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Simulations for any mechanistic electrochemical scheme: construction of KISSA-1D and KISSA-2D software : Overview of main publications

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Abstract. We consider here shortly the numerical computational approaches and strategies for the best accuracy of calculations for solution of complex electrochemical problems which we applied during the last 20 years constructing and using conformal and quasi-conformal mappings for different microelectrodes geometries. Our best knowledge and expertise led us to developing KISSA-1D and KISSA-2D software.

Introduction

Applied mathematics with all specific its tools and apparatus in coupling with computer simulation is a great motor for modern experimental science. Number of numerical methods and approaches for analysis, simulation, optimization and fitting procedures allows to use mathematical models for description of any complex experimental situation and search the best mathematical approach for accurate and fast solution of these models. Comparison results obtained by different mathematical and numerical methods allow to get correct solution at the end after analysis of solutions obtained by different ways or improve the initial mathematical models.

The theoretical investigation of electrochemical processes is complicated by specific features, which need to take in account for creation of models and choice of numerical approach for their solution. The first and main feature it is discontinuity of conditions in space coordinate. For example, that is a finite size of active biological elements or discontinuous flux at the electrode-insulator interface or stepwise change of driving force potential at the electrode/solution interface. Second is an extremely different time scales of coupled processes.

In real experimental conditions we have a very different reaction or diffusion rates, or time constants of potential scan and diffusion/reaction, etc.. The respective mathematical models are then no more amenable to analytical treatment and thus must be solved using approximate numerical methods. The choice of numerical method for simulation is very important also.

Within our research, we proposed the numerical approach with automatically created computational grid which we called “adaptive” grid. That is allowed to provide an accurate and precise simulation of electrochemical systems of any complexity in sense of reaction mechanisms. We considered the models described in one (1D) and two (2D) spatial dimensions.

On the first stage we developed the numerical approach with the adaptive computational grids in 1D space coordinates in the combination of special time grid for electrochemical simulations. This numerical strategy was practically completed and implemented in the computer software KISSA-1D (for one-dimensional models). This general strategy was based on an original approach for tracking reaction fronts both near the electrode and in the bulk of the solution and quick concentration changes due to varying driving force of heterogeneous electrochemical processes. The numerical space grid may be then automatically adjusted to ensure sufficiently high node density within such zones while using expanding grid between them to minimize the overall number of grid points and hence the computational time involved [1-4] for finalized results (values of concentration of all species in each grid point and electrochemical currents).

On more complicated stage it was a development of KISSA- 2D for two-dimensional electrochemical simulations for disk and a single band microelectrode. Our idea was to apply the construction of conformal and (quasi)conformal mappings for creation of computational grid at disk and at band electrodes. In coupling with finite difference method (ADI) for simulation of partial differential equations [5].

We had a huge experience in the conformal mapping construction of various electrode geometries for numerical solution of different mathematical models and experimental situations where mass transport including active and inactive surfaces and the ensuing diffusional patterns [6-26]. Great advantages of the (quasi)conformal computational grid is that the grid lines closely follow to the flux lines and those of equal concentration/potential for uncomplicated electron transfer reactions providing excellent resolution in the vicinity of singularities (e.g. electrode edges and/or corners of the simulation domain. Table 1 demonstrates the real space of diffusion distribution at the electrode surface in colors and a space of simulations for different electrode

geometries, and also mathematical formulas for coordinate transformations and computational grid for calculations.

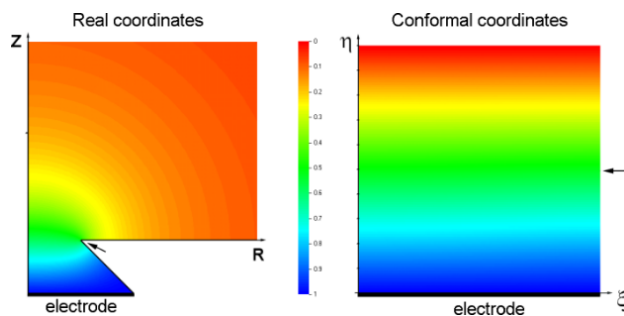


Fig. 1. Simulated concentrations shown in real and conformal coordinates at a disk microelectrode.

Apart from that, an extremely contorted semi-infinite initial space region of interest can be mapped onto a resulting closed transformed computational space, where concentration and potential distributions are much smoother, which greatly simplifies numerical procedures. In our case for disk it is allows obtaining analytical accurate solution. Fig. 1 shows the diffusional pattern generated by a disk microelectrode in a conical insulating well of the real and the conformal artificial space created by applied quasi-conformal transformation [14,15].

Thus, such mathematically designed approach gives a more accurate results with minimum computational expenses in comparison with the application of some software which based on application of the finite element method together with the “adaptive” generated triangles-based grids (Fig.2) relying on typical requirements which are generally fitted to usual physical problems (e.g., aero- or hydrodynamics, engines, etc.) but which were not specifically developed to involve discontinuous boundary conditions since this is seldom encountered outside of electrochemistry.

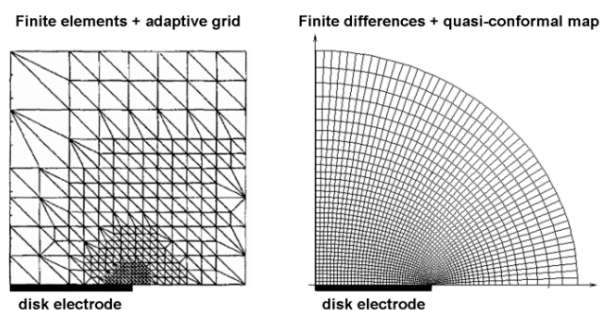


Fig. 2. Using different numerical techniques for computational grids construction for application of finite element method and finite difference method.

Conversely, conformal and quasi-conformal grid formulation encompasses already the main features of the sought solution through its mathematical definition. This ensures that the grid nodes are optimized intrinsically for the problem at hand. For example, the Fig. 2 on the left side compares a disk electrode mesh generated using an adaptive finite-element method (left-hand-side) to that produced mathematically by the quasi-conformal map representing the optimum numerical grid (right-hand-side) for uncomplicated diffusion [6]. This shows immediately that the flux lines and equiconcentration lines are already tracked rather satisfactorily by the quasi-conformal mesh while they are not by the triangle-generated one.

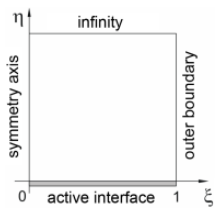
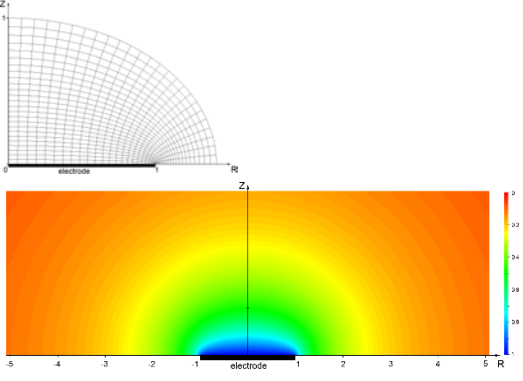
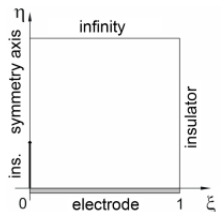
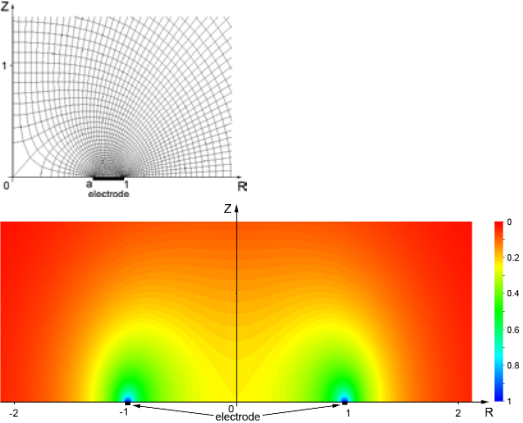
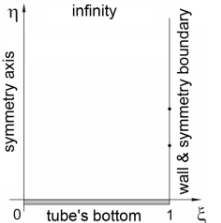
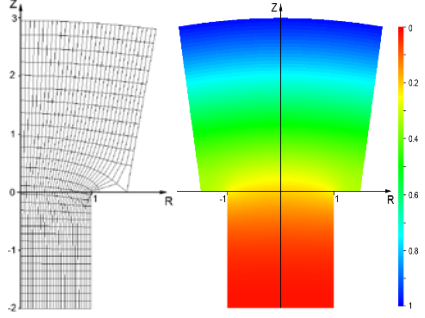
However, even though conformal space transformations bring a number of invaluable advantages listed above, they have a limited ability to represent sharp reaction fronts away from the electrode surface. Therefore, in order to create a general simulation approach effective for arbitrary reaction mechanisms the resulting conformal grid must be further adjusted to account for possible zones of rapid concentration changes in the solution bulk caused by fast homogeneous interactions. The exact strategy of this adaptation was developed and implemented in KISSA-2D for a number of widely employed electrode geometries allowing two-dimensional formulations of mass transport-reaction problems. This user-friendly interface software allows to introduce any reaction scheme in chemical formulation by the users, so as to allow them to treat any sought kinetic problem.

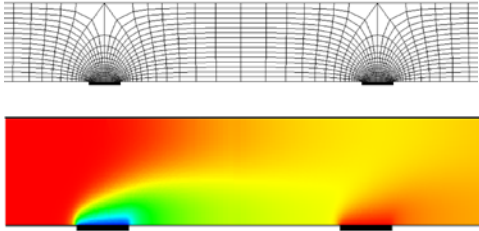
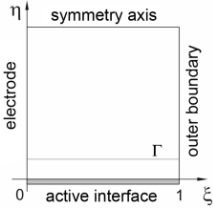
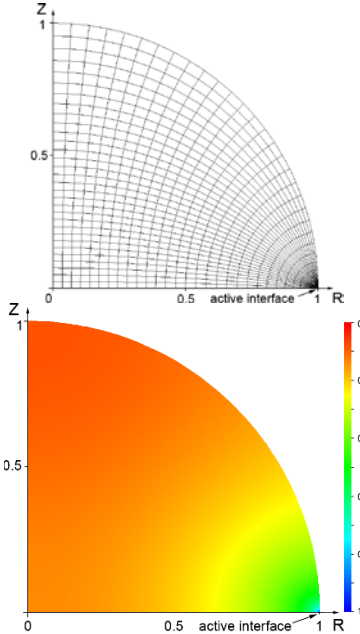
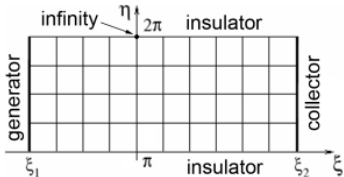
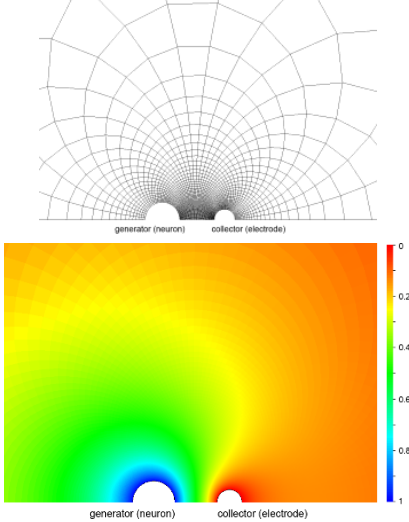
Conformal mappings constructed for 2D symmetrical microelectrode geometries

Our many years expertise allows to tell that application of the conformal mapping for simulation of reactive mechanisms at symmetrical electrode geometry gives the best result which often can be obtained on a very small space grids and it has a logical explanation. Grid in real coordinates repeating the distribution of species concentration by diffusion process (see Table 1).

Table 1 contains the conformal and quasi-conformal mappings we developed for efficient simulation of diffusion and diffusion-convective mass transport in micro-scale physicochemical systems with references to our corresponding papers [6-26]. It should be underlined that for some electrode geometries (e.g. disk) application of the conformal mapping allows to get simulations equals to mathematically analytical results, i.e. maximal accuracy which are possible. The reason of that follows from the excellent properties of the conformal mappings. For disk geometry this conformal transformation was constructed from the analytical expression for steady state behavior concentration at disk electrode [6, 7, 14, 15].

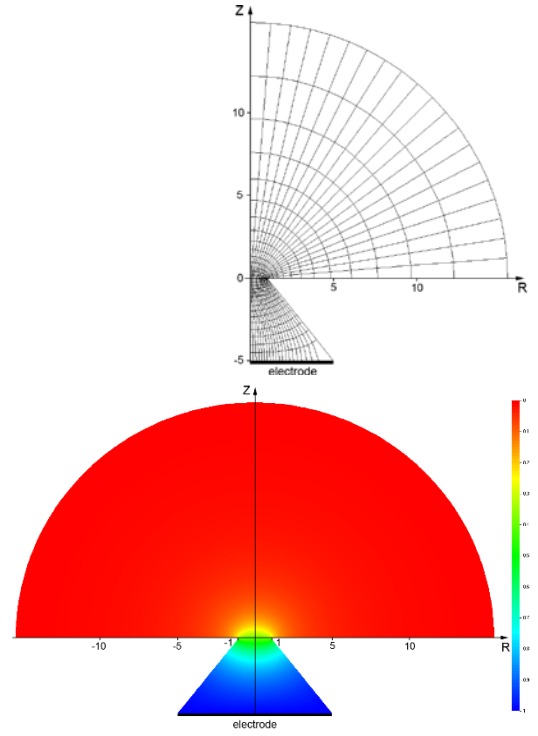
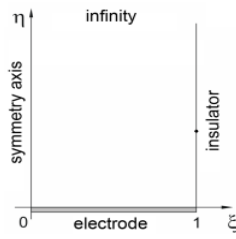
Table 1. Coordinate transforms which correspond to the electrode geometry and computational grids with calculated concentrations shown in the real space.

Electrode geometry	Coordinate transformation, artificial space for calculations	Computational grid, simulated concentration in real coordinates
<p>Disk</p> <p>refs. [6]</p>	$R = \sin\left(\frac{\pi}{2}\xi\right) / \cos\left(\frac{\pi}{2}\eta\right)$ $Z = \cos\left(\frac{\pi}{2}\xi\right) \tan\left(\frac{\pi}{2}\eta\right)$ 	
<p>Ring</p> <p>refs. [7]</p>	$X = \sqrt{(1-a^2) \sin^2\left[\frac{\pi}{2}\omega\right] + a^2}$ 	
<p>Nanotube cavity, ref. [18]</p>	$X = 1 + \frac{(-\zeta_3)^{1-\beta}}{\pi\sqrt{\zeta_2}} \int \frac{\omega \sqrt{e^\omega - \zeta_2}}{\ln \zeta_2 (e^\omega - \zeta_3)^{1-\beta}} d\omega$ 	

<p>Two bands in channel, ref. [11]</p>	$Z = \frac{i}{\pi} \arccos \left[a - b \cos \left(\pi \left\{ \xi + i \frac{\eta}{1-\eta} \right\} \right) \right]$	
<p>Droplet-modified electrode or vesicle, ref. [12]</p>	$R = -\frac{\sinh \left[\frac{\pi}{2} \tan \left(\frac{\pi}{2} \eta \right) \right]}{\cosh \left[\frac{\pi}{2} \tan \left(\frac{\pi}{2} \eta \right) \right] - \sin \left(\frac{\pi}{2} \xi \right)};$ $Z = \frac{\cos \left(\frac{\pi}{2} \xi \right)}{\cosh \left[\frac{\pi}{2} \tan \left(\frac{\pi}{2} \eta \right) \right] - \sin \left(\frac{\pi}{2} \xi \right)}$ 	
<p>Two hemi-cylinders assembly; neuron-electrode refs. [8, 10]</p>	$X = \frac{a e^{-\xi} - (a-b) \cos \eta + b e^{\xi}}{2(\cosh \xi - \cos \eta)};$ $Y = \frac{(a-b) \sin \eta}{2(\cosh \xi - \cos \eta)}$ 	

**Nanopore,
recessed
electrode
refs. [14-16]**

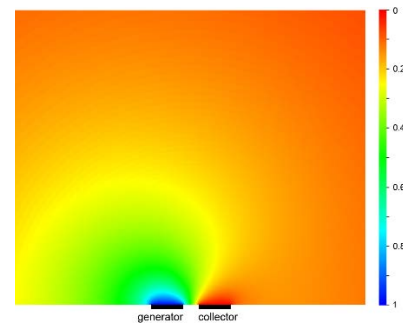
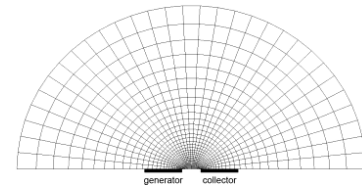
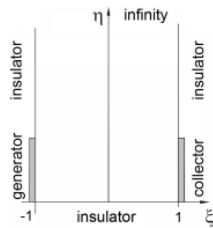
$$X = -iH_p + C \int_0^\omega \frac{1}{\sin\left(\frac{\pi}{2}\omega\right)} \left[\frac{\sin^2\left(\frac{\pi}{2}\omega\right) - u_3}{\sin^2\left(\frac{\pi}{2}\omega\right) - 1} \right]^{1-\alpha/\pi} d\omega$$

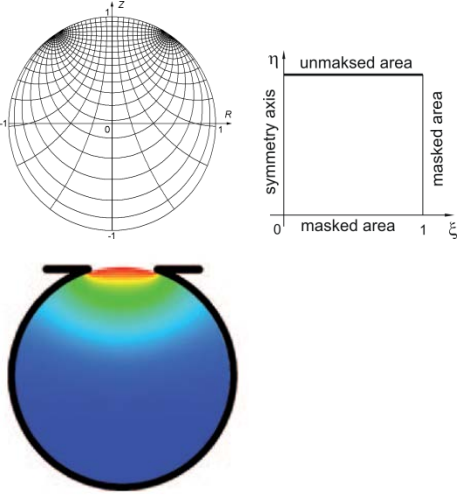


**Two microbands
assembly,
refs. [9,17]**

$$X = \sin\left(\frac{\pi}{2}\xi\right) \cosh\left(\frac{\pi}{2}\eta\right) ;$$

$$Y = \cos\left(\frac{\pi}{2}\xi\right) \sinh\left(\frac{\pi}{2}\eta\right)$$



<p>Vesicle (or partially masked spherical body)</p> <p>refs. [27, 28]</p>	$\omega^* = K \int \prod_{i=1}^m \left(1 - \frac{\zeta}{X_i} \right)^{\gamma_i - 1} d\zeta ;$ $\omega = \xi + i\eta = \xi^* + f(\eta^*)$	
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All these constructed by authors conformal and quasi-conformal transformations we applied for solution of real experimental electrochemical situations and published in our articles [1-34]. All these geometries of considered models have electrode symmetry and that allows to solve numerically only half of electrode surface saving CPU time.

Table 1 demonstrates our results published in the corresponding articles and allows to make some important conclusions:

- conformal mappings transform highly-curved the flux lines and equiconcentration lines onto straight (or almost straight) lines;
- conformal mappings transform usually encountered a half-infinite space onto a close one;
- the shape of the simulation area in transformed space is much more convenient for numerical simulation compared to the physical space;
- the above features result in highly accurate and extremely effective numerical approaches which require few grid nodes;
- in some case the conformal mappings allow obtaining analytical solutions for the steady-state regime (for example, disk) [6, 14, 15].

Development of KISSA-1D and KISSA-2D software

The main problems encountered in electrochemical simulations for 1D and 2D problems are

- large discrepancy between the extent of the diffusion layer and widths of kinetic fronts

of fast chemical reactions requires very large numerical grids;

- semi-infinite simulation space;
- edge effects (singularities) at microelectrodes.

Using our previous knowledge of application conformal mappings and numerical simulation strategy of adaptive grid we constructed KISSA-1D software for planar, spherical and cylindrical microelectrode geometry.

We created two different programs:

- KISSA-1D for simulating one-dimensional problems at planar, (hemi)sphere or (hemi)cylinder electrode geometries; [1-4, 29]
- KISSA-2D for simulating two-dimensional problems at disk or band microelectrode geometries [5].

Description of main general features and functions of our software listed below.

KISSA-1D software [1-4] is designed for automatic simulation of electrochemical reaction mechanisms of any complexity involving any number of reactants and elementary (electro)chemical steps yielding following computational results:

- electrochemical currents (CV, LSV, chronoamperometry, double potential step, etc.);
- concentration distributions of all species;
- surface coverage of adsorbed species;
- intensity of electrochemiluminescence (ECL) emission.

Physicochemical Models solved by KISSA-1D may include:

- heterogeneous electron transfer (ET) steps including any numbers of electrons and complex ET with adsorption;
- homogeneous chemical reactions of any order, including those leading to ECL [40,41];
- kinetically controlled adsorption-desorption;
- reactions in the adsorbed state and between adsorbed and solution species, i.e. dynamic adsorption steps [30,34,39];
- natural convection limiting the extent of the diffusion layer [29];
- system pre-equilibration that takes into account finite duration of the pre-equilibration period and finite reaction rates [29];
- self-assembled monolayer [26]

The Computational Strategy of KISSA-software includes :

- a novel algorithm for automatic adaptation of the computational grid using a kinetic criterion for cases of fast homogeneous kinetics (and possibly travelling reaction fronts) [1-4];

Algorithm of adaptive tracking of reaction fronts shows Fig.3 for EEE mechanism with fast comproportionation in KISSA-1D at planar electrode. This picture shows why it is important correct numerical solution in points where concentrations of species A, B, C, D reach its maximum and then falling down.

- use of conformal or quasi-conformal coordinate transforms for adequate tracking of diffusional propagation and resolution of edge effects at microelectrodes (disk and band) in software KISSA-2D.

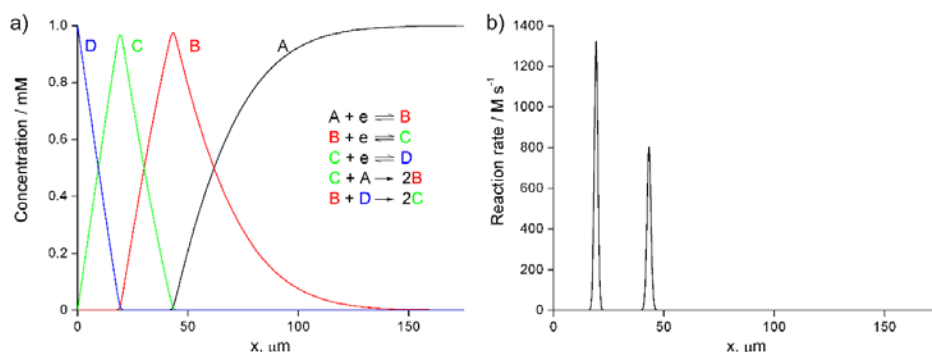


Fig. 3. Concentration profiles (a) and overall reaction rate (b) during an EEE sequence with fast comproportionation at a planar electrode. Narrow and intense reaction fronts result in rapid variations in concentrations.

Program Interface offers for KISSA-1D and KISSA-2D

- convenient entry of a reaction mechanism and parameters;
- graphical output of computed currents, concentration distributions, surface coverages and ECL intensity;
- export of simulation results into a file;
- import of experimental electrochemical currents for comparison with simulation;
- printing of all graphics of calculations.

Fig. 4 shows the windows of KISSA-1D interface for DISP simulation. Opened windows of Parameters, calculated CV of simulated current, distribution of simulated concentrations of all species and possibility to open and save graphics, data if file and print them. Fig. 5 demonstrates the windows of KISSA-2D for EEE mechanism with the corresponding parameters, calculated concentration at disk in real and transformed space coordinates.

Table 2 demonstrates the Cyclic Voltammetry for several reaction mechanisms calculated at disk and band electrodes on the adjusted computational grids around reactive front moving zones. In the last version of KISSA-2D we improved interface for calculation at disk and band electrodes by including possibility to make a user choice between two different grids applied to

simulation : the conformal map or adaptive front reaction grid, or using both together (see Table 2). That allows to save a time for calculation for concrete problem.

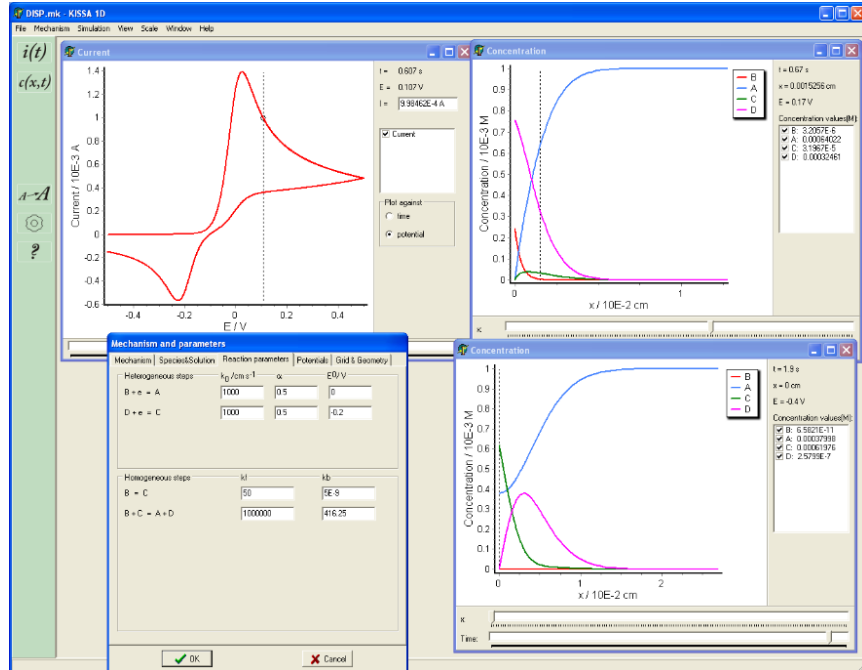


Fig. 4. The window of KISSA-1D software with example of simulation of DISP mechanism.

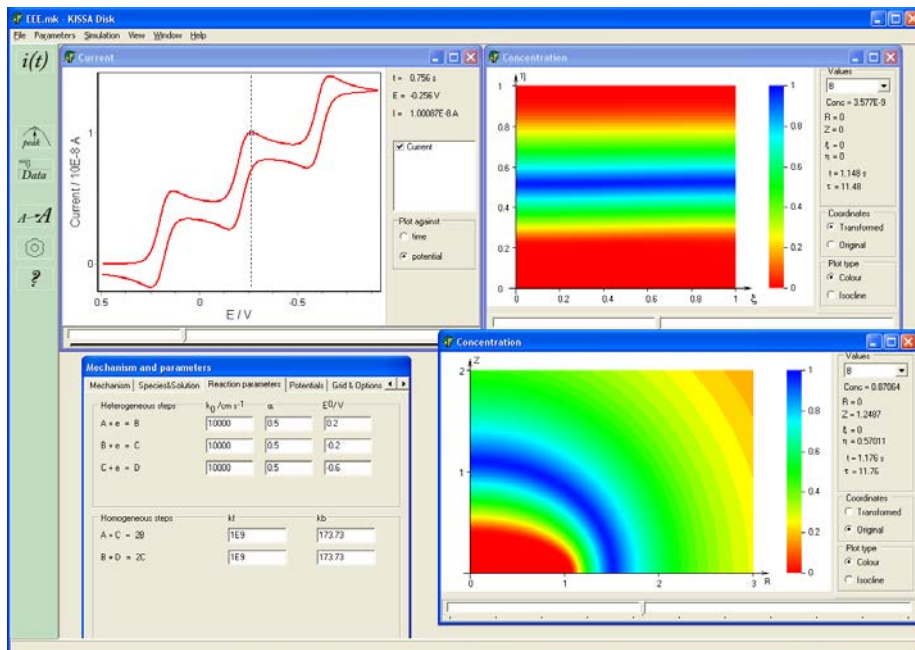
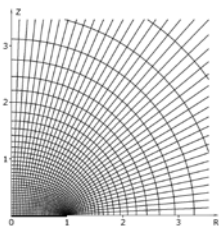
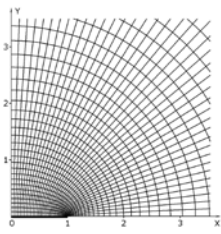
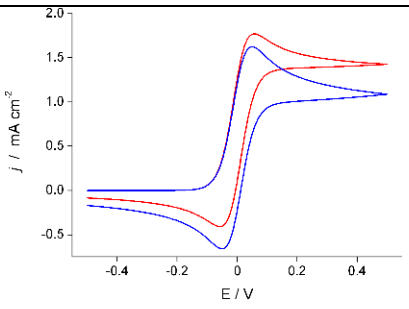
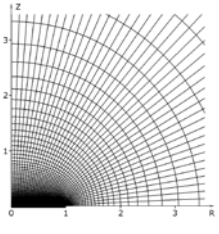
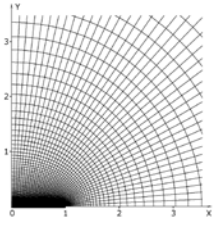
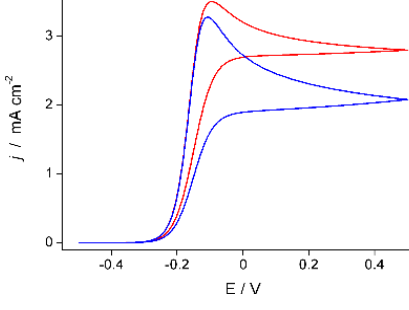
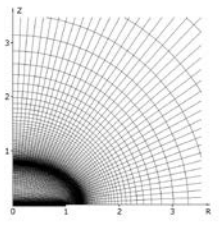
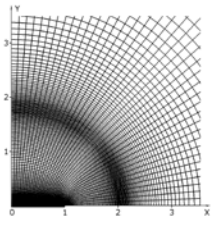
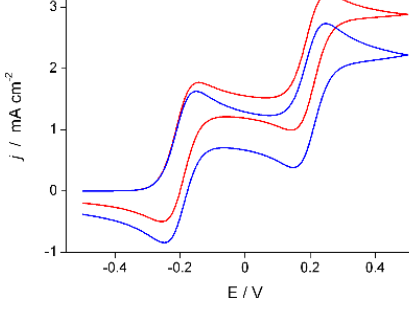
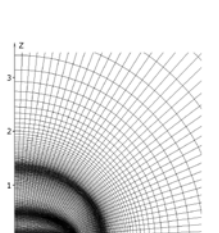
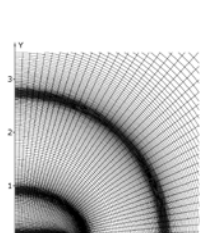
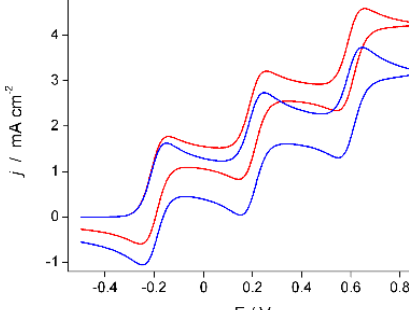


Fig. 5. Window KISSA-2D with results of EEE mechanism (current), parameter values and simulated concentrations in real and conformal space.

Table 2. Simulated reaction mechanisms and computational grids corresponding to very fast homogeneous reactions. The last column shows a comparison of current densities at *disk* (red curves) and *band* (blue curves) microelectrodes under Cyclic Voltammetry [5].

Mechanism	Disk	Band	Cyclic Voltammetry
E $A \pm e \rightleftharpoons B$			
EC_rE $A \pm e \rightleftharpoons B$ $B \rightleftharpoons C$ $C \pm e \rightleftharpoons D$			
EE $A \pm e \rightleftharpoons B$ $B \pm e \rightleftharpoons C$ $A + C \rightleftharpoons 2B$			
EEE $A \pm e \rightleftharpoons B$ $B \pm e \rightleftharpoons C$ $C \pm e \rightleftharpoons D$ $A + C \rightleftharpoons 2B$ $B + D \rightleftharpoons 2C$			

All parameters (initial concentrations, rate constants, diffusion coefficients etc) were the same in both case of calculations for disk and band for correct comparison of results.

Implementation of our strategy for automatic computational grid construction allowing to develop a software for computational electrochemistry for 1d and 2d simulations (KISSA-1D and KISSA-2D) and found solution of the many interesting experimental problems including simulation of different types of adsorption-desorption processes [30,34-36,39]; complex reaction mechanisms leading to ECL emission [40-42], and a lot of other specific experimental situations. The last version of KISSA-1D is presented on our information site [43].

Conclusions

Simulation approach based on (quasi)conformal mapping complemented with kinetically imposed adaptive grid, as developed by authors of in this work, allows obtaining very accurate solutions for electrochemical mechanisms of arbitrary complexity, even in the presence of extreme kinetic difficulties, which encompass the most severe experimental situations. This approach was realized in KISSA-2D for disk and band geometries. In the last version of software we added the possibility to make a choice to use two grids at the same time or any of them separated that to allow us save time of calculations for simple problems and get preliminary results on the initial stage of investigations when the mechanism and all parameters are not defined yet finally.

Acknowledgements

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