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ON-LINE RESEARCHER'S DATABASE ON THE ELECTRICAL DOUBLE LAYER CONSTRUCTED WITH A USER-ORIENTED DATABASE MANAGEMENT SYSTEM COOD

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On-line researcher's databases on the electrical double layer (ELDOL and ELCHEM) have been constructed with a user-oriented database management system COOD (Conversationally Organized Database Management System). Numerical data together with bibliographic informations were stored in these databases. They are supported by graphic display facilities.

There exist a number of database management systems for large scale and/or specially designed databases.[1] Those management systems, however, are too sophisticated for a personal use or a construction of researcher's database of relatively small size for a small group of researchers.

Recently, a user-oriented database management system COOD (Conversationally Organized Database Management System)[2] was developed, which has been implemented on an ACOS 77/900 Time Sharing System at the Computer Center of Tohoku University. The system COOD provides a tool for an easy construction and use of databases to researchers who are not specialist of the computer systems.

In this study an attempt was made to construct a database on the Electrical Double Layer (ELDOL) by using some of the basic facilities of the system COOD.[3] Data concerning the electrical double layer are widely used in the field of electrochemistry and electroanalytical chemistry and provide important information in understanding electrode kinetics.[4] Researcher's database consists of databases ELDOL and ELCHEM. The ELDOL contains electrocapillary data, differential capacity data and surface charge data, which are collected mainly from literatures already published. The references and bibliographies are stored in the database ELCHEM.

Both the databases are connected with each other with the relational key and the reference number.

Procedures to construct the ELDOL and ELCHEM are as follows:[5] (i) define the database with the Data Description Language (DDL), (ii) define the file characteristics with the File Description Language (FDL), (iii) accumulate data in the database with the Conversational Data Manipulation Language (CML). Figure 1 shows a description of the database ELDOL. Data for each item are difined with a format statement given in a bracket, which are the same as those given in the FORTRAN except J format conversions.

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DDL;
  DATABASE ELDOL : Database on Electrical Double Layer;
    TABLE CAPIL
       : Investigation of electrical double layer;
      NO          (I4) UNIQUE : Serial number;
      KIND        (A70)       : Kind of data;
      ELECT       (A70)       : Electrode;
      MEDIUM(5)   (A70)       : Medium;
      TEMP        (J10)       : Temperature (degree in Centigrade);
      PZERO       (J10)       : Point of zero charge(PZC) (V);
      SUBST(5)    (A40)       : Substance(s) used;
      CONCN(5)    (J10)       : Concentration of substance (M);
      NDATA       (I2)        : Number of data;
      POTL(30)    (J7)        : Potentials;
      DATA(30)    (J7)        : Data values;
      UNIT(2)     (A16)       : Unit used;
      REMARKS(3)  (A70)       : Remarks;
      REGNO(5)    (A10)       : CAS registry number;
      REFNO(2)    (A60)       : Reference number;
      COMPILER    (A70)       : Compiler;
END-DDL;


FDL;
  DATABASE ELDOL;
           PERMISSION READ;
    TABLE CAPIL;
           MAX 200;
END-FDL;
```

Fig. 1. Description of database structure and file characteristics of the system ELDOL.

```
SYSTEM ? COOD

COOD-PROCESS ... ? CML
?USE ELDOL/CAPIL;
EXPLAIN ITEMS OF ELDOL, YES OR NO ? NO
?STORE NEW CAPIL FROM CDATA;

***      50 DATA STORED.

?USE ELCHEM/LITFL;
EXPLAIN ITEMS OF ELCHEM, YES OR NO ? NO
?STORE NEW LITFL FROM RDATA;

***      20 DATA STORED.
```

Fig. 2. Storage of data to new tables from preliminarily prepared data files.

A specification of the form Jw such as J7 and J10 (Fig. 1) is used to transmit real values retaining significant figures.

The storage and the retrieval of data are easily performed with CML. Examples of storage are given in Fig. 2, where data are stored from the sequential file CDATA to the table CAPIL of the database ELDOL and from the sequential file RDATA to the table LITFL of the database ELCHEM. Figure 3 shows examples of retrieval. The first question is a request of data on "capacity of 0.1 M KBr", and then the user requests "LITFL 0002", which has been found by the retrieval of the table CAPIL.

Another feature of the system ELDOL is the data-display facility which utilizes some of the basic functions of the system DRAFTER.[6] This facility has been developed to display numerical data from the ELDOL onto a graphic display terminal or onto a drafter instrument at the Computer Center. The program is written with the FORTRAN language and the Data Manipulation Language (DML) of the system COOD. Picking up the data from the database is very easy as shown in Fig. 4: the necessary data are obtained by only issuing a few statements, such as .USE,

```
SYSTEM ? COOD

COOD-PROCESS ... ? CML
?USE ELDOL/CAPIL;
EXPLAIN ITEMS OF CAPIL, YES OR NO ? NO
?SELECT CAPIL WHEN(PART(KIND)='CAPACITY' & SUBST='KBR' & CONCN=0.1);
*** END OF TABLE

***       1 DATA FOUND.
OUTPUT DATA, YES OR NO ? YES

*TABLE  CAPIL    IN ELDOL
DISPLAY, NAME(N) OR EXPLANATION(E) ? NAME

NO      :    3
KIND    : 3 Differential capacity
ELECT   : Mercury
MEDIUM  : 0.1 M KBr
TEMP    : 25
PZERO   : -0.530
SUBST   : KBr
CONCN   : 0.1
NDATA   : 22
POTL    :
  -0.141   -0.149   -0.168   -0.188   -0.211   -0.242   -0.277   -0.316
  -0.358   -0.399   -0.441   -0.485   -0.530   -0.584   -0.650   -0.739
  -0.846   -0.965   -1.088   -1.202   -1.328   -1.440
DATA    :
  186.0    144.2    100.8    80.40    67.44    60.19    52.96    49.43
  48.18    47.78    46.91    45.37    41.38    33.73    25.76    20.12
  17.49    16.32    16.15    16.69    17.53    18.43
UNIT    : V(SCE)
          micro F/sq.cm
REMARKS : V(SCE) = volt vs. saturated calomel electrode
REGNO   : - - -
REFNO   : LITFL0002
COMPILER: A. YAMADA

?USE ELCHEM/LITFL;
EXPLAIN ITEMS OF LITFL, YES OR NO ? NO
?SELECT LITFL WHEN(NO=2);
*** END OF TABLE

***       1 DATA FOUND.
OUTPUT DATA, YES OR NO ? YES

*TABLE  LITFL    IN ELCHEM
DISPLAY, NAME(N) OR EXPLANATION(E) ? NAME

NO      :    2
AUTHOR  : Holmqvist P.
TITLE   : Measurement of differential capacity of electrode double
          layer by a derivative chronopotentiometric method
JOURNAL : J. Electroanal. Chem., vol. 68, p. 31
YEAR    : 1976
REMARKS : University of Uppsala
KEY     : Differential capacity
          Derivative chronopotentiometry
          Aniline
          Halogen ion
RELKEY  : CAPIL0002, CAPIL0003
```

Fig. 3. An example of storage and retrieval by the system COOD.

```
SUBROUTINE PICKUP (NUM,KIND,NDATA,XX,YY,IND)
        DIMENSION  XX(50), YY(50)
PRINT,     'DATA NO. TO DISPLAY'
READ,                NUM
.USE ELDOL/ CAPIL(NO,KIND,NDATA,POTL,DATA);
.OPEN CAPIL FOR RETRIEVAL;
   IND=0
.FIND CAPIL WHEN(NO.EQ.NUM);
.IF END(CAPIL), GO TO 9;
   IND=1
.GET KIND, NDATA, POTL, DATA;
                    DO 10 I=1,NDATA
                    XX(I)=POTL(I)
                    YY(I)=DATA(I)
                    CONTINUE
10
 9 .CLOSE CAPIL;
RETURN
END
```

Fig. 4. A program example using Data Manipulation Language.

.OPEN, .FIND, .IF, .GET, and .CLOSE. Figure 5 gives an example of the display on a graphic display terminal.

The system ELDOL has proved to be very useful for the interpretation of electrode kinetics especially for on-line simulations.[7,8] In conclusion, although this system is implemented mainly for studying the electrochemical data, its application is not limited to this particular field. It may be applied to other subjects in which both numerical data and graphic processing are of importance. The system can be used from any place via a public telephone network.

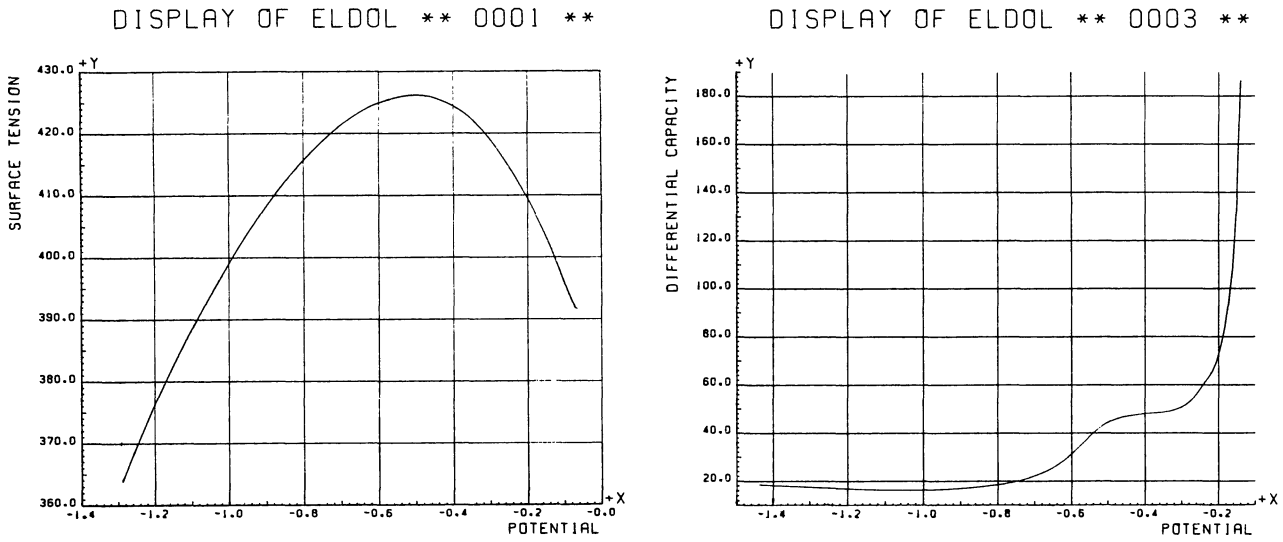

Fig. 5. Examples of display on graphic display terminal.

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Reference and Notes

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