

SOFTWARE FOR CHEMFET SENSOR DATA PROCESSING AND VISUALISATION

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ABSTRACT: Characterisation and quality assessment of newly developed CHEMFET sensors demands flexible and efficient data processing environment. The paper presents design and implementation of a software tool CEDaR (Chemfet sensor Evaluator for Design and Resarch) that meets the expectations. CEDaR imports data from XML measurements files, allowing not only for simple data queries and visualisation, but also for manual, automatic or mixed data filtering in order to eliminate noisy or faulty data. Higher level data processing includes: calculation of chemical responses from chemical-electrical measurements, optimisation-based characterisation of different sensor models. Unique to CEDaR is uniform handling of all data objects, including data processing algorithms and their parameters. CEDaR has been developed and tested using real measurement data¹.

INTRODUCTION

Characterisation of CHEMFET sensors is necessary for assessment of their suitability for environmental monitoring of ions. Characterisation of newly developed (and so constantly changing) sensors requires flexible and reliable data processing and visualisation environment. A need for such environment arose also in the EU SEWING project [9], oriented at design and manufacturing of water monitoring systems.

Analysis of user expectations revealed that the software is needed for two interrelated, yet distinct purposes. First, it should assist in assessment of CHEMFET sensor quality – providing fast estimates of standard sensor parameters (sensitivity, selectivity). Second, it should be a flexible, interactive, algorithmically rich environment for research on CHEMFET sensor modelling and for design of measurement systems.

The software was expected to handle the following user-accessible objects:

- Raw measurement data, e.g. transfer and output CHEMFET characteristics – imported from a sensor measurement stand [4] (currently via XML files) after some preliminary “data sanity check”.
- Data processing algorithms - such as filtering, calculation of chemical characteristics from I/V CHEMFET characteristics, model fitting
- Models of CHEMFET sensors, e.g. a combination of chemical models, such as Nikolsky-Eisenmann [1] (NE), super-Nikolski-Eisenmann (SNE) [7, 8], as well as electrical models, such as modified Merckel [4-6,8] model.
- Parameters of algorithms and models

- Output data – produced by algorithms, e.g. chemical responses, models parameters

Apart from standard store/query/retrieve database operations on all the above data objects, it was expected to provide other actions:

- setting up and running data processing algorithms
- visualisation of ad-hoc defined relations between objects, e.g. dependence of fitted model parameters on measurement conditions, sensor operating point, sensor age etc.

ARCHITECTURE OF CEDAR

To satisfy the above specifications a specialised software tool, called CEDaR, has been designed and implemented in MATLAB [10] environment. CEDaR uses a relational database (RDB) as its central data repository (see fig. 1). Currently MS ACCESS database

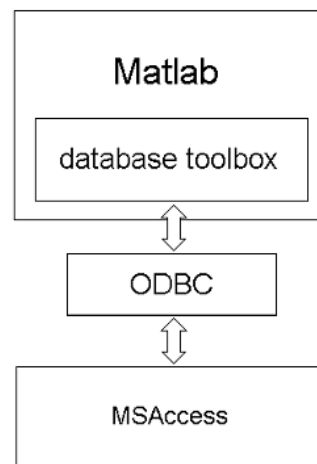


Fig.1. Main components of the CEDaR program

¹ This work was supported by the 5-th EU Framework Programme SEWING [9]

is operated from MATLAB via the Database Toolbox [10] using Open Database Connectivity driver (ODBC)

Measurement data are imported to database from XML data files which contain full description of the measurement session:

- session description
- description of the measured sensors
- stabilized parameters description and value
- independent parameters description and values
- dependent parameters description
- raw measurement data of dependent parameters

Data, e.g. subsets of measurement sessions, can be subject of user selected transformation, then visualised and possibly stored.

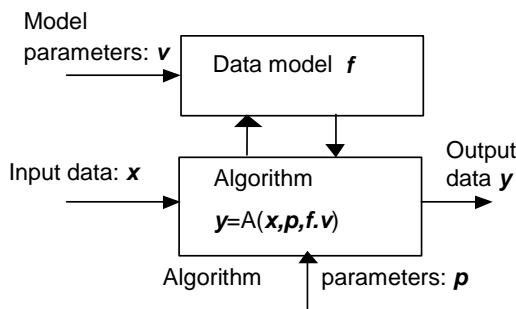


Fig.2. Basic data processing schema for CEDaR

Data processing model implemented in CEDaR is presented in fig. 2. Full specification of data processing operation in general consists of:

- specification of input data set x ,
- a data processing algorithm A , and possibly a data model f .
- values of model parameters (v) and algorithm parameters (p) – e.g. requested accuracy for optimisation based algorithms.

CEDaR was designed to store not only results of data processing steps y , but also the full specification of each data processing step, i.e. (x, A, p, f, v) in fig. 2. That way it is possible to determine upon user's request relationships between any data item and any detail of the measurement session or a data processing step it relied upon. A simplified ERD schema for the relational database of CEDaR is shown in fig. 3.

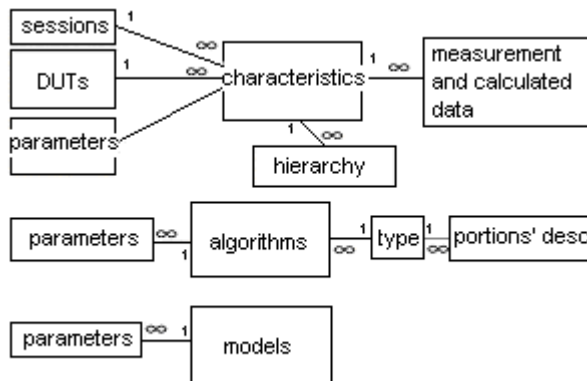


Fig.3. Simplified ERD schema of relational database

To standardise interface of data visualisation and data processing function a generic data handling engine was implemented. A user-selected portion of data is taken from the relational database (RDB) and kept in memory as a cell matrix. Data from the matrix are projected into two-dimensional subspaces, and subsequently plotted (see fig. 4). This method of

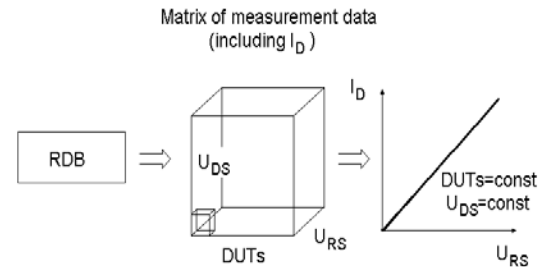


Fig.4. Data visualisation schema

visualization is essential for visual exploration of relationships between dependent data object. For example it is possible to investigate dependence of sensor selectivity on operating point, temperature or sensor age.

Preparation of input data for data processing algorithms is more complicated, since different algorithm/data model require different input data subsets. For illustration fig. 5 demonstrates steps that are required to evaluate dependence of sensor chemical responses on the operating point voltage (U_{DS}) for different sensor devices under test, (DUTs). In this example the original

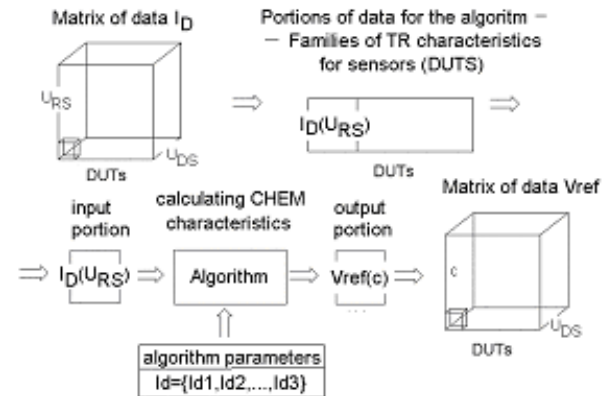


Fig. 5. An example of data processing flow

data are transfer electrical characteristics (denoted here as $I_D(U_{RS})$), measured for selected sensors, ionic content of water c , and U_{DS} biasing voltage. An algorithm (to be detailed later on) evaluates chemical characteristics (denoted as $V_{ref}(c)$) and stores the output data internally in a form of a multi dimensional matrix.

The main advantage of the proposed (internally complicated) data handling schema is flexibility. This feature is priceless when there is a need for adding new data processing algorithms, models or visualisation modules. The flexibility is very useful also when searching for dependencies of sensor properties on

different factors. One should note that structural flexibility of CEDaR is enhanced by intrinsic flexibility of interactive MATLAB environment, that offers many specialised high quality powerful toolboxes [10].

DATA PROCESSING ALGORITHMS

Fitting Models of CHEMFETs

One of most important characteristics features of CEDaR is its ability to fit complex CHEMFET models. Fig. 6 shows a structure of CHEMFET sensor devices and a structure of a useful class of separable models for these devices. Value of the voltage source U_{GR} is dependent on ion concentration in the tested solution. dFET denotes electrical model of a gateless FET that is a part of any CHEMFET device (as seen in the upper part of fig. 6).

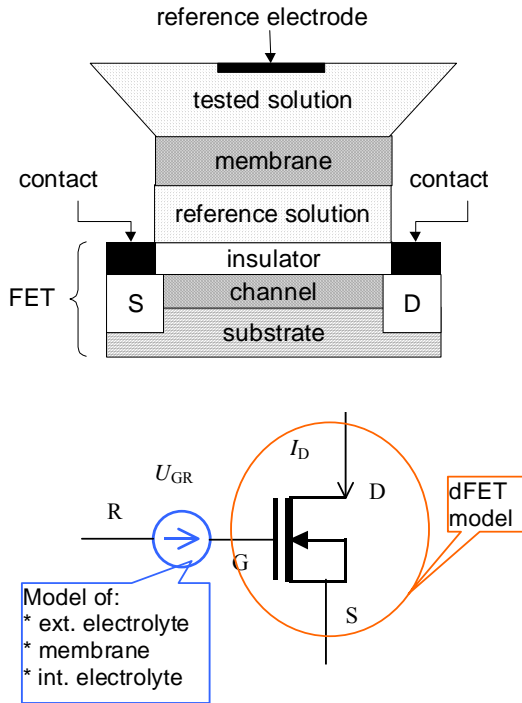


Fig. 6. Structure of a CHEMFET sensor device and its separable model

Such separable CHEMFET models have been also implemented in CEDaR. Currently the U_{GR} value is calculated using Nikolsky-Eisenmann [1] (NE) or Reduced super-Nikolsky-Eisenmann (RSN) [7,8] model. For the NE model:

$$U_{GR} = U_N + U_{N0}, \text{ where} \quad (1a)$$

$$U_N = N \frac{V_T}{z_0} \ln \left(a_0 + \sum_{j=1}^{m-1} K_j a_j^{z_0/z_j} \right) \quad (1b)$$

where U_{N0} is a membrane technology dependent constant; a_0, z_0 denotes activity and valency of the main ion, while a_j, z_j – activities and valencies of interfering ions. For a fixed operating point (I_D, U_{DS}) the reference electrode to source voltage of the NE model can be expressed as follows:

To accurately describe electrical behaviour of CHEMFET devices in a wide range of operating points

$$U_{RS} = U_0 - N \frac{V_T}{z_0} \ln \left(a_0 + \sum_{j=1}^{m-1} K_j a_j^{z_0/z_j} \right) \quad (2)$$

For the RSN model and a fixed operating point:

$$a_0 \tilde{e}_B^{z_0} + \sum_{j=1}^{m-1} \tilde{K}_j a_j \tilde{e}_B^{z_j} = 1, \text{ where} \quad (3a)$$

$$\tilde{e}_B = \exp \left(\frac{U_{RS} - \tilde{U}_0}{N V_T} \right) \quad (3b)$$

we use a Merckel model modified by Opalski [4, 5, 6, 8] to represent electrical properties of the internal gateless FET. Fitting of these complex electro-chemical models is performed using MATLAB optimisation toolbox [10] with mini-max, least squares or least absolute value fit quality measures.

Calculation of Chemical Responses

In our current measurement practice full (i.e. extensive) characterisation of sensors is frequently implemented by measurement of their transfer (or output) electrical characteristics for different ionic content and temperature. Thus evaluation of chemical responses of sensors needs some data processing as shown in fig. 5, and 7.

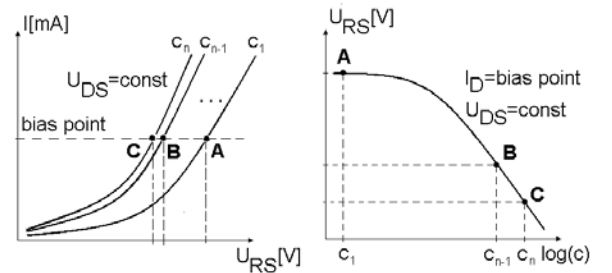


Fig. 7. Calculation of a chemical response of a CHEMFET sensor from transfer I/V curves

Mathematically this particular data processing is just a calculation of implicitly defined relationship between sensor output voltage U_{RS} (see also fig. 7) and the main ion activity c from the following equation:

$$I_D(U_{RS}, U_{DS}, c) = I_{D0} \quad (4)$$

where $I_D(U_{RS}, U_{DS}, c)$ is a chemical-electrical model of CHEMFET device, while $U_{DS} = U_{DS0}$ and I_{D0} denote operating point.

It is possible, in principle, to use any – even the most complex (and accurate) model of the sensor to evaluate $I_D(U_{RS}, U_{DS}, c)$ function. Since calculations of the chemical response involve very small changes of electrical conditions (I_D current, since U_{DS} is fixed for transfer I/V curves) it is reasonable, for sake of efficiency, to use a local approximation to the sensor I/V curves (for fixed c), i.e. $I_D(U_{RS}, U_{DS}, c)$. In our

actual implementation CEDaR offers several types of approximations of $I_D(U_{RS}, U_{DS}, c)$.

- For local polynomial approximation values of coefficients p_j are calculated by least-squares fitting of a p -th degree polynomial

$$\sum_{j=0}^p p_j * U_{RS,i}^j - I_{D,i} = 0$$

using $N > p$ data points, $U_{RS,i}$, $I_{D,i}$ for each ionic activity value c . Then equation (4) is solved for each selected operating point current and each selected ionic activity to give a point of the chemical response (fig. 7). Experimentally it was found that $p=3$, $N=4$ gives acceptable results, except when data points (interpolation nodes) are very close.

- Cubic spline interpolation – is organised similarly to the polynomial approximation, except that it uses global interpolation with cubic splines to interpolate dependence of the drain current I_D on the reference electrode to source voltage U_{RS} . In effect resulting curves are more smooth than for the first algorithm.
- Spline approximation – uses spap2 spline toolbox function [10] that approximates dependence of I_D on U_{RS} in the weighted mean-square sense. This technique allows for smoothing out local data errors and also automating elimination of outliers.

Characterisation of Chemical Responses

Chemical responses provide most important data for fast evaluation of CHEMFET sensors. Basic quantitative measures of any CHEMFET response are sensitivities of sensor output to the main ion (i.e. the ion the sensor is designed to be most sensitive to), sensitivity to other (disturbing) ions, and range of sensing. Instead of sensitivity to disturbing ions selectivity coefficients are frequently used, even though the coefficients are not always uniquely defined and meaningful (see [2] for details).

There are two approaches to characterisation of sensor model parameters.

1. In the first approach one assumes separability of CHEMFET model and fixed operating point. The fitting of NE, RSN or other models uses chemical CHEMFET response – e.g. calculated as visualised in fig. 5.
2. Second approach fits a global chemical-electrical CHEMFET model which does not have to be separable. Currently a mixture of NE or RSN models with a modified Merckel is mostly used – as it allows for quite accurate global modelling of CHEMFET (see [5] for details).

The first approach is common to evaluation of CHEMFET quality for a fixed measurement setup, while the second is useful for model research and for design of measurement circuitry.

In current CEDaR implementation both characterisation techniques are available. To accommodate local

modelling of temperature sensitivity of CHEMFET currently linear dependence of the offset voltage is assumed, but a more complicated model (e.g. as proposed in [6]) can be used as well. That way for a constant I_D and U_{DS} the NE model has a form:

$$U_{RS} = (U_{0nom} + c_u(T - T_{nom})) - \frac{NV_T}{z_0} \log(a_0 + K_s a_s^{z_0/z_s})$$

where c_u denotes a temperature sensitivity of the offset voltage. Altogether NE has four parameters: U_{0nom} , N , K_s , c_u . The same number of parameters is used by the RSN model.

EXAMPLES OF PROGRAM USAGE

Sample visualisation presented in this section are intended only as a preview of CEDaR visual capabilities. Most calculations and visualisations are presented for the same NO_3 selective CHEMFET sensor device. In the last visualisation a NH_4 sensitive CHEMFET sensor data were used – just to show that CEDaR works correctly also for cation selective sensors.

Raw and Processed Data Visualisation

Fig. 8 presents visualization of transfer electro-chemical characteristics. It is easy to identify specified characteristic or to plot them separately. A separate window presents description of the presented data, so that operator can learn which measurement sessions and data processing steps have been involved in producing the data.

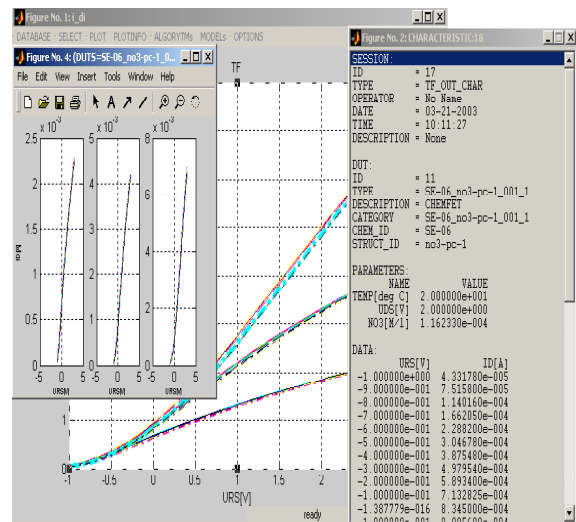


Fig. 8. Electro-chemical CHEMFET characteristics ($UDS=[0.5;1;2]$, $NO_3=[3.5e-7; 1.1e-6; 2.3e-6; 1.1e-5; 3.5e-5; 1.2e-4; 2.5e-4]$, $TEMP=20$)

Chemical Responses – Calculation and Visualisation

Calculation of chemical characteristics requires selection of the following items: a modelling algorithm (here spline interpolation was used, that did not require additional parameters), solver of equation (4) with its parameters (the selected algorithm required only one parameter I_{D0} – the bias current) and input data (here a one-parameter family of transfer characteristics were chosen with concentration of NO_3 as a parameter). The result of the operation is shown in Fig. 9. The transfer characteristics of the sensor were converted to chemical characteristics for three drain current values: $I_{D1}=0.5\text{mA}$, 1mA , 2mA .

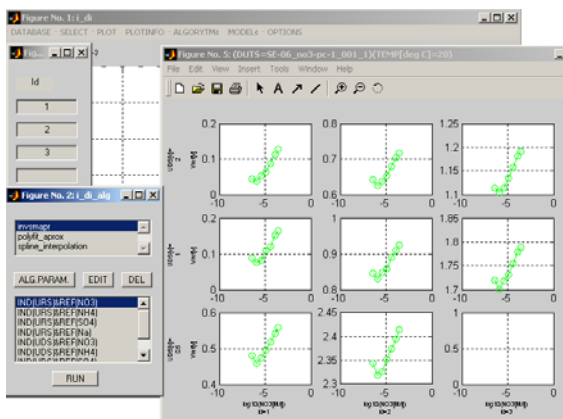


Fig. 9. Chemical characteristics ($U_{DS}=[0.5;1;2]$, $I_{D1}=[1;2;3]$, $TEMP=20$) (Note: lower-right corner axes are empty because bias point is out of measurements range)

Model Characterization

Fig. 10 shows results of mini-max fitting of the mixed NE + modified Merckel CHEMFET model (solid lines) to measurements (at markers).

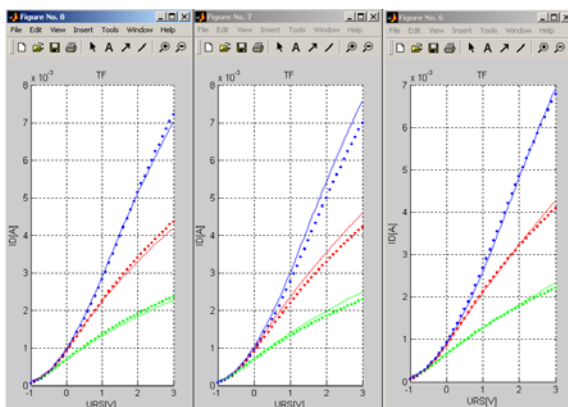


Fig. 10. The chemo-electrical CHEMFET model fitting for $TEMP=10\text{C}$ (left), $TEMP=20\text{C}$ (middle), $TEMP=30\text{C}$ (right)

Joint approximation of transfer electrical characteristics for seven activity levels of the main ion variable 10^{-6} mol/l up to 10^{-4} and three temperatures is shown. The composite model exhibits a maximum relative error 6.1% for the whole range of concentrations' variations and three temperature values. The mean squared error is below 3.7%.

Fig. 11 shows results of NE model characterisation for a

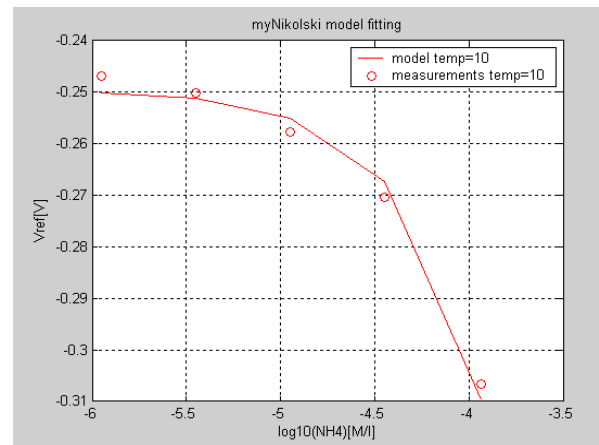


Fig.11. Example fit of the NE model to a CHEMFET sensor response

development-grade NH_4 -sensitive CHEMFET sensor at one operating point ($I_{D1}=0.5\text{mA}$, $U_{DS}=2\text{V}$).

CONCLUSIONS

This paper reports design and implementation of an original software tool CEDaR oriented at visualization and data processing of CHEMFET measurement data. The tool can assist in quality assessment of a substantial number of sensor devices. Due to its generic database model and MATLAB environment, that is used for implementation, CEDaR is flexible and convenient for research in the area of sensor modelling. Flexibility means not only, that it can handle ad-hoc searches for relationships in raw and process data, but also - that new data processing or visualisation modules may be easily added if a need arises.

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