Design of an Expert System for Emergency Response to a Chemical Spill. 2. ERexpert Module Design and Development

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The requirements for standardized procedures, systematic documentation, and rapid response from personnel with different levels of training make the application of computer-based expert system technology a promising approach in the development of software that can aid in planning the response to chemical spills. In this paper, the development of a modular expert system is described. ERexpert, which was developed for use in the Microsoft Windows 3.1 environment, can be used to guide the nonexpert user through the emergency response process. The knowledge base of this program consists of two functional groups, a database of factual information and a rule base of heuristic expertise. The factual database, named Factbase, was developed using the Microsoft Access 1.0 relational database system. Spill related information was mapped into a set of subject-oriented tables. In the Rulebase, heuristic knowledge is first organized into a knowledge matrix, and the results are then converted into rules that can be used by the inference engine in solving problems with incomplete information. A multilayer knowledge domain matrix format has been designed to aid in the representation of complex decision-making processes. Microsoft Visual Basic 3.0 program language was used to develop the graphical user interface that provides quick and efficient control of the program. The implementation procedures and results are fully discussed together with a description of the program.

1. INTRODUCTION

For any chemical spill accident, the potential for environmental damage and time are linked through an exponential relation that puts a premium on response practices that can be enacted immediately.[1] This requires both highly efficient reporting systems and quick deployment of a complex set of countermeasures, yet each spill is an individual situation. In practice, not only are these requirements often beyond the capability of a single human expert but also, because of the unpredictable nature of an accident as to time and location, experienced personnel and the necessary referential information may not be available. On the other hand, computer-based expert systems, which can provide availability and consistency together with increased task performance, are ideal tools to address complicated problems that require prior knowledge to be applied under stress and time constraints, such as in planning the response to a chemical spill.

Kollig *et al.*[2] pointed out that the quickest and least expensive way of obtaining environmental information is by accessing a database. Such databases may be capable of furnishing the user with literature reports, however, in many cases the problem is that the lack of consideration of the environmental reality makes such information hard to be implemented easily in a real situation. Literature data and previous case-history records cannot be applied under new circumstances unless the heuristic knowledge of the field experts on how to use these data could be captured and reapplied properly to interpret the difficulties found in the re-application processes.

The specific actions required for the clean up of chemical spills are determined by a combination of the physical, chemical, geological, and biological properties of the released compounds in the complex matrix of the natural environment. It is, of course, imperative that information used for planning such a response is valid for the micro environmental surrounding the spill. Yet, a literature search revealed that little human expertise has been documented that can be used to help in solving the difficulties regarding the use of the rather massive amount of information that is available on techniques, regulations, and procedures involved in the response to a chemical spill. Certainly, the lack of effective software that can be used to capture such complex heuristic knowledge is one of the reasons that the extrapolation of available spill response technology to the environmental reality is extremely difficult.

Expert systems are computer programs that give the appearance of human-like reasoning for problems ordinarily requiring special expertise.[3] The aim of an expert system is not merely to capture a static representation of a knowledge domain but to simulate the particular problem-solving task (or tasks) carried out within that domain.[4] A generic set of such tasks has been identified by Hayes-Roth *at al.*,[5] among them, interpretation and diagnosis are the two task-categories that analytical chemists are most familiar with and have been the subject of many implementations of expert system technology. Recent programs include the ESCA project for liquid chromatography described by Buydens *et al.*,[6] an expert system concerned with trace metals analysis by voltametric methods,[7,8] data interpretation for petroleum based volatiles by GC-MS analysis,[9] diagnostic and automation in atomic absorption spectrometry,[10-12] and diagnosis of faulty data in gas chromatography.[13] In the environmental area, applications started to emerge in the mid-1980s[14] and have shown a steady increase ever since.[15] Applications

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include the U.S. EPA's environmental monitoring system, that was developed to increase the accuracy, timeliness, and cost-effectiveness of field sampling, chemical analysis, and data validation,[16] the GEOTEX expert system for hazardous waste site investigations,[17] the ES-EPA program for environmental pollutant analysis developed in Japan,[18] and a risk assessment model for chemical constituents of hazardous waste.[19] However, to our knowledge applications in the field of emergency response to chemical spills have not yet been reported.

This paper describes the development and implementation of the ERexpert modular expert system, a program that incorporates the knowledge acquisition results, obtained through a causal analysis of the appropriate heuristic knowledge, in the form of a Knowledge Domain Matrix.[20] This decision-making system uses both static and conceptual data to support the strategies to be followed by the user in order to select the most favorable response countermeasures using supplementary information required for the chemicals involved in the spill. A graphical user interface has been developed that provides essential communication between the system user and the knowledge base. Finally, the possibility of integration of the ERexpert module into the SPILLexpert frame is discussed.

2. COMPUTER ENVIRONMENT

All the computer work was carried out on an Intel 80386, 20 MHz computer, with 8 megabyte of RAM, two 150-megabyte hard disks, a 1.44-megabyte floppy disk, and a super VGA graphic monitor.

The ERexpert program is designed for use in the Microsoft Windows 3.1 environment. Software chosen for the development of this project are all MS Windows based applications. Microsoft ACCESS (version 1.0), an interactive relational database system, was utilized for factual data management. EAshell is a Windows based expert system shell developed in our laboratory[21] that provides the inference engine. Microsoft Visual Basic (version 3.0) was used as the programming language for the development of the graphical user interface; the inference processes are initiated by calls to EAengine, which is compiled as a dynamic linked library (dll).

3. COMPONENTS IN THE EREXPERT SYSTEM

Expert systems are integrated computer programs. In general, an expert system contains three fundamental components:[35,36] (i) a knowledge base in which the domain knowledge is embedded, (ii) an inference engine that manipulates the knowledge, and (iii) a user interface that provides access to the system utilities.

3.1. The Knowledge Base. ERexpert allows different knowledge representation formats to be used simultaneously. The overall knowledge base in this program contains both a Rulebase and a Factbase. The Rulebase is an ASCII file in which heuristic knowledge is coded as production rules that are associated with a number of goal variables. The Factbase comprises a number of subject-oriented tables in which factual information is stored as either text or numbers.[20] During execution, the heuristic module containing "IF condition THEN conclusion" rules can be used to offer the user advice based on the facts provided, while a search of the Factual database provides information specific to the case that can supplement the conclusion(s) reached during an inference process.

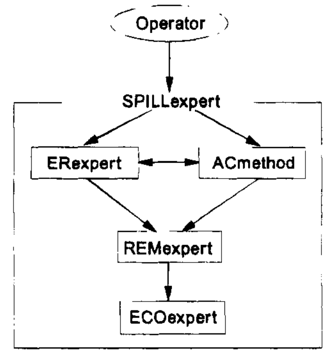

Figure 1. The SPILLexpert frame in which a set of interconnected modular expert systems focus on a single subdomain of the overall problem domain.

3.2. The Inference Engine. The inference engine, EAengine, which is a part of EAshell,[21] supports three inference strategies, namely forward, backward, and mixed chaining. Forward chaining, also called data-driven reasoning, starts by examining the premise of rules and fires those that are complete, 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 backwards through the Rulebase in an attempt to find evidence that could support the hypothesis selected from the Rulebase. Mixed chaining refers to an inference strategy that uses both forward and backward reasoning with a single knowledge base. This mode starts in the forward chaining mode and when a situation arises for which insufficient evidence is encountered to support a hypothesis, the inference engine automatically switches to the backward chaining mode. Through this strategy, additional support may be found for the hypothesis by asking the user more goal-driven questions.

3.3. The User Interface. One of the major problems to be solved in the development of an expert system is the requirement for an effective and easy-to-use user interface that allows efficient use of the different modules. The object of the ERexpert system is to make planning the spill response faster and more accurate, so the design of the user interface is a critical feature of the program. There are two layers of communication in ERexpert: (i) between the modular expert systems and (ii) between the system user and the program. MS Windows is a powerful operating system that provides communication functionality through dynamic data exchange (DDE), object linking and embedding (OLE), dynamic linking libraries (DLL), and the multiple-document interface (MDI). We have previously developed a graphical user interface (GUI) for the ERexpert system.[22] This interface was written using Microsoft Visual Basic (version 3.0).

4. DESIGN FOR THE EREXPERT MODULE

4.1. The SPILLexpert Frame. The primary objective was to design a structure that would enable the separate yet correlated development of a series of knowledge-based modules. Emphasis was paid to the feasibility and effectiveness of the integration of such independently developed modules into this general structure. As shown in Figure 1, the SPILLexpert frame was developed so that all the technical elements involved in a spill response were incorporated into a number of modular expert systems. The following modules are invoked in a session using SPILLexpert: ERexpert, for planning the emergency response following a hazardous material spill, emphasizes the containment and deployment

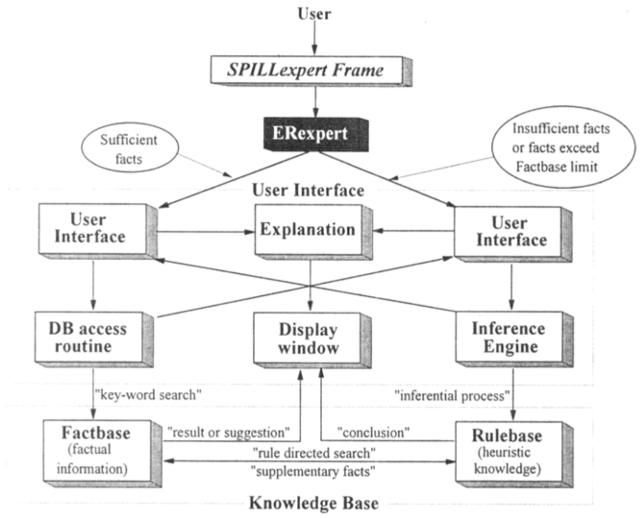

Figure 2. Design of ERexpert. The diagram shows the interactions between each of the components and how information flows inside the program.

of primary remedial actions; ACmethod directs the selection of sampling and analysis methods to be used to identify and qualify the hazardous chemical(s) in the complex environmental matrix; REMexpert provides instructions for the next phase of cleanup operations once a spill is under control and has been contained, for further remediation; and ECOexpert offers advice related to risk assessment and environment restoration.

4.2. The ERexpert Module. As a module in the SPILLexpert frame, ERexpert emphasizes the subdomain of emergency response to a chemical spill. ERexpert uses both production rules and a database of facts to represent the expertise of the domain experts. Figure 2 shows the design adopted for the development of the ERexpert module. The user interface section encompasses an I/O program that provides the functions of evidence inquiry (user input), explanation/display (system output), the routines used for database access, and for inference processes. The knowledge base section consists of both a Factbase and a Rulebase that can be used by the program interchangeably. The program first uses the static knowledge of the Factbase in an effort to solve a problem. If the facts about a particular spill are not sufficient or exceed the limitations of the Factbase, the system then considers this problem to be an incomplete case and will launch the inference process to try and solve the uncertainties using the conceptual knowledge in the Rulebase. In ERexpert, both the database search process and the inductive procedures are computer subroutines embodied in the user interface that are controlled by the user.

4.3. The Knowledge Encoding Scheme. The Knowledge Domain Matrix (KDM) method has been fully discussed previously[12,20] and is only briefly summarized here. In this form of knowledge encoding, a two-dimensional matrix is employed to code the knowledge set which is obtained from causal analysis of the domain problem and expressed in terms of a set of conditions and conclusions. The premises of an action are recognized as **conditions** and listed as the first column in KDM. Similarly, the actions resulted from a set of conditions are termed as **conclusions** and listed as the first row of the same matrix. Finally, the logic connections are made possible by filling in the corresponding cells with "T(rue)" and "F(alse)" values.

In reality, however, the decision-making process may often require multiple inferential processes to be performed at different levels, and each of these levels may require the use of previous conclusions, together with additional observations as new conditions, to carry the reasoning process on further.[20] The diagnostic procedures necessary to solve a fault in an hyphenated instrument, such as GC-MS, requires, at a minimum, a two-step inferential processes to be performed in tandem. In terms of the KDM, this multistep inference process cannot be represented by a single two-dimensional matrix. In Figure 3, we show a multilayer matrix structure designed to address such a complication in

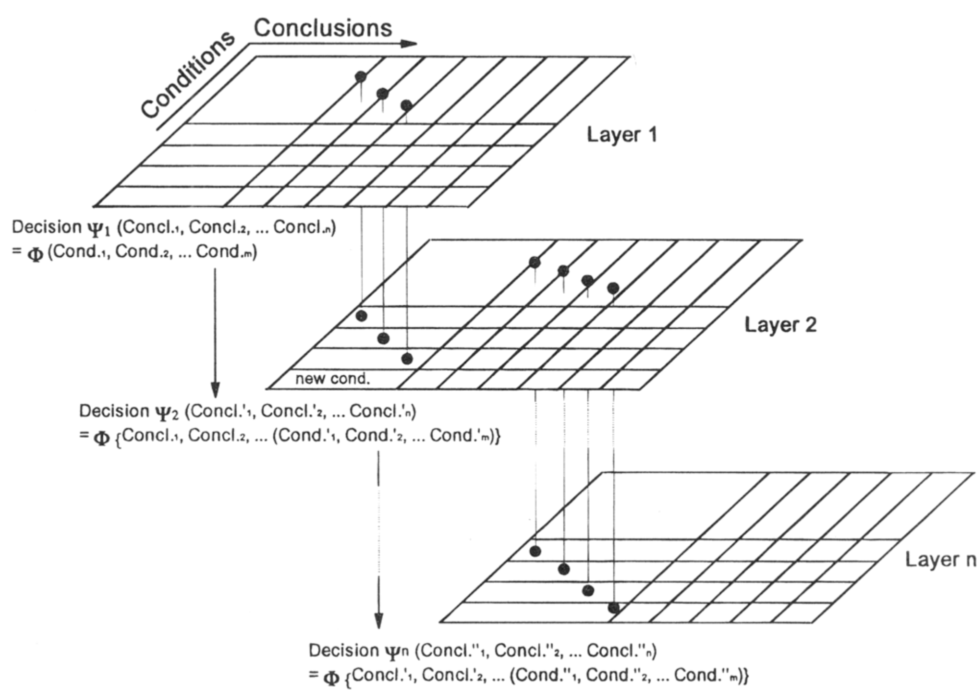

Figure 3. This multilayer knowledge domain matrix is designed to represent complex inference processes in which many layers of induction are involved. Between these knowledge layers, the conclusions obtained from the previous round of reasoning may be used as the conditions in the next round. The vertical lines represent the transfer of one or more conclusions from an upper layer to a deeper layer. The conclusions then become conditions of the deeper layer. This is represented by the logic statements Y_1, Y_2, and Y_n.

Comp ID	Category ID	CAS No.	Comp Name	Phase	Family	Synonyms	Method ID
5	1A; 2B	71-43-2	Benzene	VAPOR; LIQUID	Aromatic compound	Benzol; Phenyl hydride; Coal naphtha; Benxole; Cyclohexatriene	Reserved
36	1A; 2B	110-54-3	Hexane	VAPOR; LIQUID	Aliphatic hydrocarbon	None	Reserved
65	1B	7782-50-5	Chlorine	VAPOR	Halogen	Bertholite	Reserved
84	2A; 4E	108-95-2	Phenol	VAPOR,SOLID	Aromatic alcohol	Carbolic acid; Phenic acid; Phenylic acid; Phenyl hydrate; Hydroxybenzene; Monohydroxybenzene	Reserved
93	1C; 4B	7664-41-7	Ammonia, anhydrous	VAPOR; LIQUID	Ammonia	Ammonia	Reserved
98	1D	74-82-8	Methane	VAPOR	Aliphatic hydrocarbon	Mash gas; Methyl hydride	Reserved
144	3A	309-00-2	Aldrin	SOLID	Halogenated aromatic compound	1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-1,4,5,8-dimethano naphthalene	Reserved
264	3B; 4A	7726-95-6	Bromine	LIQUID	Halogen	None	Reserved
290	4A	7664-93-9	Sulfuric acid	LIQUID	Mineral acid	Oil of vitriol; Spirit of sulfur; Hydrogen sulfate. Sulfuric acid (fuming) is known as oleum.	Reserved
299	4B	1310-73-2	Sodium hydroxide	SOLID	Alkali hydroxide	Caustic soda; Caustic alkali; Caustic flake; Sodium hydrate; Soda lye; White caustic	Reserved
353	2C	107-21-1	Ethylene glycol	LIQUID	Alcohol	Glycol; Ethylene alcohol; Glycol alcohol; 1,2-Ethanediol	Reserved
400	3B	67-68-5	Dimethyl sulfoxide	LIQUID	NA	Methyl sulfoxide; DMSO; Gamasol 90	Reserved
401	4C	7761-88-8	Silver nitrate	SOLID	Salt	Lunar caustic; Silbernitrat	Reserved
402	4D	6484-52-2	Ammonium nitrate	SOLID	Salt	None	Reserved
403	2E	124-18-5	Decane	LIQUID	Aliphatic hydrocarbon	None	Reserved

Figure 4. The "Compound List" table of the current Factbase contains 17 characteristic chemicals (RHCs) that each represents a subgroup of chemicals for one of the 17 behavioral categories available to ERexpert. These RHCs are used to mirror the whole community of hazardous chemicals for which ERexpert can respond.

the knowledge domain. In this figure, the domain knowledge is represented by separate knowledge matrices that each focus on one subdomain of the target. For example, in order to represent the knowledge related to the diagnosis of faulty analysis by GC-MS, the knowledge domain can be arranged into two KDMs in which the first concentrates on diagnosis of analysis by gas chromatography, and the second focuses on diagnosis of MS-related problems. Determining the most appropriate response to a chemical spill is a multistep decision process, and we have developed this multilayer KMD mechanism to represent the domain knowledge used in the development of ERexpert.

5. IMPLEMENTATION OF THE DESIGN

5.1. Implementation of the Database Structure. The factual database integrated into the ERexpert module, called Factbase, was developed using the MS ACCESS database system. This Factbase, as described in the previous paper,[20] consists of a set of internally connected, subject-oriented fact tables. The current Factbase of ERexpert contains 17 characteristic chemicals, called representative hazardous chemicals (RHCs), where each one represents one of the 17 subgroups of chemicals that exhibit the behavioral categories identified by the system.[20] These RHCs are used to mirror the whole community of hazardous chemicals for which ERexpert is designed to respond. RHCs are stored in the "Compound List" table of the Factbase (Figure 4). In this same table, a group of pre-defined indices are included in association with the chemicals. These indices, called identification numbers (IDs), were employed to realize the connections among different factual tables. The internal connections between the tables are described in the diagram shown in Figure 5. According to this structure, related information for those chemicals listed in the "Compound List" table are mapped into separate subjective tables. The Factbase of ERexpert is furnished with query functions developed using the MS ACCESS BASIC language. In conjunction with the ID numbers, these queries provide accessibility to the factual data stored elsewhere in the Factbase. On execution, the database module runs as a

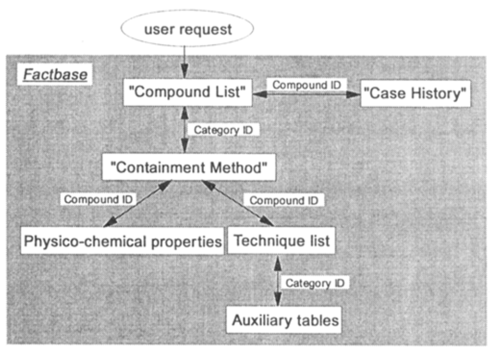

Figure 5. The structure of the Factbase, a database designed to encompass the factual information used in response to chemical spill accidents. The Factbase consists of a set of internally connected, subject-oriented fact tables. A group of predefined indices are employed to enable the connections between the different fact tables.

background task. The database receives commands through the user interface to perform required operations and returns the results to the front-end. Additional factual information can be added fairly easily into the database according to the design, and, as is to be expected, the more the facts, the better the performance. However, the principal information set of the RHCs provide this database module with sufficient flexibility to cover a range of hazardous chemicals if the target chemical can be categorized into one of the 17 behavioral groups. Production rules defined to identify the chemical categorization are integrated into ERexpert and can be used to help with the identification if users have difficulty in determining the identity of a target compound.

As shown in Figure 5, in addition to the information supplied by the subject-oriented tables, the ERexpert Factbase is also equipped with a "Case-History" subdatabase in which individual cases of responses to spills have been recorded and connected to the main database through the Compound ID index. This "Case-History" subdatabase serves two primary purposes. First, the records of previous responses to similar spill provide a valuable reference when planning response actions for the current situation. Second, this database provides an archive medium for effective docu-

Conditions / Conclusions	Volatile chemicals							Solid chemicals					
	1. Correct mechanic failure; close valve, clog leaks, shut down pump. To clean up, decide chemical type (Category ID), run KB again.	2. Avoid spark. Inert foam coverage with mist knock down.	3. Avoid spark. Cryogenic condensation, air dilution (fans/blowers).	4. Avoid spark. Encapsulation.	5. Inert foam coverage with mist knock down.	6. Cryogenic condensation, or air dilution using fans or blowers.	7. Encapsulation.	8. Solid chemicals are usually self contained. Recovery by shoveling or	9. Fluidized solids will be treated as liquids, concern is to prevent run off into watercourse/sewage, assign a liquid category ID to the target.	10. Treat as Category 2A/3A chemicals on dry surface.	11. Treat as fluidized Category 2A/3A chemicals.	12. No spark. Inert foam/plastic sheet, earthen dike, excavation, trench, pump/vacuum in auxiliary tank/sump, remove bottom, direct to paved surface/sealant to slow penetration. Temp. burial for later treatment.	13. Earthen dike, trench, excavation, pump/vacuum to auxiliary tank/sump, remove bottom, direct to paved surface/sealant to slow penetration. Temporary burial to contain for later treatment.
1. Mechanical failure	T												
2. Category 1A chemicals*		T	T	T									
3. Category 1B chemicals*					T	T	T						
4. Category 1C chemicals*						t							
5. Category 1D chemicals			t										
6. Sheltered area			T			T							
7. Calm area (air/water surface)		T	T	T	T	T	T						
8. Limited spill size				T			T						
9. Category 2A chemicals*								T	T				
10. Category 3A chemicals*								t	t				
11. Spill happened on land								T	T	T.	T	T	T
12. Dry ground surface								T	F	T	F		
13. Category 2B chemicals*												T	
14. Category 2C chemicals*													T
15. Category 2D chemicals*													
16. Category 2E chemicals*													
17. Category 3B chemicals*													
18. Flat surface													
19. Soft surface/river bottom												T	T
20. Flammable													
21. Volatile													
22. Liquid state										F	F		
23. Spill in watercourse													
24. Category 4A chemicals*										T	T		
25. Category 4B chemicals*										t	t		
26. Category 4C chemicals*										t	t		
27. Category 4D chemicals*										t	t		
28. Category 4E chemicals*										t	t		
29. Category 4F chemicals*										t	t		
30. Natural barrier exists													
31. Geographically feasible area													
32. Small removable volume													
33. Clear area													

Insoluble liquid/solid chemicals

14. Inert foam/plastic sheet, excavation, earthen dike, trench to contain, pump/vacuum in auxiliary tank/sump, remove bottom, direct to paved surface/sealant to slow penetration. Temp. burial for later treatment.											T				T				T														
15. No spark contac. Earthen dike, trench, excavation, pump/vacuum in auxiliary tank/sump, remove bottom, direct to paved surface/sealant to slow penetration. Temporary burial for later treatment.											T					T			T														
16. Avoid spark. Inert foam/plastic sheet,, foamed polyurethane, concrete dike to contain, pump/vacuum collect in auxiliary tank/sump, direct to paved surface/surface sealant. Temp. burial for later treatment.											T		T					T	F														
17. Foamed polyurethane/concrete dike, pump/vacuum in auxiliary tank/sump, direct to paved surface/sealant. Or temporary burial.											T			T				T	F														
18. Inert foam/plastic sheet, foamed polyurethane, concrete dike to contain, pump/vacuum in auxiliary tank/sump, direct to paved surface/sealant. Temporary burial to contain for later treatment.											T				T			T	F														
19. Avoid spark contact. Foamed polyurethane, concrete dike to contain, pump/vacuum in auxiliary tank/sump, direct to paved surface/ surface sealant. Temporary burial to contain for later treatment.											T					T		T	F														
20. Treat as Category 2B chemicals.											T						T			T	T												
21. Treat as Category 2C chemicals.											T						T			F	F												
22. Treat as Category 2D chemicals.											T						T			F	T												
23. Treat as Category 2E chemicals.											T						T			T	F												
24. Natural dike/excavation, pump recover in auxiliary tanks/temp. burial.										t							T						T							T			
25. Under water dikes, excavations, dredging, or temporary burial.										t							T		T				T										
26. Curtain barriers contain spill and pump to recover.							T			t							T						T										
27. Avoid spark. Booms, weirs, pneumatic barriers contain spill, skimmer/ vacuum collector recovery into auxiliay tank.							T						T			t							T										
28. Booms, weirs, or pneumatic barriers to contain. Recovery by skimmers/vacuum collector into auxiliay tank.							T		t					T	t								T										
29. No effective method to contain, use burning to cleanup spill.													T			t							T								T		
30. No effective method to contain/clean up floating chemical spill. Water dilution/biodegradation process.									t					T	t								T										

	Soluble liquid chemicals																	
31. Removable volume of insoluble chemicals, pump to auxiliary tank/sump, centrifuge separation/solvent extraction to treat spill.	32. Treat as Category 2B chemicals.	33. Treat as Category 2C chemicals.	34. Treat as Category 2D chemicals.	35. Treat as Category 2E chemicals.	36. No effective containment for dissolving chemical spills in large, open watercourse, water dilution and biodegradation.	37. For removable volume of soluble chemicals (4A-4F), pump to auxiliary tank/sump, solvent extraction/gelation separation.	38. Sealed boom in limited, calm water area, neutralization except HCN. Also ion exchange or adsorption.	39. Limited size/flow water, diversion spill, neutralization except HCN, adsorption or ion exchange.	40. Sealed booms contain spill in limited, calm water area. $NaHCO_3$, CO_2 neutralization. Adsorption or ion exchange.	41. Limited spill size/flow water, diversion spill, neutralization, adsorption (activated carbon), ion exchange (process resin.)	42. Sealed booms contain, precipit., adsorp. or ion exchange.	43. Limited size/flow water, diverse spill, precip., adsorp., ion exchange.	44. Sealed booms contain, oxidation for cyanide salt, adsorption, ion exchange for other salts in this group.	45. Diversion spill, oxidation (CN salt), adsorp./ion exchange for others.	46. Sealed booms to contain, adsorption or ion exchange.	47. Limited size/flowing water, diversion spill, adsorption, ion exchange.	48. Sealed booms to contain, adsorption, ion exchange.	49.Limited size/flowing water, diversion spill, adsorption ion exchange.
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Figure 6. The Knowledge Domain Matrix (KDM) for the second knowledge layer in ERexpert is displayed. As part of the entire KDM used in ERexpert, the knowledge encoded in this matrix is the knowledge subdomain applicable to the selection of containment techniques and/or primary remedial methods for chemical spills. Those conditions denoted by asterisks are conclusions from a previous round of inference. The heuristics in ERexpert have been encoded into a three-layer knowledge matrix including (i) compound categorization, (ii) containment and remedial method selection, and (iii) treatment site selection. Depending on the scope of the target problem, these layers of knowledge can be applied separately or in conjunction with each other. "t"s represent the "parallel" cases in the KDM that are parallel to the "T" in the above adjacent cells.

mentation of the actions taken and reasons for those actions for each spill. Obviously, such a systematic recording of the actions taken in response to a spill will greatly aid in the sharing of experience. We anticipate that with the use of the ERexpert system, this subdatabase will grow larger and play an increasingly more important role in the process of planning responses.

5.2. Implementation of the Knowledge Encoding Results. A multilevel KDM structure has been implemented in this study for the first time to represent the complex layers of knowledge involved in planning the appropriate response actions following a chemical spill emergency. In the previous paper,[20] we described a KDM for the knowledge subdomain used in the classification of hazardous chemicals into different environmental behavioral categories. Figure 6 illustrates the contents of the second KDM layer that forms part of the complete KDM currently employed by the ERexpert system. The knowledge set encoded in this KDM is the knowledge subdomain used in selection of proper containment techniques and/or primary remedial methods. As shown in Figure 6, a number of these conditions (denoted by asterisks) are conclusions from the previous round of inference. At the present stage, the heuristic knowledge in the ERexpert module has been encoded into a three-layer knowledge matrix, which includes the knowledge subareas of (i) compound categorization, (ii) containment and remedial methods selection, and (iii) treatment site selection. Depending on the scope of a domain problem, these layers of knowledge can be applied separately or in conjunction with each other in the problem-solving process.

The coded heuristic knowledge in a multilayer KDM structure needs to be reformatted before EAengine can perform the required inductive processes. In this study, the results obtained from knowledge matrices are converted into a set of conditional statements, known as production rules, in which the heuristics are represented in the form of a series of IF condition(s) THEN conclusion(s) statements. A tool kit (Rule-Editor) has been developed in our laboratory to convert a filled KDM into a knowledge file of rules (KBF) for use by EAengine.[21] A KBF file consists of three major sections: a goal section, a logical expression section, and a user query section. The goal section provides information about goals used for backward chaining and contains a set of goal-related variables. The logical expression part is the main section in which heuristics are represented in *IF...-[AND/OR]... THEN...* statements, an explanation (*EXP*) statement is also given for conclusions of each rule. Finally, the user query section asks questions related to the facts and provides options as answers for identification. An example KBF file and a brief explanation are given in Table 1, in which CateID, ContTech, and TrmtSite are goal variables that represent the knowledge subdomains in the KBF file. CateID represents the knowledge subdomain used for categorization of chemicals based upon their environmental behavior, ContTech is a knowledge subdomain that deals with containment and remedial actions, and TrmtSite describes the heuristic knowledge used in selection of the treatment site. It is important to note that when both AND and OR are used in a rule, OR takes precedence over AND as if parentheses surround expressions connected by OR. This rule (named 29) is applicable if the spill happened on an unpaved surface (highway side, farm land, etc.), and solid chemicals were involved that either float or sink if they encounter water. The conclusion suggests that if the ground is wet, the target chemical(s) should be treated as liquid chemicals and the major work should be directed toward preventing run off into the watercourse or sewage system.

Table 1. An Example of a Rule File and a Brief Explanation of the Meaning of Variables

KBF Example	Explanation
Goal Section **FIND** CateID, ContTech, TrmtSite; :	Starts with ***FIND***, ends with ";". Goal variable **CateID** is for the assignment of a categorisation ID to a compound; **ContTech** for selection of containment techniques; and **TrmtSite** for selection of treatment site.
Logic Expression Section RULE 29 **IF** Variable11=YES **AND** Variable12=NO **AND** Variable9=YES **OR** Variable10=YES **THEN** ContTech=As liq./Pre.run-off/Assg.liq.ID; **EXP** "Fluidized solids shall be treated as liquids. The major concern is to prevent the solid from running off into the watercourse or sewage system. Response methods may be obtained by assigning a proper liquid category ID to the target." :	This block begins with keyword ***IF***, the premises are connected by ***AND***s or ***OR***s, and the pointer ";" ends the block. Corresponding content of each variable is given by the ASK sentence in the Query Section. The content after Keyword ***THEN*** is the conclusion part of a rule block, and a full explanation of the result is given in a ***EXP*** block immediately after that rule block.
User Query Section **ASK** Variable11 "Spill happened on land?" **OPTION** YES, NO; **ASK** Variable12 "Dry ground surface?" **OPTION** YES, NO; **ASK** Variable9 "Category 2A compound?" **OPTION** YES, NO; **ASK** Variable10 "Category 3A compound?" **OPTION** YES, NO;	The ***ASK*** keyword begins a query block while a ";" ends it. ***OPTION*** clause provides available answers to a particular question.

5.3. Development of the ERexpert Module. Figure 7 shows the graphical user interface developed for the SPILLexpert project. This interface was written in the MS Visual Basic language within the MS Windows 3.1 environment. A user with little computer knowledge can easily become familiar with the operation of each of the graphical features, such as the content of the menus and the intuitive icons. Part A in Figure 7 shows the main window of the SPILLexpert program in which five icons connect to five stand-alone modular expert systems embodied in the main frame. Clicking on the icon ER activates the ERexpert module. In part B of Figure 7, the first screen of ERexpert is displayed in which an icon set is illustrated and briefly explained. This icon set provides the user with full access to the embedded functions in ERexpert. The operational sequence of ERexpert is described in the flowchart given in Figure 8. The sequence starts with a database search for the target compound that the user provided. Based on the result of this process, different routines can be initiated that will deduce information about the chemical.

To run the ERexpert module, the user needs first to provide the system with a set of primary data about the spill. The template shown on as Figure 9A is the input dialogue box. In the next step, ERexpert employs this information set to search the Factbase. If the target compound can be found in the database, the search results are assigned to a set of variables and ERexpert informs the user through the "System Reminder", a text bar at the bottom of the window (B), that a successful search process has been completed. By clicking on appropriate icons, the system is prompted to show corresponding information about the target chemical in a display window (B). Figure 9B shows a report sheet of the

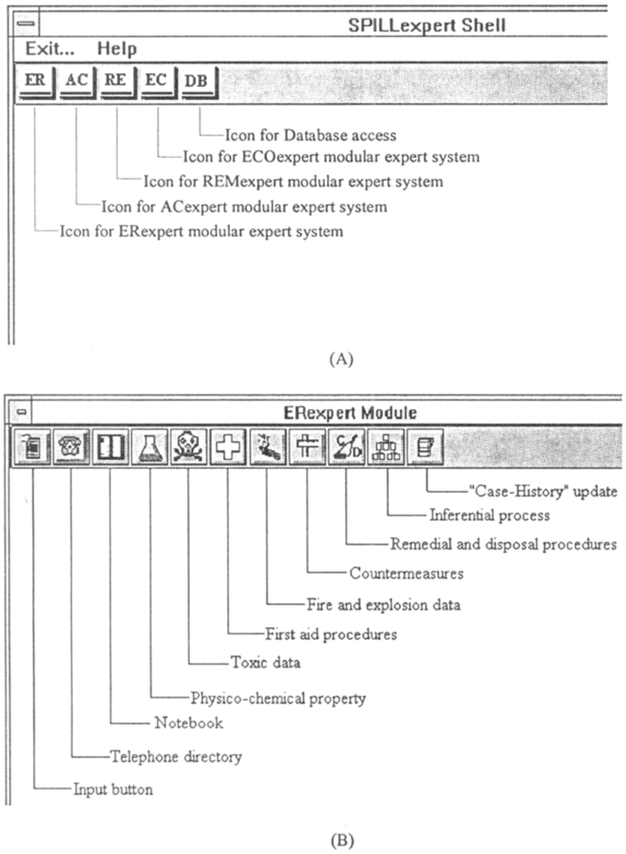


Figure 7. The graphical user interface developed for SPILLexpert operates in MS Window 3.1 environment. Part A shows the main window of the SPILLexpert program in which five icons connect to five stand-alone modular expert systems embodied in this main frame. In part B, the first screen of ERexpert is displayed in which an icon set is illustrated and briefly explained. This icon set provides the user with a full access to the embedded functions.

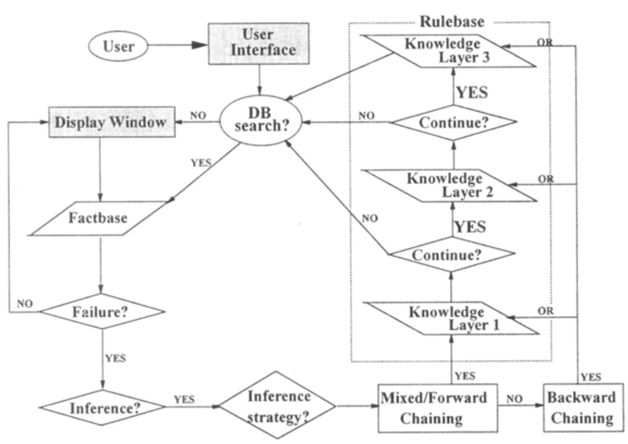


Figure 8. The operational sequence of ERexpert. First, a database search process, followed by inference processes. Three inference strategies, forward backward and mixed chaining, are incorporated into the program, the chaining mode needs to be selected at the beginning of each inference process.

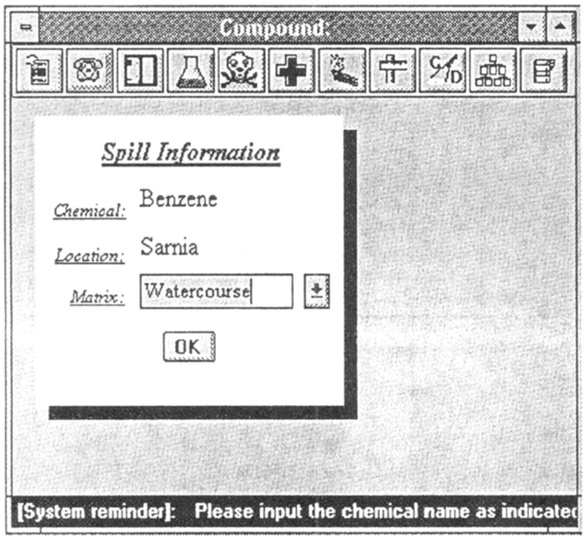
physico-chemical properties of the target compound (i.e., benzene). Customized report sheets were designed as the output medium to show the results of Factbase search in a more organized and easy to read format.

On the other hand, if the target compound is not currently included in the Factbase, ERexpert returns a failure message for the Factbase search process and prompts the user to start an inference process. As shown in Figure 8, one of the three inference strategies incorporated into the program, mixed chaining, forward chaining, and backward chaining, needs to be selected at the beginning of each inference process. In practice the mixed chaining mode is the most commonly used inference strategy.

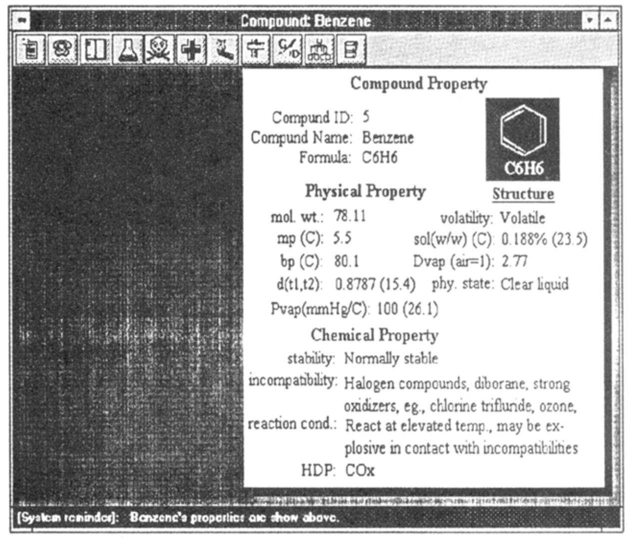
The template shown in Figure 9C is the window designated for the mixed chaining mode. In this mode, a set of questions will be prompted by the system. The order of the questions presented by ERexpert is dynamic in that it is decided by statistical analysis of the knowledge matrix based on the answers to the previously asked questions. Once a unique set of questions has been answered, the particular conclusion that satisfies this question set is identified by the inference engine and displayed in a result dialogue box. The forward chaining mode can be fast but is only appropriate if the user is certain that all the symptoms can be identified correctly. In this process, the system will present an entire selection of symptoms to the user, from those selected the engine will conduct its reasoning based on the answers without further questioning. The backward chaining mode is the best choice if part of the knowledge matrix can be identified as the causes of a problem. This inference process is made possible because the arrangement of the knowledge in KDM is goal oriented. Significantly fewer questions will be asked in this mode because only those questions that are related to the selected goal variable need to be answered. EAengine is capable of making suggestions even if incomplete information is used. In order to do this, the inference engine counts the number of hits (Q) in a partially fulfilled inferential process and compares this number to the number required to fire the rule (C). Then it calculates the probability of the suggested conclusion(s) and displays the result(s) as confidence factor [$CF=(Q/C)\times 100\%$]. In the final display, the suggested answers are ranked according to the CFs. Once an inference process has been completed following the operation sequence shown in Figure 8, the user can either apply the suggestions to direct another search of the Factbase to gather more factual information or use them directly in the response planning.

A number of specific functions have been built into the ERexpert module. For example, as shown in Figure 7B access is provided to a directory of the regional response centers (RRCs). A notebook is available for recording information important to the response process; once clicked, a template will appear on the screen, and the text written there can be systematically backed-up or saved-on-exit as files using *date* plus extension *txt* as filenames in a subdirectory in the ERexpert main directory (..\Diary). The multitasking ability inherent in MS Windows enables this notebook to be left open and accessed during the whole response operation. The textual information written in the notebook can be readily integrated into the "Case-History" subdatabase as a record of an individual case, and an update function is embodied in the user interface for this purpose. These case records result from use of the ERexpert program and therefore shall be evaluated against their application significance to decide whether to be included into the Case-History subdatabase. This is a quick upgrade that only modifies the "Case-History" subdatabase; the subject-oriented factual tables in the Factbase will not been changed. A full scale update of the Factbase requires the user to perform a series of integration on each of the subject-oriented tables. This process requires not only the collection of factual information but also the knowledge on both MS ACCESS and the design of ERexpert database. Unlike the quick update of the "Case-History" subdatabase, the full scale

(A)



(B)



(C)

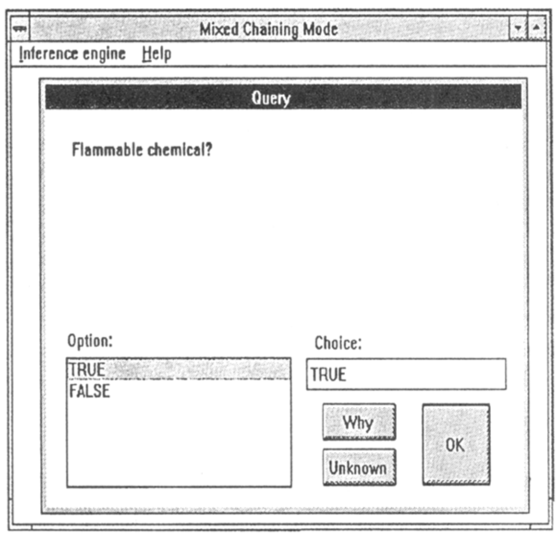


Figure 9. Three examples of screens from the graphical user interface of ERexpert. (A) is the information input dialogue box; (B) is a display window; here the database search result is reported; and (C) is a report from the inference engine; here the mixed chaining inference mode is shown in which questions prompted by EAengine are listed on the top, the option window provides user choices for the questions, the right text box shows the current choice, and the three buttons below are the command buttons for user to confirm the choice.

integration must be conducted by a knowledge engineer. A separate module (***DB***) is built and can be accessed through the SPILLexpert main window (Figure 7A).

5.4. An Example Session of ERexpert. This session assumes an accident involving TOLUENE occurred on unpaved ground near the side of a highway under normal weather condition. According to the operation sequence in Figure 8, ERexpert first searches the Factbase and because TOLUENE is not included in the current database, this search fails. If the inductive process is initiated and the mixed chaining mode is chosen, the user needs to answer a set of questions prompted by the system. The question sequence is as follows:

Knowledge Layer 1 (*CateID*):

Q1: Highly volatile chemical?

A1: NO

Q2: Liquid chemical?

A2: YES

Q3: Density (liquid/solid) less than water?

A3: YES

Q4: Flammable chemical?

A4: YES

Therefore, the inference process based on Knowledge Layer 1 reaches a conclusion, and the system prompts for further reasoning through a dialogue box. As demonstrated in Figure 8, if further reasoning is required, the inference engine combines the current conclusion that the CateID is equal to Cate2B (category for flammable liquid chemicals), with new conditions in an effort to identify further conclusion(s).

Knowledge Layer 2 (ContTech):

Q5: Mechanical failure?

A5: NO (or previous mechanical failures have been fixed)

Q6: Spill happened on land?

A6: YES

Q7: Dry surface?

A7: Unknown (do not care since a liquid chemical was involved in the accident)

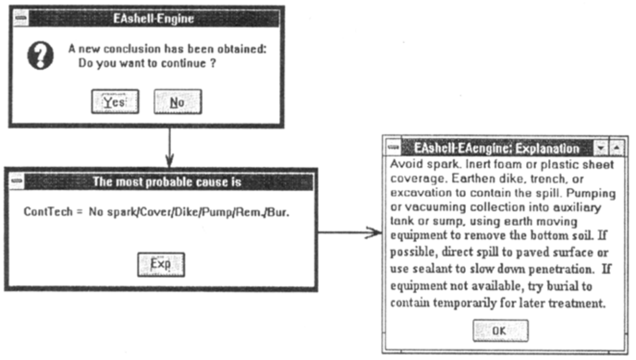


Figure 10. Dialogue boxes for the inference process used in ERexpert. The top dialogue provides communication between the inference engine and the user and allows the user to decide whether a further search is required. The conclusion box shows a brief conclusion, and the dialogue box gives a more detailed explanation of the conclusion.

Q8: Cate2B chemical?
A8: YES (the previous inferential result)
Q9: Soft ground/river bottom?
A9: YES

Since TOLUENE belongs to a group of less volatile and flammable liquid chemicals, ERexpert suggests that it is possible that fire and explosion may occur following such an accident; therefore, if possible, proper coverage of the spill site is recommended to minimize the spreading of the vapor, and no sparks should be allowed in the accident area. Next, possible containment and clean up procedures for the spill are given: these include a combination of the construction of earthen dikes and trenches and the removal of bottom soil. Figure 10 shows the dialogue boxes in which the conclusion and explanation are given. Detailed instructions about the usage of equipment and possible precautions may be found in the auxiliary tables in the Factbase accessed by the CateID.

It is important to note that the way in which the system proposes subsequent questions is based on a statistical analysis of the knowledge matrix; therefore, the order of the rules in the KBF file is a significant factor in deciding with the overall performance of the inference engine. The general principle is to place the rules in the order of importance, the rules that are most frequently used should be put at beginning of the KBF file. EAengine accepts three answer options: positive confirmation (YES, TRUE), negative confirmation (NO, FALSE), and no confirmation (UNKNOWN, DON'T KNOW). Sometimes, the last option can be interpreted as DON'T CARE. It is found that the way a question is answered may affect the number of questions asked by the inference engine though the final conclusion stays the same. This is because in order to completely represent the domain expertise, the same condition may occasionally be presented twice in the knowledge matrix. Therefore, in the inference process, especially when multistep induction is involved, one question can appear more than once. Depending on the nature of the question, such questions can be answered differently. For example, the answer to question 7 in the example above can be either "YES" (we had assumed normal weather condition for this session) or "UNKNOWN" (don't care), but we find that the two different answers result in two totally different sequences of questions. A "YES" to Q7 will generate a question sequence consisting up to 17 questions instead of five listed above when the answer was UNKNOWN in the second round of reasoning (Knowledge

Table 2. Relationship between the Answers Chosen and the Question Sequences in a Study Session Using the TOLUENE Spill Case[e]

Sequence 1 [a] *(Random RULE order)*	Sequence 2 [b,1] *(Structured RULE order)*	Sequence 3 [b,c] *(Structured RULE order)*
Q1: Mechanical failure?	Q1: Mechanical failure?	Q1: Mechanical failure?
A1: NO	A1: NO	A1: NO
Q2: Category 1A chemicals?	Q2: Spill happened on land?	Q2: Spill happened on land?
A2: NO	A2: YES	A2: YES
Q3: Sheltered area?	Q3: Dry ground surface?	Q3: Dry ground surface?
A3: NO	A3: YES	A3: YES
Q4: Category 1B chemicals?	Q4: Category 2A chemicals?	Q4: Category 2A chemicals?
A4: NO	A4: NO	A4: NO
Q5: Spill happened on land?	Q5: Category 3A chemicals?	Q5: Category 3A chemicals?
A5: YES	A5: NO	A5: NO
Q6: Dry ground surface?	Q6: Liquid state?	Q6: Liquid state?
A6: YES	A6: YES	A6: UNKNOWN (don't care)
Q7: Category 2A chemicals?	Q7: Flammable?	Q7: Category 2B chemicals?
A7: NO	A7: YES	A7: YES
Q8: Category 3A chemicals?	Q8: Volatile?	Q8: Soft ground surface?
A8: NO	A8: YES	A8: YES
Q9: Liquid state?	Q9: Category 4A chemicals?	
A9: YES	A9: NO	
Q10: Flammable?	Q10: Category 4B chemicals?	
A10: YES	A10: NO	
Q11: Volatile?	Q11: Category 4C chemicals?	
A11: YES	A11: NO	Sequence 4 [b,d,2]
Q12: Category 4A chemicals?	Q12: Category 4D chemicals?	*(Structured RULE order)*
A12: NO	A12: NO	Q1: Mechanical failure?
Q13: Category 4B chemicals?	Q13: Category 4E chemicals?	A1: NO
A13: NO	A13: NO	Q2: Spill happened on land?
Q14: Category 4C chemicals?	Q14: Category 4F chemicals?	A2: YES
A14: NO	A14: NO	Q3: Dry ground surface?
Q15: Category 4D chemicals?	Q15: Category 3B chemicals?	A3: UNKNOWN (don't care)
A15: NO	A15: NO	Q4: Category 2B chemicals?
Q16: Category 4E chemicals?	Q16: Category 2B chemicals?	A4: YES
A16: NO	A16: YES	Q5: Soft ground surface?
Q17: Category 4F chemicals?	Q17: Soft ground surface?	A5: YES
A17: NO	A17: YES	
Q18: Category 3B chemicals?		
A18: NO		
Q19: Category 2B chemicals?		
A19: YES		
Q20: Soft ground surface?		
A20: YES		

[a] Unstructurted RULES in a random order in the KBF file. As a result, irrelevant questions are asked by the system. [b] Structured RULES placed in the order of importance in the KBF file. This improves the system's performance by eliminating the irrelevant questions asked in Sequence 1. [c] An answer of UNKNOWN (DON'T CARE) to any one of Q6 ~ Q8 of the questions asked in Sequence 2 will force the system to an abandon unnecessary "deeper" reasoning loop to select the most obvious conclusion(s). [d] This is the best answer sequence and was illustrated in the text because it clears any ambiguity in the answers to force the system to identify the most obvious conclusion. [e] Superscripts 1 and 2: these two question sequences are used as examples in the text.

Layer 2), although the final conclusions are identical. We investigated why this happened by examining the chemical significance of the two different answers to the same question. In this example, a "YES" to Q7 implies that the dryness of the ground becomes a significant factor in considering potential response actions. Such a possibility forces EAengine to search deeper reasoning loops to consider the physical state of the spilled chemical(s), because solid chemicals may be fluidized by the wet ground and that may alter the selection of the response actions. On the other hand, wet ground may not affect the response dramatically for liquid chemicals. As a result, more questions are asked in order to get a clearer definition of the spilled chemical. In Table 2, more detailed results are listed from a thorough study of the relationship between the answer options and question sequences. The results also show that the order of the ASK in the user query section of a KBF file does not affect the question sequence chosen by the inference engine.

6. DISCUSION AND CONCLUSIONS

6.1. Task Characterizations. A number of expert systems have been developed in the chemistry domain.[37,38] These systems are concerned with three large fields of research: instrumental diagnosis, data interpretation and structure elucidation, and synthesis planning. Instrumental diagnosis deals mainly with verbal expression of human expertise, and the target domains are bound to specific instrumentation and are, therefore, clearly defined.[12,13,23,24] On the other hand, data interpretation and structure elucidation expert systems deal largely with numerical data in which a specific analytical instrument is involved and interdiscipline overlaps are not often observed.[25-28] Traditional planning-type expert systems in the chemistry domain have a similar character, for example, the determination of synthetic pathways for a given organic compound.[29-31] Recently, Olivero *et al.*[32] have described the development of an expert system to assist in the selection of experimental plans that ranks 13 types of experimental design according to the suitability to the proposed project.

Nevertheless, the planning task by its nature can be a much more complicated process because it often involves factual information of both textual and numeric formats as well as heuristic knowledge. While response to a spill is typically a planing task, it becomes more difficult because interdisciplinary fields are involved and human experts in this area are specialized in only one of the many aspects and thus are only proficient in one side of the problem. Consequently, for the SPILLexpert project, which aims at the development of an expert system capable of solving all planning tasks in response to spills, the development process becomes more difficult because the knowledge overlap magnifies an already complicated situation. Perhaps the solution to this difficulty is to use segregated development and a systematic integration scheme, an approach first described by Kateman.[33] Using such a scheme, the general expert system framework may consist of many stand-alone modules, and the number is dependent on the application, in which each subsystem focuses on solving a subproblem area of the problem domain. Van den Bogaert *et al.*[34] have also discussed the possibility of building an expert system incrementally by constructing separately developed subsystems into a general framework. The ESCA project has shown that such a process is possible. However, the need to fill the knowledge gap between different stand-alone expert systems may be difficult.[6] The development work on ERexpert has demonstrated that this scheme can be useful in reducing the complexity of a development target, especially when faced with a multidisciplinary domain problem.

6.2. System Update and Knowledge Base Expansion. The knowledge base of the current ERexpert module employs 97 rules that are mainly used to deal with problems from three aspects, including chemical categorization, containment methodology, and treatment-site selection. The menu-item "HELP" is designed to allow users to request definitions of unfamiliar terms used by ERexpert. If ERexpert is to find its way into environmental applications, the program must be flexible and easy to integrate. It should be possible to add new knowledge or adapt the system according to changes in the application environment. The ERexpert prototype can be updated through separate refurbishing of the knowledge base without changing the master computer code. As discussed in the previous paper,[20] the knowledge base developed using the KDM encoding scheme is relatively easy to validate, and one may change the logical relations in certain parts of the knowledge base without upsetting the rest. An expert with little computer skill can modify the knowledge base by adding more knowledge or by rewriting an unclear part.

6.3. Limitations and Perspectives. The ERexpert modular system is still very much in the research phase. The program currently covers most of the containment countermeasures and primary remedial actions in handling spill accidents. However, remedial procedures can be rather complicated and often involve dynamic processes that require mathematical modeling in order to simulate the processes of distribution, degradation, and detoxification of chemicals in the natural environmental. The current ERexpert model does not consider the effects of a complex environmental matrix or weather factors, and, therefore, it is incapable of simulating the response processes dynamically. While mathematical modeling may be an effective approach in the prediction of the distribution of spilled chemicals, we expect to see major research advances to be made in the environmental research area so that the environmental behavior of chemicals, their disruptions to the ecosystem, and their degradation processes in the environment can be more quantitatively described. Kollig *et al.*[2] wrote that experimental conditions cannot be extrapolated to environmental conditions without considerable mathematical manipulation. Nevertheless, our study is valuable because ERexpert not only is a reference tool for field professionals dealing with chemical spills but also provides the possibility for integration of domain expertise and relevant research progress into an expert system in which few applications have been reported. Although, the ERexpert modular system deals with only one subdomain within the spill domain, we expect that the design protocol and knowledge encoding scheme developed through this study are generally applicable for subsequent development of other modular systems in the SPILLexpert project. In the next phase of project development, we plan to implement this protocol into the development of the AC-method modular system. We anticipate that with the multitasking ability of MS Windows, the difficulty in linking the different modular systems can be easily solved.[13]

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