Data Extraction: 40 Chemicals from 18 Sources

Report for the NDWAC CCL Work Group

Plenary Meeting

September 17-18, 2003

Attribute Scoring Data Set

- Purpose: extract and organize data for testing proposed attribute scoring approaches for PCCL to CCL classification
- 40 chemicals with a range of data availability
- 18 data sources with a range of data types and formats
- Identify data extraction issues

Attribute Scoring Data Set - 10 chemicals randomly selected from:

- CCL Universe Example Data Set
  - Gate 1
  - Gate 4
  - Chemicals With No Health Effects or Occurrence Data/Info
- National Reconnaissance of Emerging Contaminants (NREC)
  - Now in CCL Universe Example Data Set

Attribute Scoring Exercise Chemicals

Gate 1	Gate 4	Outside Gates	NREC
1,3-Dichlorobenzene	Carbonyl sulfide	(E)-2-Hexenyl butyrate	17a-Estradiol
Boron	1,2-Dibromo-2,4-dicyanobutane	2-Propanol, 1-(tert-dodecylthio)-	5-Methyl-1H-benzotriazole
Chloroethane	2,3,7,8-Tetrachlorodibenzofuran	alpha-Damascone	bis-Phenol A
Dicamba	Aluminum oxide	C.I. Pigment yellow 119	Cimetidine
n-Butylbenzene	Ethylene	Dimethyl trisulfide	Diethylphthalate
Methane, dibromo-	Ethane, 1-chloro-1,1-difluoro-	Flamprop	Equilin
Hexachlorobutadiene	Heptachlorodibenzo-p-dioxin	Isobutyric acid	Lincomycin
Zinc	Isocyanic acid, methyl ester	Naphthalene, 1,2,3,4-tetrahydro-	Phenanthrene
Metolachlor	Phosgene	Phthalide, 6-(dimethylamino)-3,3-bis[p-(dimethylamino)phenyl]-	Tetracycline
Vanadium	Diazomethane	Sodium acid pyrophosphate	Warfarin

Occurrence Sources

- Agency for Toxic Substances and Disease Registry (ATSDR) - Internet HazDat
- United States Geological Survey (USGS) - National Water Quality Assessment (NAWQA) Program
- USGS - National Reconnaissance of Emerging Contaminants (NREC)
- NLM - Hazardous Substance Databank (HSDB)

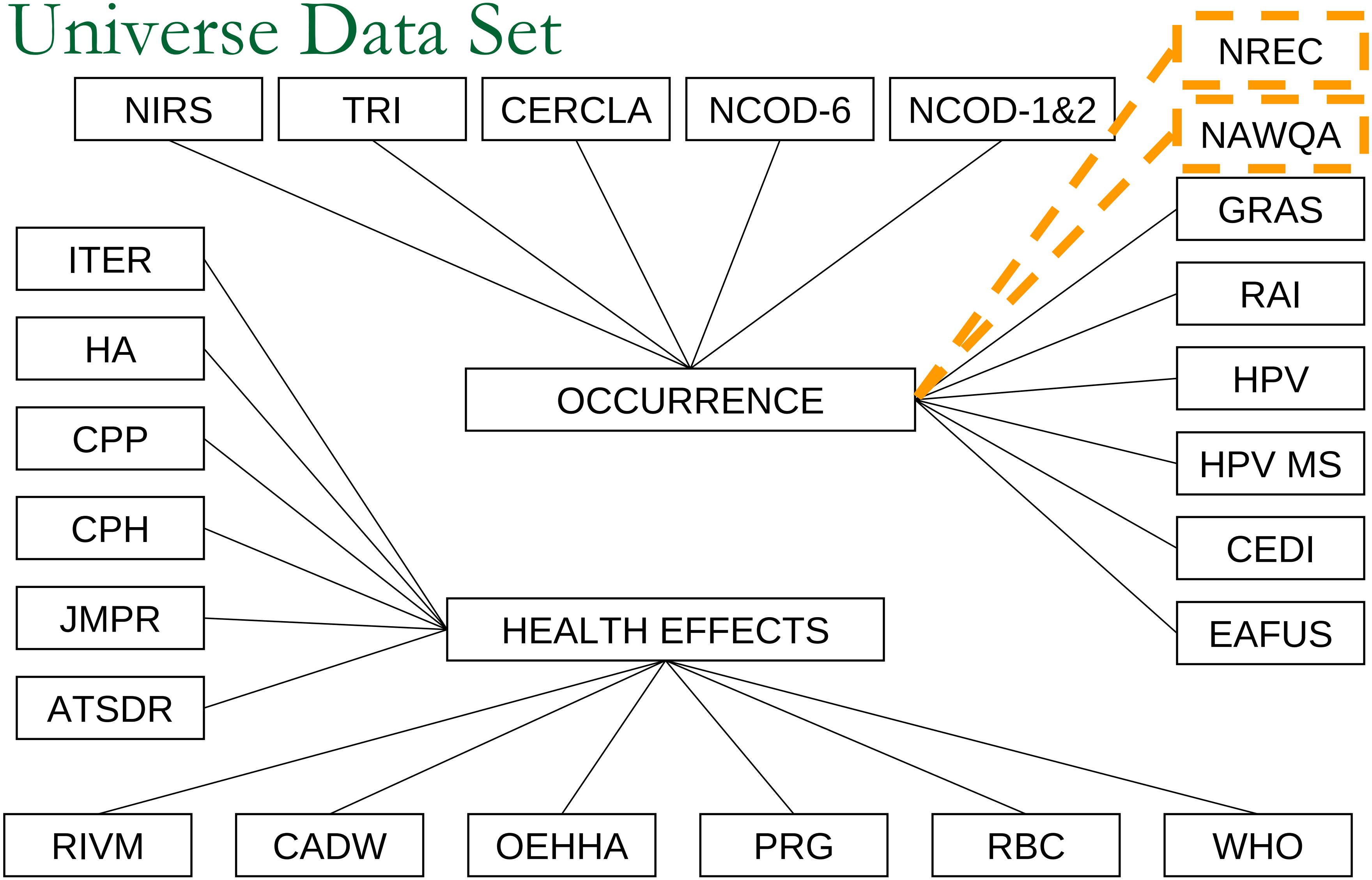
Chemical Property Sources

- National Library of Medicine (NLM) - ChemIDplus
- National Center for Manufacturing Sciences - Solv DB
- Syracuse Research Corporation (SRC) - PHYSPROP database
- NLM - Hazardous Substance Databank (HSDB)

Health Effects Sources

- ATSDR - Toxicological Profiles
- NLM - Chemical Carcinogenesis Research Information System (CCRIS)
- International Programme on Chemical Safety (IPCS) - Concise International Chemical Assessment Documents (CICADs)
- NLM - Developmental and Reproductive Toxicity (DART)
- NLM - Genetic Toxicity (GENETOX)
- NLM - Hazardous Substance Databank (HSDB)
- USEPA - Integrated Risk Assessment System (IRIS)
- IPCS - Joint Expert Committee on Food Additives (JECFA)
- IPCS - Joint Meeting on Pesticide Residues (JMPR) - Monographs
- National Toxicology Program (NTP) - Toxicity & Health/Safety Reports
- Risk Assessment Information System (RAIS) - Toxicity Factors (and supporting data)
- Registry of Toxic Effects of Chemical Substances (RTECS)
- NLM - TOXLINE

25 Data Sources from Example CCL Universe Data Set



Data/Information Downloading

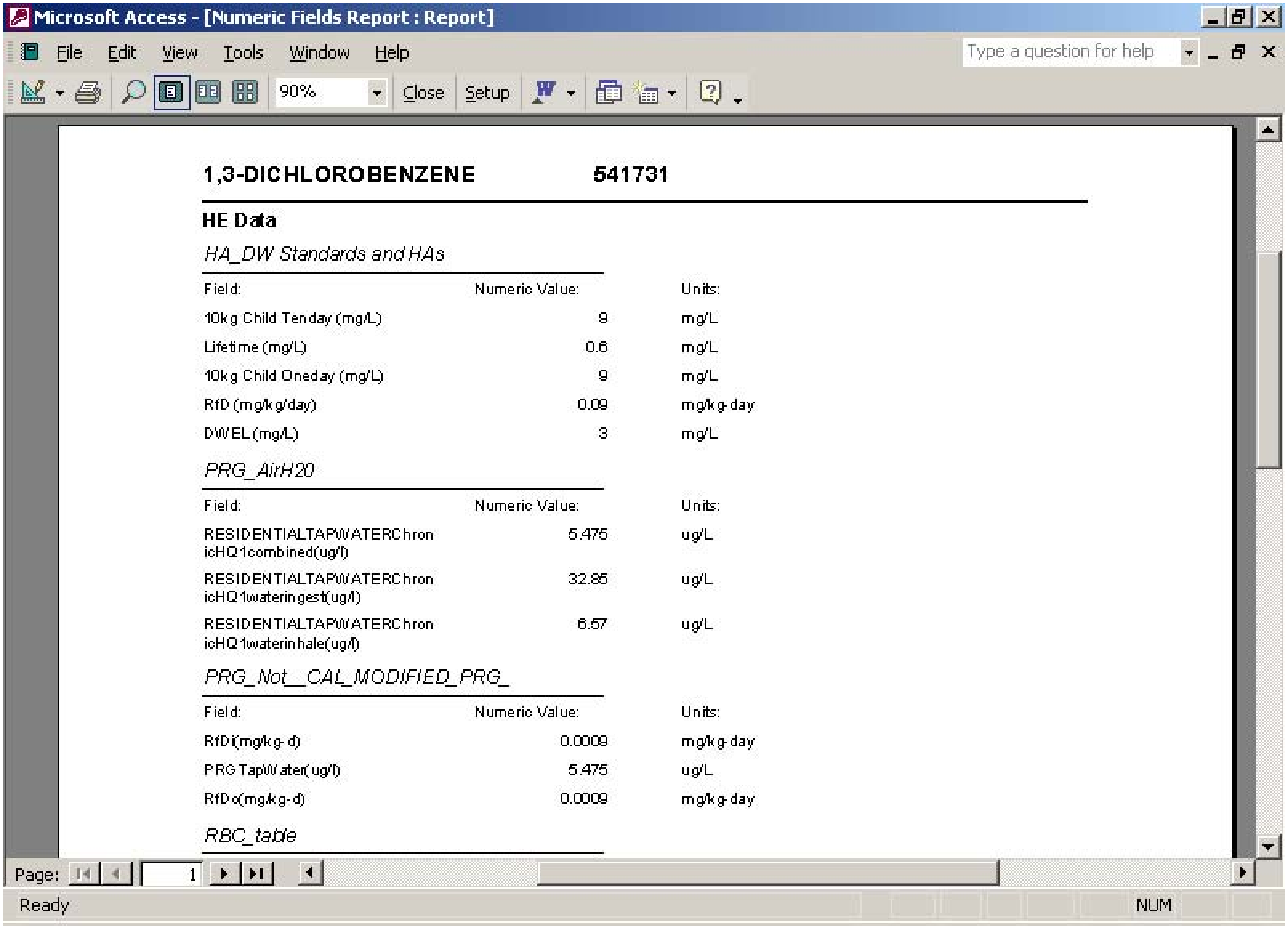
- Tabular Sources (e.g., NAWQA)
  - Downloaded to MS Excel
  - Developed summary statistics
  - Imported to MS Access
- Monographic Sources (e.g., JECFA)
  - Text and data cut and pasted into Access as textual memo fields
- Bibliographic Sources (e.g., TOXLINE, DART)
  - Downloaded to Endnote

Types of Data Elements Obtained

- Health Effects
  - RfD, SF, UR, LO(A)EL, NO(A)EL, LD_{50}
  - Supporting study data (e.g., dose, duration)
  - Absorption, excretion, metabolic data (not obtained)
  - Inhalation-based data (not obtained)
- Occurrence
  - Obtained/developed summary statistics
    - Mean, maximum, ranges, frequency of detection
  - Obtained production/use information
- Chemical property data
  - e.g., solubility, Henry’s Law
  - Half-lives (not found)
  - Production (not found - except HPV list)

Example of Data -1

1,3-Dichlorobenzene - Health Effects Data



1,3-DICHLOROBENZENE 541731

HE Data

HA_DW Standards and HAs

Field:	Numeric Value:	Units:
10kg Child Tenday (mg/L)	9	mg/L
Lifetime (mg/L)	0.6	mg/L
10kg Child Oneday (mg/L)	9	mg/L
RfD (mg/kg/day)	0.09	mg/kg-day
DWEL (mg/L)	3	mg/L

PRG_AirH20

Field:	Numeric Value:	Units:
RESIDENTIALTAPWATERChronicHQ1combined(ug/l)	5.475	ug/L
RESIDENTIALTAPWATERChronicHQ1wateringest(ug/l)	32.85	ug/L
RESIDENTIALTAPWATERChronicHQ1waterinhale(ug/l)	6.57	ug/L

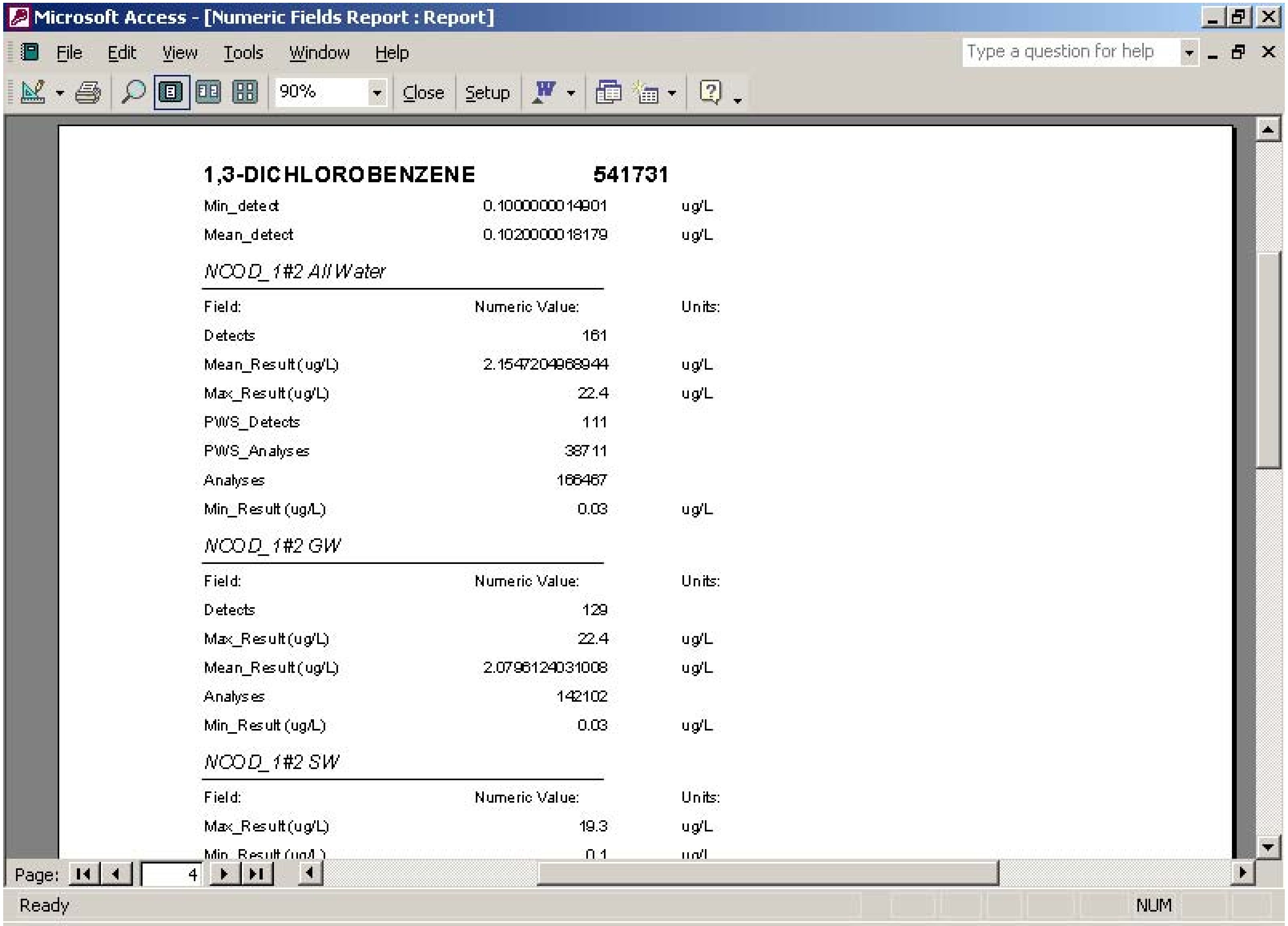
*PRG_Not__CAL_MODIFIED_PRG_*

Field:	Numeric Value:	Units:
RfDi(mg/kg-d)	0.0009	mg/kg-day
PRG TapWater(ug/l)	5.475	ug/L
RfDo(mg/kg-d)	0.0009	mg/kg-day

RBC_table

Example of Data -2

1,3-Dichlorobenzene - Occurrence Data



1,3-DICHLOROBENZENE 541731

Min_detect	0.100000014901	ug/L
Mean_detect	0.102000018179	ug/L

NCOD_1#2 All Water

Field:	Numeric Value:	Units:
Detects	161	
Mean_Result (ug/L)	2.1547204968944	ug/L
Max_Result (ug/L)	22.4	ug/L
PWS_Detects	111	
PWS_Analyses	38711	
Analyses	166467	
Min_Result (ug/L)	0.03	ug/L

NCOD_1#2 GW

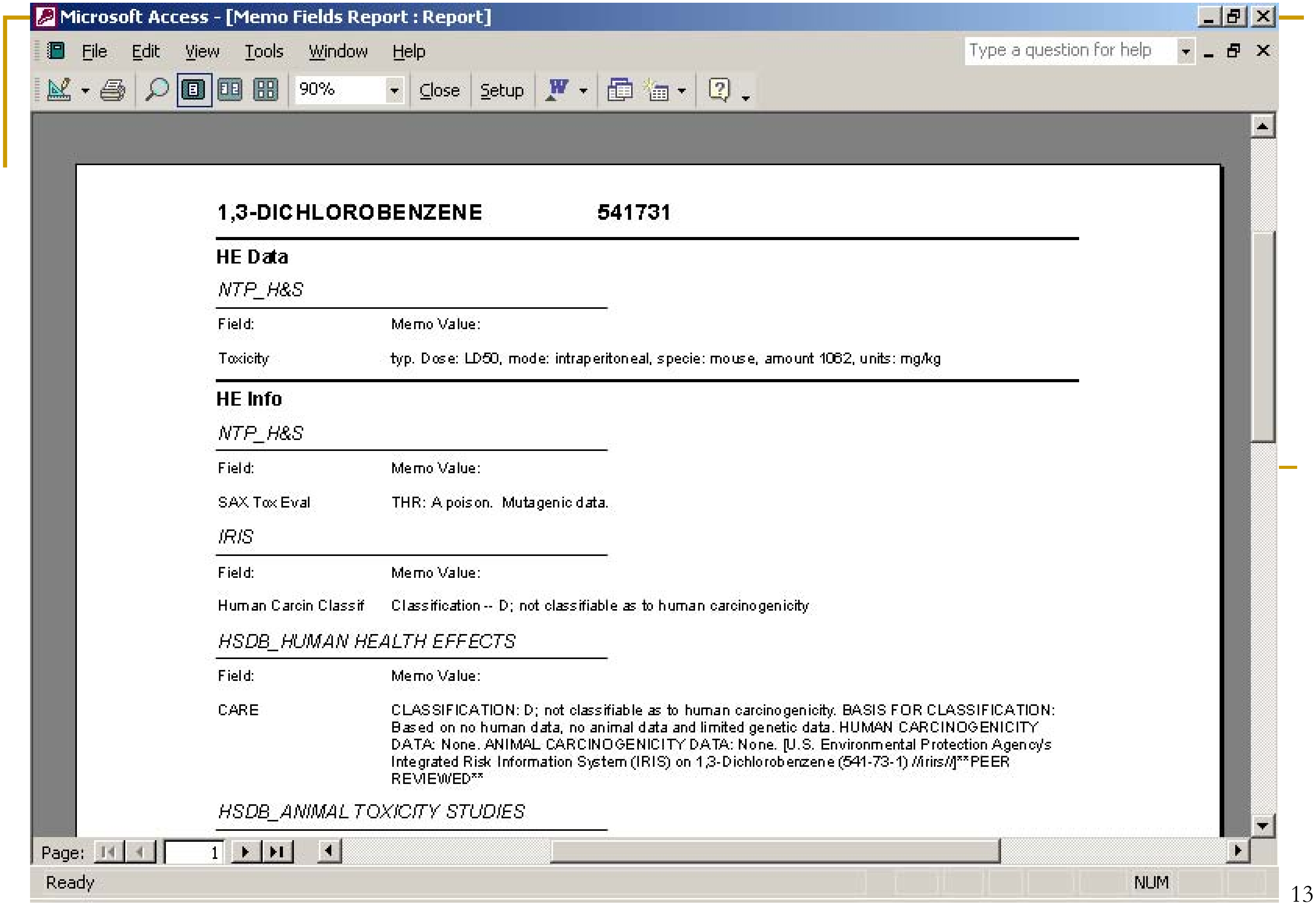
Field:	Numeric Value:	Units:
Detects	129	
Max_Result (ug/L)	22.4	ug/L
Mean_Result (ug/L)	2.0796124031008	ug/L
Analyses	142102	
Min_Result (ug/L)	0.03	ug/L

NCOD_1#2 SW

Field:	Numeric Value:	Units:
Max_Result (ug/L)	19.3	ug/L
Min_Result (ug/L)	0.1	ug/L

Example of Data -3

1,3-Dichlorobenzene – Data from text sources



1,3-DICHLOROBENZENE 541731

HE Data

NTP_H&S

Field:	Memo Value:
Toxicity	typ. Dose: LD50, mode: intraperitoneal, specie: mouse, amount 1062, units: mg/kg

HE Info

NTP_H&S

Field:	Memo Value:
SAX Tox Eval	THR: A poison. Mutagenic data.

IRIS

Field:	Memo Value:
Human Carcin Classif	Classification -- D; not classifiable as to human carcinogenicity

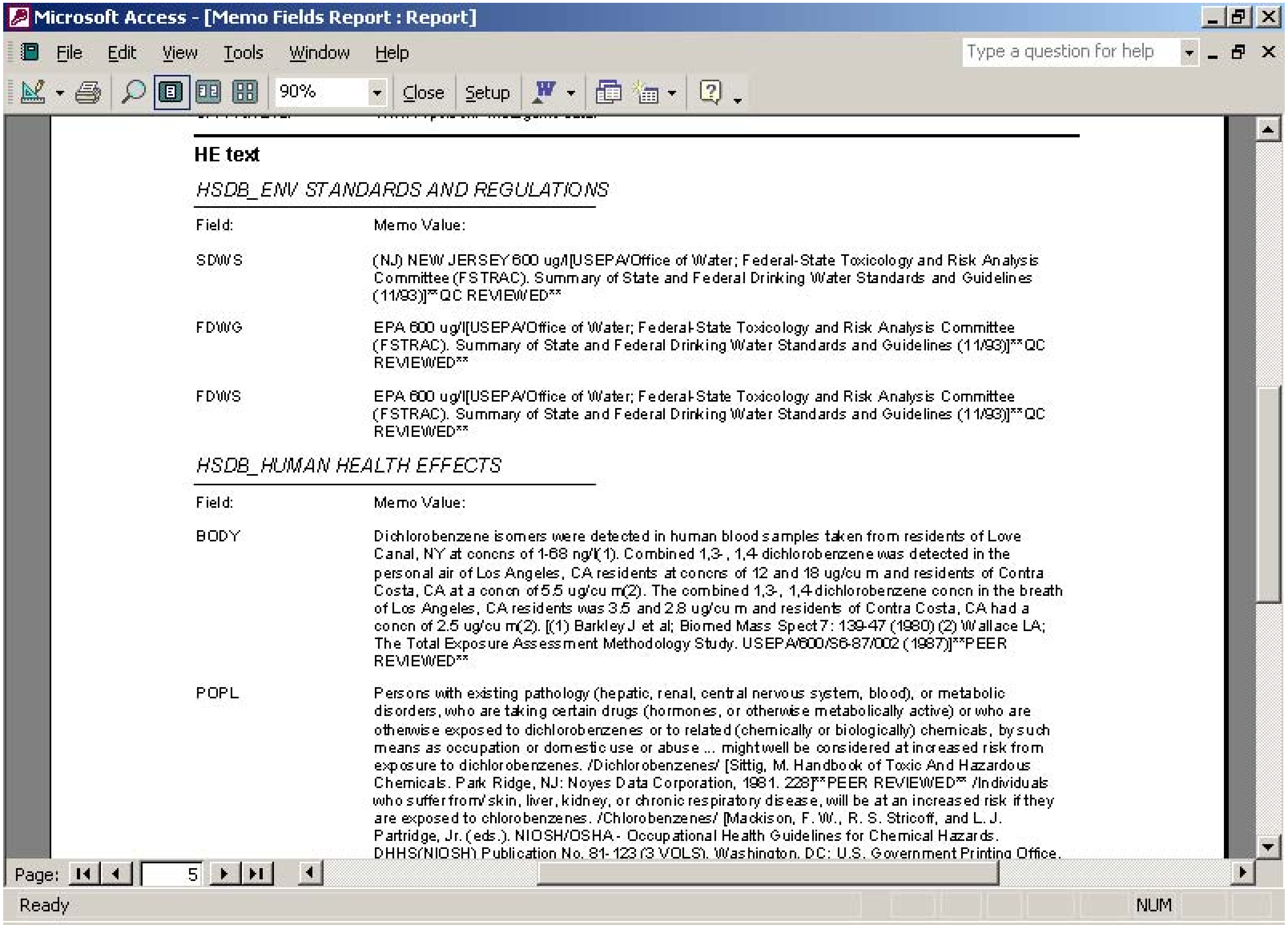
HSDB_HUMAN HEALTH EFFECTS

Field:	Memo Value:
CARE	CLASSIFICATION: D; not classifiable as to human carcinogenicity. BASIS FOR CLASSIFICATION: Based on no human data, no animal data and limited genetic data. HUMAN CARCINOGENICITY DATA: None. ANIMAL CARCINOGENICITY DATA: None. [U.S. Environmental Protection Agency's Integrated Risk Information System (IRIS) on 1,3-Dichlorobenzene (541-73-1) /Iris/]**PEER REVIEWED**

HSDB_ANIMAL TOXICITY STUDIES

Example of Data -4

1,3-Dichlorobenzene – Data from text sources (continued)


Microsoft Access - [Memo Fields Report : Report]
File Edit View Tools Window Help
Type a question for help
90%
Close
Setup
Page: 5
Ready
NUM

HE text

HSDB_ENV STANDARDS AND REGULATIONS

Field: Memo Value:

SDWS

(NJ) NEW JERSEY 600 ug/l[USEPA/Office of Water; Federal-State Toxicology and Risk Analysis Committee (FSTRAC). Summary of State and Federal Drinking Water Standards and Guidelines (11/93)]**QC REVIEWED**

FDWG

EPA 600 ug/l[USEPA/Office of Water; Federal-State Toxicology and Risk Analysis Committee (FSTRAC). Summary of State and Federal Drinking Water Standards and Guidelines (11/93)]**QC REVIEWED**

FDWS

EPA 600 ug/l[USEPA/Office of Water; Federal-State Toxicology and Risk Analysis Committee (FSTRAC). Summary of State and Federal Drinking Water Standards and Guidelines (11/93)]**QC REVIEWED**

HSDB_HUMAN HEALTH EFFECTS

Field: Memo Value:

BODY

Dichlorobenzene isomers were detected in human blood samples taken from residents of Love Canal, NY at concns of 1-68 ng/l(1). Combined 1,3-, 1,4 dichlorobenzene was detected in the personal air of Los Angeles, CA residents at concns of 12 and 18 ug/cu m and residents of Contra Costa, CA at a concn of 5.5 ug/cu m(2). The combined 1,3-, 1,4 dichlorobenzene concn in the breath of Los Angeles, CA residents was 3.5 and 2.8 ug/cu m and residents of Contra Costa, CA had a concn of 2.5 ug/cu m(2). [(1) Barkley J et al; Biomed Mass Spect 7: 139-47 (1980) (2) Wallace LA; The Total Exposure Assessment Methodology Study. USEPA/600/S6-87/002 (1987)]**PEER REVIEWED**

POPL

Persons with existing pathology (hepatic, renal, central nervous system, blood), or metabolic disorders, who are taking certain drugs (hormones, or otherwise metabolically active) or who are otherwise exposed to dichlorobenzenes or to related (chemically or biologically) chemicals, by such means as occupation or domestic use or abuse ... might well be considered at increased risk from exposure to dichlorobenzenes. /Dichlorobenzenes/ [Sittig, M. Handbook of Toxic And Hazardous Chemicals. Park Ridge, NJ: Noyes Data Corporation, 1981. 228]**PEER REVIEWED** /Individuals who suffer from/ skin, liver, kidney, or chronic respiratory disease, will be at an increased risk if they are exposed to chlorobenzenes. /Chlorobenzenes/ [Mackison, F. W., R. S. Stricoff, and L. J. Partridge, Jr. (eds.). NIOSH/OSHA - Occupational Health Guidelines for Chemical Hazards. DHHS(NIOSH) Publication No. 81-123 (3 VOLS). Washington, DC: U.S. Government Printing Office.

Data Extraction Level-of-Effort

Varies greatly

- Extraction method
- Tabular, monographic, bibliographic
- Complexity of format
- Number of chemicals in source data/information
- Number of data elements in source

TYPE	Data Extraction/ formatting time	Example
Tabular	0.25 to 5 days	SRC Physprop
Mono-graphic	1 to 5 days	HSDB
Biblio-graphic	1 to 10 days	DART

Example - Registry of Toxic Effects of Chemical Substances - RTECS

- RTECS is a bibliographic source with a twist: reports data values from various studies
- Each RTECS field is designated with a tag at the start of the line, and a tag for the start of different sections
- Wrote a program to gather specific data
- Data of interest [e.g. Lowest Observable Adverse Effect Level (LOAEL) from multiple dose studies] was automatically entered into tables

Issues with RTECS Importing

- Not all rows began with a tag (e.g. study title)
- Some sections contained extraneous data
- Data was within text, though in a standardized format
- Not every file had the same group headers or the same fields for each entry – some missing
- Units are as cumulative dose, rather than customary daily dose

Solutions to the RTECS Importation

- A parsing program was customized to:
  - Recognize that non-tagged rows went with the previous field
  - Recognize when fields or groups were not provided
- Text fields with data were parsed using string functions
  - Followed a particular pattern 99% of time
  - Remaining values were extracted manually

Data Extraction Issues: Compiling Monographic Data and Information

- Textually-formatted data/information not well suited for entry in a tabular format
  - Data contained in textual passages
  - Requires individual data source programs
  - We’re learning – programmers have had successes segregating values from text
  - Continue to evaluate and consider alternatives
  - Requires careful review post processing

Data Extraction Issues: Elemental and Inorganic Contaminants

- Metals
  - Data/information for elemental and inorganic forms is voluminous
  - Various oxidation states
    - Differences in toxicity (e.g., Cr^{+3}, Cr^{+6})
    - Differences in chemical properties (e.g., Na^0 vs. Na^+)
- Analytical Methods
  - Speciate by oxidation state
  - Do not report individual inorganic compounds
    - May not match CAS # for compounds

Lessons Learned on Data Extraction

- Demonstrated it is feasible to extract and develop data
- Level of Effort to obtain data ranges from hours to days
  - An option for the more difficult text sources is a placeholder table with candidate identifiers, letting the user know information on candidate exists in the source
- Developing programs to obtain data from text sources
  - Requires flexibility in programs to account for exceptions to patterns
  - May still require some manual entry, but will be limited to a set of sentences rather than entire file

Recommendations/Next Steps

- Develop a hierarchical approach for CCL data gathering
  - Avoid gathering duplicate/extraneous data
  - Update knowledge on elements for each contaminant before going to additional sources
  - Identify desired elements in each source in advance
- Continue to develop and test parsing programs to obtain the data needed
- Develop approach for inorganics
- Create and track a consistent approach