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USE OF SIMPLE THERMODYNAMIC AND STRUCTURAL PARAMETERS TO PREDICT SELF-REACTIVITY HAZARD RATINGS OF CHEMICALS*

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Summary

A major problem in the transportation, transfer and storage of bulk chemicals is the problem of catastrophic instability under unforeseen situations. Numerous calculated thermodynamic, experimental, and structural parameters were evaluated for their ability to predict in advance the stability (self-reactivity) of such chemical substances in order to be able to avoid the undesirable situations. It was concluded that the relationship between the parameters considered and chemical stability is too obtuse for ready conventional statistical analysis. Subsequently, pattern recognition techniques were employed for statistical analyses and 13 of the more promising parameters were evaluated with considerable success. Total under- and overestimation error was less than 10% relative to generally accepted consensus grading into three stability categories: (1) explosive, (2) hazardous polymerization or decomposition, and (3) nonhazardous. The methods, therefore, seem to have great potential for use in minimizing hazards in the transportation, transfer and storage of chemicals.

Introduction

The original purpose was to evaluate and optimize existing computer codes based on classical thermodynamics in regard to their ability to predict chemical stability. Although a number of computer codes, and in a few cases combinations of calculated and experimental parameters, have been suggested [1—5] for hazard prediction, there has been no systematic effort to evaluate the relative power of these approaches in predicting the self-reactivity hazard posed by chemicals. This study had special interest in chemicals currently transported in bulk on U.S.A. waterways, but the approach can be more generally applied.

A number of benefits would occur if a computerized predictive approach for hazard evaluation of chemical systems could be demonstrated. First,

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substantial savings in time and cost could be realized in testing of new chemicals and the task of evaluating the astronomical number of combinations between nearly 1000 chemicals now or soon to be transported in bulk. Also it has been estimated that over a hundred thousand new organic chemicals [6] are synthesized each year in the U.S. While only a fraction of these ever become sufficiently useful to be shipped in bulk, a low-cost way to estimate potential hazard at the R and D stage of development (which might entail transportation of relatively small, but still highly hazardous, quantities of material) would be valuable.

Second, simplification and improvement of hazard rating systems could be undertaken. Many of the current systems are arrived at by consensus, are quite subjective, and may thereby impose unnecessary restrictions (*e.g.*, transportation cost penalties) on some chemicals while allowing others to present excessive risks to human life, the environment, transportation facilities, and equipment. The cost and time penalties for such errors in current hazard rating systems could be reduced by an impartial but accurate computer assessment of hazard.

Finally, unanticipated hazards, which might slip through an experimental hazard test program due to, for instance, critical sample geometry effects such as those frequently encountered, might be identified if a successful computer prediction method is possible.

In all these potential benefit areas, even partial success of a computer simulation might be useful in that it could serve as a screening tool which would concentrate the comparatively expensive experimental evaluations on those chemicals which pose the greatest hazard.

Assessment of self-reactivity energy hazard potential of chemicals has historically been accomplished by:

(1) consulting consensus ratings, which incorporate inputs from full-scale experience, intuition, and laboratory data; or

(2) interpretation of data from laboratory-scale experiments, only recently incorporating round-robin testing and standardization.

Full-scale experiments are generally precluded due to experimental difficulties, environmental impact, and especially costs. Recently, a number of computational approaches have also been attempted.

Background

A number of recent studies have attempted to use thermodynamic evaluations to predict chemical hazard as defined by the National Fire Protection Association (NFPA) "reactivity" rating [1,5] or experimental shock sensitivity data [2]. No attempt has been reported to date, however, to correlate these predictions with other consensus rating systems or to assess the relative power of the various parameters (both calculated thermodynamic quantities and Arrhenius equation experimental data) which have been proposed. Since previous studies have all claimed some degree of success in estimating hazard, an unbiased means of comparison is desirable. Further, since it was previously noted [2] that some combination of four numerical parameters from the American Society for Testing and Materials computer code (CHETAH) seemed to possess substantially better hazard correlation than could be obtained by considering only one or two at a time, a comparison technique capable of simultaneously considering a reasonable number of parameters and rating the relative power of each would be useful.

For the most part, previous hazard correlation studies have not attempted rigorous statistical analysis because classical techniques would have indicated, for the reasons previously discussed, less favorable results than could be intuitively drawn from the authors' graphical presentations or simple rankings.

Although not considered in this study or in previous, comparable studies [1—5] hydrodynamic computer codes developed primarily within the weapons industry have achieved some success in evaluating the response of explosives to varying stimuli. However, their use of non-ideal gas equations of state requires extensive experimental data as input (*e.g.* elastic constants and C_p for the condensed phase), thus precluding or severely limiting use of these codes in screening new chemicals.

Procedure

Consensus hazard rating system

Current hazard rating systems exhibit a marked difference in the definition of terms like "reactivity", a large difference in the degree of subjectivity required to assign a given chemical to a particular hazard class, and in some cases a lumping of more than one type of hazard into the same rating system to facilitate use by a particular group.

To exemplify the diversity of these hazard rating systems, the National Academy of Sciences—National Research Council (NAS—NRC) [7] system breaks reactivity into five distinct rating systems:

"Other chemical"
"Binary compatibility"
"Water"
"Self" and
"Fire",

whereas the National Fire Protection Association (NFPA) [8] lumps many of the same considerations into two rating systems:

"Reactivity"	(shock sensitivity, decomposition or polymerization, reaction with water)
"Flammability"	(ignition and explosive dusts).

For the purposes of this study, the consolidations and equivalences shown in Table 1 were made between the NAS—NRC "Self" rating system and the NFPA "Reactivity" system. Whenever reactivity with water was felt to influence the NFPA rating, the NAS—NRC "Water" rating was consulted and appropriate interpretations considered. It is felt that these consolidations

TABLE 1

Consolidated rating system for NAS—NRC and NFPA reactivity

Characterization in this study*	NAS—NRC Self	NFPA Reactivity
(1) Nonhazardous	0, 1	0
(2) Hazardous decompositions or polymerizations	2, 3	1, 2
(3) Explosives	4	3, 4

* Subjective due to inherent characteristics of consensus rating systems.

are more than justified after consideration of the relative lack of discrimination between NAS—NRC "Self" grades 0 and 1 (both nonhazardous reactions) and grades 2 and 3 (reflecting the stabilizer requirement more than the severity of the chemical reaction), and between NFPA "Reactivity" grades 1 and 2 (both capable of hazardous reactions but not explosions) and grades 3 and 4 (both capable of explosion at unspecified levels of initiation conditions). It was noted, however, that there was still no complete reconciliation between the ratings, and differences among several of the chemicals encountered in this study created difficulties especially in regard to the statistical analysis. The methodology used was, by computerized thermodynamic models, to predict whether a compound was reactive or not and then to assign it a rating based upon statistical pattern recognition and compare the rating thus obtained with consensus ratings.

Thermodynamic reactivity calculations

The overall flow of input thermodynamic data, calculated parameters, and experimental data is shown schematically in Fig. 1. The various thermodynamic computer programs indicated on this chart have been described elsewhere [1—5, 9—12], except for EQUICA, which was developed at Battelle based on the work of Cruise [13]. However, an overall comparison has not been previously accomplished. In terms of the algorithm used to compute

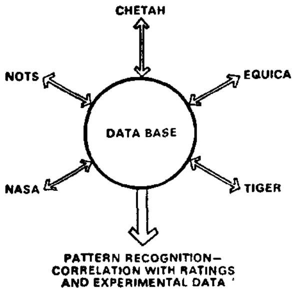

Fig. 1. Flow of input data, calculated parameters and experimental data.

the thermodynamic equilibrium conditions, these codes can be categorized as using minimization of Gibbs free energy (designated ΔG min.), the modified equilibrium constant approach (designated "mod. K"), or enthalpy maximization (designated ΔH max.), as indicated in Table 2. CHETAH also calculates two additional hazard criteria, oxygen balance and enthalpy of combustion.

TABLE 2

Categorization of thermodynamic codes

Code	Characteristic		
	ΔG min.	mod. K	ΔH max.
(A) Classical thermodynamic			
NASA	X		
NOTS		X	
TIGER		X	
EQUICA		X	
(B) Modified thermodynamic			
CHETAH			X

The comparative flexibility of these codes is shown in Table 3. In order to cover the possible range of types of calculations, either the NASA or TIGER codes plus CHETAH are indicated. Since only enthalpy—pressure (*HP*) calculations and enthalpy maximization (CHETAH) have been employed in hazard modeling in the past however, NOTS could also be used.

TABLE 3

Comparative flexibility

Type calculation*	NASA	TIGER	NOTS	CHETAH	EQUICA
TP	X	X	X		X
HP	X	X	X		
SP	X	X			
TV	X	X	X		
UV	X	X			
SV	X	X			
H max.				X	

*The symbols T, P, H, S, U, and V relate to the conventional thermodynamic properties shown as follows: T: Temperature (K); P: Pressure (atm); H: Enthalpy (kcal/mole); S: Entropy (kcal/mole-K); V: Specific volume (m^3/kg); U: Internal energy (kcal/mole).

Specification of any two in the pairs shown defines the thermodynamic system. In order to select which code(s) to use on this study, other criteria were also considered (Table 4).

TABLE 4

Criteria used to select code(s) for this study

Code for reactivity calculations	Ease of use	Public availability
NASA—LRC	1	1
NOTS	2	2
EQUICA	2	3
TIGER	3	3
CHETAH	1	1

Key: 1 = good; 2 = fair; 3 = bad.

Theoretically, it would be expected that each code would give identical results for the same type of calculation regardless of the algorithm used. To confirm this, representative compounds were run on various codes and comparisons of predicted decomposition temperatures (Table 5), equilibrium composition (Table 6), and other parameters were made. NASA code was subsequently selected for use in this study (in conjunction with CHETAH) for the following reasons:

(1) Maximum flexibility;

(2) Superior ease of use and compatibility with Battelle's Control Data Computer system;

(3) Superior public availability (National Technical Information Service);

(4) Incorporation of a "trace" option enabling prediction of low concentration combustion products.

Minor modification of this code (< ~ a dozen additional FORTRAN statements) was required to calculate pressures for the reaction products at equilibrium temperatures in a molar volume using the ideal gas equation of state and reaction enthalpies (ΔH_R):

$$\Delta H_R = \sum_{i=1}^{NP} C_i H_i - \sum_{j=1}^{NR} C_j H_j$$

TABLE 5

Comparison of temperatures and decomposition, T_D, calculated by NOTS and NASA codes

Chemicals	NOTS T_D, K	NASA T_D, K
Nitroethane	1161	1161
Epichlorohydrin	1042	1042
Acrylonitrile	1896	1891
Nitrobenzene	1540	1538
Acetic acid	652	655
Butyraldehyde	800	801
Propylene oxide	951	951

TABLE 6

Comparative equilibrium composition calculation (thermal decomposition of acrylonitrile at 1300 K and 1 atm pressure)

Species	Concentration of species (moles)	
	EQUICA	NASA
HCN	3.459×10^{-5}	3.5258×10^{-5}
NH_3	1.746×10^{-5}	1.6047×10^{-5}
C(s)	6.004×10^{-1}	6.0034×10^{-1}
H_2	2.970×10^{-1}	2.9756×10^{-1}
N_2	1.004×10^{-1}	1.0032×10^{-1}
CH_4	2.121×10^{-3}	1.7257×10^{-3}
H	4.503×10^{-7}	3.7969×10^{-7}
C_2H_2	1.789×10^{-7}	2.0284×10^{-7}
CH_3	4.831×10^{-8}	5.1507×10^{-8}
H_2N	2.699×10^{-10}	3.0380×10^{-10}

where NP = number of products, NR = number of reactants, C = moles of species, H = enthalpy of formation of species at 298 K from elements in standard states.

Decomposition and stoichiometric oxidation reaction calculations were accomplished in the CHETAH and NASA codes, inputing 1 mole quantities of each of the 20 chemicals selected for reactivity study. Whenever available, enthalpies of formation for the compound's transportation state (solid, liquid or gas) were used as input to the NASA code for the HP-type calculation; however, it was noted that the calculated parameters were highly dependent on the state and associated enthalpy of formation. It was discovered that calculated parameters were dependent on the precision carried through the calculations and also on the species considered. For example, identical results were achieved as previous studies [1] when the same precision and products were considered, but when more product species and greater mathematical precision were employed, results differing as much as 5% were obtained. For the most part, however, virtually identical results were obtained as shown in Table 7 for acetylene.

Statistical evaluation

Early in the course of this study, it was recognized that the relationship of hazard with the calculated and experimental parameters was too subtle to be amenable to standard statistical evaluation. Hence, pattern recognition techniques were employed in the statistical evaluations of this study.

The basic premise of pattern recognition is that the samples can be considered in an abstract mathematical sense as points in an n-dimensional space (hyperspace), with coordinates which are related to the measured or calculated parameters [14—18]. The objective is then to determine if the parameters are

TABLE 7

Results obtained for acetylene using NOTS and NASA codes

Property*	Units	Definition	NOTS	NASA
T_D	K	Temperature of decomposition	2898.3	2900
H_D	kcal/mole	Enthalpy of decomposition	−48.3	−48.2514
P_D	atm	Pressure of decomposition	10.3	10.2514
T_O	K	Temperature of oxidation	3341.4	3341
H_O	kcal/mole	Enthalpy of oxidation	−116.9	−116.9132
P_O	atm	Pressure of oxidation	49.6	49.623

*Same species as Stull [1].

sufficient to properly place the samples in unique classes and which parameters are most important for this classification.

A comparison of pattern recognition *versus* classical statistics reveals a number of common elements and several elements of artificial intelligence unique to pattern recognition (Table 8). In general, classical statistics is preferred because of the concept of "confidence levels", which can be applied to most data sets being evaluated. However, when the relationship between the variables is obtuse, the greater power of pattern recognition will enable useful relationships to be derived whereas the classical approaches will fail. The subjective confidence criteria based on experience in the case of pattern recognition analysis imposes additional concern that a "representative" sample as large as possible be used in the analysis.

TABLE 8

Comparison of pattern recognition and classical statistics

PATTERN RECOGNITION VERSUS CLASSICAL STATISTICS

Common elements

Variance
Covariance
Principal component analysis
Linear discriminant classification

Unique elements of artificial intelligence in P.R.

Linear learning matching
  (negative feedback training)
Piece-wise continuous threshold logic units

↓

Adaptive learning networks

↓

Pattern recognition classification

Findings

Previous work evaluation

Reevaluation of previous computational approaches to model the NFPA reactivity rating [1,4] resulted in considerable scatter using this study's consolidated rating system. The $(T_O - T_D)$ *versus* T_D plot, as originally proposed by Stull [1] to place chemicals into risk categories where the risk is proportional to the zone number, shows a characteristic degree of scatter for 45 chemicals listed in Table 9 when only these two variables are considered (Fig. 2) and the same scatter was noted on the original plot. Especially disconcerting about this is the degree to which explosive chemicals (NFPA grades of 3 and 4) are intermixed with the nonexplosives. However, upon instituting the pattern recognition techniques [16] and using all 6 variables simultaneously (T_D, H_D, P_D, T_O, H_O *and* P_O) for the same 45 NFPA-graded chemicals, only 3 classification errors remained using binary linear classification [16]:

Compound	Actual Grade	Computed Grade
Acetylene	3	2
1,3—Butadiene	2	1
Styrene	2	1

This corresponds to about 7% underestimation of hazard, nil overestimation, and 7% total error. The relative power of the variables was evaluated by the pattern recognition program and found to be

H_O	0.77,	P_D	0.60,	H_D	0.25,
P_O	0.70,	T_D	0.44,	T_O	0.08.

It should be noted that only monomers were incorrectly classified.

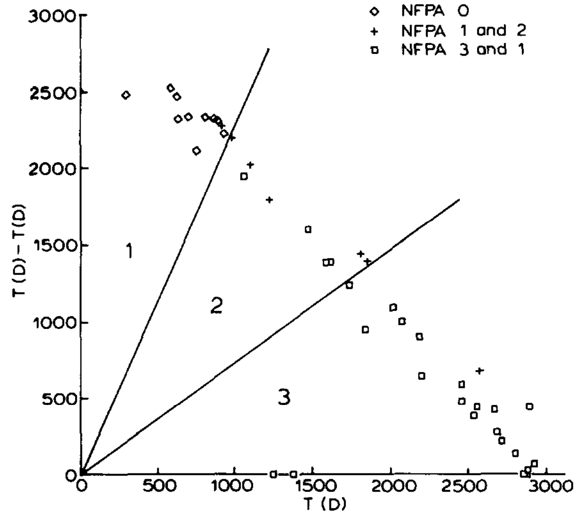

Fig. 2. Scatter in hazard data using plot of $T_O - T_D$ *versus* T_D and consolidated NFPA rating.

TABLE 9

NFPA-rated chemicals originally evaluated by Stull [1]

Glycol dinitrate
Nitrocellulose 14.14%
Manitol hexanitrate
Dipentaerythritol hexanitrate
Gylcerolmonolactate trinitrate
Nitroglycerine
Polyvinyl nitrate
Tetryl
Beta HMX
Cyclonite RDA
1,3,5—Triamino—2,4,6—trinitrobenzene
1,3—Diamino—2,4,6—trinitrobenzene
Metriol Trinitrate
Nitroguanidine
Ethylenedinitramine
Ammonium picrate
2,4,6—Trinitroaniline
1,2,4—Butanetrioltrinitrate
Ammonium perchlorate
Picric acid
Ammonium nitrate
Diethyleneglycol dinitrate
Triethyleneglycol dinitrate
2,4,6—Trinitrotoluene
2,4—Dinitrophenol
Acetylene
Nitroethane
Hydrogen cyanide
Allene
Methylacetylene
1,3—Dichloropropene
1,3—Butadiene
Styrene
4—Nitroaniline
Cyclopropane
Biphenyl
Benzene
Butene—1
Aniline
1,3—Dichloropropane
Acetone
Propane
Octane
Cellobiose (wood)
Acetic acid

Current work

In view of the lack of clear discrimination (clustering tendency) between the hazard grades, it was decided to increase the sample size as much as possible beyond the 20 compounds originally selected for this study (Table 10).

TABLE 10

Original chemicals for reactivity study

Acetaldehyde
Acrylonitrile
Adiponitrile
Epichlorohydrin
Ethylene oxide
Ethylenimine
Hydrazine
Hydrogen peroxide, 50%
Methyl vinyl ketone
Mononitrobenzene
Nitroethane
Nitromethane
Nitropropane
Propargyl bromide
Styrene
Sulfur dioxide (liquid)
Tetraethyl lead
2,4—toluene diisocyanate
Vinylidene chloride
White phosphorus

Consideration of the 20 chemicals originally selected for this study plus the 45 of Stull [1] just discussed resulted in the errors shown in Table 11 using the binary linear classification method of pattern recognition.

TABLE 11

The errors resulting using the binary linear classification method of pattern recognition on the six Stull [1] parameters

Compound	Consensus grade	Pattern recognition computed grade
Acetylene	3	2
1,3—Butadiene	2	1
Styrene	2	1
Tetraethyl lead	3	2
Total underestimated	4	
Hydrogen cyanide	2	3
Hydrazine	2	3
Epichlorohydrin	2	3
Adiponitrile	1	2
Total overestimated	4	
1,3—Dichloropropene	2	ND*
4—Nitroaniline	2	ND*
Propargyl bromide	3	ND*
Total ND*	3	

*No decision.

Calculation of errors thus gives about 6% underestimated, 6% overestimated, and about 12% total combined error. Again, a significant portion of the total error was due to monomers. The relative power of the six parameters on this data set was found to be essentially the same as before:

H_O	0.66,	P_D	0.45,	H_D	0.27,
P_O	0.64,	T_D	0.36,	T_O	0.22.

Other previous work [4] to model the NFPA reactivity rating using a "reaction hazard index" (RHI) based on the parameters of temperature of decomposition (T_D) and activation energy (E_A) of the Arrhenius equation also shows considerable scatter. For example, an RHI of 3.5 in that work could be interpreted as an NFPA reactivity rating of 0, 1, 2, 3, or 4. Using pattern recognition of these same parameters and 43 of the same compounds, the errors shown in Table 12 were observed using binary linear classification pattern recognition.

All kinetic data were taken from critically assessed compilations by Stull [4] or Benson [22].

This corresponds to about 20% underestimation error and about 15% overestimation error for a total error of about 35%. The relative power for the parameters was:

T_D	0.85,
E_A	0.38.

TABLE 12

The errors observed using binary linear classification pattern recognition on T_D and E_A

Compound	Consensus grade	Pattern recognition computed grade
Underestimated		
Acetic acid	2	1
Diethyl carbonate	2	1
Isopropyl ether	2	1
Ethylene oxide	3	2
Nitroethane	3	2
1—Nitropropane	3	2
Tert-butyl peroxide	3	2
Tert-butyl hydroperoxide	3	2
Diethyl peroxide	3	2
Total underestimated	9	
Overestimated		
Formic acid	1	2
Cyclopropane	1	2
1-Butone	1	2
Toluene	1	2
Dicyclopentadiene-endo	2	3
Vinyl allyl ether	2	3
Total overestimated	6	

Incorporating an additional term of the Arrhenius rate equation, the pre-exponential log A factor, along with T_D and E_A on these same 43 compounds gave the errors shown in Table 13 using binary linear classification.

The incorporation of the log A factor thus improves the underestimation error to about 15% from 20%, the overestimation error to about 10% from 15% and the overall error to 25% from 35%. The relative power of each of these parameters was:

T_D	0.85,
E_A or E_D	0.38,
$\log A$	0.29.

Using CHETA parameters, NAS—NRC ratings, and 26 chemicals selected for this study plus 19 from another recent study [9], the errors shown in Table 14 were observed using binary linear classification.

These result in about 7% overestimated and 13% underestimated for a total error of 20%. With the CHETAH parameters nearly all the error was again associated with monomers. All four parameters seemed to have about equal weight as shown below:

TABLE 13

The errors found by adding log A to T_D and E_A, using binary linear classification classification

Compound	Consensus grade	Pattern recognition computer grade
Underestimated		
Acetic acid	2	1
Propylene	2	1
Iso-propyl ether	2	1
Ethylene oxide	3	2
Nitroethane	3	2
1-Nitropropane	3	2
Total underestimated	6	
Overestimated		
Cyclopropane	1	2
1-Butene	1	2
Tert-amylacetate	1	2
Dicyclopentadine	2	3
Total overestimated	4	

TABLE 14

The errors found using binary linear classification on four CHETAH parameters

Compound	Consensus grade	Pattern recognition computed grade
Underestimated		
Ethylene oxide	3	2
Epichlorohydrin	2	1
Methyl vinyl ketone	2	1
Nitrobenzene	1	2
Styrene	2	1
Vinyl acetate	2	1
Total underestimated	6	
Overestimated		
Hydrazine	2	3
Vinylidene chloride	2	3
Vinyl chloride	2	3
Total overestimated	3	

CHETAH criterion	Parameter	Relative power
1	$H_{\mathrm{max.}}$	0.56
2	H_C–$H_{\mathrm{max.}}$	0.56
3	O_2 bal.	0.68
4	Mod. $H_{\mathrm{max.}}$	0.58

In order to elucidate the monomer classification problem, the six equilibrium parameters of Stull [1] were coupled with a free radical resonance stabilization factor and heat of polymerization [19—21] for the 45 compounds treated by Stull [1] plus 20 selected for this study. Errors were found to consist of those shown in Table 15.

TABLE 15

The errors using binary linear classification on six Stull [1] parameters plus resonance stabilization and heat of polymerization

Compound	Consensus grade	Pattern recognition computer grade
Acetylene	3	2
Toluene—2,4—diisocyanate	2	1
Total underestimated	2	
Hydrogen cyanide	2	3
1,3—dichloropropene	2	3
Hydrazine	2	3
Epichlorohydrin	2	3
Total overestimated	4	
4—nitroaniline	1	ND*
Acetaldehyde	2	ND*
Vinylidene chloride	2	ND*
Adiponitrile	1	ND*
Tetraethyl lead	3	ND*
Total ND*	5	

*No decision.

Projection of the sample points in n-dimensional space into two dimensions, as shown in Fig. 3, provides a means of subjectively evaluating relative "clustering" of sample points. This has no bearing on classification and is merely a visual input to assist in interpretation of the complexity of the problem The two axes of such mappings are linear functions of the input parameters, but the numerous and variable processing steps make each mapping unique for the particular case under study.

The pattern recognition yielded about 3% underestimation and 6% overestimation for a total error of less than 10%. It was noted that substantially

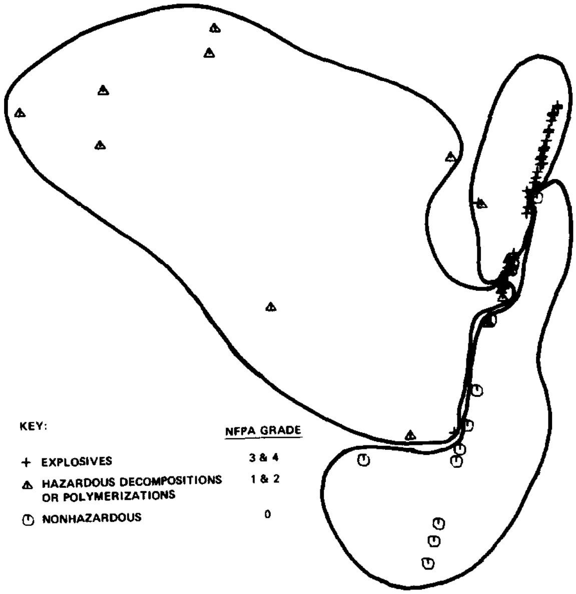

Fig. 3. Mapping - - Stull [1] parameters, heat of polymerization and resonance stabilization factor.

greater clustering occurred on the mapping than on previous cases, and, overall, the separation of explosives, hazardous self-reactive chemicals, and non-hazardous chemicals was quite good.

The relative power of the parameters considered on this case was:

Resonance stabilization	1.15,
P_O	0.64,
H_O	0.63,
P_D	0.39,
T_D	0.31,
H_D	0.24,
H_{poly}	0.24,
T_O	0.17.

Conclusions

It is concluded that a new technique is in the process of development for the prediction of hazards associated with chemicals' self-reactivity. On the basis of the reactivity studies performed in this study, it is also concluded that the thermodynamic parameters originally proposed by Stull and those of CHETAH have approximately the same power to differentiate explosive, hazardous, and nonhazardous chemicals. The relatively small sample size makes further comparison between these two highly subjective. Coupling Arrhenius factors with thermodynamic parameters seemed to have substantially less power than these other approaches, however. Classification of the various parameters considered on the basis of predictive power is somewhat subjective in view of the variation observed from one data set to another, but three categories can be delineated (see Table 16).

TABLE 16

Relative predictive power of parameters for self-reactivity hazard

Predictive power	
High	Resonance stabilization of free radical P_O H_O Four CHETA parameters
Medium	P_D T_D H_D $H_{\text{polymerization}}$
Low	T_O E_A $\log A$

Considering the overall error of less than 10% using less than half of the high power parameters simultaneously, it is felt that even more favorable accuracy can be achieved in modeling consensus self-reactivity hazard class assignment. It is recommended that experimental data be used whenever possible to test hazard models in order to eliminate the subjectiveness and occasional contradiction which exist in varying degrees in the current hazard rating systems. It is felt that most of the nondecisions revealed in this study will be eliminated as the sample size is increased (as the pattern recognition program can better "learn" what a hazardous chemical is), and as more of the significant parameters can be simultaneously considered.

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