

15. CELL EQUILIBRIA

The screenshot shows the 'Cell Equilibrium' software window. At the top, there is a menu bar with 'File', 'Edit', 'View', 'Insert', 'Delete', 'Format', 'Units', 'Calculate', and 'Help'. Below the menu bar is a spreadsheet with the following data:

	SPECIES Formula	Temper. C°	Amount kmol	%
1	Hydrogen	25.000	22.400	
2	H2(g)	25.000	22.400	
3	Platinum	25.000	1.000	
4	Pt	25.000	1.000	
5	e-(Pt)	25.000		
6	PHASE 3:	25.000	69.500	
7	H2O	25.000	55.500	
8	H(+a)	25.000		
9	OH(-a)	25.000	7.000	
10	K(+a)	25.000	7.000	
11	Platinum	25.000	1.000	
12	Pt	25.000	1.000	
13	e-(Pt)	25.000		
14	Air	25.000	105.400	
15	N2(g)	25.000	83.000	
16	H2O(g)	25.000		
17	O2(g)	25.000	22.400	
18				
19				
20				
21				

On the right side of the window, there are several control panels:

- Phase Data:** Header: Platinum; Capacitance: 100000.000; Type: Metal; Electrode: Cathode.
- Heading:** This is input file for the CELL program.
- Extra Balances:** A list of values: 13 1, 17 -4, 0 0.
- Temperature:** 25.000 C; **Pressure:** 1.000 bar.
- File Path:** C:\Hsc5\Cell\Fucell.ice

At the bottom, there are buttons for 'Exit', 'Ins Row', 'Del Row', 'Ins Phase', 'Del Phase', 'Save', and 'Cell'.

Fig. 1. Input data for the Cell program.

The CELL module calculates the equilibrium composition of an electrochemical cell using the same calculation method as the GIBBS-solver. However, the CELL module is especially designed for electrochemical cell calculations.

In addition to the phase compositions it also gives the electrochemical potentials of the electrodes. The user gives input data for the CELL program in the Cell Equilibrium window, see Fig. 1.

Brief Instructions:

In the Cell Equilibrium window you can give the input data required for the calculations and save the input data for the CELL program. You can see examples of the data by selecting **Open** from the **File** menu. Please do this before making your own input files for CELL.

1. You can move in the spreadsheet using the mouse or arrow keys.

- If you want to edit the cell double click with the mouse or simply start typing. Use **Esc** key to undo typing.
- When you are satisfied with the formula or number, press **Enter**, **Down** or **Up** keys. You can also click another cell with the mouse.
- Type the name of the first species into the Species column. Note that you must start filling in the spreadsheet from the first row.
- You can first type all species and then edit the temperature and amount values, or you can give these values after every species name input.
- You can toggle between degrees Celsius and Kelvins by selecting **C** or **K** from the Units menu and from moles to kilograms (or Nm^3 for gases) by the **mol** selection.
- You must divide the species into phases in the same way as described in normal equilibrium calculations, see examples in Chapter 15.2.
- Every phase must have its own phase row. All species under this phase row until the next phase row belong to this same phase.
- For every phase you must at least specify its **Type** (Gas, Liquid, ...). You must also specify the Anode and Cathode phases. You can also give a name and capacitance for the phases.
- If you want to change the order of species, simply use **Insert Row**, Copy and Paste or the Drag and Drop technique described in Chapter 20. *Diagram Graphics*.
- You can also insert and delete rows by pressing **Ins Row** and **Del Row**.
- You can give **Extra Balances** as a table or matrix in the Extra Balances Box. For example:

13	1	' Species 13: Oxidation number of e-(Pt)
17	-4	' Species 17: Oxidation number of O2(g)
Q	0	' Discharge amount: Q/F (mol)

Extra Balances makes it possible to calculate potentials of electrodes and chemical compositions of phases at different discharge states of an electrochemical cell.

You must first define the species numbers, which react at the anode or cathode, as well as their oxidation numbers. In the example oxygen gas O2(g) is decomposed on a cathode, its oxidation number is $2 * (-2) = -4$. The oxidation number of an electron is always 1.

The discharge amount defines the amount of electricity, which is transferred from anode to cathode in the equilibrium. By changing the discharge amount you can calculate potentials and compositions at different discharge states of the cell. Note:

Q = Amount of electricity in As (charge)

F = Faraday's constant, 96487 As/mol

- When you are satisfied with the data, save it by pressing **Save**.
- After saving you can go to the CELL-program by pressing **Cell**.

Additional Information:

You can obtain more information on the CELL program and the thermodynamics in the background using **Help** as well as from the original publications of the authors^{7,8}.

15.1 Cell Module

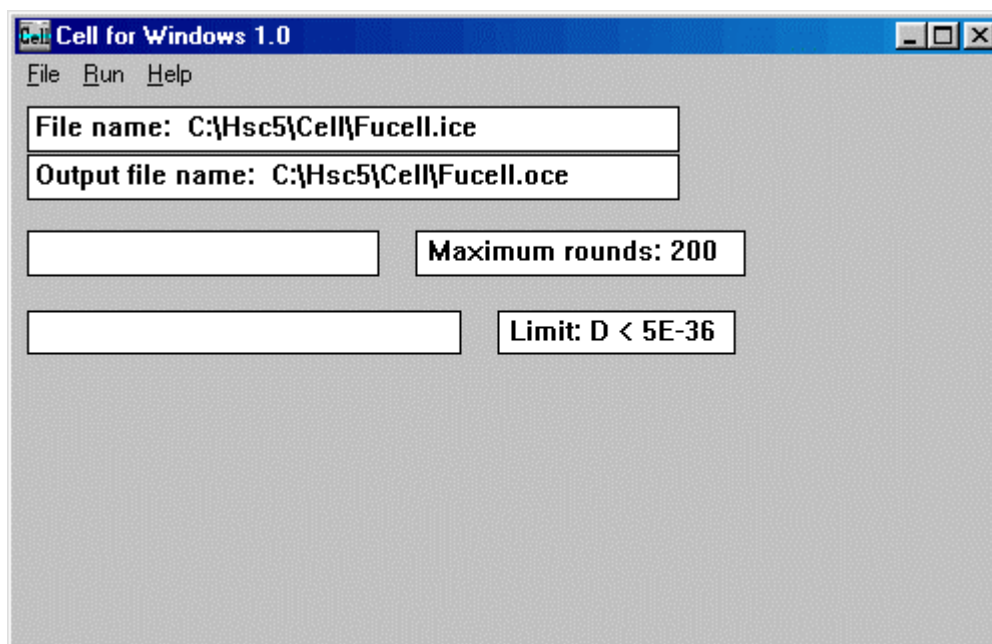


Fig. 2. Cell program.

The CELL-program calculates the equilibrium configuration of chemical and electrochemical systems and cells, half cells, fuel cells, as well as secondary and primary batteries.

For a complete cell with two or more electrodes, the total charge and the amount of atoms present in the system are not sufficient conditions of equilibrium. The additional constraint used in the CELL routine is the so-called DISCHARGE EQUATION. This describes how much charge can be transferred from the cathode to the anode due to the redox reactions taking place in the cell before the equilibrium state is reached from the initial equilibrium state, see the example fucell.ice. These constraints can be defined in the **Extra Balances** box, see Fig. 1.

Running the program:

1. Open input data file with the option "**File|Open...**"
2. Select the option "**Run|Calculate**". The program will then calculate the equilibrium state. If you want to change the number of iterations, choose the "Run|Maximum rounds" option which gives the new number of iterations. The default value is 200. You may interrupt the calculation by pressing any key or the mouse button.

Antti Roine

August 10, 2006

06120-ORC-T

3. Answer YES to the question "Do you want to save equilibrium data?" if you want to save results in input data file format on the file "Equil.ice". Otherwise select NO.
4. You can return to the HSC Main menu by selecting "**File|Exit**".

With the options "**File|View** input file" and "**File|View** output file" you can view the input file and output file, respectively. You may also send files to the printer with the **Print** option in the viewing window.