and Amyotte, 2007] Khan, F. I. and Amyotte, P. R. (2007). Modeling of /bp texas city/ refinery incident. *Journal of Loss Prevention in the Process Industries*, 20(4–6):387 – 395. Sixth International Symposium on Hazards, Prevention, and Mitigation of Industrial Explosions.

[Kletz, 2009] Kletz, T. A. (2009). Accident reports may not tell us everything we need to know. *Journal of Loss Prevention in the Process Industries*, 22(6):753 – 756. Papers Presented at the 2007 and 2008 International Symposium of the Mary Kay O'Connor Process Safety Center and Papers Presented at the WCOGI 2007.

[Knegtering and Pasman, 2013] Knegtering, B. and Pasman, H. (2013). The safety barometer: How safe is my plant today? Is instantaneously measuring safety level utopia or realizable? *Journal of Loss Prevention in the Process Industries*, 26(4):821–829.

[Knublauch et al., 2004] Knublauch, H., Fergerson, R. W., Noy, N. F., and Musen, M. A. (2004). The protégé owl plugin: An open development environment for semantic web applications. In *International Semantic Web Conference*, pages 229–243. Springer.

[Laskey, 2008] Laskey, K. B. (2008). Mebn: A language for first-order bayesian knowledge bases. *Artificial Intelligence*, 172(2):140 – 178.

[Laskey et al., 2010] Laskey, K. B., Costa, P. C., and Janssen, T. (2010). Probabilistic ontologies for multi-int fusion. *Ontologies and Semantic Technologies for Intelligence*, 213:147.

[Laskey et al., 2011] Laskey, K. B., Haberlin, R., Carvalho, R. N., and da Costa, P. C. G. (2011). Pr-owl 2 case study: A maritime domain probabilistic ontology. In *STIDS*, pages 76–83.

[Lykourentzou et al., 2011] Lykourentzou, I., Papadaki, K., Kalliakmanis, A., Djaghloul, Y., Latour, T., Charalabis, I., and Kapetanios, E. (2011). Ontology-based operational risk management. In *Commerce and Enterprise Computing (CEC), 2011 IEEE 13th Conference on*, pages 153–160.

[Mannan, 2004] Mannan, S. (2004). *Lees' Loss Prevention in the Process Industries: Hazard Identification, Assessment and Control*. Number v. 1 in Chemical Petrochemical & Process. Butterworth-Heinemann.

[Matsumoto et al., 2011] Matsumoto, S., Carvalho, R. N., Ladeira, M., da Costa, P. C. G., Santos, L. L., Silva, D., Onishi, M., Machado, E., and Cai, K. (2011). Unbbayes: a java framework for probabilistic models in ai. *Java in Academia and Research*, page 34.

[McCoy et al., 1999] McCoy, S., Wakeman, S., Larkin, F., Jefferson, M., Chung, P., Rushton, A., Lees, F., and Heino, P. (1999). Hazid, a computer aid for hazard identification. *Process Safety and Environmental Protection*, 77(6):317 – 327.

[McGuinness et al., 2004] McGuinness, D. L., Van Harmelen, F., et al. (2004). Owl web ontology language overview. *W3C recommendation*, 10(10):2004.

[Melik-Merkumians et al., 2010] Melik-Merkumians, M., Zoitl, A., and Moser, T. (2010). Ontology-based fault diagnosis for industrial control applications. In *Emerging Technologies and Factory Automation (ETFA), 2010 IEEE Conference on*, pages 1–4.

[Musen, 1989] Musen, M. A. (1989). *Automated generation of model-based knowledge-acquisition tools*. Elsevier.

[Musen and Team, 2015] Musen, M. A. and Team, t. P. (2015). The protégé project: A look back and a look forward. *AI matters*.

[Nakayama et al., 2016] Nakayama, J., Sakamoto, J., Kasai, N., Shibutani, T., and Miyake, A. (2016). Preliminary hazard identification for qualitative risk assessment on a hybrid gasoline-hydrogen fueling station with an on-site hydrogen production system using organic chemical hydride. *International Journal of Hydrogen Energy*, 41(18):7518 – 7525.

[Noy et al., 2001] Noy, N. F., McGuinness, D. L., et al. (2001). Ontology development 101: A guide to creating your first ontology.

[Paltrinier et al., 2013] Paltrinier, N., Tugnoli, A., Buston, J., Wardman, M., and Cozzani, V. (2013). Dynamic procedure for atypical scenarios identification (DyPAISI): A new systematic HAZID tool. *Journal of Loss Prevention in the Process Industries*, 26:683–695.

[Paltrinier et al., 2015] Paltrinier, N., Villa, V., and Cozzani, V. (2015). Overview on dynamic approaches to risk management in process facilities. *Chemical Engineering Transactions*, 43:2497–2502.

[Paltrinieri et al., 2014] Paltrinieri, N., Wilday, J., Wardman, M., and Cozzani, V. (2014). Surface installations intended for carbon capture and sequestration: Atypical accident scenarios and their identification. *Process Safety and Environmental Protection*, 92(1):93–107.

[Pradeep et al., 2012] Pradeep, Y., Khaparde, S., and Joshi, R. (2012). High level event ontology for multiarea power system. *Smart Grid, IEEE Transactions on*, 3(1):193–202.

[Prem et al., 2010] Prem, K. P., Ng, D., and Mannan, M. S. (2010). Harnessing database resources for understanding the profile of chemical process industry incidents. *Journal of Loss Prevention in the Process Industries*, 23(4):549 – 560.

[Saud et al.,] Saud, Y. E., Israni, K. C., and Goddard, J. Bow-tie diagrams in downstream hazard identification and risk assessment. *Process Safety Progress*, 33(1):26–35.

[Seligmann et al., 2012] Seligmann, B. J., Németh, E., Hangos, K. M., and Cameron, I. T. (2012). A blended hazard identification methodology to support process diagnosis. *Journal of Loss Prevention in the Process Industries*, 25(4):746–759.

[Sánchez et al., 2007] Sánchez, D. M., Cavero, J. M., and Martínez, E. M. (2007). The road toward ontologies. In Sharman, R., Kishore, R., and Ramesh, R., editors, *Ontologies : A Handbook of Principles, Concepts and Applications in Information Systems* , chapter 1, pages 3–20. Springer, Springer US.

[Vahid Ebrahimipour, 2015] Vahid Ebrahimipour, S. Y. (2015). *Ontology Modeling in Physical Asset Integrity Management*. Springer International Publishing, Springer International Publishing Switzerland, first edition.

[Venkatasubramanian and Vaidhyanathan, 1994] Venkatasubramanian, V. and Vaidhyanathan, R. (1994). A knowledge-based framework for automating hazop analysis. *AIChE Journal*, 40(3):496–505.

[Villa et al., 2016] Villa, V., Paltrinier, N., Khan, F., and Cozzani, V. (2016). Towards dynamic risk analysis: A review of the risk assessment approach and its limitations in the chemical process industry. *Safety Science*, 89:77–93.

[Wells, 1996] Wells, G. (1996). *Hazard identification and risk assessment*. IChemE.

[Wiesner et al., 2008] Wiesner, A., Morbach, J., Yang, A., Bayer, B., and Marquardt, W. (2008). Chemical process systems. Technical report lpt-2008-29, Aachener Verfahrenstechnik.

[Wilday et al., 2011] Wilday, J., Paltrinieri, N., Farret, R., Hebrard, J., and Breedveld, L. (2011). Addressing emerging risks using carbon capture and storage as an example. *Process Safety and Environmental Protection*, 89(6):463–471.

[Wu et al., 2013] Wu, J., Zhang, L., Lind, M., Liang, W., Hu, J., Jørgensen, S. B., Sin, G., and Khokhar, Z. U. (2013). *Hazard Identification of the Offshore Three-Phase Separation Process Based on Multilevel Flow Modeling and HAZOP*, pages 421–430. Springer Berlin Heidelberg, Berlin, Heidelberg.

[Xin et al., 2017] Xin, P., Khan, F., and Ahmed, S. (2017). Dynamic hazard identification and scenario mapping using bayesian network. *Process Safety and Environmental Protection*, 105:143 – 155.

[Yu, 2011] Yu, L. (2011). *A Developer's Guide to the Semantic Web*. IT Pro. Springer Berlin Heidelberg.

[Zhao et al., 2009] Zhao, J., Cui, L., Zhao, L., Qiu, T., and Chen, B. (2009). Learning hazop expert system by case-based reasoning and ontology. *Computers and Chemical Engineering*, 33(1):371 – 378.

[Zhou et al., 2015] Zhou, A., Yu, D., and Zhang, W. (2015). A research on intelligent fault diagnosis of wind turbines based on ontology and fmeca. *Advanced Engineering Informatics*, 29(1):115 – 125.

Appendix A

Local Probability Distributions

Local Probabilistic Distributions are Actually the Probabilistic logics and values declared to generate the Bayesian network. UnBBayes software MEBN plug-in calculates the probabilistic values for random variable states. A probabilistic scenario is declared through simple "$If...Else...$" logics and predefined Probabilities.

A.1 Demonstration: Simple Hazard Model

The Local Probability Distributions(LPDs) for the simple h azard model has been based on logical expressions for three different nodes. The declarations are listed in following sub-sections.

A.2 Dynamic Hazard Identification: The Hazard Scenario Model

A.2.1 Input Nodes:Default LPD Values

Default State values for The Hazard Scenario Model can be found from following table.

The LPD distribution logics based on each node can be found below.

A.2.2 *'causePraimaryEvent'* Node LPD

```
  if any Sc have (ReactiveProcess= true & HasCapacity = LowCapacity)
   [if any Sc have (HasFlowRate = HighFlowRate )[
    Overflow = 0.15,
    MechanicalFailure = 0.05,
    NormalOperation = 0.05,
    ReactionRunaway = 0.75
 ] else [
    Overflow = 0.05,
    MechanicalFailure = 0.10,
    NormalOperation = 0.60,
    ReactionRunaway = 0.25
 ]
 ] else if any Sc have
 (ReactiveProcess= false & HasCapacity = LowCapacity)
  [if any Sc have (HasFlowRate = HighFlowRate )[
    Overflow = 0.85,
```

```
    MechanicalFailure = 0.05,
    NormalOperation = 0.05,
    ReactionRunaway = 0.05
] else [
    Overflow = 0.15,
    MechanicalFailure = 0.10,
    NormalOperation = 0.60,
    ReactionRunaway = 0.15
]
] else if any Sc have ( HasStrengthOfMaterials = LowStrength)
 [if any Sc have (HasFlowRate = HighFlowRate )
  [if any Sc have ( HasPressure = HighPressure )
  [ if any Sc have ( HasTemperature =  HighTemperature )[
    Overflow = 0.05,
    MechanicalFailure = 0.8,
    NormalOperation = 0.13,
    ReactionRunaway = 0.02
] else [
    Overflow = 0.10,
    MechanicalFailure = 0.37,
    NormalOperation = 0.50,
    ReactionRunaway = 0.03
]
]  else [
    Overflow = 0.05,
    MechanicalFailure = 0.25,
```

```
    NormalOperation = 0.65,
    ReactionRunaway = 0.05
 ]
 ]else  [
    Overflow = 0.05,
    MechanicalFailure = 0.20,
    NormalOperation = 0.70,
    ReactionRunaway = 0.05
 ]] else [
    Overflow = 0.03,
    MechanicalFailure = 0.10,
    NormalOperation = 0.85,
    ReactionRunaway = 0.02
 ]
```

A.2.3 *'causeSecondaryEvent'* Node LPD

```
 if any Sc have (HumanError = true)
 [if any Sc have ( HasMatState = Dust | HasMatState = Solid)
 [
  MaterialRelease = 0.85,
   NoRelease = 0.15
] else [if any Sc have ( CausePrimaryEvents = MechanicalFailure)
[
   MaterialRelease = 0.95,
   NoRelease = 0.05
] else if any Sc have ( CausePrimaryEvents = Overflow)
```

```
 [
MaterialRelease = 0.80,
   NoRelease = 0.20
] else if any Sc have (CausePrimaryEvents = ReactionRunaway)
[if any Sc have (SufficientOverHeatRemoval =false)
[
   MaterialRelease = 0.95,
   NoRelease = 0.05 ]
else[
   MaterialRelease = 0.60,
   NoRelease = 0.40
]
]else [
   MaterialRelease = .65,
   NoRelease = .35
]
]
]else [if any Sc have ( CausePrimaryEvents = MechanicalFailure)
[if any Sc have ( HasMatState = Vapor )
[ if any Sc have ( HasPressure = HighPressure ) [
  MaterialRelease = 0.8,
   NoRelease = 0.2
] else if any Sc have (HasPressure = NormalPressure ) [
   MaterialRelease = 0.50,
   NoRelease = 0.50
] else [
```

```
    MaterialRelease = 0.20,
    NoRelease = 0.80
]
] else  if any Sc have ( HasMatState = Liquid )
[ if any Sc have ( HasPressure = HighPressure ) [
    MaterialRelease = 0.7,
    NoRelease = 0.3
] else if any Sc have (HasPressure = NormalPressure ) [
    MaterialRelease = 0.40,
    NoRelease = 0.60
] else [
    MaterialRelease = 0.15,
    NoRelease = 0.85
]
] else  [ if any Sc have ( HasPressure = HighPressure ) [
    MaterialRelease = 0.5,
    NoRelease = 0.5
] else if any Sc have (HasPressure = NormalPressure ) [
    MaterialRelease = 0.20,
    NoRelease = 0.80
] else [
    MaterialRelease = 0.05,
    NoRelease = 0.95
]]
] else if any Sc have ( CausePrimaryEvents = Overflow)
 [if any Sc have ( HasMatState = Vapor ) [
```

```
MaterialRelease = 0.30,
   NoRelease = 0.70
] else  if any Sc have ( HasMatState = Liquid )  [
   MaterialRelease = 0.80,
   NoRelease = 0.20
] else [
   MaterialRelease = 0.06,
   NoRelease = 0.94
]
] else if any Sc have (CausePrimaryEvents = ReactionRunaway)
 [ if any Sc have (SufficientOverHeatRemoval =false) [
   MaterialRelease = 0.90,
   NoRelease = 0.10 ]
else[
   MaterialRelease = 0.40,
   NoRelease = 0.60
]
]else [
   MaterialRelease = 0.02,
   NoRelease = 0.98
]
]
```

A.2.4 *'causeTertiaryEvent'* Node LPD

```
  if any Sc have (HasReleaseContainement = false )
  [if any Sc have ( CauseSecondaryEvents = MaterialRelease )
```

```
[ if any Sc have ( HasMatState = Vapor )
[ if any Sc have ( HasAtmConditions = UnstableWeather )
[ if any Sc have ( HasLocation = Rural ) [
   Dispersion = 0.80,
   NoDispersion = 0.02,
   VaporCloudFormation = 0.18,
   DustCloud = 0.00
]  else [
   Dispersion = 0.63,
   NoDispersion = 0.02,
   VaporCloudFormation = 0.35,
   DustCloud = 0.00
]
] else [
   Dispersion = 0.30,
   NoDispersion = 0.05,
   VaporCloudFormation = 0.64,
   DustCloud = 0.01
]


] else if any Sc have ( HasMatState = Liquid )
 [ if any Sc have ( HasVapPressure = LowVapPressure)
 [ if any Sc have ( HasAtmConditions = UnstableWeather)
 [ if any Sc have ( HasTemperature = HighTemperature) [
   Dispersion = 0.68,
```

```
    NoDispersion = 0.02,
    VaporCloudFormation = 0.30,
    DustCloud = 0.00
] else [ Dispersion = 0.40,
    NoDispersion = 0.10,
    VaporCloudFormation = 0.50,
    DustCloud = 0.00
]
] else [ if any Sc have ( HasTemperature = HighTemperature) [
    Dispersion = 0.250,
    NoDispersion = 0.05,
    VaporCloudFormation = 0.70,
    DustCloud = 0.00
] else [ Dispersion = 0.20,
    NoDispersion = 0.15,
    VaporCloudFormation = 0.65,
    DustCloud = 0.00
]
]
]else [ if any Sc have ( HasTemperature = HighTemperature) [
    Dispersion = 0.30,
    NoDispersion = 0.15,
    VaporCloudFormation = 0.55,
    DustCloud = 0.00
] else [ Dispersion = 0.10,
    NoDispersion = 0.45,
```

```
    VaporCloudFormation = 0.45,
    DustCloud = 0.00
]]



] else if any Sc have (HasMatState = Dust)
[ if any Sc have ( HasAtmConditions = UnstableWeather)[
    Dispersion = 0.33,
    NoDispersion = 0.02,
    VaporCloudFormation = 0.05,
    DustCloud = 0.60
] else [
    Dispersion = 0.10,
    NoDispersion = 0.15,
    VaporCloudFormation = 0.05,
    DustCloud = 0.70
]

] else [ Dispersion = 0.10,
    NoDispersion = 0.65,
    VaporCloudFormation = 0.05  ,
    DustCloud = 0.20
] ]



else [
```

```
    Dispersion = 0.10,
    NoDispersion = 0.85,
    VaporCloudFormation = 0.05
  ]
  ]else [
    Dispersion = .1,
    NoDispersion = .8,
    VaporCloudFormation = .1
  ]
```

A.2.5 *'HasHazardof'* Node LPD

```
if any Sc have ( HasMaterialToxicity = true)
[if any Sc have
(CauseTertiaryEvents = Dispersion |CauseTertiaryEvents = DustCloud)
[ if any Sc have ( HasCombustibility = true)
[ if any Sc have (HasIgnition = true )
[ if any Sc have ( HasConfinement= true ) [
    FireHazard = 0.08,
    ExplosionHazard = 0.60,
    ToxicHazard = 0.30,
    NoHazard = 0.02
  ] else [
    FireHazard = 0.60,
    ExplosionHazard = 0.10,
    ToxicHazard = 0.28,
    NoHazard = 0.02
```

```
]
]else [
   FireHazard = 0.10,
   ExplosionHazard = 0.10,
   ToxicHazard = 0.75,
   NoHazard = 0.05
]
]else  [
   FireHazard = 0.10,
   ExplosionHazard = 0.10,
   ToxicHazard = 0.75,
   NoHazard = 0.05
]
]else if any Sc have ( CauseTertiaryEvents = VaporCloudFormation )
 [ if any Sc have ( HasCombustibility = true)
 [ if any Sc have (HasIgnition = true )
 [ if any Sc have ( HasConfinement= true ) [
   FireHazard = 0.08,
   ExplosionHazard = 0.70,
   ToxicHazard = 0.20,
   NoHazard = 0.02
]  else [
   FireHazard = 0.15,
   ExplosionHazard = 0.65,
   ToxicHazard = 0.18,
   NoHazard = 0.02
```

```
]
]else [
   FireHazard = 0.10,
   ExplosionHazard = 0.10,
   ToxicHazard = 0.75,
   NoHazard = 0.05
]
]else  [
   FireHazard = 0.10,
   ExplosionHazard = 0.10,
   ToxicHazard = 0.75,
   NoHazard = 0.05
]
]else [
   FireHazard = 0.10,
   ExplosionHazard = 0.10,
   ToxicHazard = 0.65,
   NoHazard = 0.15
]
]else [if any Sc have
(CauseTertiaryEvents=Dispersion|CauseTertiaryEvents = DustCloud)
 [ if any Sc have ( HasCombustibility = true)
 [ if any Sc have (HasIgnition = true )
 [ if any Sc have ( HasConfinement= true ) [
   FireHazard = 0.30,
   ExplosionHazard = 0.65,
```

```
    ToxicHazard = 0.03,
    NoHazard = 0.02
] else [
    FireHazard = 0.65,
    ExplosionHazard = 0.25,
    ToxicHazard = 0.07,
    NoHazard = 0.03
]
]else [
    FireHazard = 0.20,
    ExplosionHazard = 0.20,
    ToxicHazard = 0.05,
    NoHazard = 0.55
]
]else  [
    FireHazard = 0.15,
    ExplosionHazard = 0.15,
    ToxicHazard = 0.05,
    NoHazard = 0.65
]
]else if any Sc have ( CauseTertiaryEvents = VaporCloudFormation )
 [ if any Sc have ( HasCombustibility = true)
 [ if any Sc have (HasIgnition = true )
  [ if any Sc have ( HasConfinement= true ) [
    FireHazard = 0.25,
    ExplosionHazard = 0.70,
```

```
    ToxicHazard = 0.03,
    NoHazard = 0.02
] else [
    FireHazard = 0.30,
    ExplosionHazard = 0.65,
    ToxicHazard = 0.03,
    NoHazard = 0.02
]
]else [
    FireHazard = 0.20,
    ExplosionHazard = 0.20,
    ToxicHazard = 0.15,
    NoHazard = 0.45
]
]else  [
    FireHazard = 0.15,
    ExplosionHazard = 0.150,
    ToxicHazard = 0.15,
    NoHazard = 0.55
]
]
else [
    FireHazard = 0.05,
    ExplosionHazard = 0.05,
    ToxicHazard = 0.05,
    NoHazard = 0.85
```

```
]
]
```

A.2.6 *'hasFireHazard'* Node LPD

```
if any Sc have ( HasHazardof = FireHazard )
[if any Sc have ( HasMatState = Vapor )
 [ if any Sc have ( HasPressure = HighPressure )
 [ if any Sc have ( HasTemperature = HighTemperature ) [
    NoFire =0.05,
    JetFire = 0.15,
    PoolFire = 0.05,
    FlashFire = 0.70,
    FireBall = 0.05
 ] else [
    NoFire = 0.05,
    JetFire = 0.55,
    PoolFire = 0.05,
    FlashFire = 0.30,
    FireBall = 0.05
 ]
 ]else if any Sc have ( HasPressure = LowPressure)
  [ if any Sc have ( HasTemperature = HighTemperature ) [
    NoFire =0.05,
    JetFire = 0.10,
    PoolFire = 0.05,
    FlashFire = 0.65,
```

```
    FireBall = 0.15
] else [
    NoFire = 0.05,
    JetFire = 0.05,
    PoolFire = 0.20,
    FlashFire = 0.45,
    FireBall = 0.25
]
] else [
    NoFire = 0.05,
    JetFire = 0.10,
    PoolFire = 0.10,
    FlashFire = 0.65,
    FireBall = 0.10
]
] else if any Sc have ( HasMatState = Liquid )
[ if any Sc have ( HasPressure = HighPressure )
[ if any Sc have ( HasTemperature = HighTemperature )
[ if any Sc have ( HasVapPressure = LowVapPressure) [
    NoFire = 0.03,
    JetFire = 0.35,
    PoolFire =0.45,
    FlashFire = 0.10,
    FireBall =0.07
] else [
    NoFire = 0.03,
```

```
    JetFire = 0.20,
    PoolFire =0.55,
    FlashFire = 0.10,
    FireBall = 0.12
]
] else [
    NoFire = 0.02  ,
    JetFire = 0.25,
    PoolFire = 0.65,
    FlashFire = 0.04,
    FireBall = 0.04
]
] else if any Sc have ( HasPressure = NormalPressure )
 [ if any Sc have ( HasTemperature = HighTemperature )
 [ if any Sc have ( HasVapPressure = LowVapPressure) [
    NoFire = 0.03,
    JetFire = 0.05,
    PoolFire =0.15,
    FlashFire = 0.70,
    FireBall =0.07
] else [
    NoFire = 0.03,
    JetFire = 0.10,
    PoolFire =0.65,
    FlashFire = 0.10,
    FireBall = 0.12
```

```
]
] else [ if any Sc have ( HasVapPressure = LowVapPressure) [
   NoFire = 0.03,
   JetFire = 0.05,
   PoolFire =0.15,
   FlashFire = 0.70,
   FireBall =0.07
] else [
   NoFire = 0.03,
   JetFire = 0.10,
   PoolFire =0.65,
   FlashFire = 0.10,
   FireBall = 0.12
]]
] else if any Sc have (HasMatState = Dust)[
   NoFire = 0.02,
   JetFire = 0.03,
   PoolFire = 0.05,
   FlashFire = 0.80,
   FireBall = 0.1
] else [
   NoFire = 0.1,
   JetFire = 0.1,
   PoolFire = .5,
   FlashFire = 0.2,
   FireBall = 0.1
```

```
]

]else [
    NoFire = 0.20,
    JetFire = 0.15,
    PoolFire = 0.35,
    FlashFire = 0.15,
    FireBall = 0.15
]
]else [
    NoFire = 0.80,
    JetFire = 0.05,
    PoolFire = 0.05,
    FlashFire = 0.05,
    FireBall = 0.05
]
```

A.2.7 *'hasExplosionHazard'* Node LPD

```
if any Sc have (HasHazardof= ExplosionHazard)
 [ if any Sc have (CauseTertiaryEvents = VaporCloudFormation) [
    VaporCloudExplosion = 0.80,
    BLEVE = 0.10,
    NoExplosion = 0.02,
    DustExplosion = 0.08
]else if any Sc have (CauseTertiaryEvents = Dispersion )
 [ if any Sc have ( HasMatState = Vapor )
```

```
  [if any Sc have ( HasTemperature = HighTemperature ) [
   VaporCloudExplosion = 0.60,
   BLEVE = 0.10,
   NoExplosion = 0.05,
   DustExplosion = 0.25
]else [
   VaporCloudExplosion = 0.70,
   BLEVE = 0.10,
   NoExplosion = 0.05,
   DustExplosion =0.15
]
] else if any Sc have ( HasMatState = Liquid )
[if any Sc have ( HasTemperature = HighTemperature ) [
   VaporCloudExplosion = 0.25,
   BLEVE = 0.70,
   NoExplosion = 0.04,
   DustExplosion = 0.01
]else [
   VaporCloudExplosion = 0.05,
   BLEVE = 0.90,
   NoExplosion = 0.04,
   DustExplosion =0.01
]
] else [if any Sc have ( HasTemperature = HighTemperature ) [
   VaporCloudExplosion = 0.02,
   BLEVE = 0.03,
```

```
    NoExplosion = 0.05,
    DustExplosion = 0.90
]else [
    VaporCloudExplosion = 0.03,
    BLEVE = 0.02,
    NoExplosion = 0.40,
    DustExplosion =0.55
] ]
] else if any  Sc have ( CauseTertiaryEvents = DustCloud)  [
    VaporCloudExplosion = 0.03,
    BLEVE = 0.02,
    NoExplosion = 0.1,
    DustExplosion =0.85
] else [
    VaporCloudExplosion = 0.1,
    BLEVE = 0.1,
    NoExplosion = 0.2,
    DustExplosion = 0.6
]


] else [
    VaporCloudExplosion = 0.10,
    BLEVE = 0.10,
    NoExplosion = 0.75,
    DustExplosion = 0.05
]
```

A.2.8 *'hazSecondaryHazard'* Node LPD

```
if any Sc have ( HasMaterialToxicity= true &
( HasHazardof= FireHazard | HasHazardof= ExplosionHazard ))
 [
    SecondaryFire = 0.05,
    SecondaryExplosion = 0.05,
    NoSecondaryHazard = 0.1,
    ToxicRelease = 0.80
 ]
 else if any Sc have
 ( HasHazardof= FireHazard &
 (HasFireHazard = FlashFire | HasFireHazard =JetFire))
 [if any Sc have (  HasMatState = Vapor ) [
    SecondaryFire = 0.05,
    SecondaryExplosion = 0.8  ,
    NoSecondaryHazard = 0.1,
    ToxicRelease = 0.05
 ] else if any Sc have (HasMatState = Liquid)
 [  SecondaryFire = 0.8,
    SecondaryExplosion = 0.1,
    NoSecondaryHazard = 0.05,
    ToxicRelease = 0.05
 ] else if any Sc have ( HasMatState = Dust )
 [  SecondaryFire = 0.05,
    SecondaryExplosion = 0.90,
```

```
    NoSecondaryHazard = 0.04,
    ToxicRelease = 0.01
]else [
    SecondaryFire = 0.3,
    SecondaryExplosion = 0.2,
    NoSecondaryHazard = 0.4,
    ToxicRelease = 0.1
]


]
else if any Sc have
(HasHazardof = ExplosionHazard & HasExplosionHazard = DustExplosion)
[if any Sc have ( HasMatState = Solid | HasMatState = Dust) [
    SecondaryFire = 0.1,
    SecondaryExplosion = 0.8 ,
    NoSecondaryHazard = 0.05,
    ToxicRelease = 0.05
] else [  SecondaryFire = 0.7,
    SecondaryExplosion = 0.2,
    NoSecondaryHazard = 0.05,
    ToxicRelease = 0.05
]
]else if any Sc have
(HasHazardof= ExplosionHazard &
HasExplosionHazard = VaporCloudExplosion)
 [if any Sc have ( HasMatState = Liquid) [
```

```
    SecondaryFire = 0.3,
    SecondaryExplosion = 0.6  ,
    NoSecondaryHazard = 0.05,
    ToxicRelease = 0.05
] else [  SecondaryFire = 0.5,
    SecondaryExplosion = 0.4,
    NoSecondaryHazard = 0.05,
    ToxicRelease = 0.05
] ]else [
    SecondaryFire = 0.05,
    SecondaryExplosion = 0.05,
    NoSecondaryHazard = 0.85,
    ToxicRelease = 0.05
]
```

Appendix B

Simulation Results

Total 45 Accident results has been listed in Chapter 4. Detailed simulation results for 5 cases are available in case studies section of Chapter 3. Rest of the simulation outputs are listed in this chapter. For some cases images of full SSBN is not provided except for the resulting events nodes.

B.1 ConAgra Natural Gas Explosion, NC, 2009

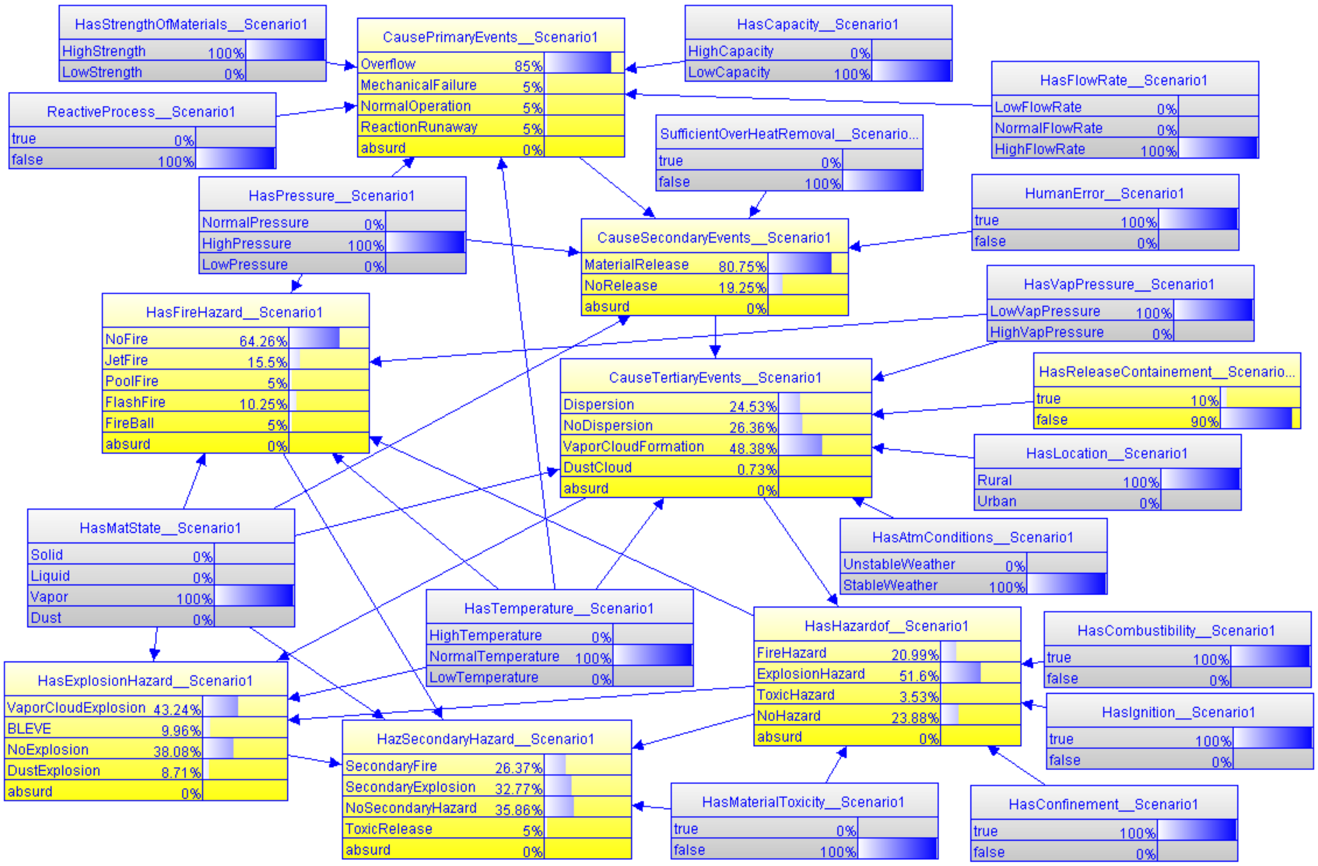


Figure B.1: Results for ConAgra Natural Gas Explosion accident.

B.2 BP Texas Refinery Explosion , 2005

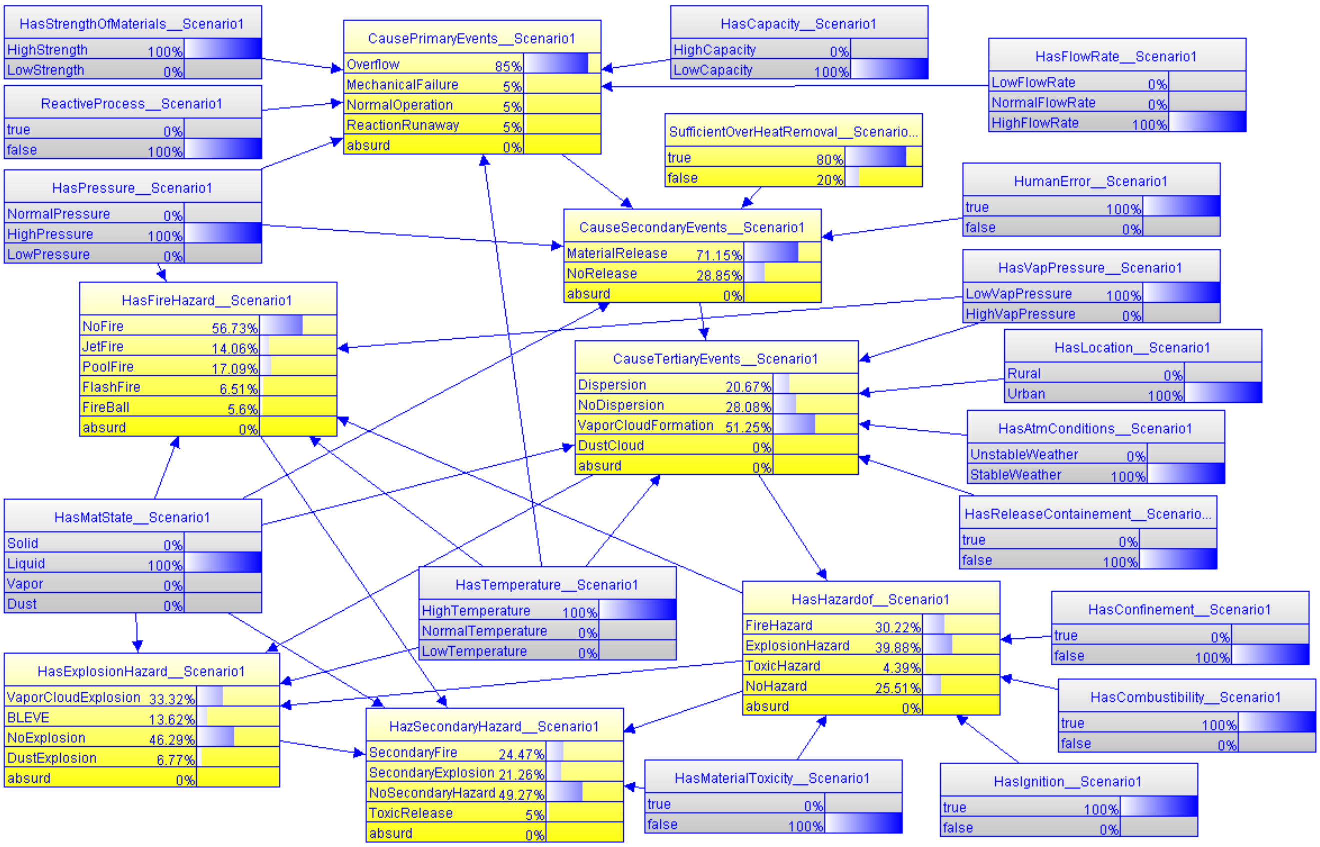


Figure B.2: Results for BP Texas Refinery Explosion accident .

B.3 WV Little General Store Propane Explosion, 2007

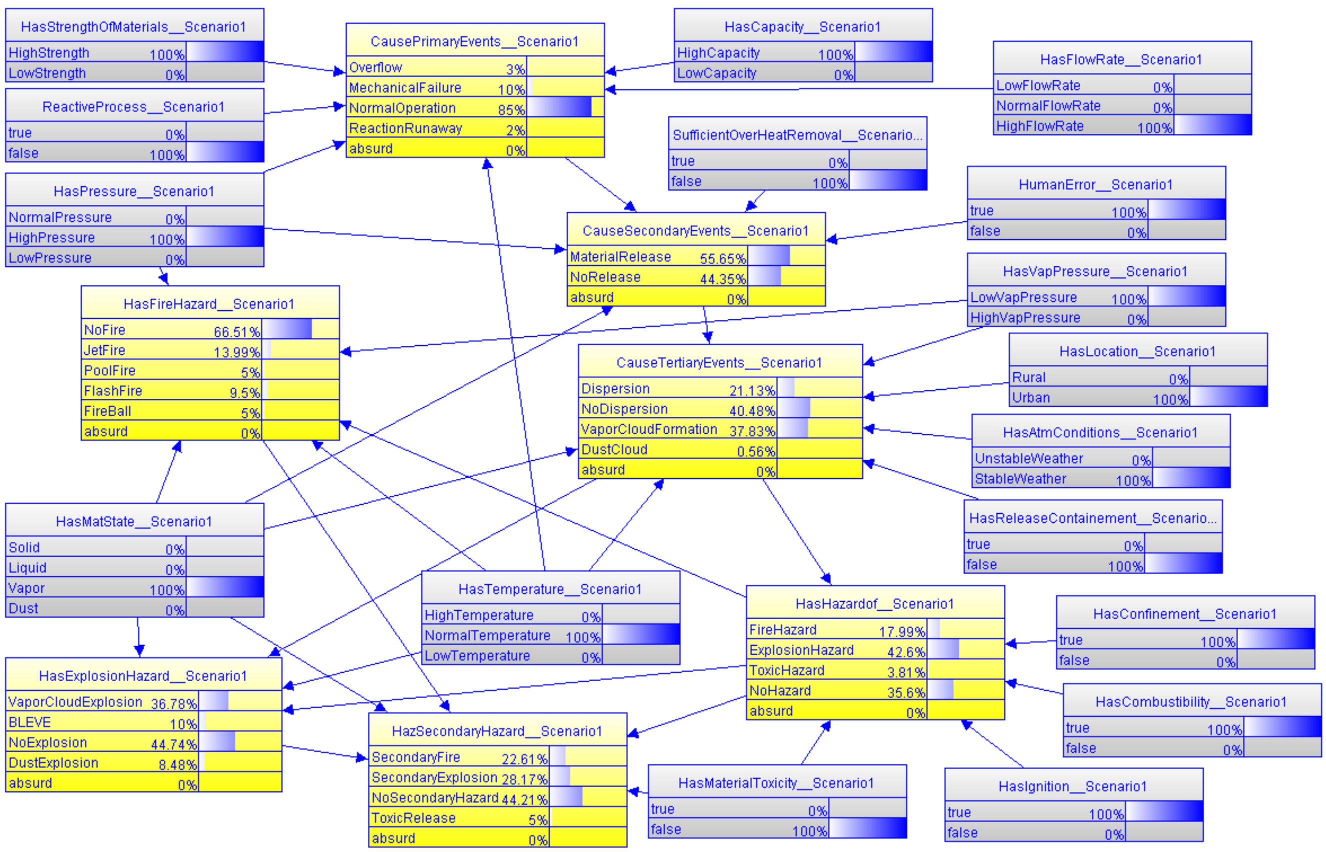


Figure B.3: Results for Little General Store Explosion .

B.4 Huston Marcus Oil and Chemical Explosion, 2004

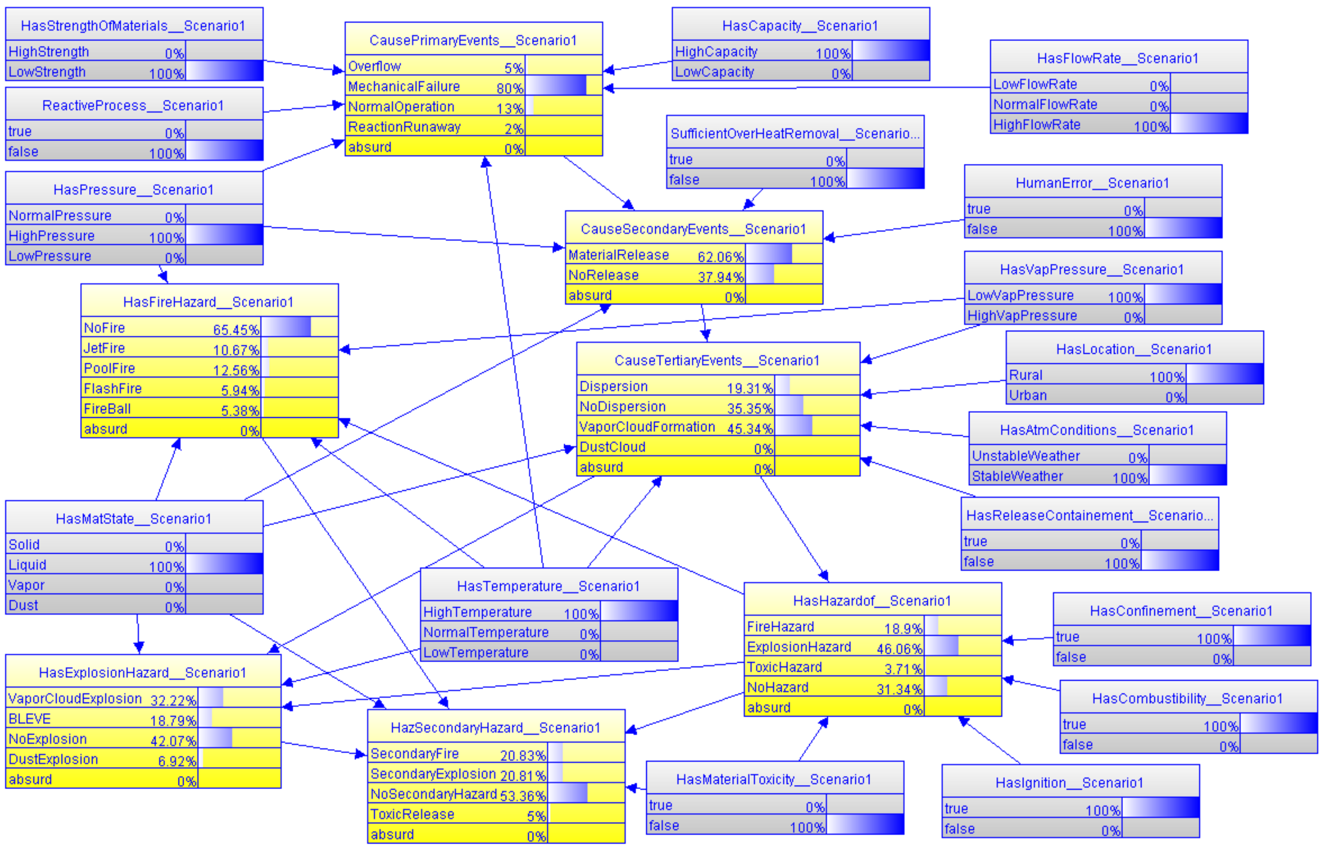


Figure B.4: Results for Huston Marcus Oil and Chemical Explosion .

B.5 West Fertilizer Fire & Explosion, Texas 2013

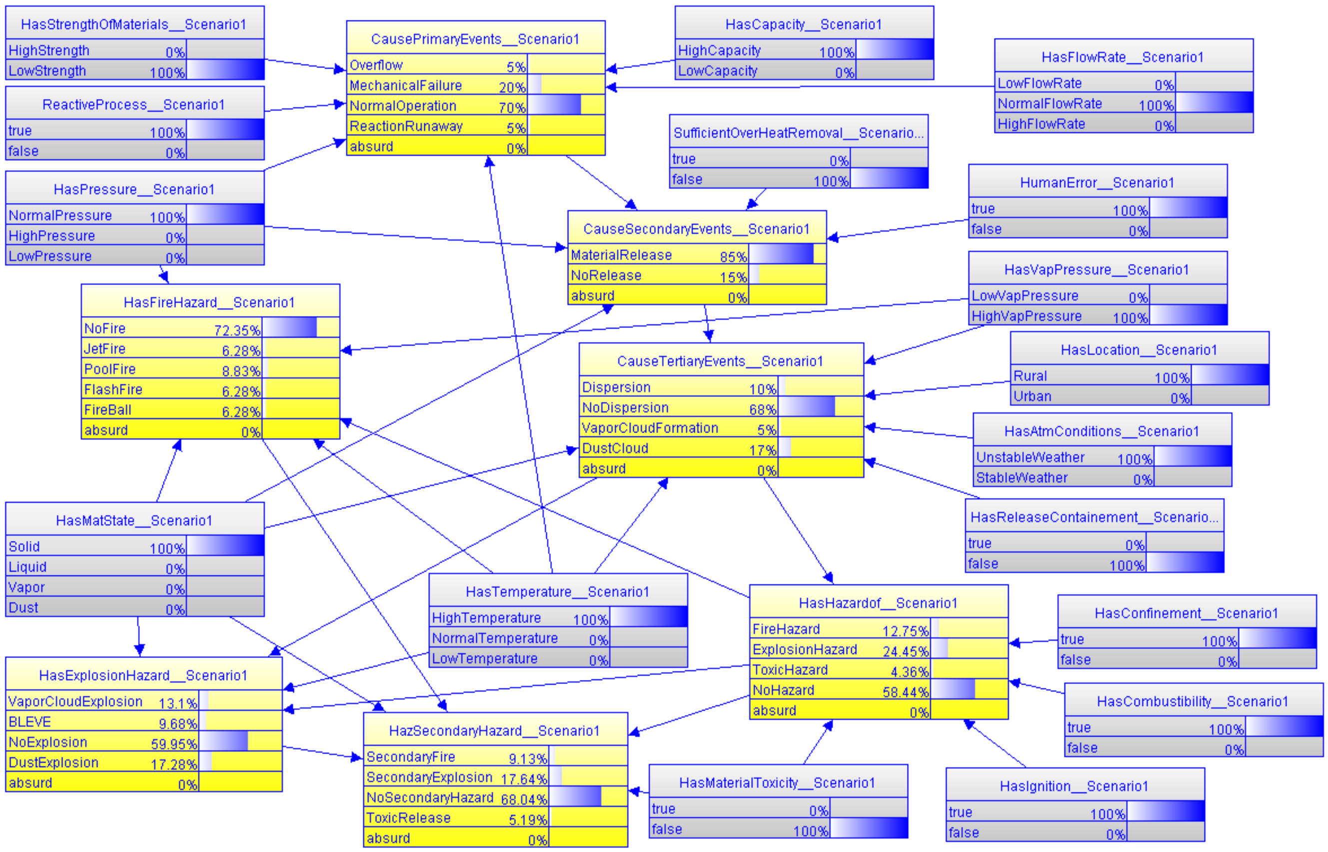


Figure B.5: Results for West Fertilizer Fire & Explosion.

B.6 Valero Refinery Propane Fire, Texas 2007

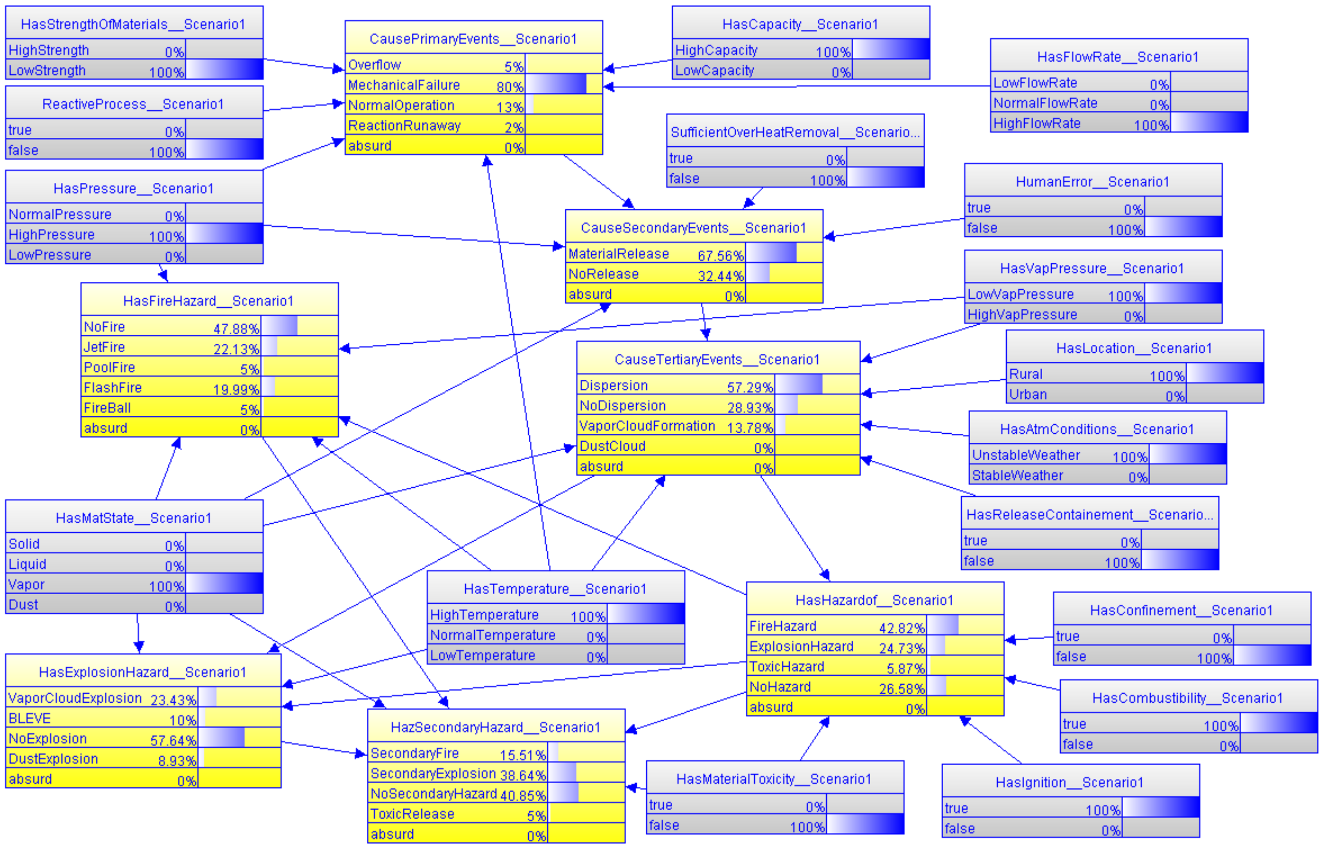


Figure B.6: Results for Valero Refinery Propane Fire.

B.7 Veolia ES Technical Solutions Fire and Explosion, Ohio 2009

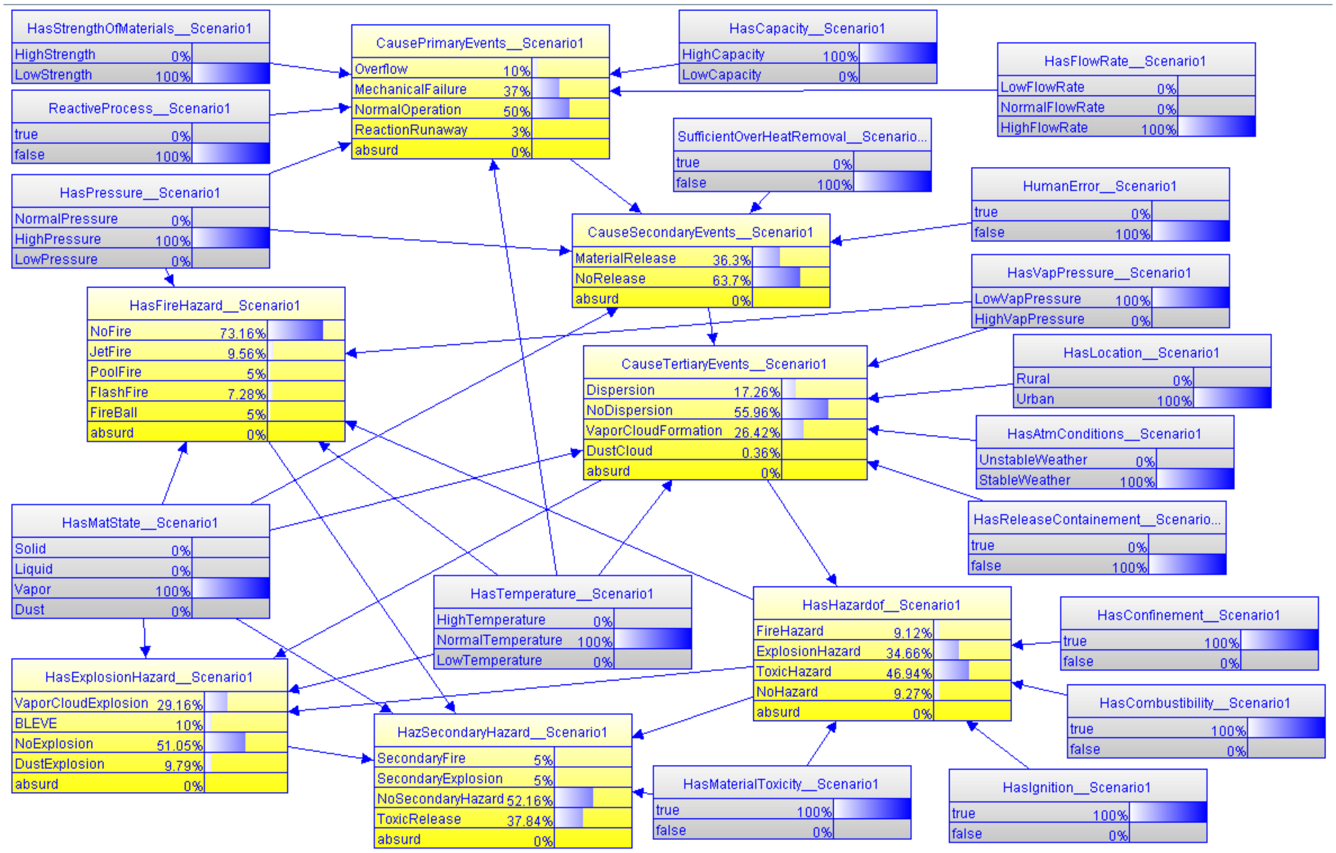


Figure B.7: Results for Veolia ES Technical Solutions Hazardous Waste Fire and Explosion.

B.8 Herrig Brothers Farm Propane Tank Explosion, Iowa 1998

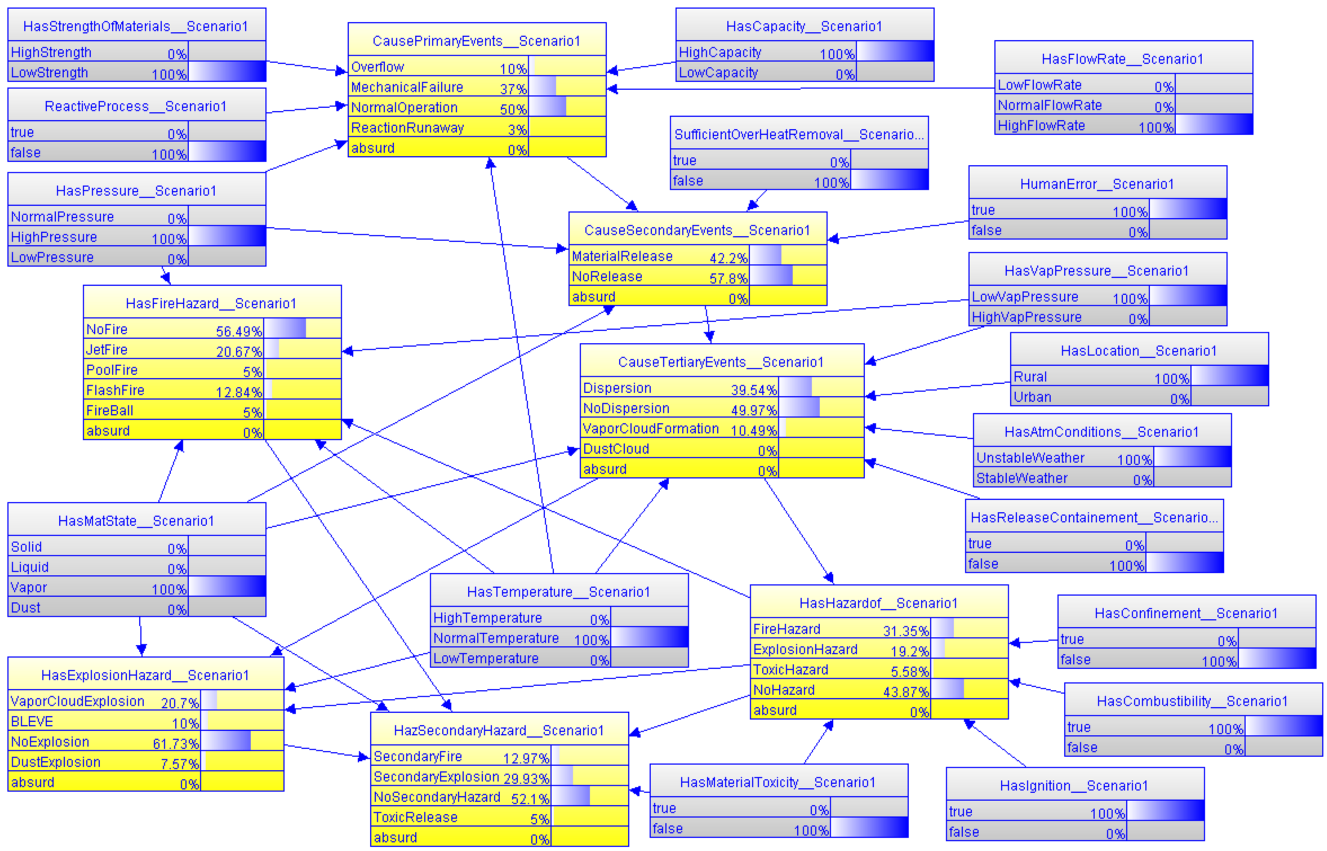


Figure B.8: Results for Herrig Brothers Farm Propane Tank Explosion, Iowa 1998 .

B.9 Silver Eagle Refinery Flash Fire and Explosion, Utah 2009

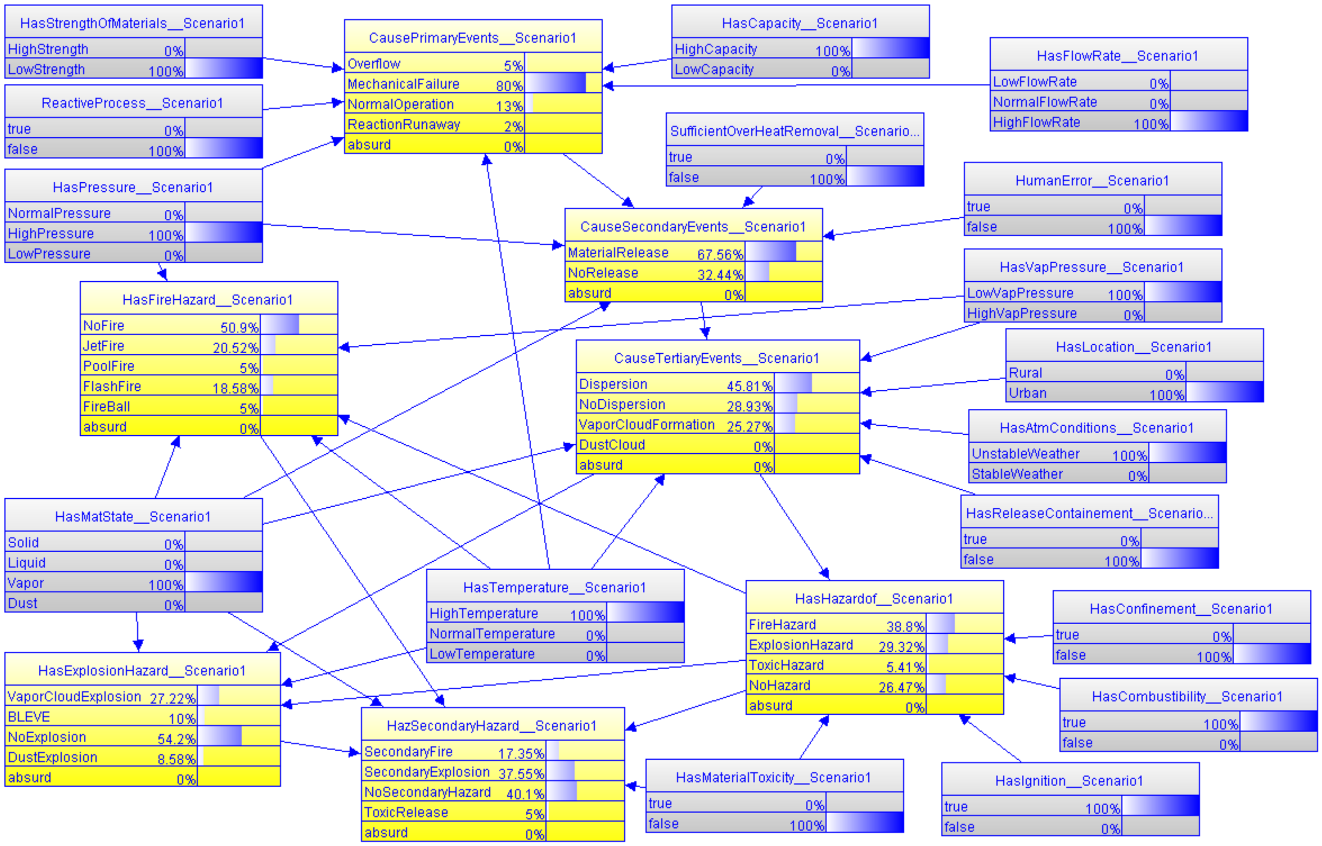


Figure B.9: Results for Silver Eagle Refinery Flash Fire and Explosion.

B.10 Carbide Industries Explosion, Louisville, Kentucky, 2011

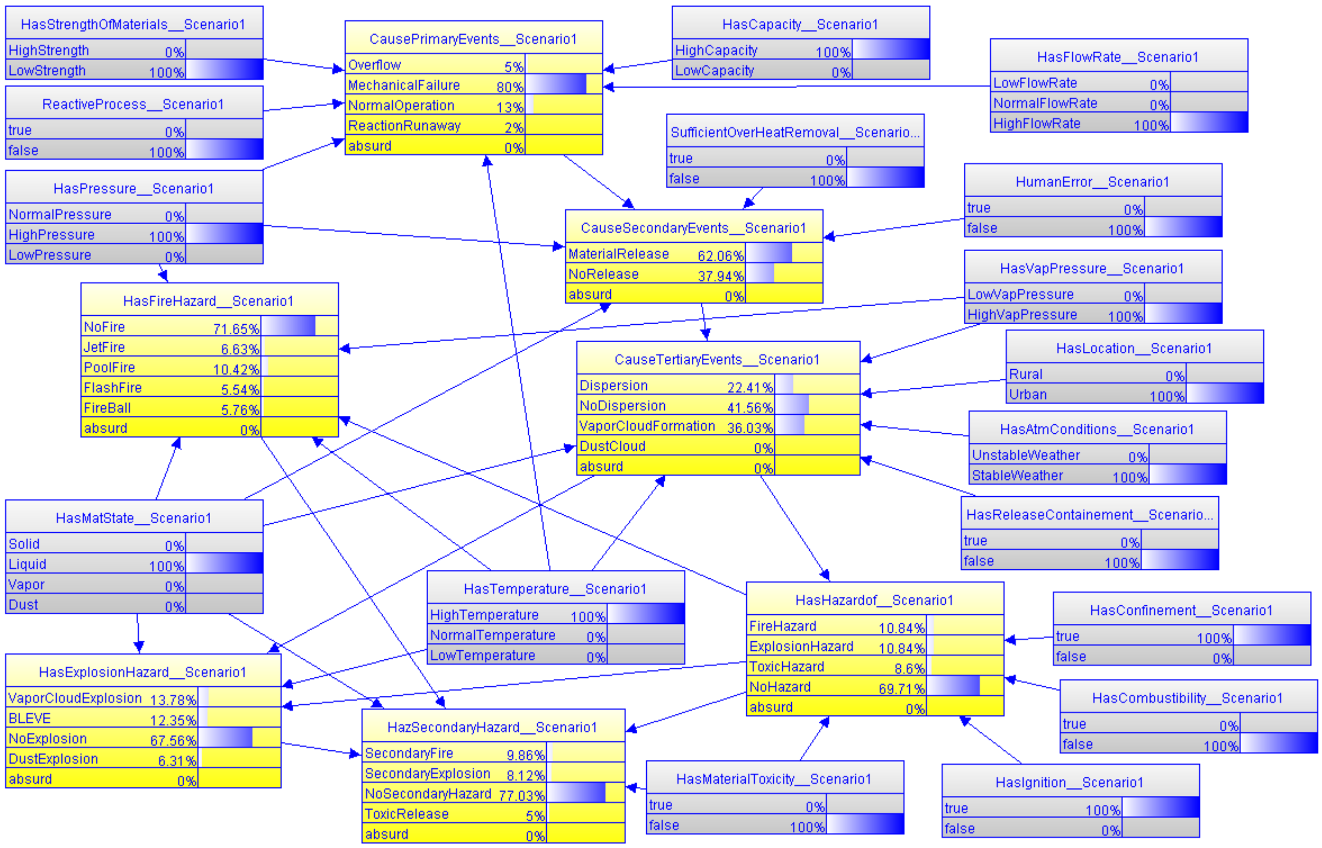


Figure B.10: Results for Carbide Industries Explosion accident.

B.11 Williams Olefins Plant Explosion, Louisiana 2013

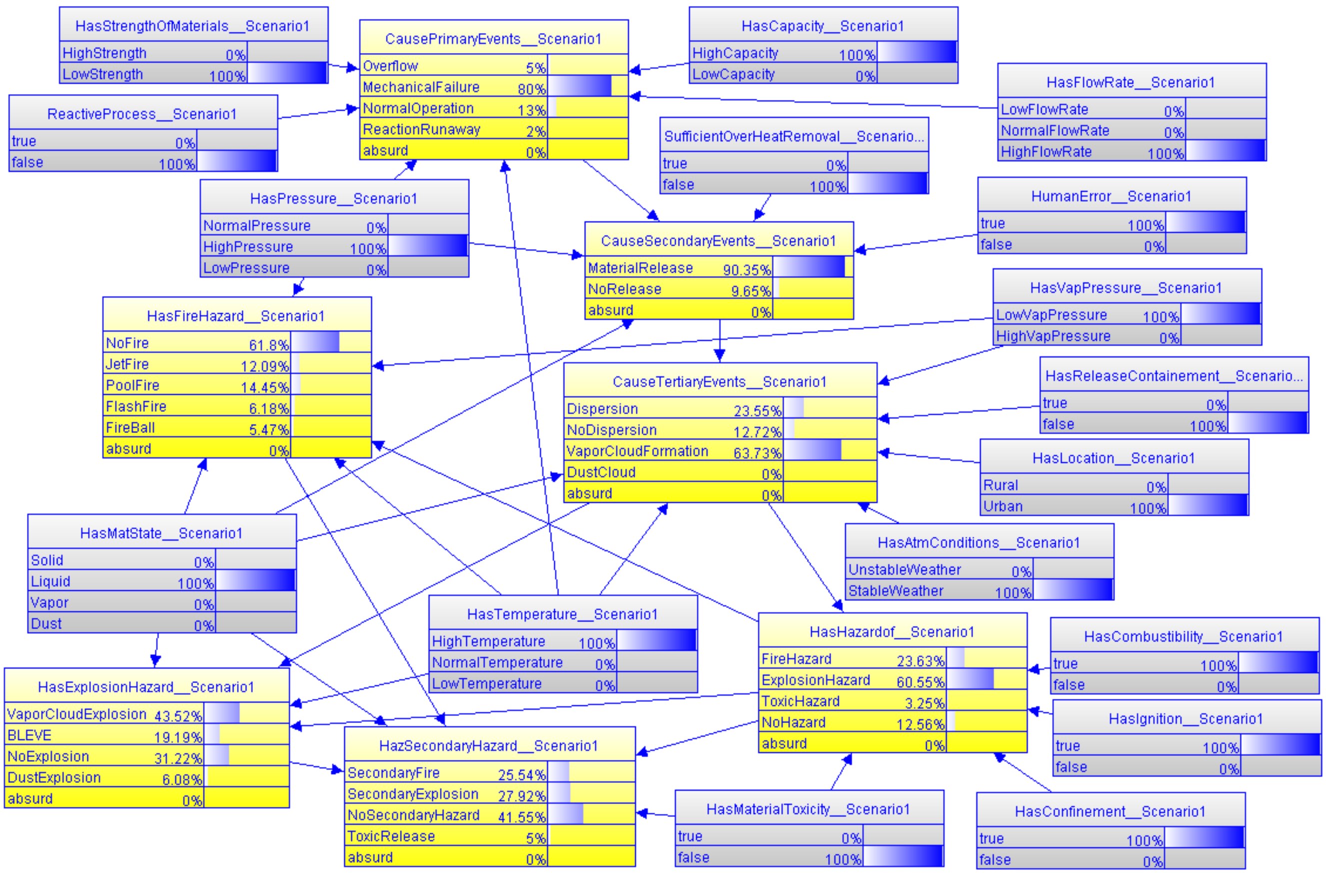


Figure B.11: Results for Williams Olefins Plant Explosion.

B.12 EQ Hazardous Waste Fire and Explosion, Apex, NC, 2006

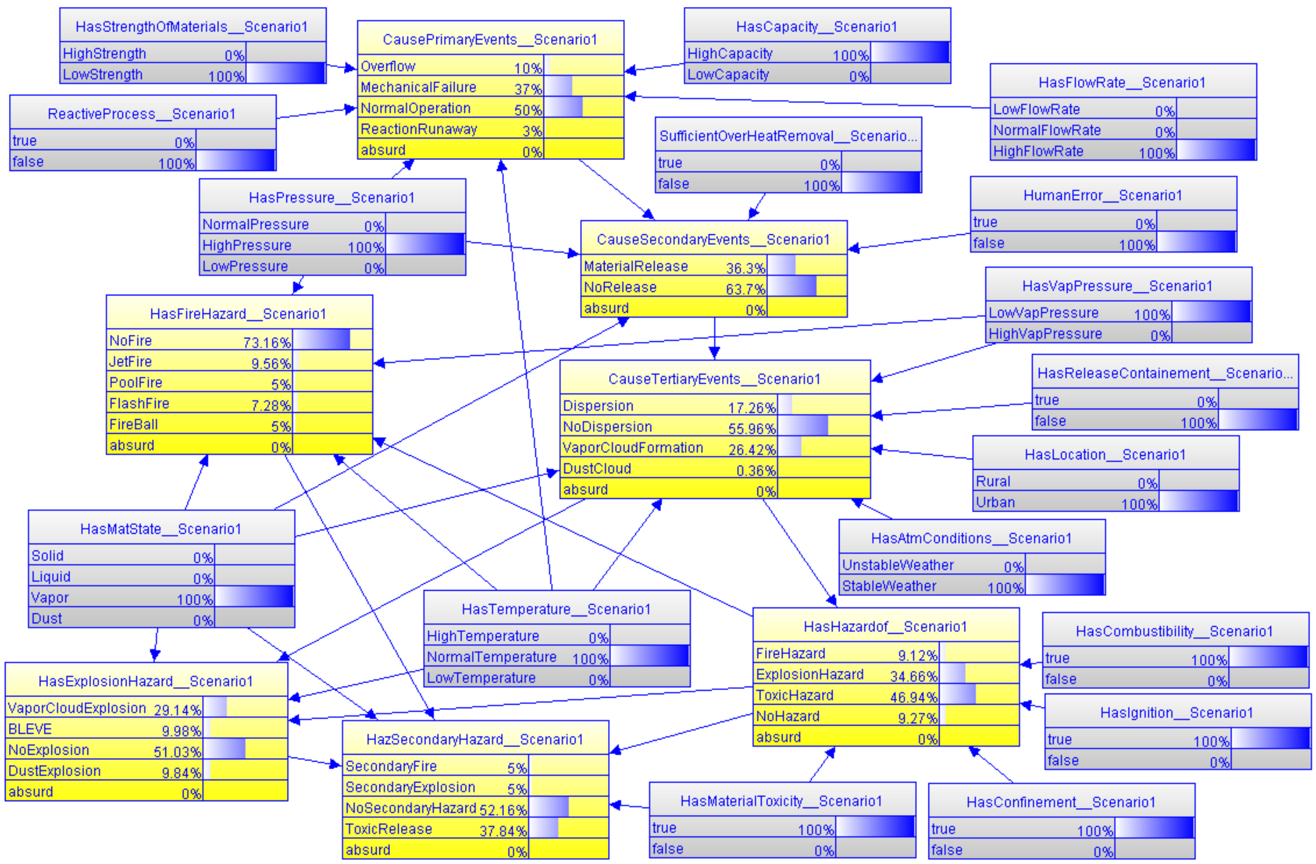


Figure B.12: Results forEQ Hazardous Waste Fire and Explosion.

B.13 Tosero Refinery Explosion, Washington 2010

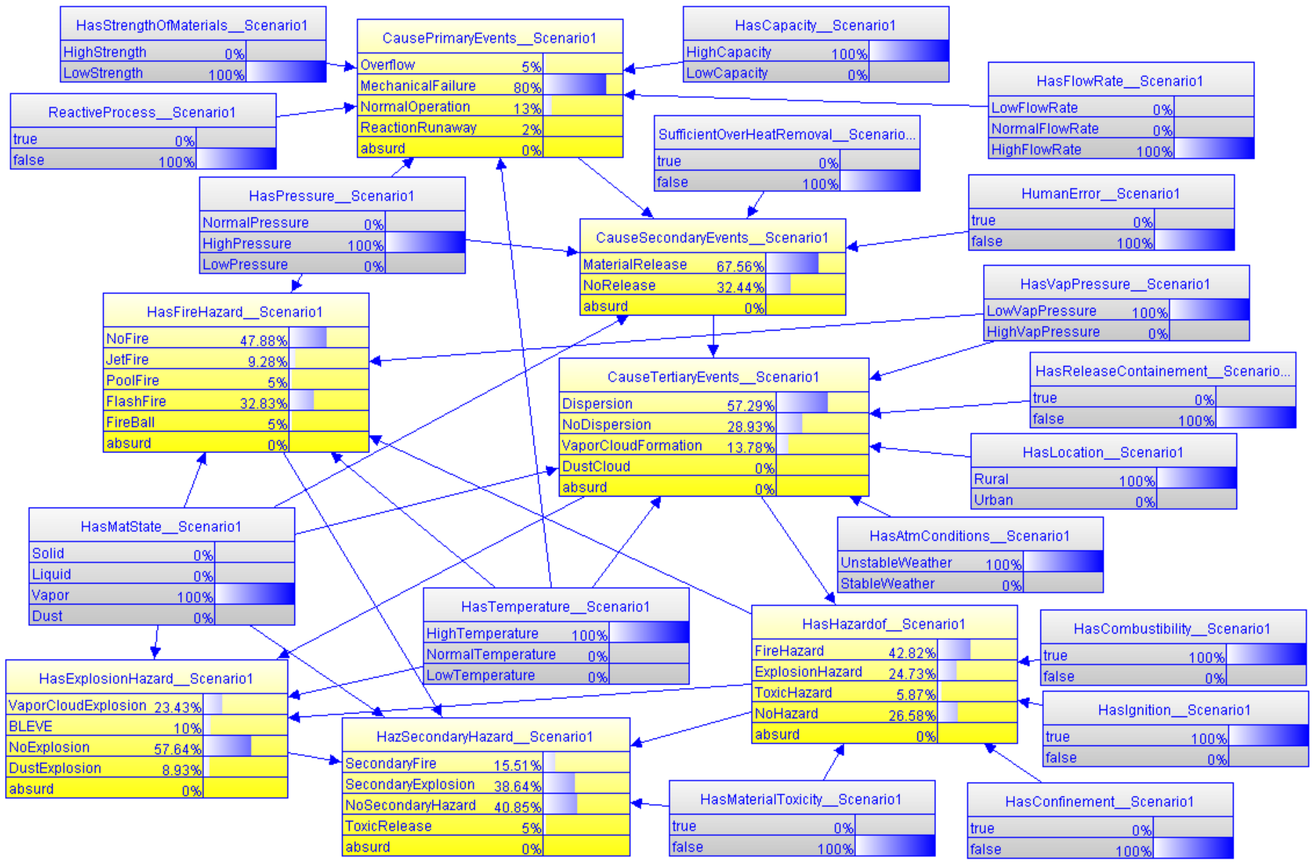


Figure B.13: Results for Tosero Refinery Explosion, Washington.

B.14 Hilton Hotel, San Diego, California, 2008

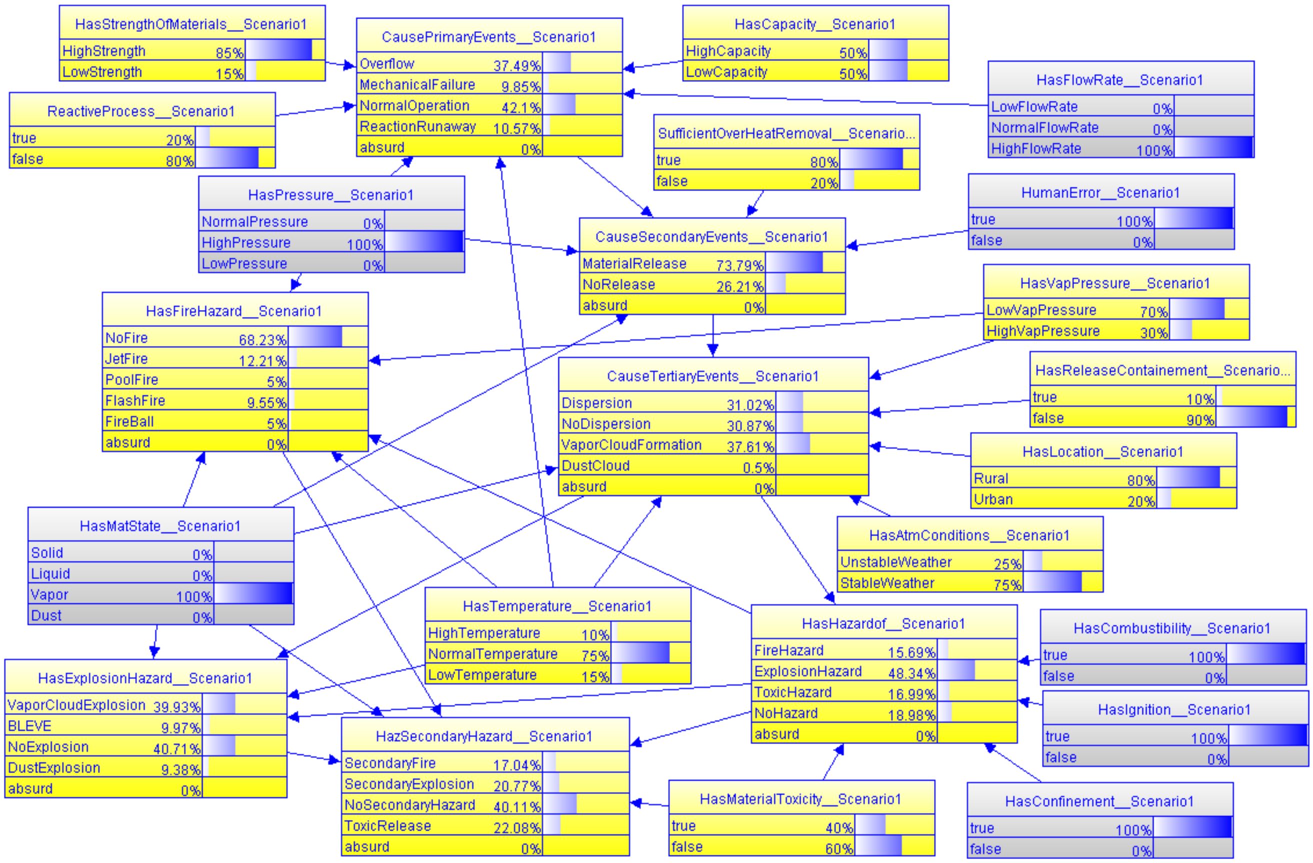


Figure B.14: Results for Hilton Hotel, San Diego, California.

B.15 Sterigenics International Ethylene Oxide Explosion, California, 2004

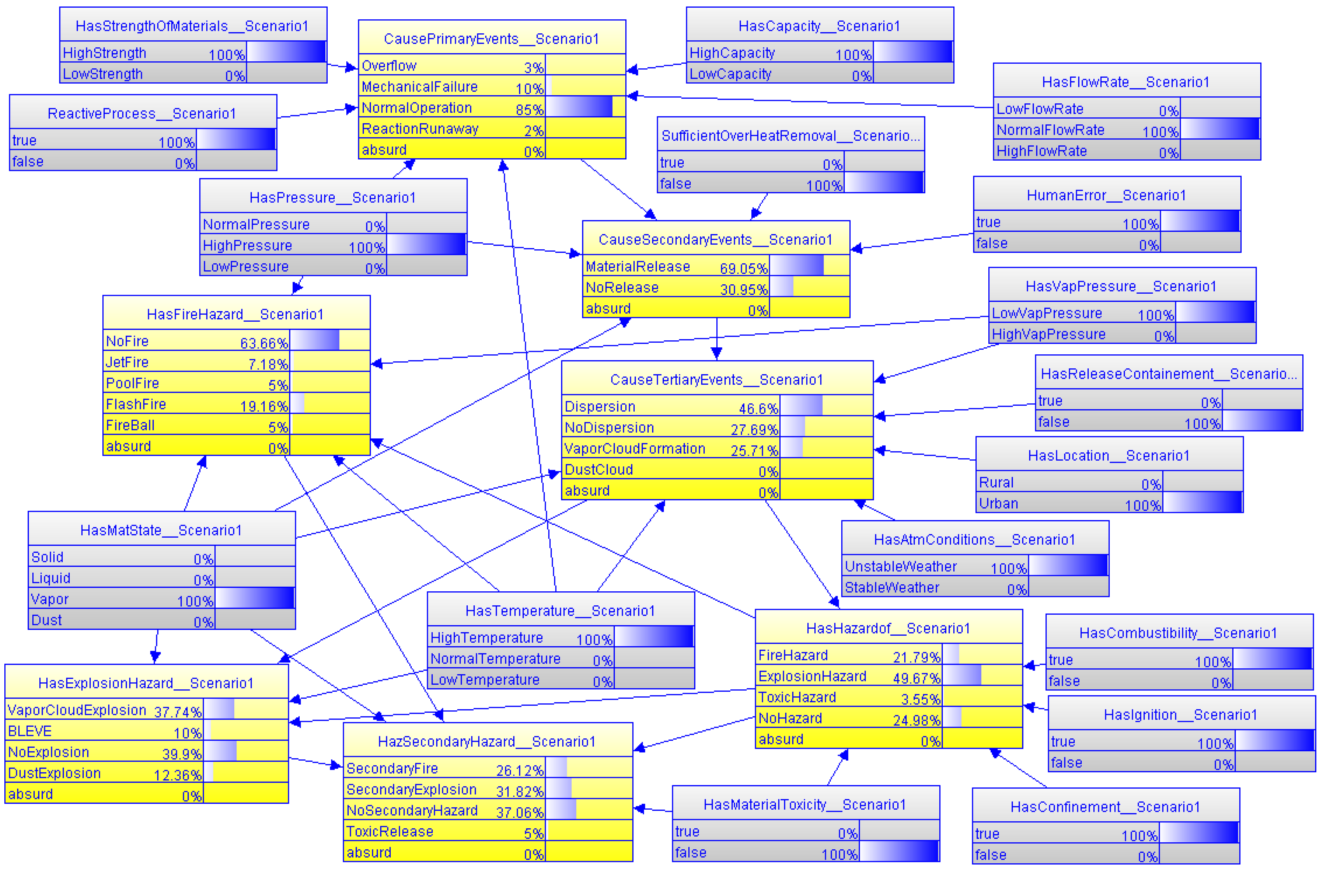


Figure B.15: Results for Sterigenics International Ethylene Oxide Explosion.

B.16 Kleen Energy Natural Gas Explosion, Middletown, CT, 2010

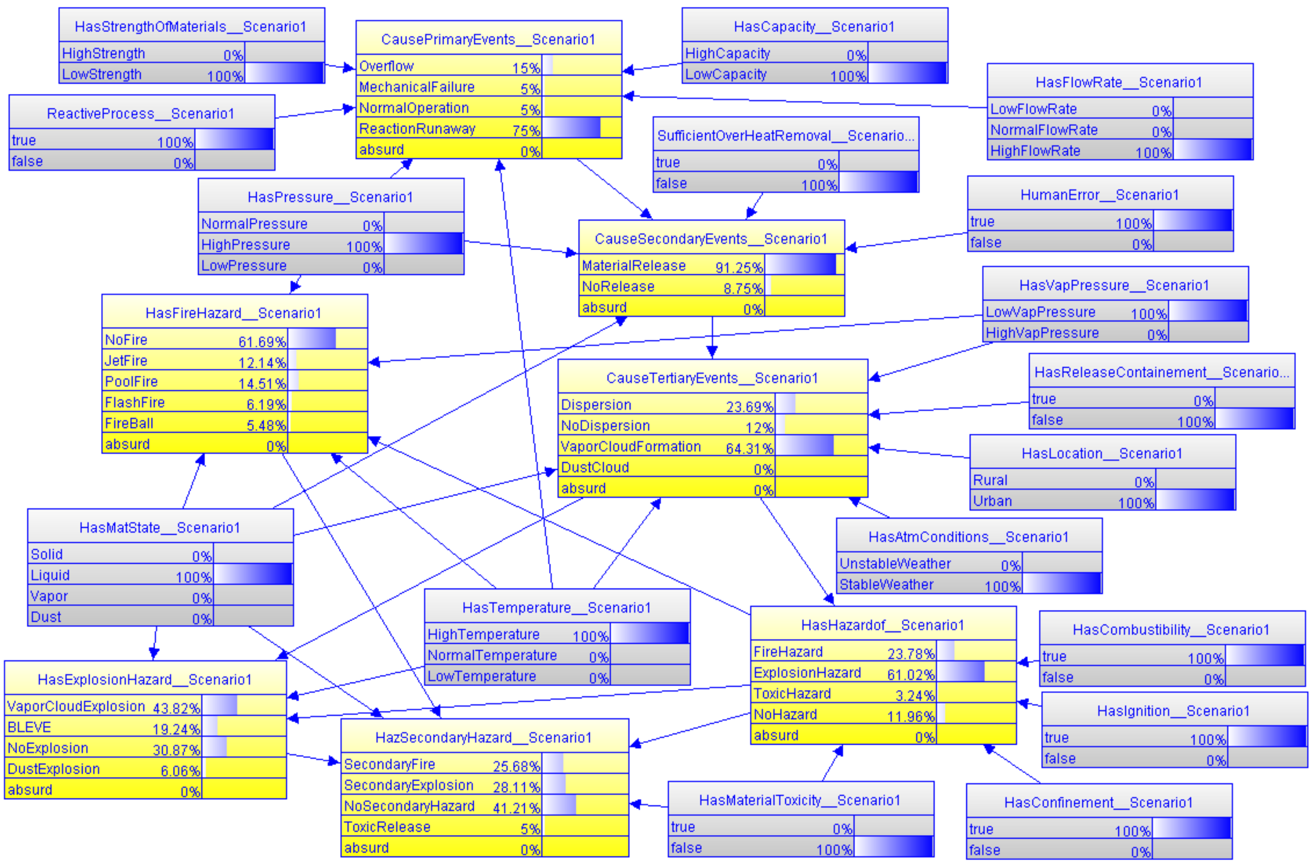


Figure B.16: Results for Kleen Energy Natural Gas Explosion.

B.17 BLSR Fire, TEXAS, 2003

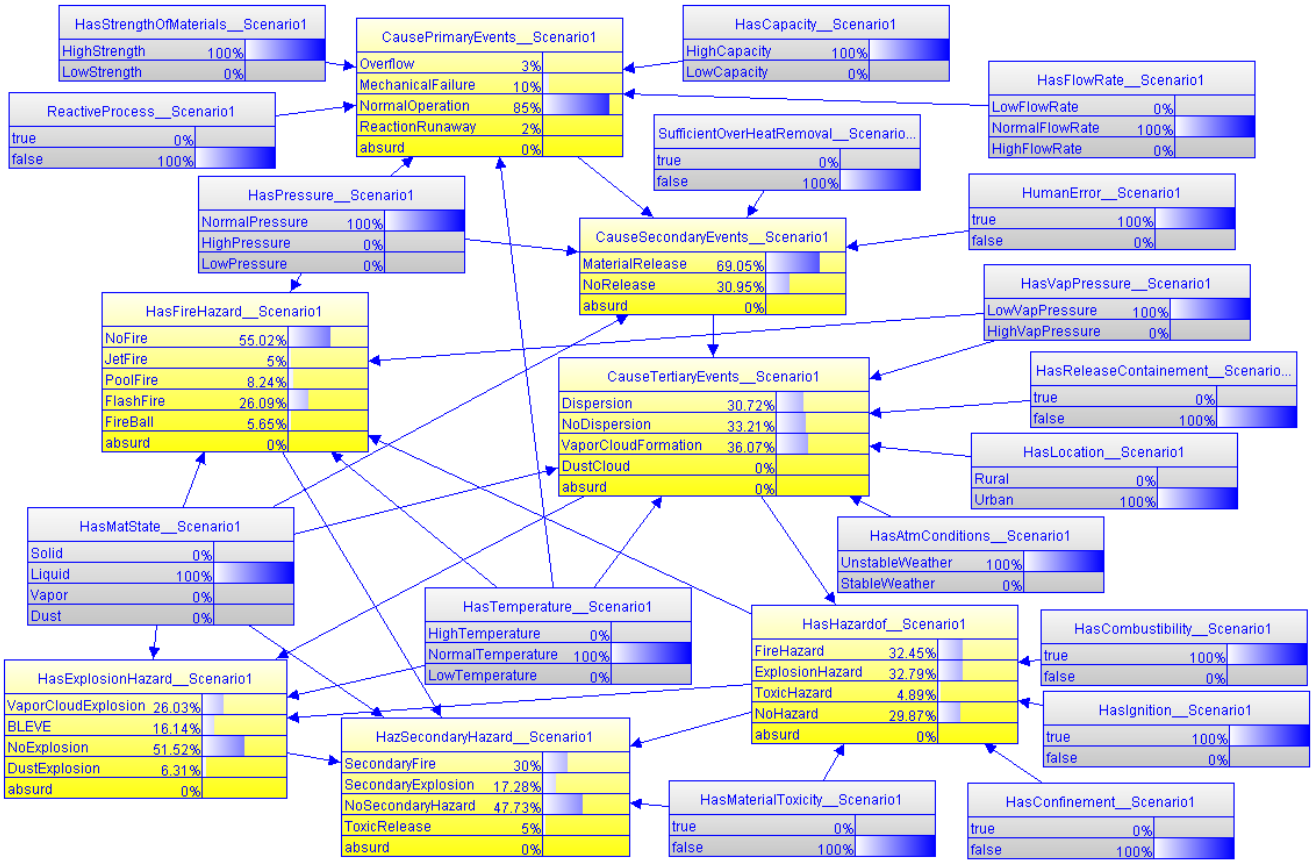


Figure B.17: Results for BLSR Fire.

B.18 Partridge Raleigh Oilfield Explosion and Fire, Missisipi, 2006

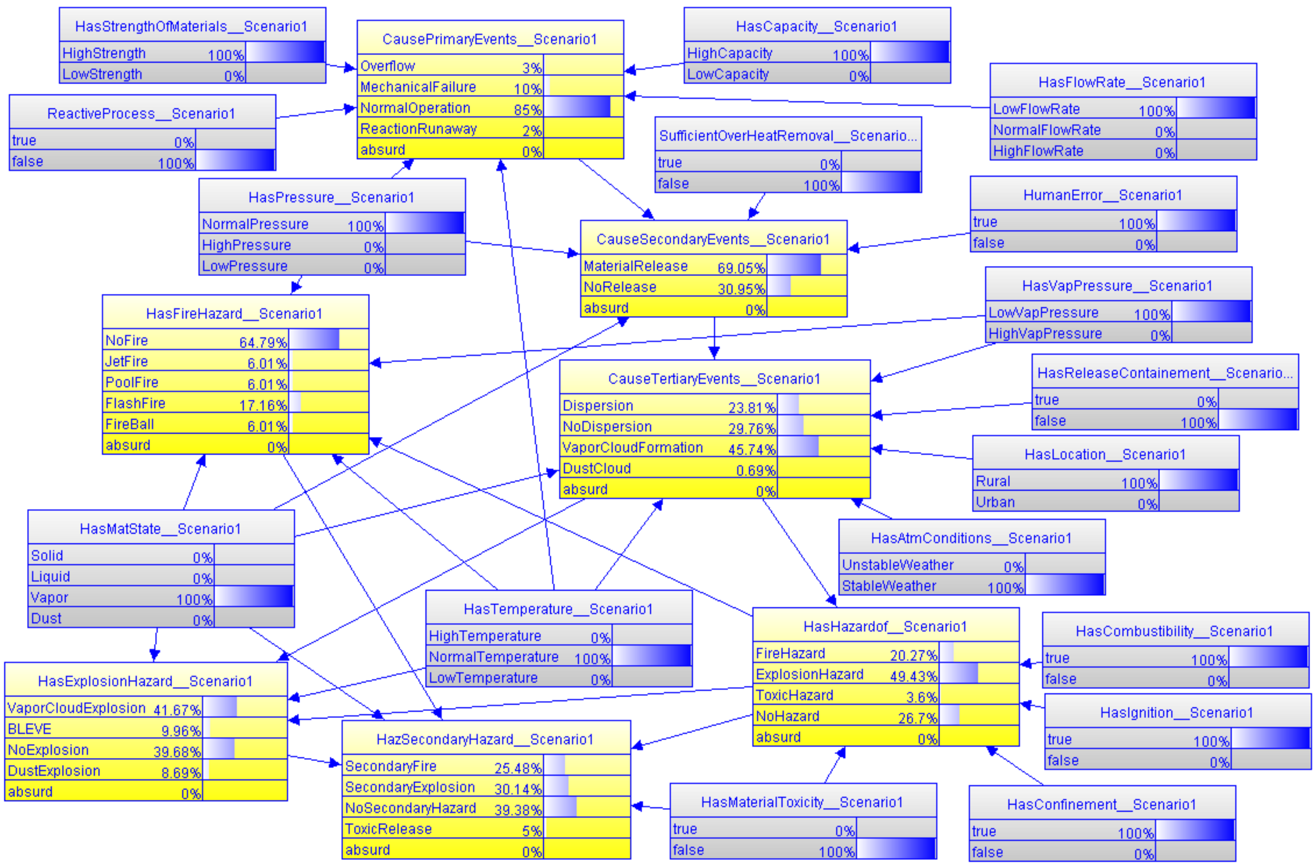


Figure B.18: Results of Partridge Raleigh Oilfield Explosion and Fire.

B.19 Formosa Plastics Corporation Explosion and Fire, Illiopolis, Illinois 2004

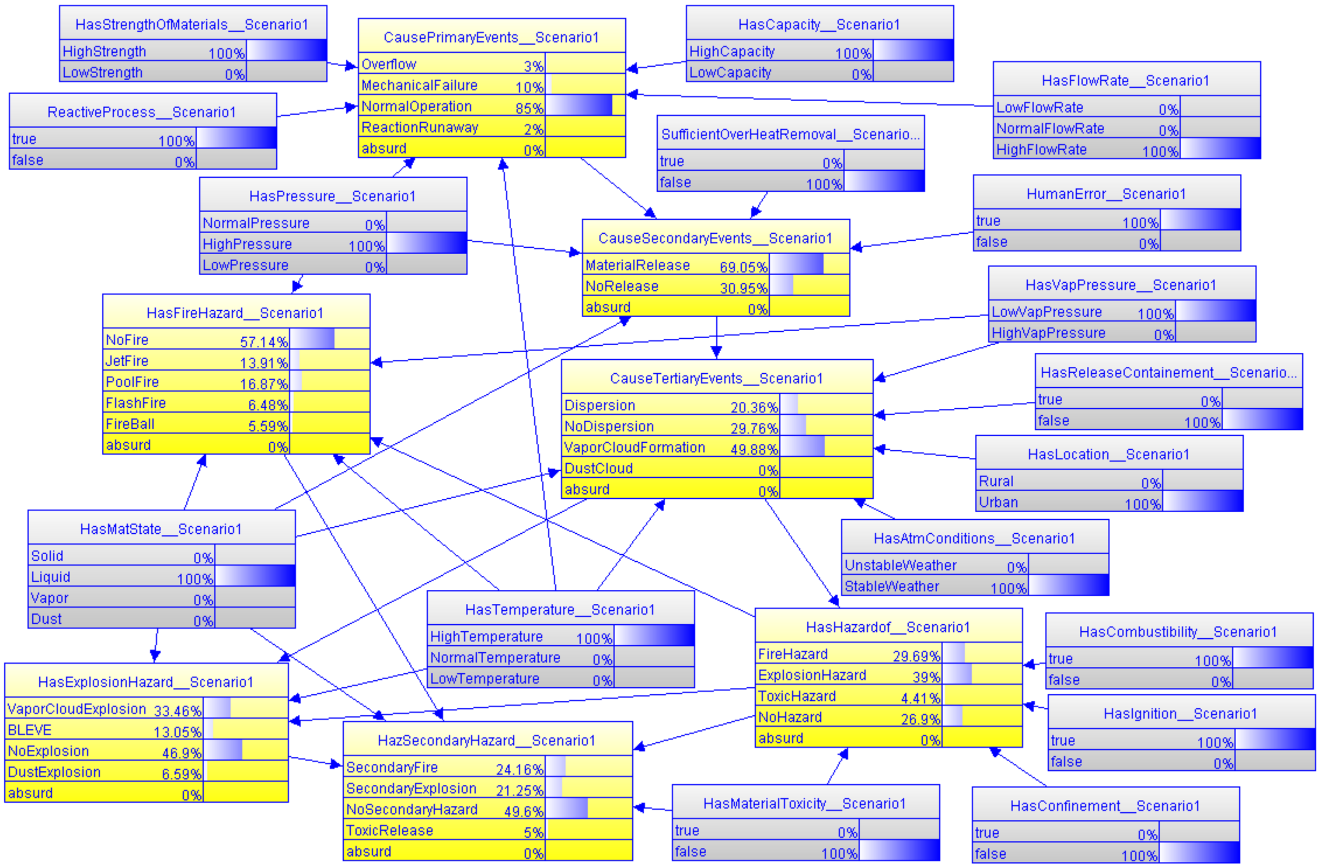


Figure B.19: Results for Formosa Plastics Corporation Explosion and Fire 2004.

B.20 Formosa Plastics Corporation Fire, Point Comfort, Texas, 2005

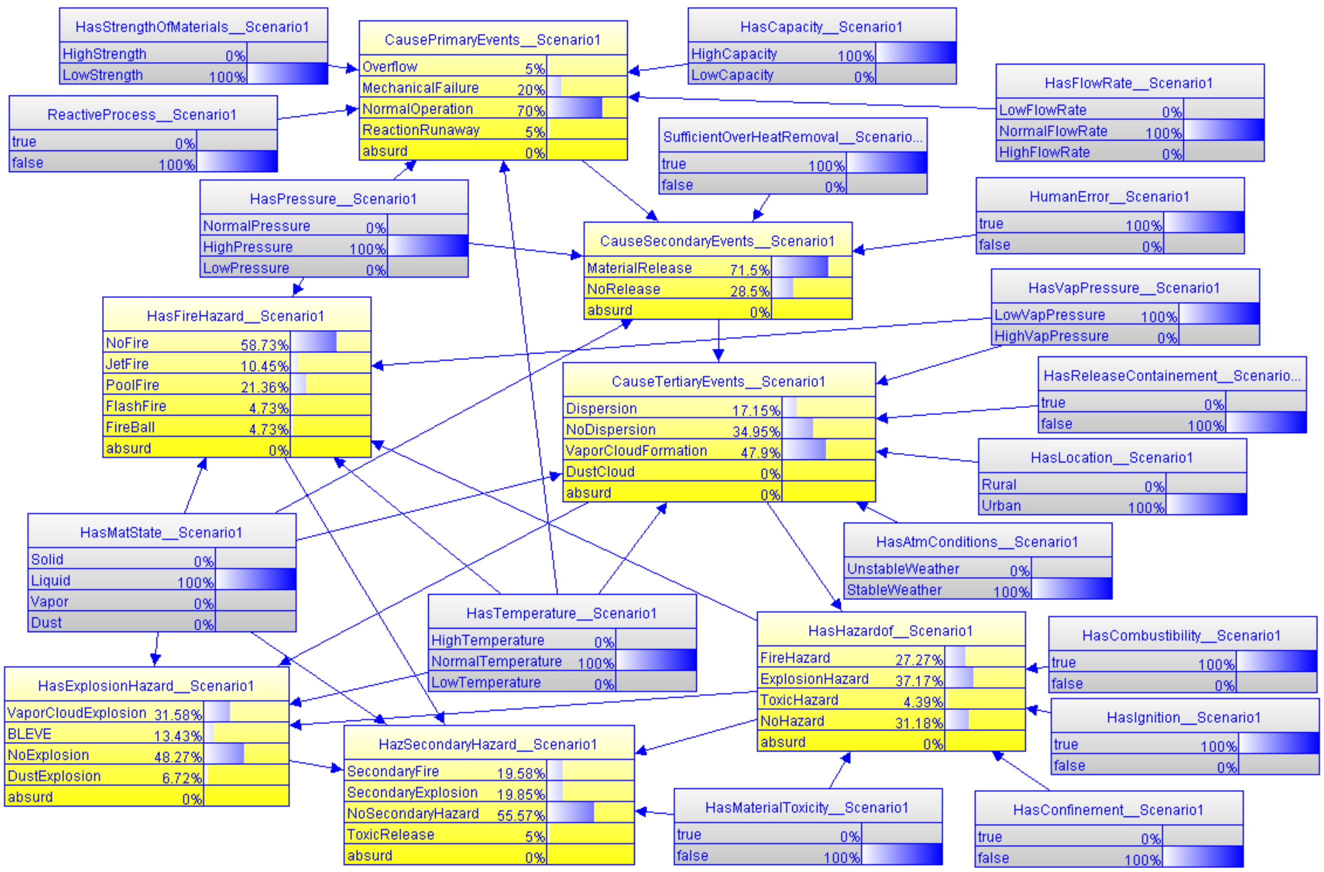


Figure B.20: Results forFormosa Plastics Corporation Fire 2005.

B.21 Praxair Propylene Cylinders Fire, St. Louis, Missouri 2005

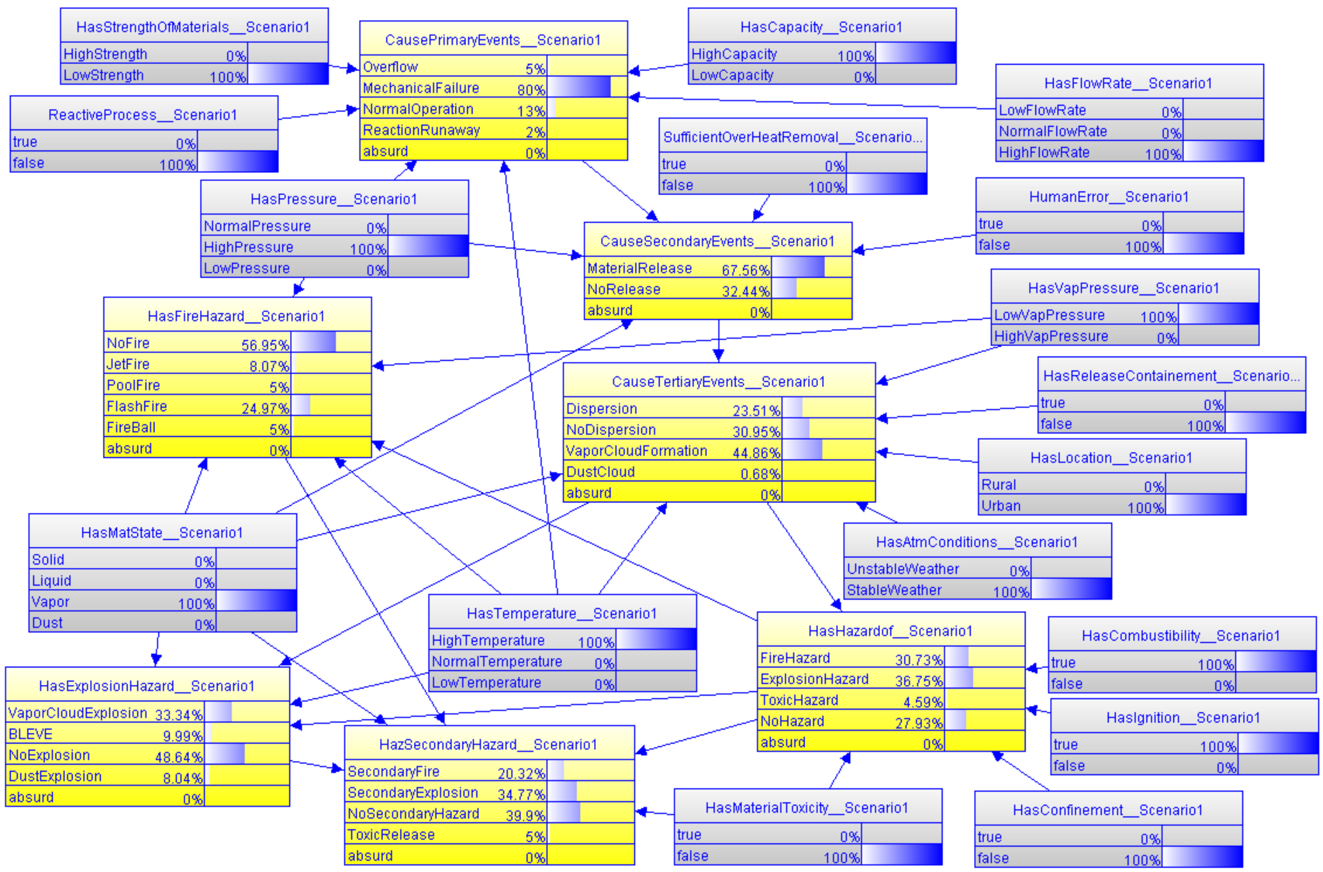


Figure B.21: Results for Praxair Propylene Cylinders Fire.

B.22 ASCO Acetylene Explosion, Perth Amboy, New Jersey 2005

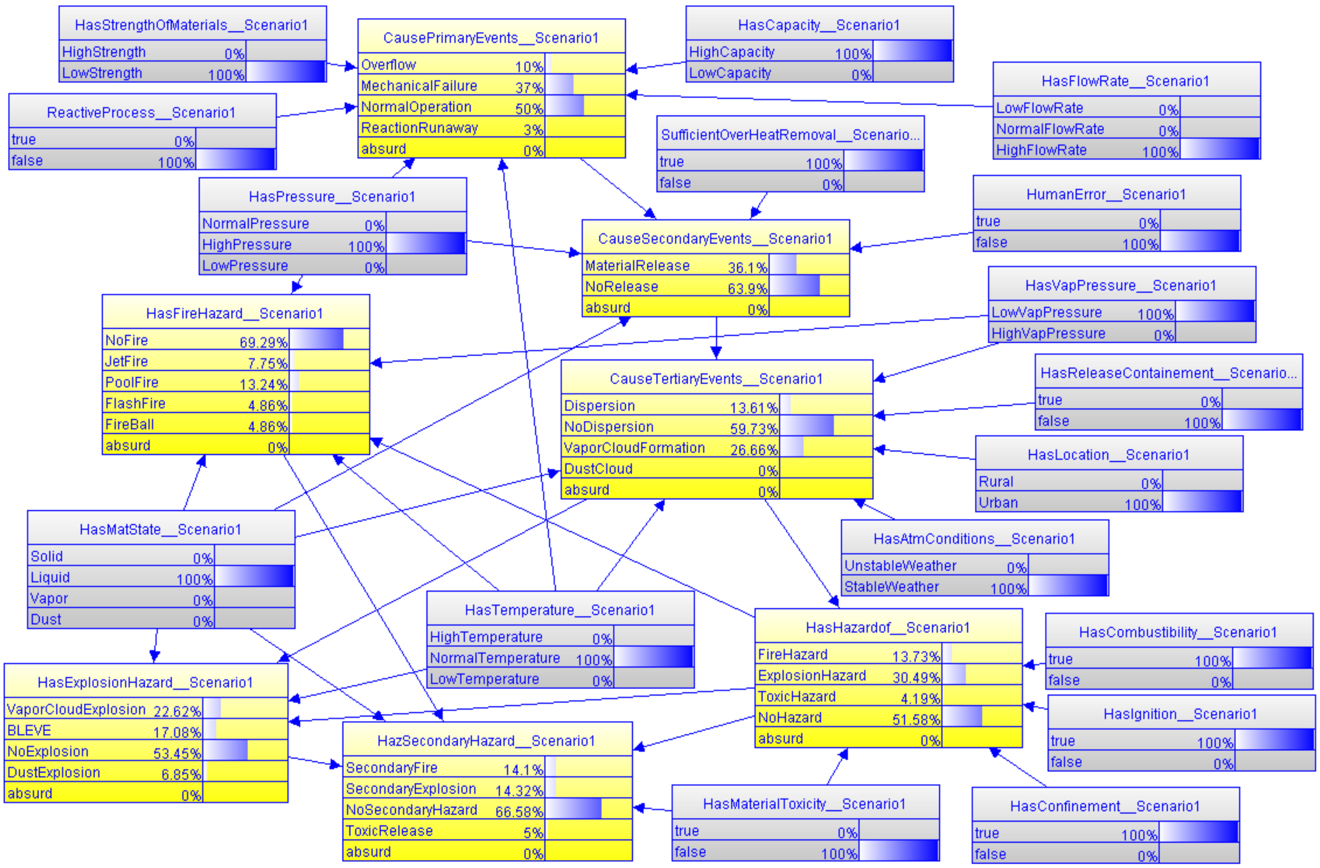


Figure B.22: Results for ASCO Acetylene Explosion.

B.23 CITGO's Corpus Christi refinery, Texas 2009

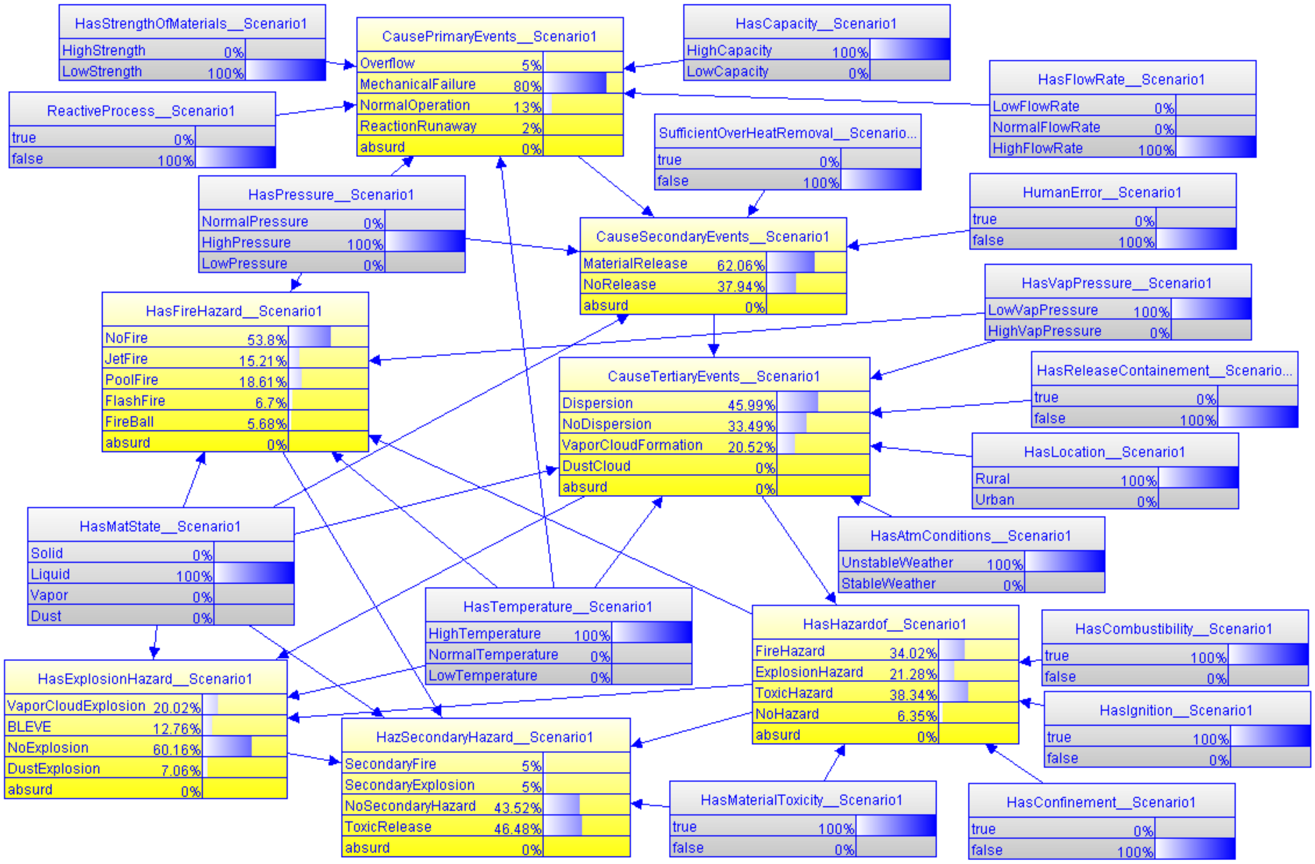


Figure B.23: Results for CITGO's Corpus Christi refinery accident (1).

B.24 Horsehead Holding Company Explosion,Pennsylvania 2010

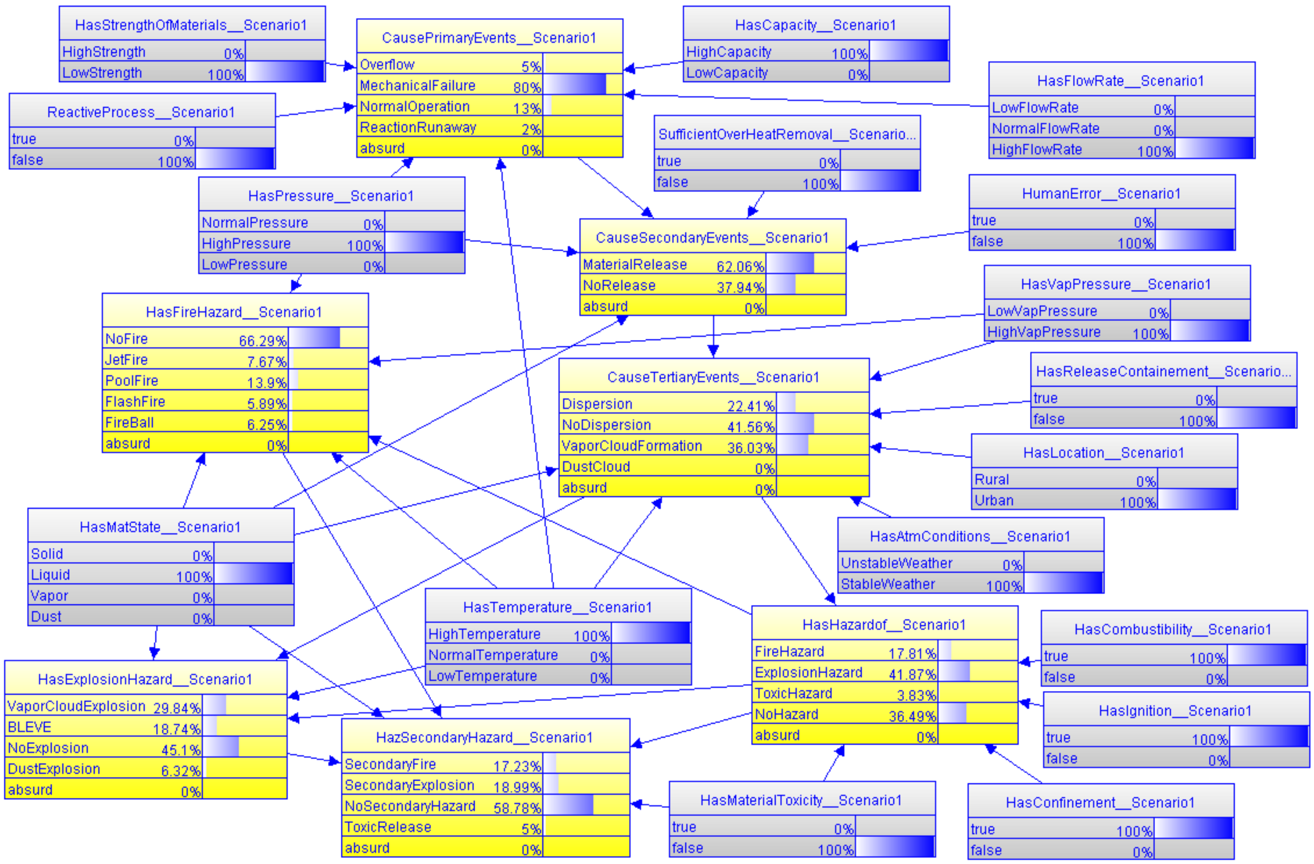


Figure B.24: Results for Horsehead Holding Company Explosion.

B.25 BP Ameco Polymers Plant Explosion, 2001

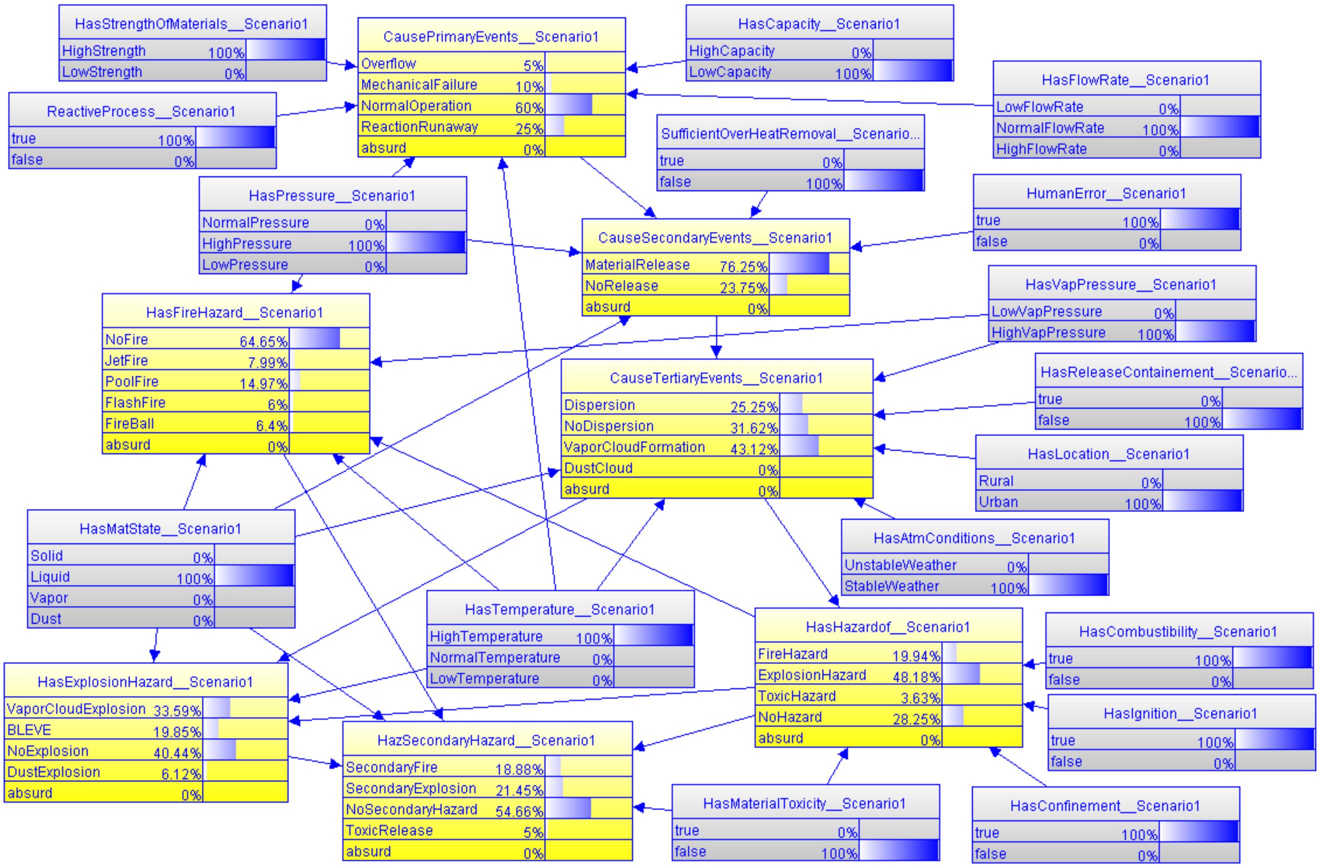


Figure B.25: Results for BP Ameco Polymers Plant Explosion.

B.26 First Chemical Corp. Reactive Chemical Explosion, Mississipi 2002

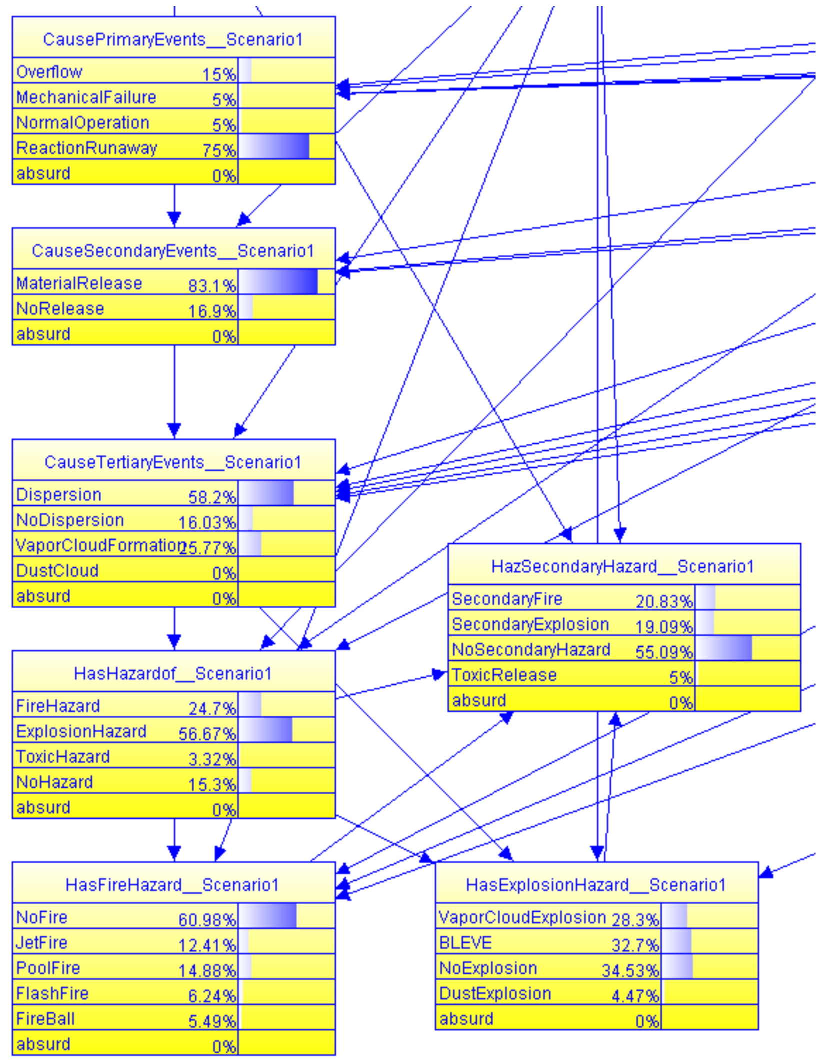


Figure B.26: Results for First Chemical Corp. Reactive Chemical Explosion.

B.27 Synthron Inc Explosion, Morganton, North Carolina 2006

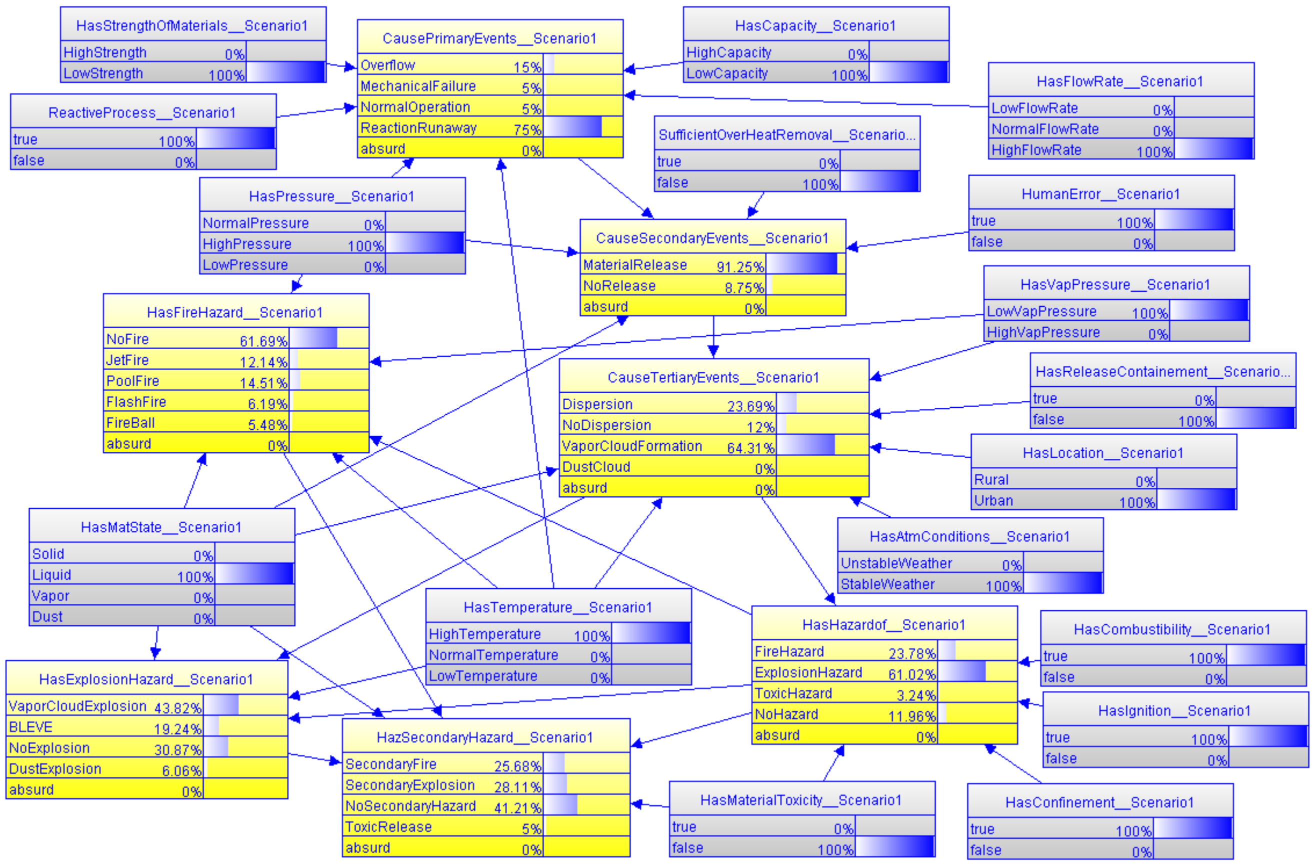


Figure B.27: Results for Synthron Inc Explosion.

B.28 T2 Laboratories Explosions, Jacksonville, Florida, 2007

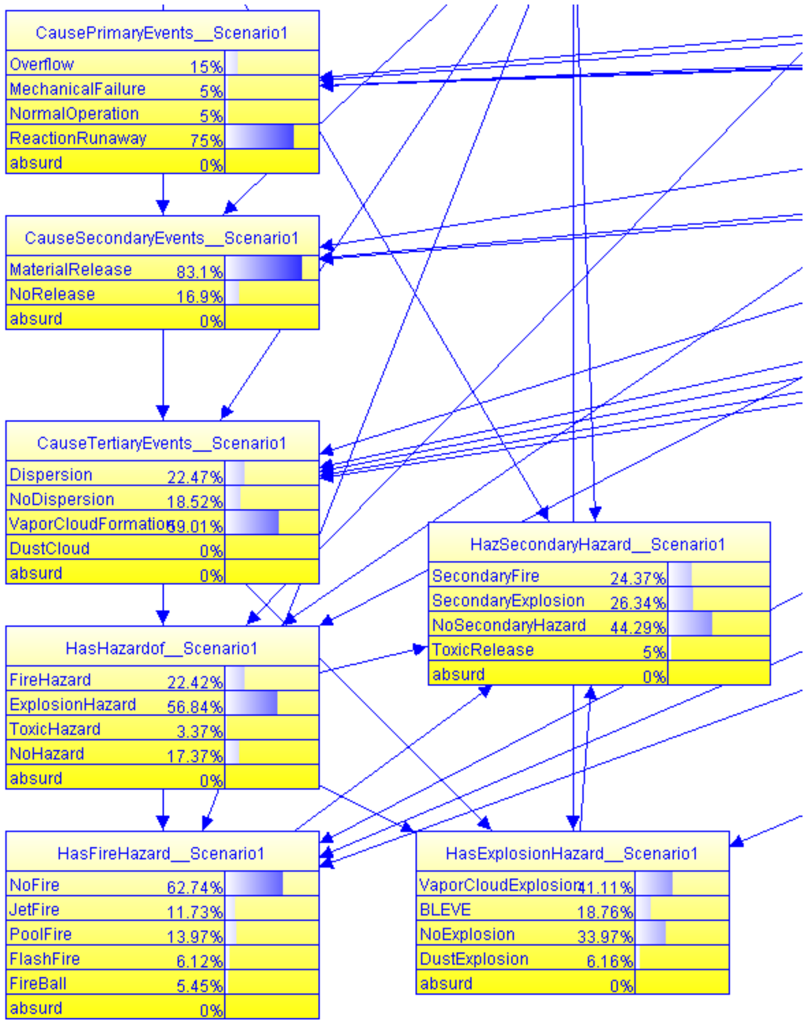


Figure B.28: Results of T2 Laboratories Explosions.

B.29 Imperial Sugar Refinery Dust explosion, Georgia 2008

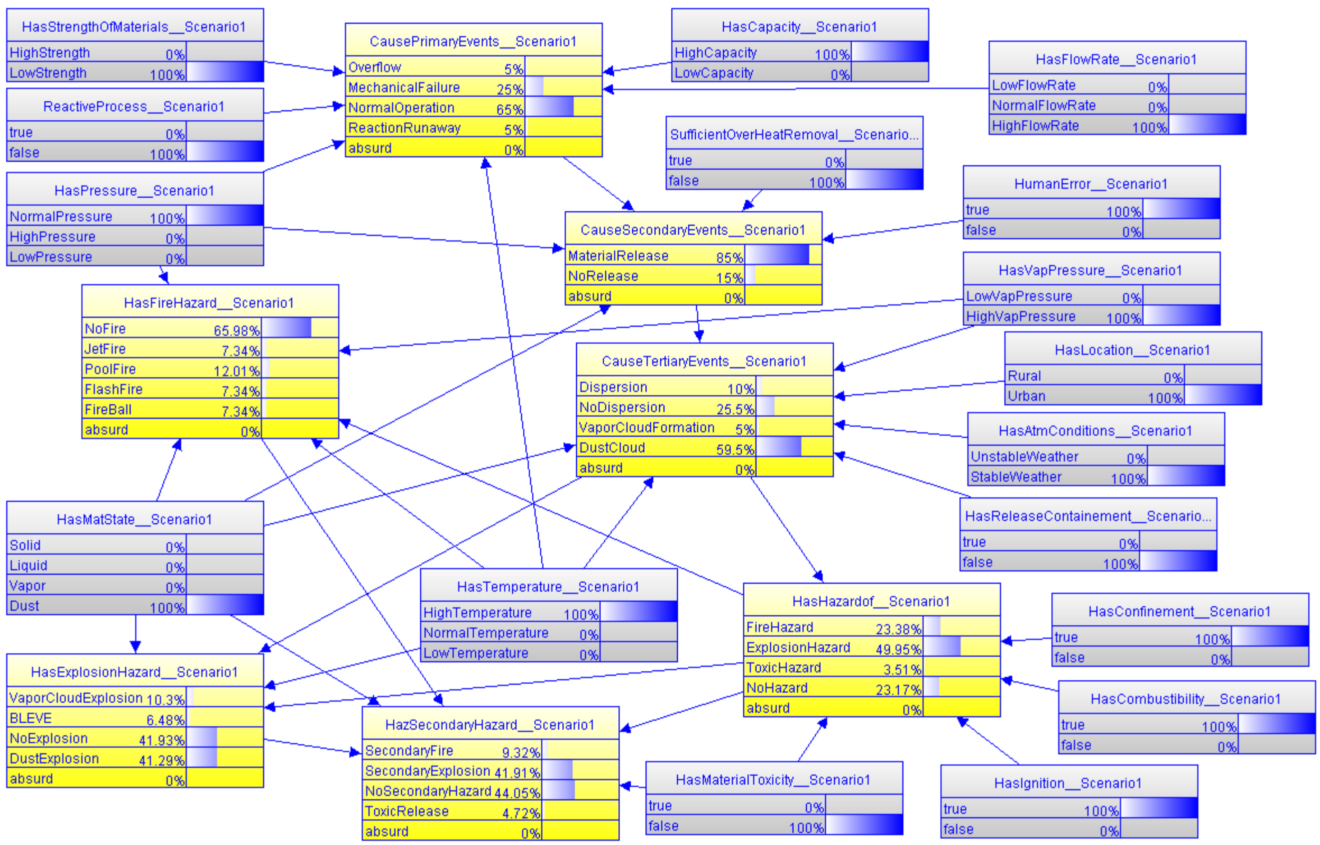


Figure B.29: Results for Imperial Sugar Refinery Dust explosion.

B.30 AL Solutions Metal Recycling, West Virginia 2007

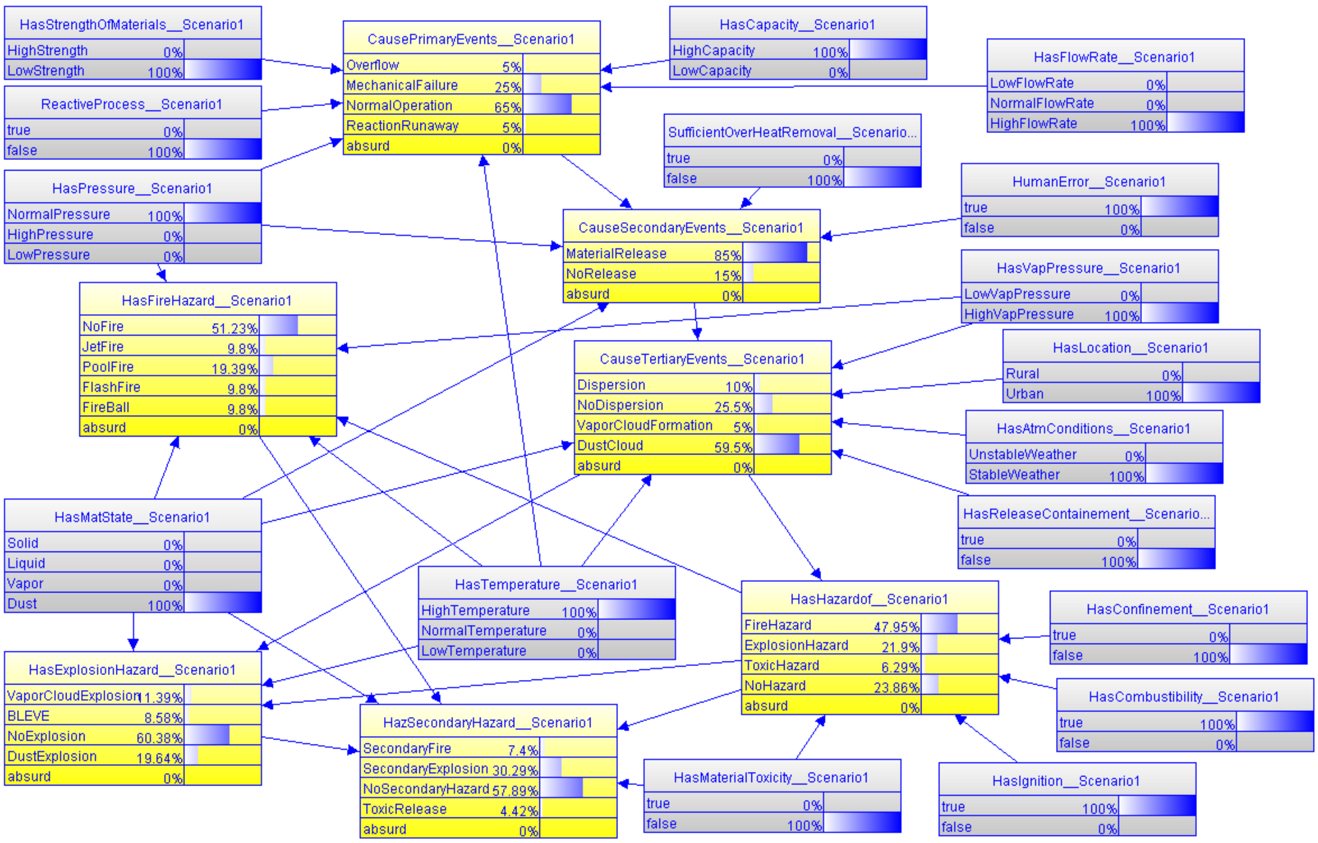


Figure B.30: Results for AL Solutions Metal Recycling accident (1).

B.31 Hoeganaes facility Flash Fires, Tennessee 2011

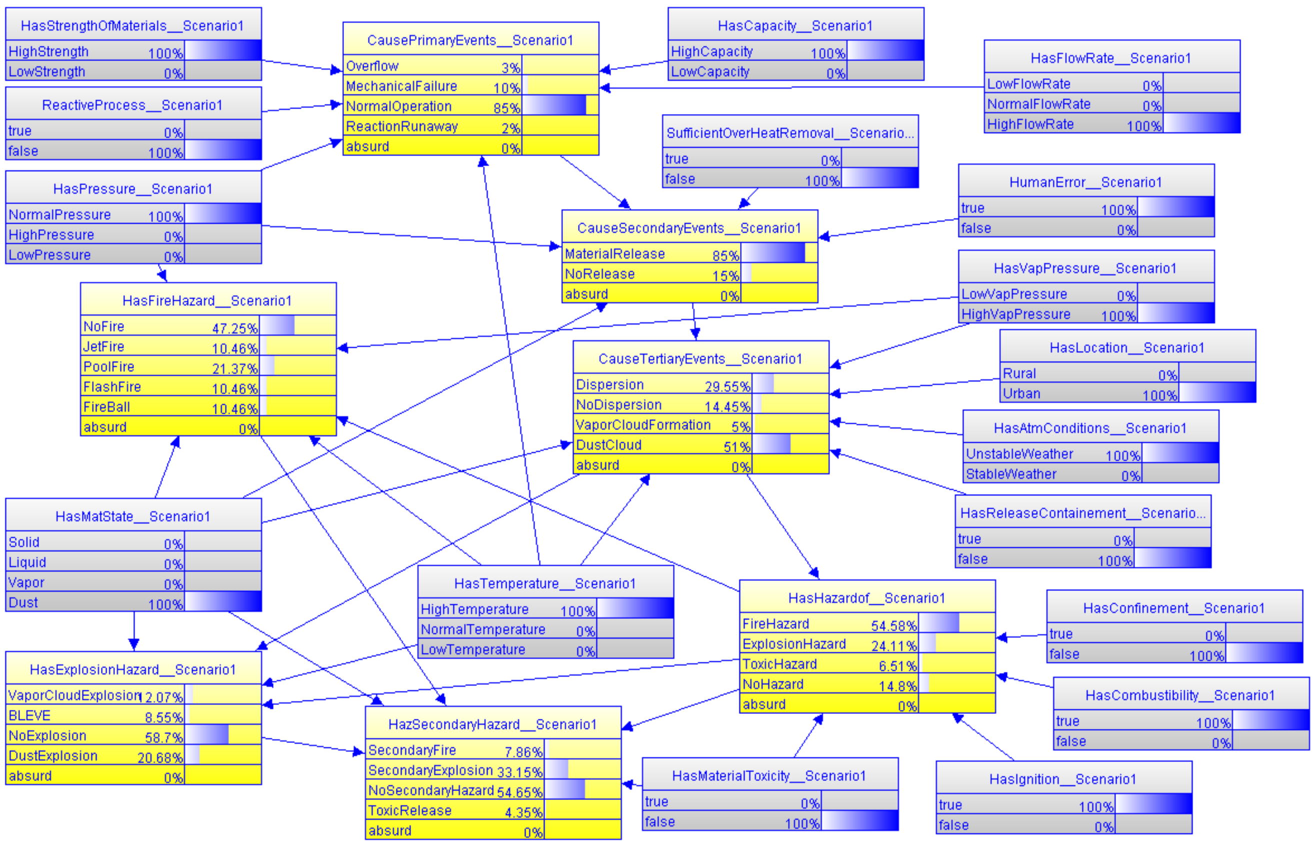


Figure B.31: Results for Hoeganaes facility Flash Fires.

B.32 West Pharmaceutical Explosion, North Carolina 2003

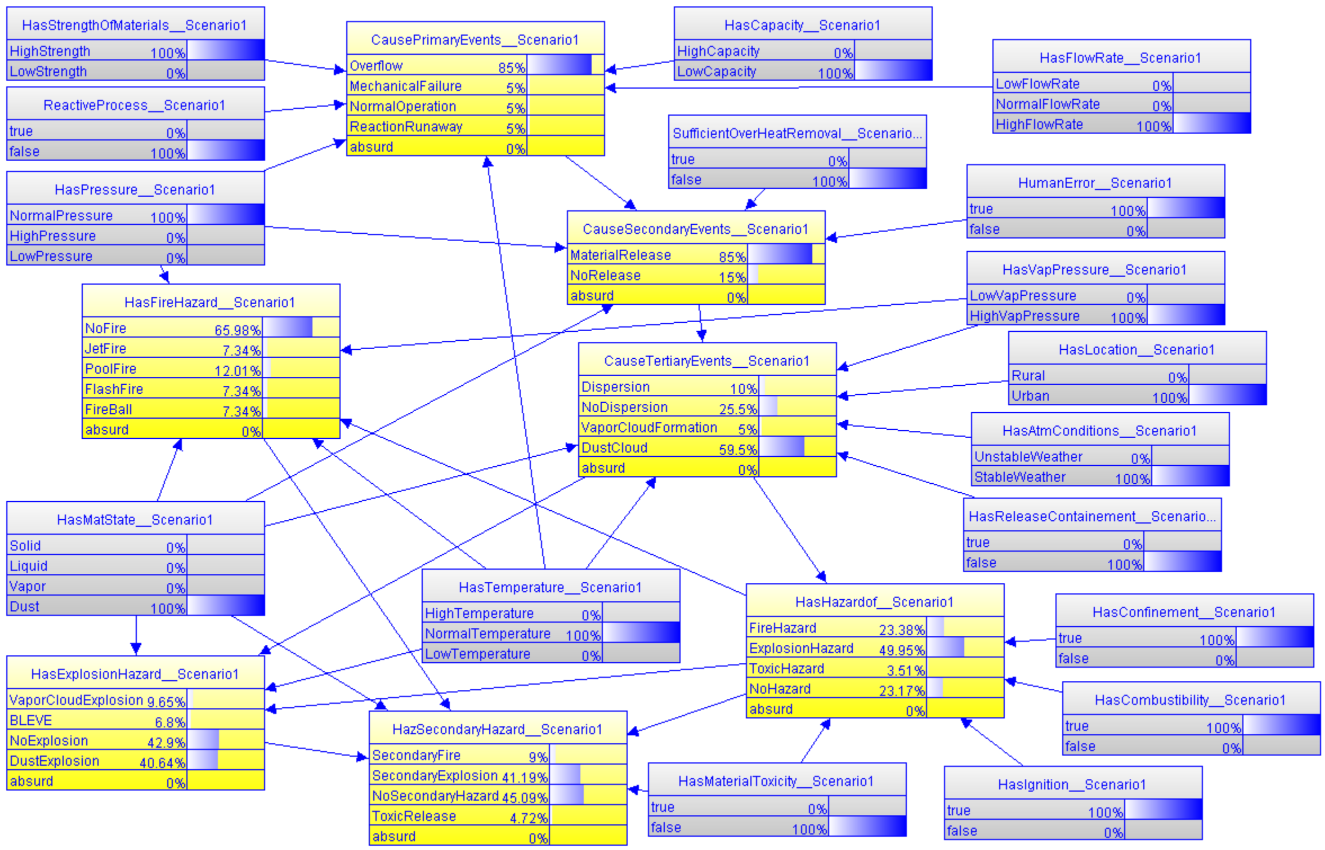


Figure B.32: Results for West Pharmaceutical Explosion.

B.33 Hayes Lemars Plant, Indiana 2003

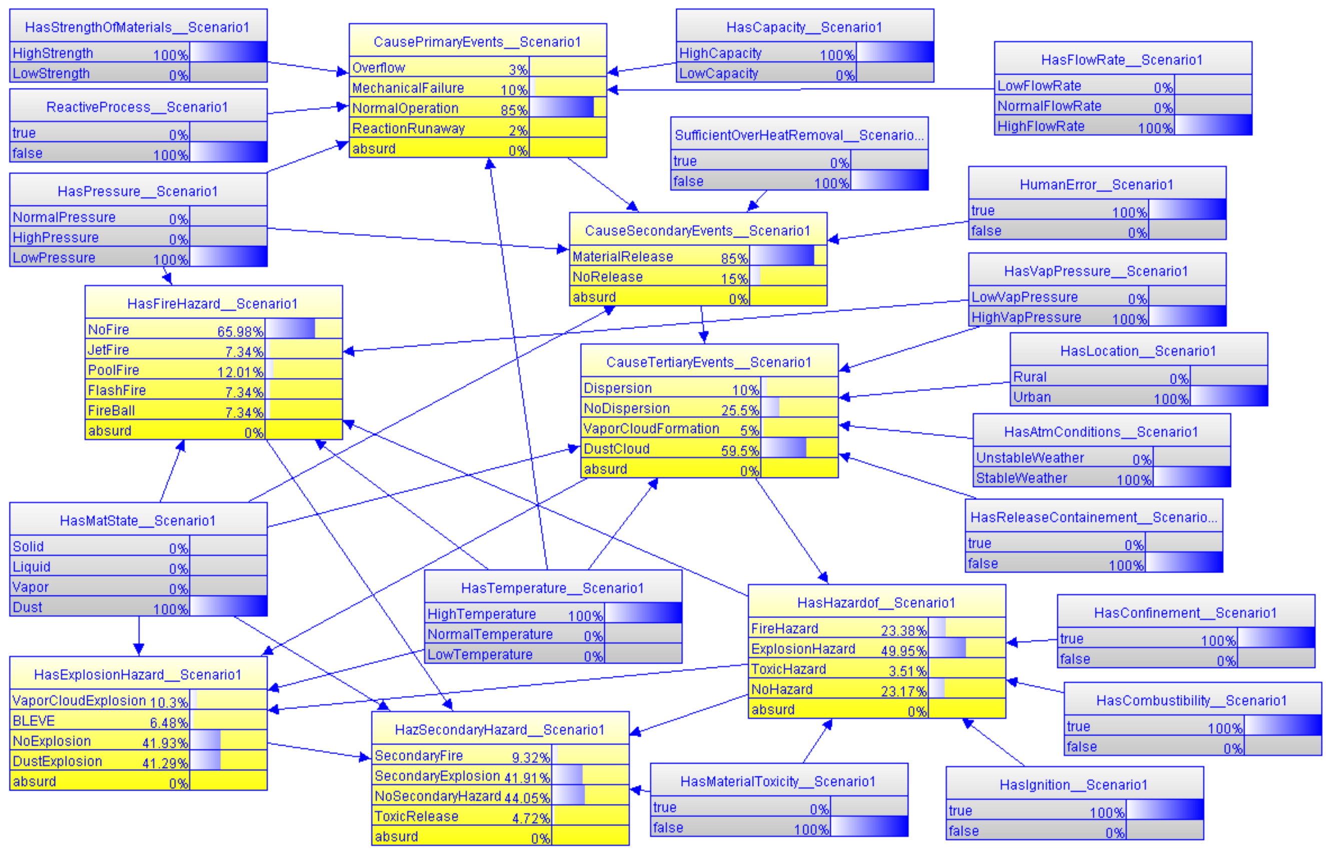


Figure B.33: Results for Hayes Lemars Plant Dust Explosion accident.

B.34 CTA Acoustics, Kentucky, 2003

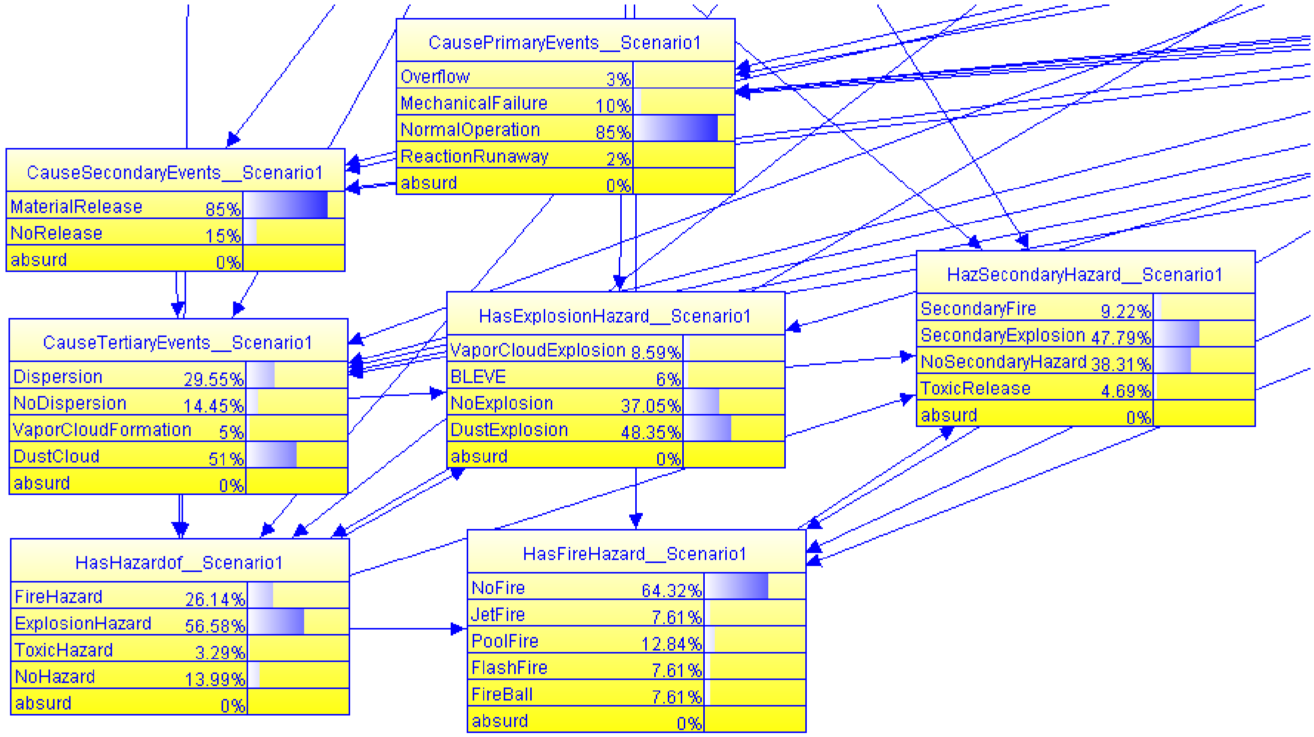


Figure B.34: Results for ConAgra Natural Gas Explosion accident (1).

B.35 DPC Enterprises Chlorine Release, Missouri 2002

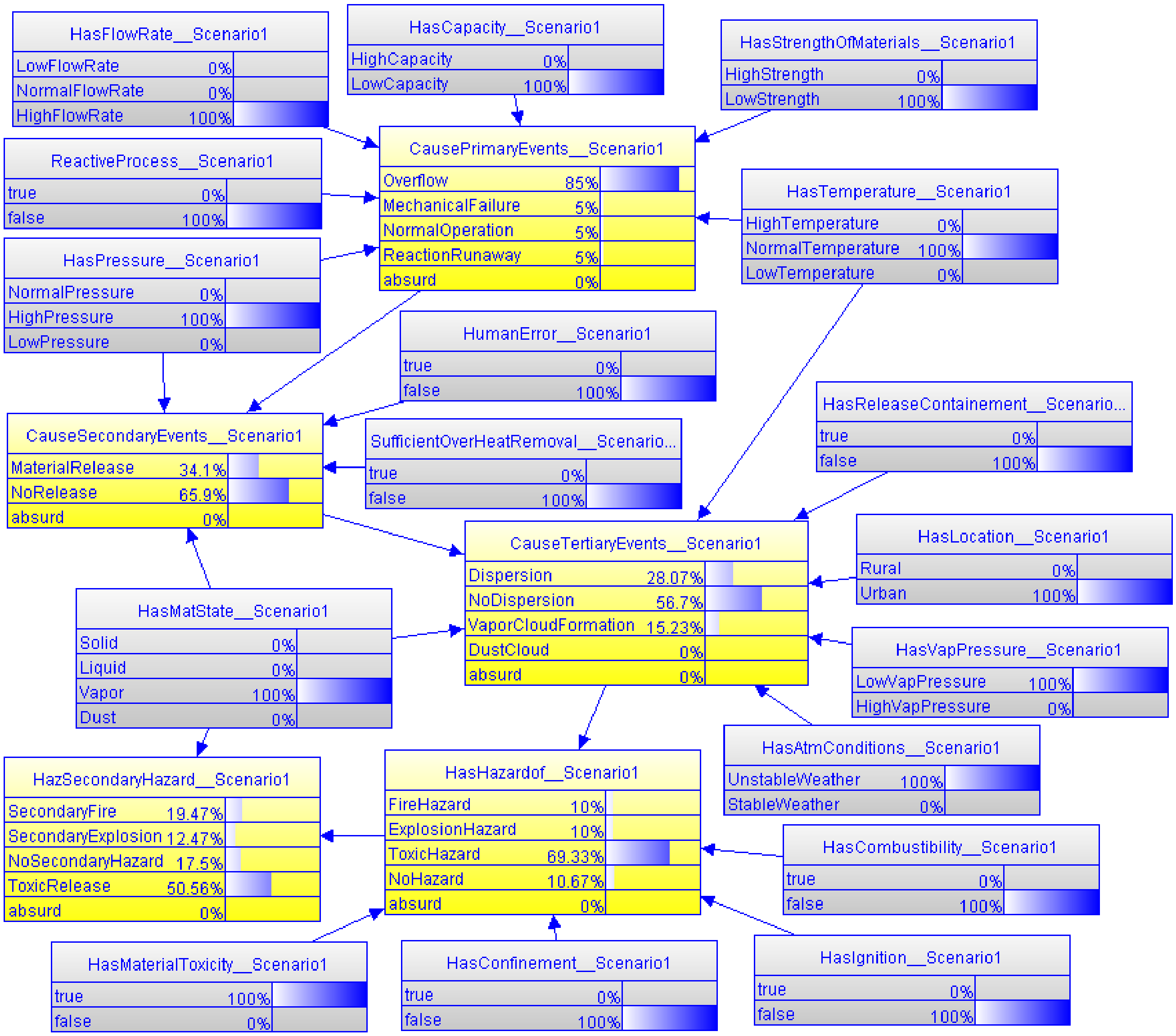


Figure B.35: Results for DPC Enterprises Chlorine Release accident.

B.36 DuPont facility Toxic Exposure, West Virginia 2008

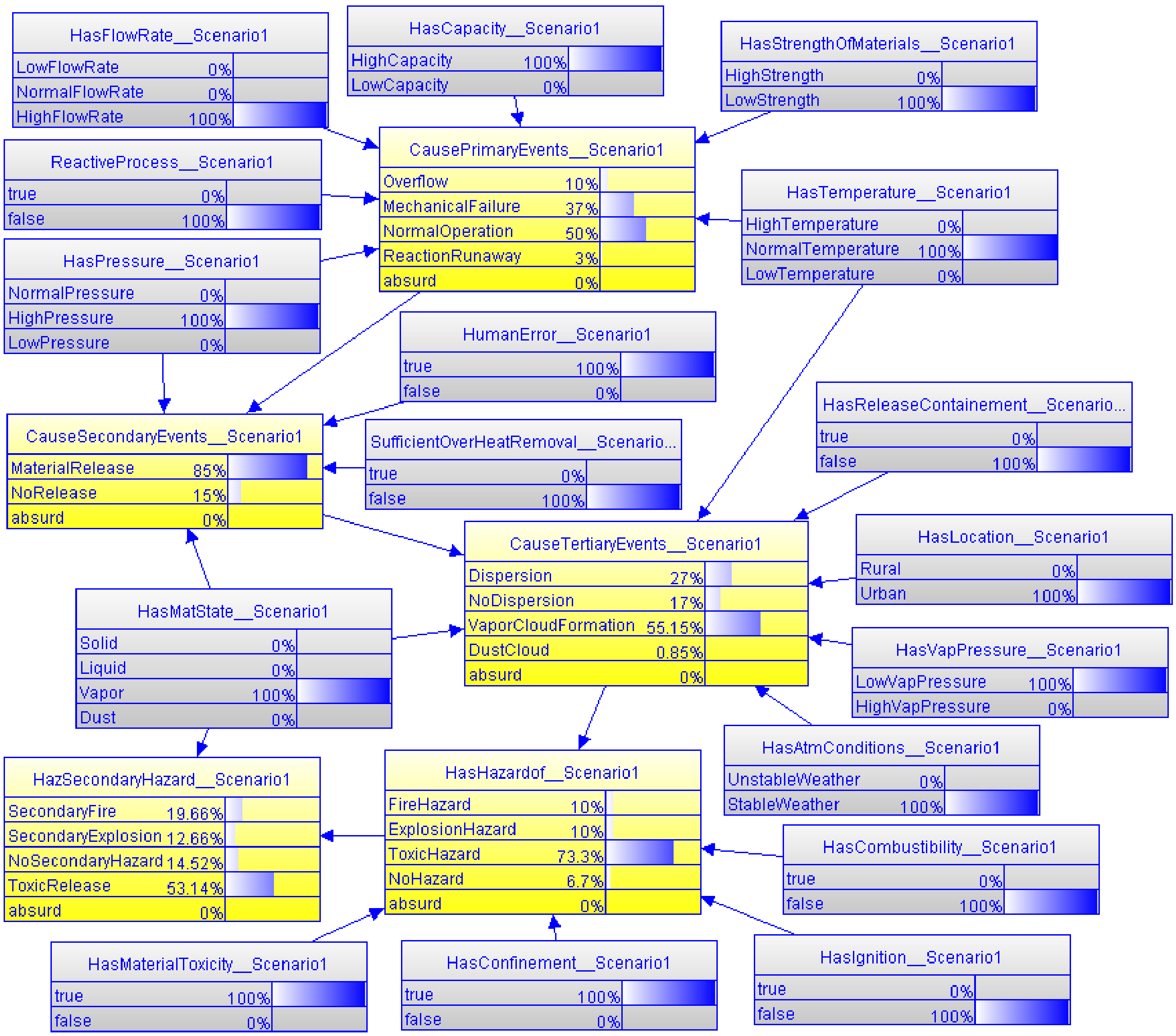


Figure B.36: Results for DuPont facility Toxic Exposure.

B.37 Bayer Crop Science, West Virginia

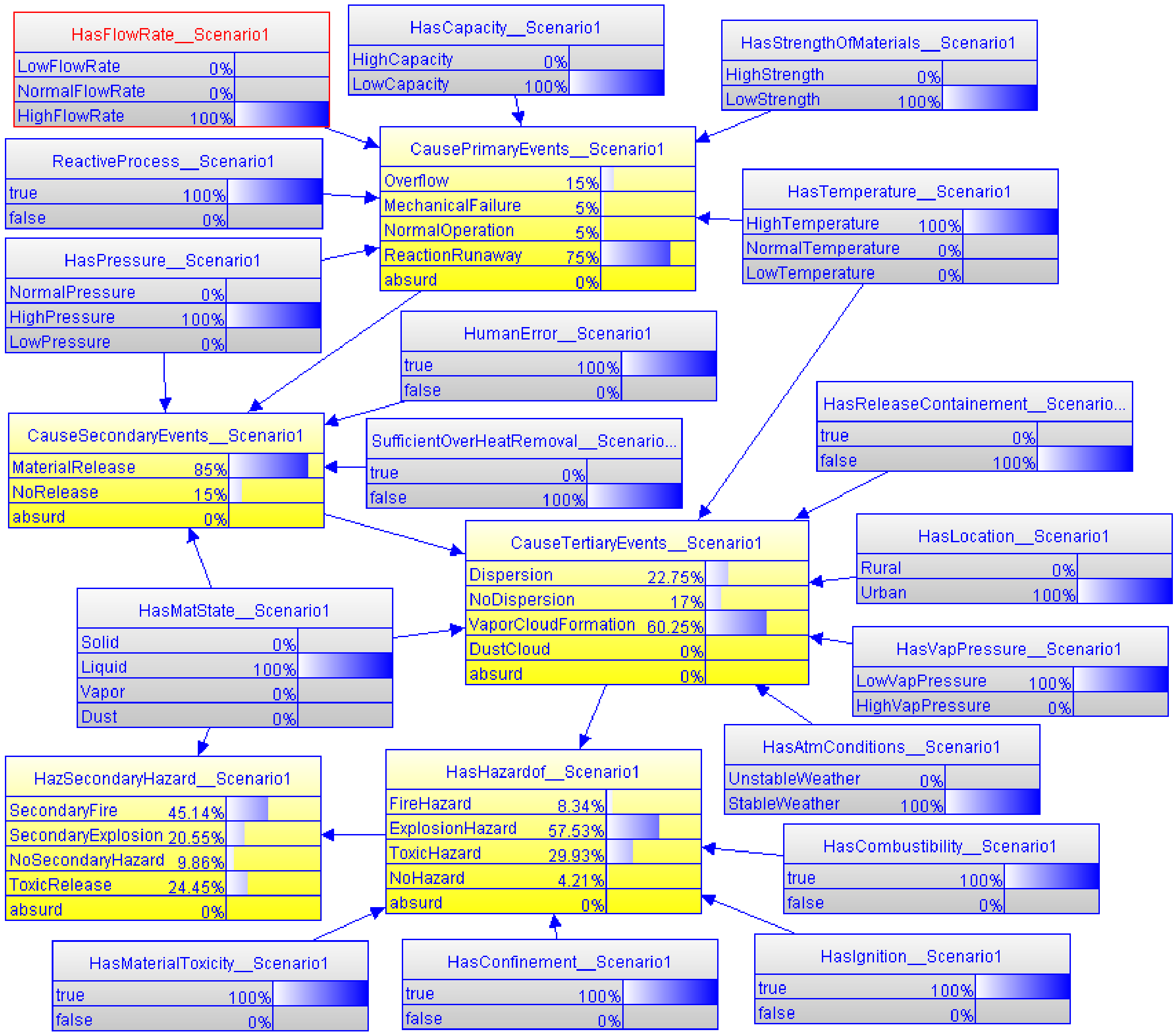


Figure B.37: Results forBayer Crop Science Toxic accident (1).

B.38 MFG Chemical Inc. Toxic Gas Release, Dalton, Georgia, 2001

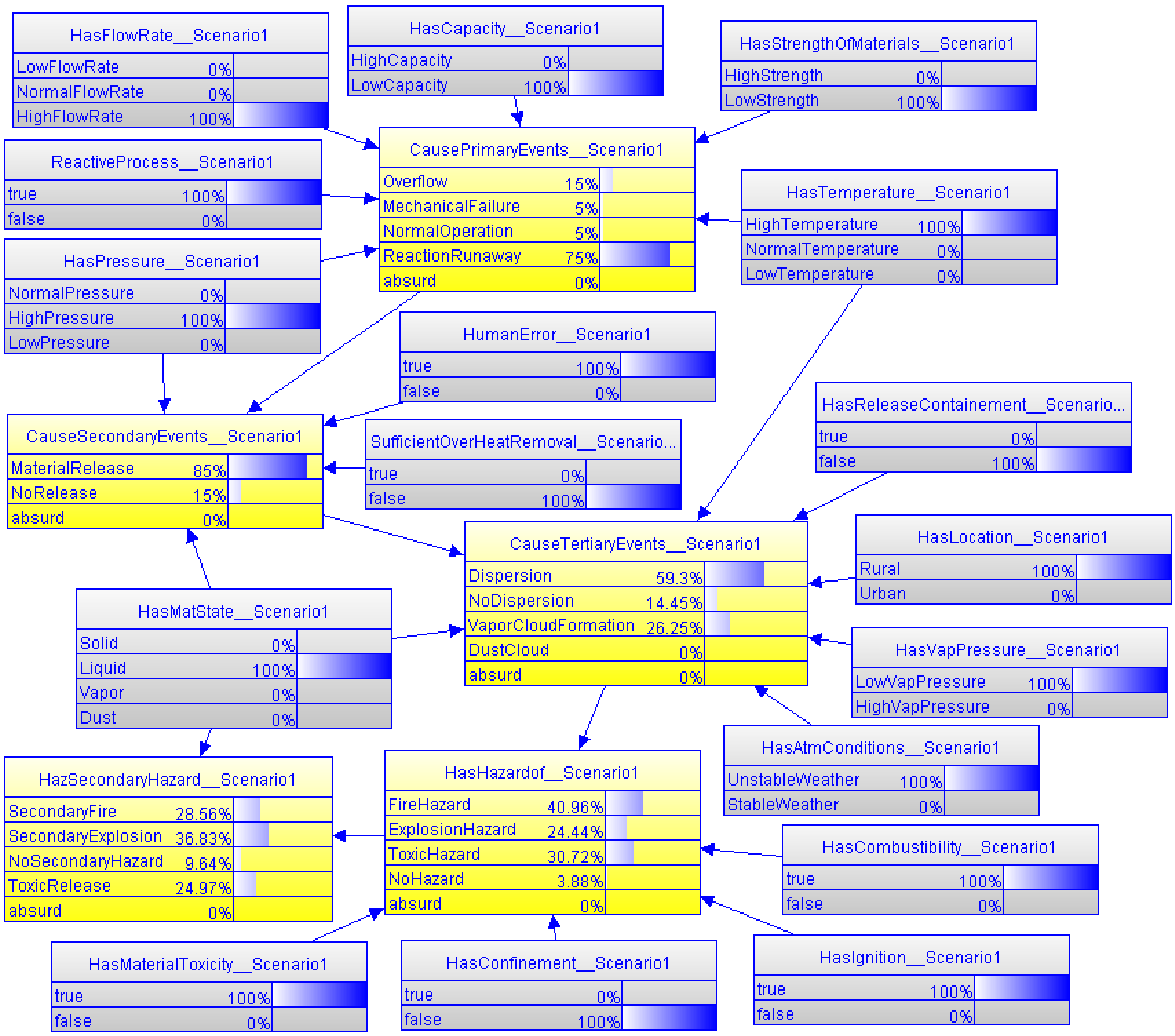


Figure B.38: Results of MFG Chemical Inc. Toxic Gas Release.

B.39 Millard Refrigerated Services Ammonia Release, AL, 2010

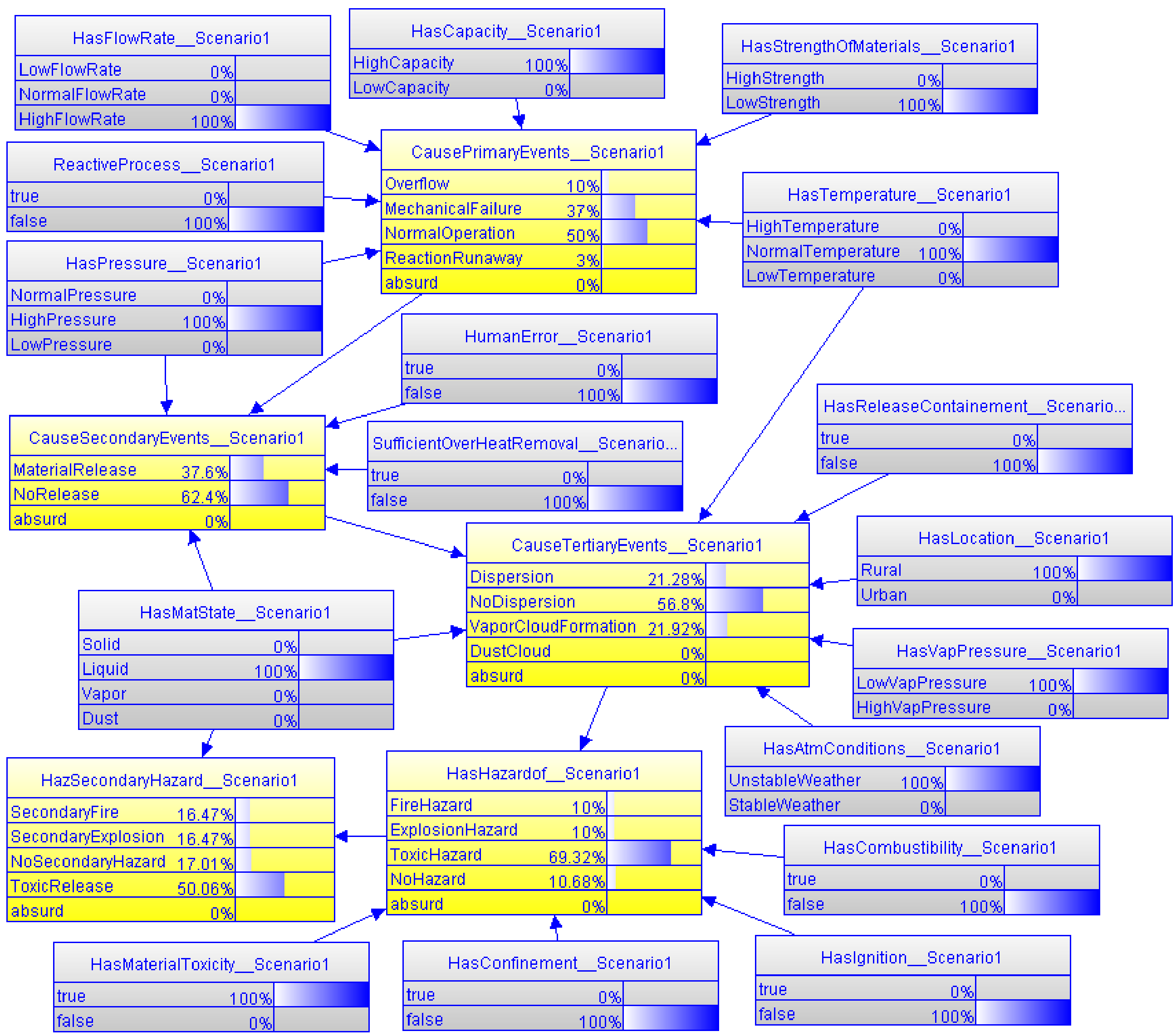


Figure B.39: Results for Millard Refrigerated Services Ammonia Release Accident.

B.40 Freedom Industries Chemical Release, WV, 2014

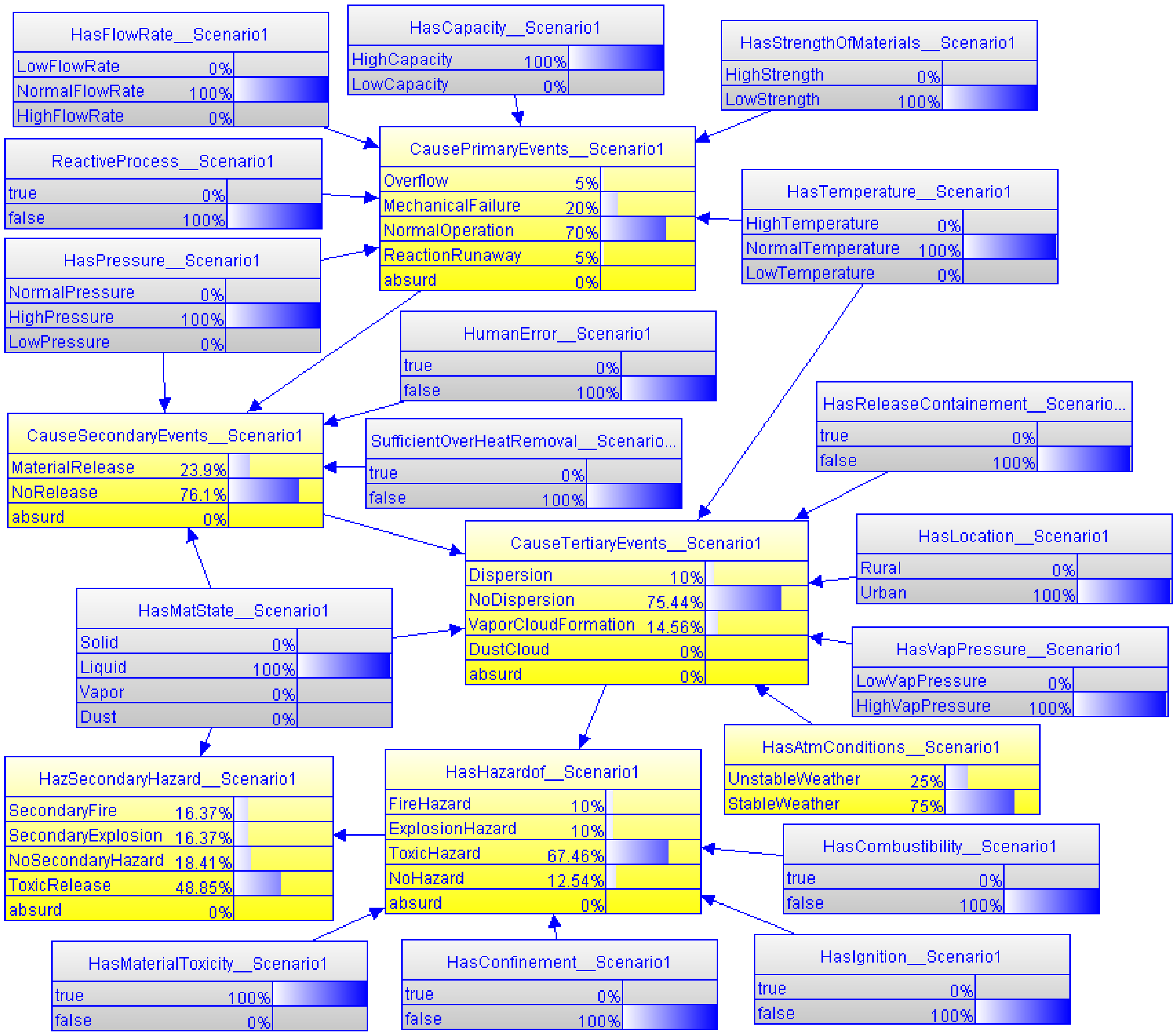


Figure B.40: Results forFreedom Industries Chemical Release accident (1).

B.41 Honeywell Plant Chlorione Release, LA, 2003

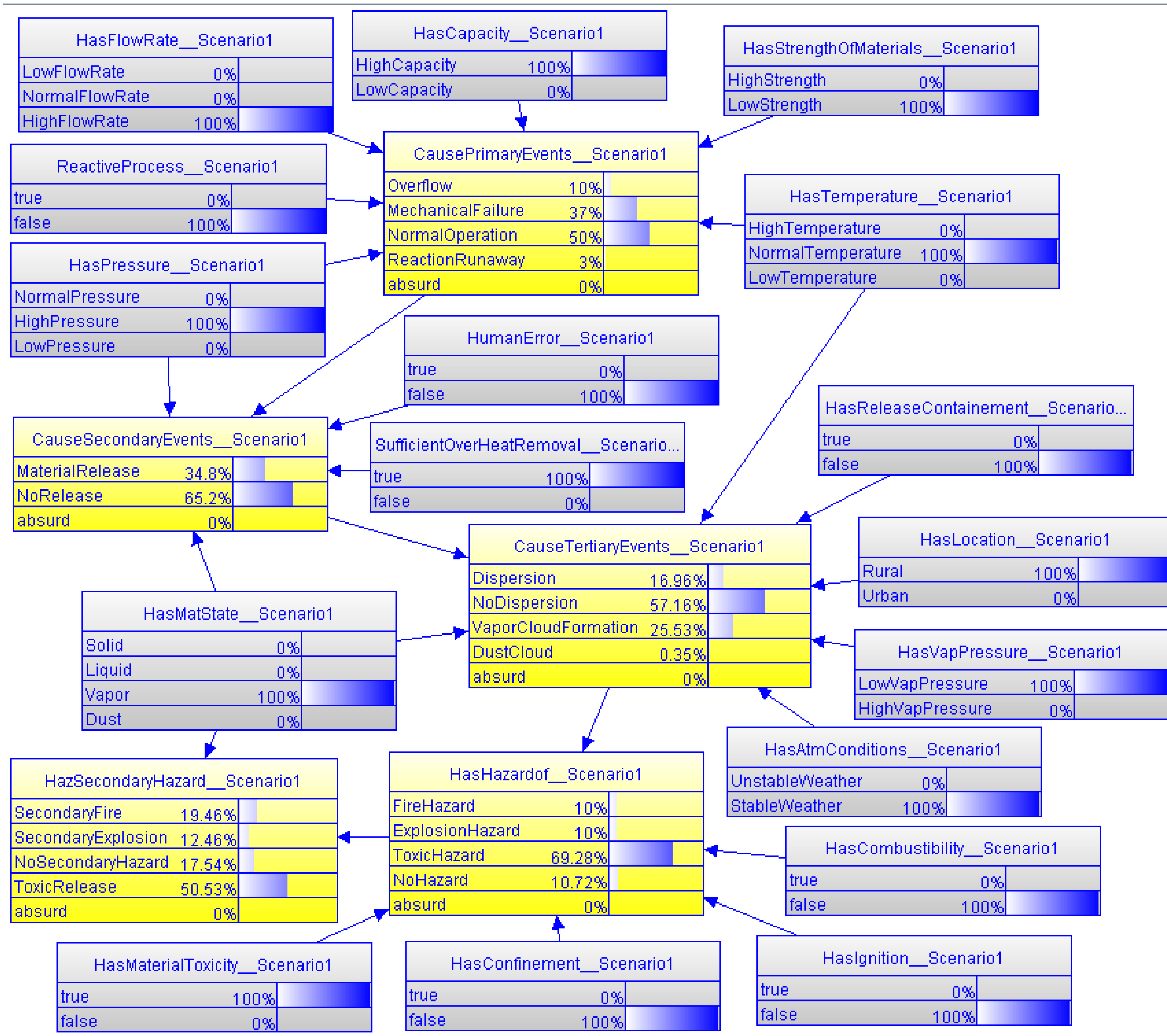


Figure B.41: Results forHoneywell Plant Chlorione Release accident (1).