Design of an Expert System for Emergency Response to a Chemical Spill. 1. Domain Definition and Knowledge Acquisition[†]

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This paper describes the knowledge acquisition stage in the development of an expert system designed to assist in planning the most appropriate response to chemical spills. A knowledge orientation analysis has been applied to the problem domain and a conceptual decision-making hierarchy has been constructed. Five primitive phases of action have been identified from this conceptual model, and these phases are followed in the subsequent development of the prototype. The knowledge base that was developed in this work consists of a database of factual information and a rulebase of heuristic knowledge. Using a subject-oriented structure, the database of information can effectively handle the large amount of literature information necessary to be considered in planning the response to a spill. The heuristic knowledge is represented as a set of production rules that help in the interpretation of the factual information. The knowledge acquisition process is referred to as a bottleneck in the development of expert system applications. For this prototype the knowledge acquisition step is carried out using an innovative knowledge encoding scheme, known as the knowledge domain matrix (KDM). A fully functional knowledge base has been developed.

1. INTRODUCTION

The development of DENDRAL 30 years ago, a system that assists in the interpretation of mass spectra data, is considered a landmark in the history of expert system applications.[1,2] Since that time expert system technology has been increasingly incorporated into many different applications and is now an accepted vehicle for providing expertise on a range of domain problems. In the field of chemistry most of the current expert system applications deal with data interpretation, structure elucidation, synthesis planning, or instrument diagnosis, all areas in which the target problems are highly domain-specific.[3−8] Nevertheless, there are situations, particularly those involving environmental chemistry, that are much less domain-specific and solving them requires multidisciplinary knowledge.

Expert systems are generally considered to be a branch of artificial intelligence (AI). An expert system is a computer program designed to emulate human experts.[9] By integrating the knowledge of the domain expert about a rather narrow field of study into a computer program, expert systems can be designed to provide specific advice based on incomplete and uncertain information.[10−12] In the environmental area, expert systems did not appear until the mid 1980s. The slow emergence of environmentally related expert systems is primarily due to the lack of a well-established scientific foundation for environmental science. Because few environmental problems can be solved using expertise from a single knowledge domain, knowledge acquisition and subsequent coding also greatly inhibited development. Thus the difficulties in trying to incorporate the domain knowledge into an expert system to deal with environmental problems are much more significant.[13] In 1987, Hushon identified 21 environmental expert systems.[14] This number has doubled in the last two years.[15] Examples of these systems include, the Soil Treatment Evaluation Program (STEP), which was developed through the use of object-oriented programming techniques.[9] STEP provides a utility that facilitates the selection of preliminary screening technologies applicable in the treatment of hazardous-waste-contaminated soils. Hanratty and Joseph have reported a comprehensive research effort to capture the knowledge used in the selection of laboratory reactors.[16] The computer-aided response technologies selector (CARTS) is an expert system designed to assist in designing the treatment train, identifying data requirements, and allowing users to evaluate different scenarios.[17] The remedial action assessment system, a computer methodology developed by Buelt *et al.*, aims at estimating remedial alternatives in terms of effectiveness, applicability, and cost.[18]

Defining the most effective methodology for the development of expert system applications in a multidisciplinary domain is challenging. In this paper, we focus on the full description of the domain, on the classification and tabulation of the decision making hierarchy, and finally on the implementation of a knowledge representation scheme that can be used to overcome difficulties previously found in the knowledge acquisition process. We document our progress made in the development of a knowledge acquisition method and the application of the scheme to the development of a modular expert system. ERexpert is a program that is designed to offer advice following an accidental chemical spill. The prototype has been constructed using a minimal set of toxic chemicals to provide proof of concept. Results from the implementation of a more extensive database and testing of this prototype in the real situations will be reported in the future. The development of ERexpert implements the following components: (i) a knowledge encoding scheme that allows a more efficient transfer of heuristic knowledge to production rules for use by an expert system and (ii) a

[†] Keyword: knowledge acquisition, chemical spill, environmental emergency, knowledge base, production rules, inference engine, knowledge domain matrix, ERexpert.

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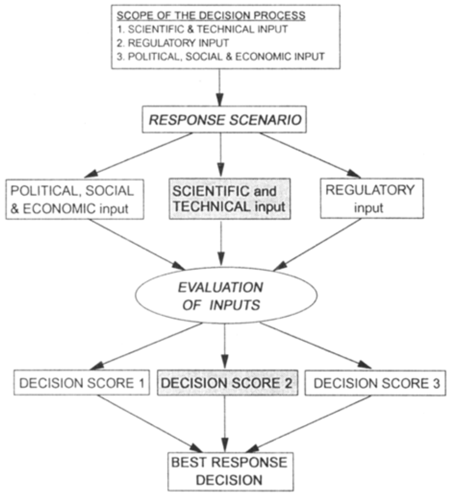

Figure 1. A description of the different aspects involved in the cleanup processes for a chemical spill accident. There are three major factors that need to be considered: (i) scientific and technological responses, (ii) regulatory constraints, and (iii) political, economic, and social demands.

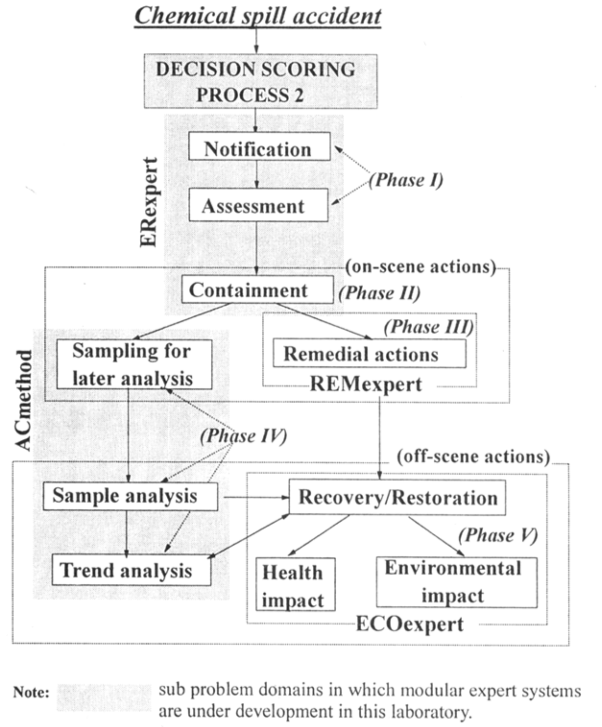

Figure 2. The decision-making hierarchy applied in response to a chemical spill accident from the scientific and technological aspect, in which five phases of response actions can be outlined.

database structure that provides an effective archival method for organization of the elaborate factual information necessary in solving problems in this domain.

2. DOMAIN PROBLEM DESCRIPTION

2.1. Chemical Spills. Hazardous materials, i.e., chemicals that are toxic, corrosive, flammable, or explosive, are a ubiquitous aspect of modern life.[19] In today's industrialized world, tens of thousands of different chemicals are produced each year. Many of these substances are not unusual materials utilized by only a few special industries, rather they are raw materials used by many manufactures in their every day production activities. These materials are manufactured and stored often in ton quantities by the producers; transported by truck, airplane, train, ship, barge, or pipeline; stored by the purchasers; and used in many manufacturing processes. At any point along this chain, a mishap may occur resulting in a hazardous materials incident. While prevention should remain as the main defense against environmental disasters, spills will inevitably occur. Accordingly, contingency plans have been and must continue to be developed for use in response to such accidents. Computer technology, especially knowledge-based expert systems, will play an increasingly important role in the environmental problem-solving process.

2.2. Definition of the Response Paradigm. Decisions are commonly made based on a set of criteria established according to a priority list. This forces the expert to focus on smaller but more tractable problem subdomains, because these subdomains are less complicated and better defined. Figure 1 presents the general aspects involved in the response to a chemical spill incident. There are three major factors to be considered in evaluating a possible protocol to be used in response to a chemical spill: (i) the scientific and technological responses, (ii) the regulatory constraints, and (iii) the political, economic, and social demands. This description is consistent with the comments made by Breshears *et al.*[20] and Levin.[21] It is obvious that a reasonable response protocol can only be constructed by considering a combination of all of these factors. In order to reduce the complexity involved, the development of the prototype expert system described in this paper has focused on the knowledge subdomains of the scientific and the technological aspects that covers response to a spill. However, despite these imposed limitations the knowledge base of the system must still incorporate expertise from a number of scientific disciplines.

2.3. The Conceptual Decision-Making Hierarchy. Establishing a conceptual decision-making hierarchy (the order of actions) that represents the problem-solving process for the target is an important step before knowledge acquisition can begin. The decision-making hierarchy outlines the logic flow and depicts possible aspects that must be considered in solving a particular domain problem. This process is described as the "knowledge orientation" step.[22] The purpose of this step is not to acquire the actual knowledge but rather to elicit the knowledge structure necessary to develop a conceptual model that the knowledge engineer can follow in the subsequent design of an application. Figure 2 shows a decision hierarchy that can be followed in response to chemical spills. This decision hierarchy consists of five relatively independent components arranged according to the order of actions taken. It is important to keep the hierarchy as simple as possible while maintaining a desired level of coverage for the problem domain. Shank and co-workers suggest that a small set of primitive actions will account for most of what must be represented in the physical world.[23] Similarly, Zhou *et al.* grouped the activities in a standard analytical laboratory into families of primitive actions and subsequently developed a robotic system to perform these operations.[24]

As shown in Figure 2, *notification and assessment* is the first step taken in response to a chemical spill. A rapid and correct assessment of the extent and the potential damage of a spill is essential information that is critical in the following phases. In some cases the response in this step might be decisive for the success of subsequent actions. *Containment* is the next and may be the most critical step in the response to a chemical spill. The aim of this step is to limit the extent of the spillage to the smallest possible area through deployment of properly chosen containment techniques. In both these phases, time is of particular importance, any delays in assessing a situation or implementing correct countermeasures may turn an accident into a disaster. *Remedial action*, the third step, includes physical removal and chemical treatment of the contaminants from the environment and the safe disposal or treatment of all collected hazardous materials. While cleanup of a contaminated environment is the real essence of the remedial action, in an emergency response to a chemical spill, it is of secondary importance because only after achieving success in the first two phases, can the remedial actions effectively minimize the environmental damage. The *sampling and trend analysis* phase is used to evaluate the success of the deployment of the previous actions. The data acquired in this phase can be used to direct subsequent actions and to document the incident for reference in the event of similar cases. *Recovery and restoration* is the final phase of the response, and during it actions are undertaken to restore the environment to its prespill conditions.

3. COMPUTING ENVIRONMENT

The computer work was carried out on an Intel 80386-based computer, AST PREMIUM/386Cwith 8 megabytes of RAM, two 150-megabyte hard disks, a 1.44-megabyte floppy disk, and SVGA graphic monitor. The prototype expert system developed in this study is designed for use in the Microsoft Windows 3.x environment. The software packages used in the development of the knowledge system are all MS Windows based applications, including Microsoft ACCESS (version 1.0), an interactive relational database system; Microsoft Visual Basic (version 3.0), the programming language; and EAshell, an expert system shell under development in our laboratory, that served as the inference engine.[25]

4. RESULTS AND DISCUSSION

The stages involved in construction of an expert system have been defined as system design and development, performance evaluation and acceptance, and system maintenance and release.[26] The results presented in this paper have focused on the knowledge acquisition phase, the process of transforming expertise into a formalism that can be used by the inference engine. The actual development of a prototype expert system using the resulting knowledge base will be presented in the companion paper. The knowledge acquisition step described here is key to system design and development. Our laboratory has developed a number of expert systems for application in analytical chemistry.[27−34,43−45] We have been successful in developing modular systems to address consultation and controlling tasks in analytical procedures. Modules that perform analytical method selection for instrumental analysis have been developed.[28e,45] Several diagnostic expert systems have been completed that help in the diagnosis of possible causes of malfunction for different analytical instruments (AA, GC, and GCMS).[32,34,43] AAcontrol is a prototype concerned with the automation of the flame AAS analysis process.[44]

We have found that knowledge acquisition is most effective when it is focused on particular cases rather than on the entire target domain. Such cases involve relatively narrow, more specific, and, therefore, less complex problem

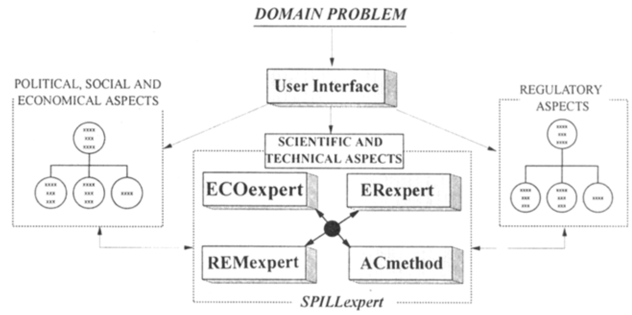

Figure 3. General structure of the SPILLexpert prototype. This is a three-frame network in which a number of subsystems are attached to each of the frame. Development has focused on the ERexpert and ACmethod modular expert systems and the user interface (shaded areas) that are part of the SPILLexpert project.

subdomains. In this project, we again experimented with this approach but now applied to a much broader and complex target domain. The subdomains involved in response to a chemical spill have been described earlier (Figure 2). Consequently the global expert system structure that is designed must encompass three frames. Each of the frames in Figure 3 comprises several members that are themselves stand-alone expert systems that perform independent tasks that are connected with the main goals of the program.

As depicted in Figure 3, SPILLexpert is the substructure corresponding to the scientific and technological subdomain that encompasses (i) ERexpert, (ii) ACmethod, (iii) REMexpert, and (iv) ECOexpert. ERexpert is a modular expert system developed to plan the emergency response following spills. The program design emphasizes the containment of the spill and deployment of remedial techniques during the primary phase of the cleanup. ACmethod is used to select appropriate sampling and analytical methods based on the matrix, sample types, and sampling conditions. In conjunction with ERexpert, REMexpert provides remedial action instructions for the next phase of the cleanup once the situation is under control and the incident has been contained. ECOexpert is a module that provides advice on actions related to restoring a ecologically balanced environment after a chemical spill. Within the SPILLexpert system, the operating sequence of these modular expert systems can be altered based upon the priority of the target problem. Each module can be operated independently. We plan to build this global expert system for chemical spill accidents incrementally by assembling a number of modular expert systems into a defined structure (a bottom-up approach).

4.1. Knowledge Base Development in ERexpert. Knowledge in most areas of specialization can be classified into two categories: factual knowledge that may be obtained from published sources and heuristic knowledge that is used by human experts in manipulating and interpreting factual knowledge.[35] Factual knowledge, such as is held in theories and in mathematical algorithms, is usually carefully defined, clearly expressed, and well documented. One can acquire this type of knowledge through learning processes. However, when faced with a real-world problem, it is common to find that the problem cannot be solved solely using factual knowledge, therefore experience or heuristic knowledge enters the problem-solving arena. Unlike factual knowledge, heuristic knowledge often does not have clear-cut values and is hard to express or document precisely. One can only acquaint oneself with heuristics through practice, a process of applying the acquired factual knowledge. Expertise as practiced by an expert is a combination of both these knowledge categories.

An expert system requires more than factual knowledge before it can be applied to solve domain problems involving uncertainty. We have found in this work that the factual information held in the knowledge base is essential to provide operational details and complete the knowledge representation for the problem domain, however, it is the heuristic knowledge in the knowledge base that extends the flexibility and applicability of a knowledge based system. Penninckx *et al.* have argued that a database of information is an extension of a knowledge system because it guarantees the completeness of the information represented.[36] As the information source of an expert system, the knowledge base containing both heuristic and factual knowledge has to be compiled into a format that will allow the inference engine to match actual conditions with the coded knowledge in order to identify a conclusion. The knowledge base used by the ERexpert prototype encompasses two components: (i) a Factbase, which is a database of factual knowledge relevant to the problem domain and (ii) a Rulebase, which uses the rule format to represent the heuristic knowledge. The inference engine used in this work manipulates the heuristic knowledge represented in rules from the Rulebase to interpret associated factual knowledge in the Factbase. The factual knowledge was obtained from published materials, and the domain expertise was extracted through interviews and discussion with field experts.

4.2. Factbase Structure and Development. Certain types of information involved in the spill response belong to the factual knowledge category. For example, the phone numbers and addresses of local environmental agencies and industrial organizations, the assessment techniques, physiochemical properties, containment equipment, etc., will not change with target chemical(s) or the geological location of an accident. Also, a collection of countermeasures used in previous spills is an important source of information for reference under the new circumstances of the current spill. Such information is referred to as static information and is organized into the Factbase to supplement facts necessary for planning response actions.

Structure. Microsoft ACCESS was chosen as the database system for construction of the Factbase. The Factbase of ERexpert consists of a number of tables, each containing a different subject relevant to the problem domain. Table 1 lists the contents of this Factbase. Three layers of fact tables exist in this database: the primary tables, the secondary tables, and the auxiliary tables.[37] Primary tables are a set of fundamental tables that determine the coverage of the current Factbase and provide records of previous cases and the general response techniques. Secondary tables consist of a property section and a containment technique section. The property section is designed to supplement each data entry in the primary level with a set of physicochemical properties as references for planning. The technical section consists of a group of tables that provide technical support for the remedial methods consistent with the target chemical(s) and the nature of the spill. The auxiliary tables provide the system user with general information and procedures necessary to handle a spill. The Microsoft ACCESS database system offers powerful query and macro functions that a system developer can use to pre-define the relationships between different tables.

Table 1. Contents of the ERexpert Factbase

Primary Tables
1. Compound List
2. Case History Database
3. Containment Techniques
Secondary Tables
Property Tables:
1. Toxicity and First Aid
2. Fire and Explosion Data
3. Chemical Property Data
4. Physical Property Data
Technique Tables for ERexpert:
1. Adsorption Techniques
2. Neutralization Techniques
3. Precipitation Techniques
4. Chelation Techniques
5. Solvent Extraction Techniques
6. Reduction/Oxidation Techniques
7. Bio-remediation Techniques
8. Incineration Technqiues
Auxiliary Tables
1. Phone Directory of Regional Response Centers
2. Shipping and Storage Requirements
3. Protective Equipment List
4. Disposal Requirements/Procedures

Figure 4 presents the structural details of the Factbase used by ERexpert. The diagram illustrates the contents of each table and how they are interrelated. In Figure 4, the "1" symbol indicates the "one" side of the relationship, and the "M" symbol indicates the "many" side of the relationship. The information stored in the fact tables is chained together through a group of identification numbers (ids). The comp ID is an id number used to connect information in the property tables and the technical tables with the primary tables. Containment and remedial techniques are organized into the technical database by order of the environmental behavior of each chemical. An index (category ID) is assigned to each behavioral group to provide connections with the primary tables. The method ID is reserved for use in the development of the ACmethod expert system module. This subject-oriented structure helps to reduce the complexity in the development of an information database designed to manage elaborate information, and it also provides the necessary flexibility in both the database development stage for knowledge input, and the post-development stage when the database needs to be upgraded. Furthermore, this subject-oriented structure is more efficient during execution since it requires less memory to load only the relevant part of the database.

Development. The inventory of chemicals changes continuously. To develop a database that can handle spills, it is neither expeditious nor practicable to attempt to develop a conventional database, one that could cover the entire chemical family, and to include every potential remediation method against each hazardous chemical. It also cannot be overemphasized that the appropriate response to a chemical spill varies from case to case, it should not be assumed that countermeasures adopted in previous cases can be used without modification under the new circumstances. A practical approach to address this conflict is to develop a categorization method that divides hazardous chemicals into different groups based on their environmental behavior so that chemicals in the same category can be assessed and similar countermeasures used. Such a categorization leads to a knowledge-based system that can be deployed to deal with the majority of hazardous chemicals.[40]

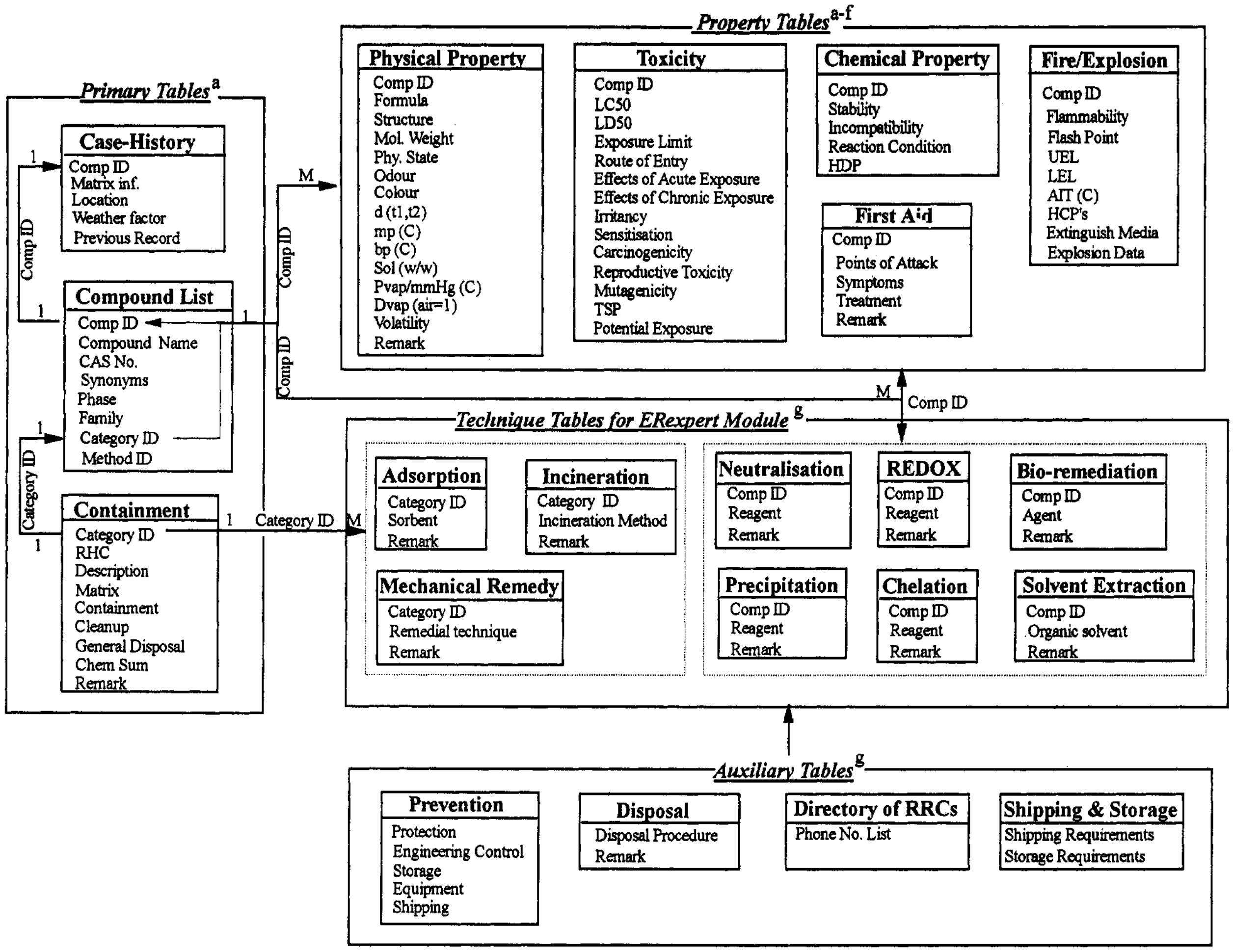

Figure 4. A diagram showing the structure of the Factbase of the ERexpert prototype. The "*1*" symbol indicates the "one" side of the relationship. The "*M*" symbol indicates the "many" side of the relationship. Accordingly, information of different sources (a−g) is arranged into this subject-oriented structure. Through embodied macro and query functions, the database is able to provide user specified information dynamically in various formats. (a) Lewis, R. J., Sr. Hazardous Chemicals Desk Reference, 2nd ed.; VNR: New York, 1991. (b) CRC Handbook of Chemistry and Physics, 75th ed.; Lide, D. R., Editor-in-Chief; CRC Press: Ann Arbor, MI, 1994/95. (c) Sittig, M. Handbook of Toxic and Hazardous Chemicals and Carcinogens, 3rd ed.; Noyes Publications: NJ, 1991; Vol. 1−2. (d) Kaye, S. Handbook of Emergency Toxicology. A Guide for the Identification, Diagnosis, and Treatment of Poisoning, 5th ed.; Charles Thomas Publisher: Springfield, IL, 1988. (e) The Merck Index. An Encyclopedia of Chemicals, Drugs, and Biologicals, 11th Ed.; Budavari, S., ed.; Merck & Co., Inc.: NJ, 1989. (f) Amdur, M. O.; Doull, J.; Klaassen, C. Casarett and Doull's Toxicology. The Basic Science of Poisons, 4th ed.; Pergamon Press: New York, 1991. (g) Hazardous Chemical Spill Cleanup, Pollution Technology Review No. 59; Robinson, J. S., Ed.; Noyes Data Corporation: NJ, 1979.

Table 2. Key Physico-Chemical Properties Used for Compound Categorization

criteria	principal behavioral group	subgroup/category ID
a. physical state	1. chemical that vaporizes (G1)	1A, 1B, 1C, 1D
b. density relative to air	2. chemical that floats (G2)	2A, 2B, 2C, 2D, 2E
c. density relative to water	3. chemical that sinks (G3)	3A, 3B
d. flammability	4. chemical that dissolves (G4)	4A, 4B, 4C, 4D, 4E, 4F
e. water solubility		
f. volatility		
g. acid/base (including those that react with water to give an acid or base)		
h. biodegradation		
i. salt containing heavy metal ion		

Table 2 lists a set of key physico-chemical properties that have been identified as criteria that can be used to categorize chemicals into different environmental behavioral groups. Using these criteria, chemicals were divided into four major categories and 17 subgroups. A training set containing 17 representative hazardous chemicals (RHCs) was identified so that each RHC represented a subgroup of compounds. Following the structure of the subject-oriented database, the Factbase was then developed. The "compound list" table of this Factbase contained the RHCs and the set of ids assigned to them. The physicochemical data for these RHCs were arranged into the property tables to construct the property section of the database. Table 3 summarizes the most commonly used containment and remedial techniques, and this information was mapped into the technical section of the Factbase.[40] Procedures for shipping, storage, disposal, protection, etc. were added to the supplementary tables to serve as the auxiliary section of the database. Queries and macros were developed to provide the necessary connections between individual tables. These functions were developed using the Microsoft ACCESS Basic language, a procedural program supplied with Microsoft ACCESS. The user

Table 3. Summary of Containment and Remedial Techniques and Specifications[a,b]

in air vapor		on land (liquid or solid)				in water (liquid or solid)					
		solid		liquid		sinking (insoluble)		floating (insoluble)		soluble and miscible	
technique	specification	technique	specification	technique	specification	technique	specificiation	technique	specificiation	technique	specificiation
dispersion, fans, blowers	very calm, sheltered areas	self-containing		dikes earthen and trench	flat or sloped surface	natural dikes & excavation	where a natural barrier exists	booms	not much current	sealed booms	limited area, contain depth
inert foam coverage	low-lying vapors and calm areas			foamed polyurethane	hard, dry surface	construction of under water dikes, excavations	if bottom can be moved	weirs	calm water surface	diversion of contaminated water	flowing water, clear area needed
cryogenic cooling	sheltered areas			foam concrete	flat ground, slow moving	curtain barriers	calm water low disperse	pneumatic barriers	shallow and calm water	diversion of contaminated water	flowing water, clear area needed
				excavation	soft ground					gelling agent	small volume
				soil surface sealing	soft gorund					water dispersion;	
mist knock down	water-soluble or low-lying vapors	shoveling and vacuuming	under normal weather conditions	correction of mechanic failure	close valve, shut down pump, pudding to pipe joint			skimmer	calm water surface	adsorption	most wide used method
air dilution using fans or blower	very calm & sheltered areas			pump or vacuum collection into auxiliary tank or sump		pump		vacuum collector	calm water surface	neutralization; ion exchange; precipitation; chelation; and redox	chemical specific methods
cryogenic condensation	very calm & sheltered areas			earth moving	removable land	dredging	bottom removable	burning	geographically right area	centrifuge separation, solvent extraction, gelation	small removable water volume
encapsulation	low-lying & limited spill size			burial	temporary mitigating measure with very limited application	burial	temporary mitigating measure with very limited application			biodegradation	less toxic chemicals

[a] Hazardous Chemical Spill Cleanup, Pollution Technology Review No. 59; Robinson, J. S., Ed.; Noyes Data Corporation: New Jersey, 1979. [b] Lewis, R. J., Sr. *Hazardous Chemicals Desk Reference*, 2nd Ed.; VNR: New York, 1991.

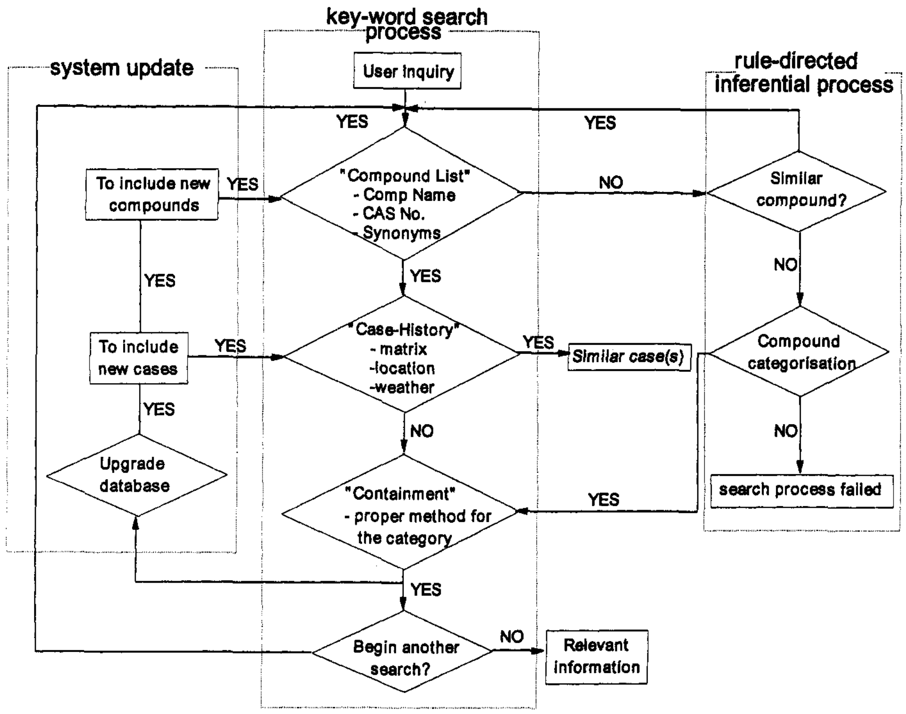

Figure 5. Operational diagram of the knowledge base, including the keyword search process, the rule-directed inferential process, and the system upgrading process.

interface that communicates between the program, the database, and the system user was developed using Microsoft Visual Basic (version 3.0). It should be mentioned that the database structure discussed above was refined several times during tests. A more detailed description of this database will be given in a separate paper.

Operation. Figure 5 is a flow chart that illustrates the search procedures used with the knowledge base. The complete process comprises a database search process based on the match of keywords, a rule-directed inferential process, and a system update procedure. A key-word search process starts with the "compound list" table to determine if there are valid database entries that could match the user-specified inquiry. The search procedure has been developed to perform searches based on unique database entries (search strategies), such as compound name, CAS no., as well as using synonyms of the target chemical. If a search strategy is fulfilled, then a set of id numbers for the target is obtained. In this way, all facts about the target chemical that are stored in various factual tables in the Factbase are made available to the user. In addition, the search program uses the [comp ID] parameter as the key word to search the "case-history" database to see whether similar case(s) have been reported previously. The "case-history" database holds descriptions of previous spills and the corresponding countermeasures adopted. This database can be upgraded to include the current plan under development using the upgrade procedure provided. In addition to the [comp ID] parameter, three common questions are asked in order to restrict the number of possible hits during the search process. The questions to be answered are as follows: Q1. the matrix in which the accident happened, Q2. the type of location of the accident, and Q3. the weather. Predetermined answers to these questions are provided as menu options to further reduce the diversities of entries. For Q1, the options are as follows: (a) watercourse, (b) loose surface, (c) paved surface, and (d) user specified. For Q2, the options are as follows: (a) urban area, (b) rural area, (c) major transportation route, and (d) user specified. For Q3, the options are as follows: (a) normal, (b) windy, (c) raining, (d) snowing, and (e) user specified.

Ideally, the result(s) reached by the end of this second round of searching should closely match the situation one is dealing with, and therefore, can be used as a guide to plan the response for the current spill. Practically, however, such occasions will be rare. Regardless of the outcome from the "case-history" database search, if the primary search did not fail, one can continue to collect relevant information for particular compound(s) in the Factbase based on the connections provided by the id numbers.

Use of the system shows that this database structure is efficient in managing the massive amounts of factual information required in arriving at an appropriate response to a chemical spill. The search subroutines were found to be sufficiently fast to be able to handle user requests and to output search results. The test results also showed that this database could be easily upgraded to include additional data entries without modification of the internal structure.

4.3. Representation and Compilation of the Heuristic Knowledge. Incomplete information or uncertainty in the knowledge is always the final dilemma when decisions have to be made. A human expert will use experience, or "rule of thumb", to resolve such predicaments. Edwards and Cooley argued that an expert system required more than factual knowledge to display expertise in a given domain.[38] What they inferred was the importance of heuristic knowledge in the problem-solving process. Kidd wrote that the aim of an expert system is not merely to capture a static representation of some knowledge domain but to simulate a particular problem-solving task carried out within that domain.[39]

As described earlier, we developed the spill-handling database using a subject-oriented structure. The role of this database is to categorize hazardous chemicals and to provide characteristic information such that chemicals in the same group can be treated similarly. Nevertheless, real-world

Table 4. Result Set from Casual Analysis of the Knowledge Used for Chemical Categorization

conclusions	conditions
1. heavier than air, flammable vapors	{group 1a chemicals: [vapor state, vapor density greater than air, flammable]}
2. heavier than iar, nonflammable vapors	{group 1b chemicals: [vapor state, vapor density greater than air, non-flammable]}
3. lighter than air, nonflammable vapors	{group 1c chemicals: [vapor state, vapor density less than air, non-flammable]}
4. lighter than air, flammable vapors	{group 1d chemicals: [vapor state, vapor density less than air, flammable]}
5. floating solids	{group 2a chemicals: [solid state, density less than water, water insoluble]}
6. floating, flammable liquids	{group 2b chemicals: [liquid state, density less than water, flammable, water insoluble]}
7. floating nonflammable liquids	{group 2c chemicals: [liquid state, density less than water, nonflammable, water insoluble]}
8. floating, spreading liquids	{group 2d chemicals: [liquid state, density less than water, water insoluble, spreading on water surface]}
9. floating, non-spreading liquids	{group 2e chemicals: [liquid state, density less than water, water insoluble, non-spreading on water surface]}
10. sinking solids	{group 3a chemicals: [solid state, density greater than water, water insoluble]}
11. sinking liquids	{group 3a chemicals: [liquid state, density greater than water, water insoluble]}
12. dissolving, acidic chemicals	{group 4a chemicals: [water insoluble, acidic chemical/react with H_2O]}
13. dissolving basic chemicals	{group 4b chemicals: [water soluble, basic chemical/react with H_2O]}
14. dissolving salts containing heavy metal ions	{group 4c chemicals: [water soluble, salt with heavy metal ion]}
15. dissolving salts without heavy metal ions	{group 4d chemicals: [water soluble, salt without heavy metal ion]}
16. biodegradable chemicals	{group 4e chemicals; [water soluble, biodegradable]}
17. nonbiodegradable chemicals	{group 4f chemicals: [water soluble, nonbiodegradable]}

situations can be so dynamic that such a database may not able to provide the diversity and resolve the complexities that arise during the problem-solving process. Thus, a knowledge-based system is necessary to extend the applicability and flexibility of the RHC database. In this project, the knowledge-based system uses a production rule format to represent knowledge. In the following section, we describe the methods used and results achieved in the development of this knowledge base.

Analysis of the Domain Knowledge. Heuristic knowledge is developed by field experts through years of practice and is used in the manipulation and interpretation of factual information to solve problems. The way in which one applies heuristic knowledge in pursuing answers towards a target problem may be represented logically by a causal analysis expression using conditions (OBServerables) and conclusions (ACTions). Such expressions can be represented as:

$$\text{decision } \psi\ (\text{ACT}_1, \text{ACT}_2, \ldots\ \text{ACT}_n) = \Phi(\text{OBS}_2, \text{OBS}_2, \ldots\ \text{OBS}_m) \quad (1)$$

Where OBS_i ($i = 1 - n$) are the observable and ACT_j ($j = 1 - n$) are the actions of the decision-making process Y. Sometimes, we observe that a set of conditions may result in a number of suggestions within which an inference engine cannot discriminate. This incomplete set of conditions together with further observations may start another decision-making process that can then produce a more precise decision. This process can be represented as

$$\text{decision } \psi'(\text{ACT}_1', \text{ACT}_2', \ldots\ \text{ACT}_p') = \Phi\{\text{decision } \psi\ (\text{ACT}_1, \text{ACT}_2, \ldots\ \text{ACT}_n)|\text{OBS}_1', \text{OBS}_2', \ldots\ \text{OBS}_q') \quad (2)$$

A production rule is a logical expression commonly used in the representation of heuristic knowledge. Therefore, when faced with incomplete information and/or uncertainties regarding the usage of factual knowledge during a problem solving process, the rules containing heuristic knowledge may be used to help users interpret the facts and reduce the ambiguity.

Knowledge Domain Matrix. If heuristic knowledge can be interpreted by causal analysis and expressed as a function of conditions and conclusions, it is possible to develop a tabular form to accommodate the causal analysis results. Such a two dimensional table is called a knowledge domain matrix (KDM). The causal analysis results can be transferred to an empty KDM in which the conditions are listed as the first row in the matrix, and the conclusions in the first column of the same matrix. At the primary level, the logical connections between conditions and conclusions in a KDM are established by filling in "True" and "False" values according to the causal analysis results. After this step, the existing logical connections are only valid between individual conditions and conclusions.

The logical relations of the entire knowledge matrix do not exist until the next step, known as the secondary knowledge encoding, is completed. At the secondary level, conditions and conclusions not related at the primary level are connected logically, thus the knowledge represented by a KDM is expanded. The knowledge in a KDM is said to be completed when all the conditions and conclusions are properly connected.

Unexpected conclusions may arise as the result of using a KDM based only on the primary and secondary knowledge encoding. This is because sometimes "parallel cases" occur when one conclusion can give rise to two sets of conditions. At the tertiary level, the final layer of knowledge is added to the KDM to differentiate between similarities that arise from parallel cases.

Blank cells in a KDM represent "no connections", neither "true" nor "false", between specified conditions and conclusions. The expertise represented by a completely filled KDM is much greater because of the knowledge contained in the off-diagonal region of the KDM that can be applied in the problem-solving process. More detailed discussion of the KDM scheme can be found in other publications by this group.[32, 33]

Compilation of Domain Knowledge. Applying the causal analysis operation to the contents in Table 2, we obtain Table 4 in which the criteria shown in Table 2 are listed as conditions and where Category IDs are identified as conclusions. These results can be readily transferred into an empty knowledge matrix. Next, the logic connections are placed in the corresponding cells in the matrix. Figure 6 shows the completed KDM that combines the knowledge shown in Table 2 and the logical connections given in Table 4. In order for the inference engine to operate, the knowledge compiled in the KDM format must be converted into a set of conditional statements, known as production rules, in which the coded knowledge is represented as a series of IF condition(s) THEN conclusion(s) sentences without using

Table 5. Global Variables and Descriptions of the Current KBF File

Goal Section	Description
1. chemical categorization *(CategoryID)*	Used to assist the user in assignment of a proper category ID for a target chemical if it is not included previously in the factbase
2. compound similarity comparison *(CompID)*	Used when the target compound is not included in the "compound list" table. This section helps the user to decide whether the target compound might resemble a "similar" compound in the data base, based on similarities among a set of physio-chemical criteria
3. containment & remedial technique *(ContTech)*	Used to assign proper containment and/or remedy methods for the target compound once this chemical's category ID is decided
4. treatment site selection *(TrmtSite)*	Used after an accident has been contained. This section helps the user to select a proper treatment site for further treatment or disposal based on the facilities, supplies and the geological location of the spill

Conditions \ Conclusions	Vapor chemicals				Insoluble chemicals (G2 & G3)							Soluble chemicals (G4)							
	1. Low lying, flammable vapors (1A)	2. Low lying, nonflammable vapors (1B)	3. Lighter than air, nonflammable vapors (1C)	4. Lighter than air, flammable vapours (1D)	5. Floating solids (2A)	6. Floating, flammable, volatile liquids (2B)	7. Floating, nonflammable, nonvolatile liquids (2C)	8. Floating, volatile, nonflammable liquids (2D)	9. Floating, nonvolatile, flammable liquids (2E)	10. Sinking solids (3A)	11. Sinking liquids (3B)	12. Acidic chemicals that dissolves in water (4A)	13.Chemicals that dissolve & react with water to give acid	14. Basic chemicals that dissolve in water (4B)	15. Chemicals that dissolve & react with water to give base	16. Water soluble salts containing heavy metal	17. Water soluble salts containing no heavy	18. Biodegradable chemicals (4E)	19. Non-biodegradable chemicals (4F)
1. Vapor state	T	T	T	T	F					F									
2. Vapor density greater than air	T	T	F	F															
3. Flammable	T	F	F	T		T	F	F	T										
4. Water soluble					F	F	F	F	F	F	F	T	T	T	T	T	T	T	T
5. Liquid state					F	T	T	T	T	F	T								
6. Volatile chemical					F	T	F	T	F										
7. Density less than water					T	T	T	T	T	F	F								
8. Acidic chemical												T	F	F	F				
9. Containing heavy metal ions																T	F		
10. Biodegradable																		T	F
11. React with water												F	T	F	T				

Figure 6. An sample knowledge domain matrix representing the causal analysis results for chemical categorization. Production rules can be readily derived from this knowledge matrix.

specific artificial intelligence language. Consequently, the containment and remedial countermeasures listed in Table 3 and the information stored in the Factbase can be selectively accessed to aid in planning the response to a spill for chemicals for which Category IDs have been identified.

Major components in a KBF file are described in Table 5, and include the following: (i) the goal section containing a list of goal variables that will be used to assign the result(s) from the inferential process; (ii) the production rule section, which is the main section where heuristic knowledge is stored in IF...AND/OR...THEN...statements; and (iii) the user query section providing the inference engine with predefined questions. In an inference process, the inference engine will only ask those questions related to the facts that the user has entered and present options for identification. The current knowledge base of the ERexpert prototype is ready for experimental testing, we expect that the 'test with cases' cycle will introduce new conditions and conclusions into the knowledge base as the system is adjusted to become more practical and applicable for use in real situations.

The rule-directed inferential process is shown in Figure 5. In this process the inference engine, EAengine, employs the knowledge stored in the Rulebase together with the supplementary information given by the Factbase to provide remediation advice following a spill. EAengine supports three inference strategies, forward, backward, and mixed chaining.[25] Forward chaining, also called data-driven reasoning, starts by examining the rule's premise and fires those rules that are satisfied, this process runs successively until all the causes are identified based on the fact(s) provided by the user. Backward chaining, or goal-directed reasoning, begins with a suspected goal, and extends from there in an attempt to find evidence from the Rulebase that matches the facts provided by the user. Mixed chaining refers to an inferential strategy that uses both forward and backward reasoning within a single knowledge base. Mixed chaining starts in a forward chaining mode and proceeds normally until the inference process stalls without selecting any conclusion. This will occur when there is insufficient evidence to identify a hypothesis. The inference engine can then switch to the backward chaining mode and will begin asking the user to supply additional information.

4.4. Maintenance of the Knowledge Base. Maintenance of an expert system, namely the need to update the knowledge base to include more knowledge and to delete redundant knowledge, is an important part of the life of an expert system. It is especially important in the early development stages that the knowledge base undergoes frequent modifications and expansions to ensure correct answers are provided. Results from using commercially available expert system shells seem not to be very promising under the perspective of both our own observations and the reports from other research groups.[32,41] We investigated the causes for this problem and found that the "decision-tree" structure adopted by many expert system shells makes maintenance difficult. Because the logical relations present in a tree-structure are rigid, any changes made to the tree may upset the whole relationship and this can only be resolved through a major revision of the decision tree from the root to the tip. Moreover, the connections in a tree-structure are behind the scene, so that the knowledge engineer is not able to see the connections, which in turn makes a change in the logical relations more difficult. The KDM process, which was adopted for this work, uses a two dimensional matrix to hold the results of the causal analysis for a given knowledge domain. Instead of using a tree-like structure, the logical relations in a KDM are made by filling in "T(rue)" and "F(alse)" values to corresponding cells in the matrix. Unlike a tree-structure in which the logical relations between conditions and conclusions are "hard-wired", the logical connections in a KDM can be edited flexibly by assigning new logical values to those cells. This type of modification is independent of the existing relationships so the structure of the KDM will not be affected. The unique advantage of the KDM scheme is that it enables the knowledge engineer to see directly the logical relations held in the knowledge matrix, so that a knowledge base developed in this way can be re-structured and expanded quite easily.[32,33]

Hypermedia is an alternative way of implementing and structuring knowledge in an expert system shell, and has recently received much attention in the development of knowledge-based systems.[42] We find the hypermedia process interesting because it provides looser connections between the conditions and conclusions so that the system user can freely change, add or delete nodes of a decision tree developed using such methodology. However, it is problematic because a naive user will find it difficult, if not impossible, to use such a knowledge system in an effective manner. In our opinion, such freedom should only be given to the knowledge engineer during the system development and upgrading processes. The results discussed in this paper suggests that the KDM process is a promising knowledge encoding method that can match the knowledge encoding requirements from a complicated domain problem, although further verification will be required to test this methodology in other applications in the future.

5. CONCLUSIONS

This study focused on the knowledge acquisition process and the development of a knowledge base for an expert system prototype intended to be used in assisting to develop appropriate emergency responses to chemical spills. In this study, we have applied the compound categorization concept to characterize hazardous chemicals into four major categories and 17 subgroups based on their environmental behavior. A subject-oriented Factbase containing the RHCs was developed using the Microsoft ACCESS rational database system. With the help of causal analysis, heuristic knowledge related to chemical categorization was extracted and compiled into the Rulebase through the implementation of the KDM process. The resulting fully functional knowledge base encompasses two parts, a Factbase that contains factual information, and a Rulebase used as a supplement to extend the coverage and applicability of the Factbase. Subsequent work regarding the implementation of this knowledge base in the development of the ERexpert prototype will be reported in part 2 of this series.

As an innovative knowledge encoding method, the KDM process has been described in detail in this paper. A KDM process includes the following three steps: (i) causal analysis of the knowledge domain, (ii) transfer of the causal analysis results into the knowledge matrix and filling in the logical connections, and (iii) conversion of a filled KDM into production rules. One of the advantages of the KDM process is that it helps the knowledge engineer to visualize logical relations between conditions and conclusions that are otherwise difficult to express. The KDM scheme also provides flexibility for future modification of the logical relations between individual conditions and conclusions without upsetting the other connections in a knowledge table. The significance of this new knowledge encoding approach can be seen through this research, however, further application of this methodology may be necessary to verify the general applicability.

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