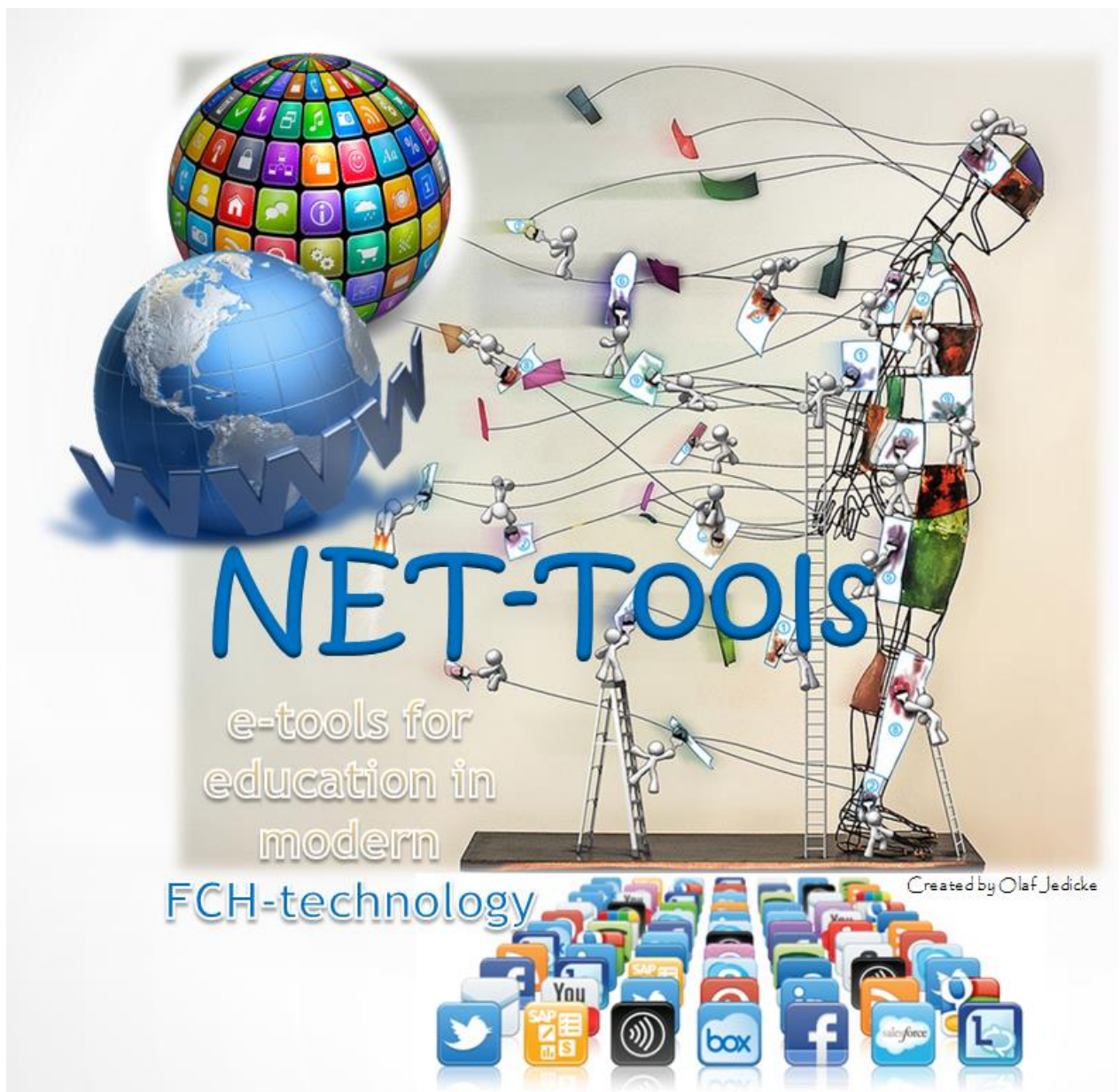


Novel Education and Training Tools based on digital applications related to hydrogen and fuel cell technologies

Deliverable D3.4:

e-Science toolbox, 1st version



D3.4: e-Science Toolbox 1st Version

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If deliverable does not get finished as scheduled in description of activity, please add a short explanatory statement. (To be done by responsible person of deliverable)

Explanatory Statement:

List of partners and short names

No	Name	Short name	Country
1	KARLSRUHER INSTITUT FUER TECHNOLOGIE	KIT	Germany
2	PERSEE	PersEE	France
3	NATIONAL CENTER FOR SCIENTIFIC RESEARCH "DEMOKRITOS"	NCSR "D"	Greece
4	UNIVERSITY OF ULSTER	UU	United Kingdom
5	DANMARKS TEKNISKE UNIVERSITET	DTU	Denmark
6	INSTITUTE OF ELECTROCHEMISTRY AND ENERGY SYSTEMS	IEES	Bulgaria
7	UNIVERSITA DEGLI STUDI DI PERUGIA	UNIPG	Italy
8	ELEMENT ENERGY LIMITED	Element Energy	United Kingdom



Document History

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30.05.2018	1.0	First draft prepared by V. Shentsov (UU)
	1.0	Tool descriptions provided by (IEES)
	1.1	Additions and changes by S. Giannissi (NCSRD)
29.06.2018	1.2	Changes provided by V. Shentsov (UU)



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1 Introduction

The content of e-Engineering was prepared before the first project meeting and delivered in milestone MS3.1 (M4). It consists of 23 tools in e-Engineering toolbox and 10 tools in e-Science toolbox summing total of 33 tools to be developed. The table of contents which was outlined in milestone MS3.1 is going to be used as a substructure for this deliverable. The content of the deliverable is formed from the tool's descriptions and realisation of them into the platform that are due in M14 as they deployed up to now based on the template for the tool's description developed and presented as an annex in MS3.1.

In the next Sections, a description of the tools in the e-Science toolbox that were delivered by M16 is provided. The description of the rest tools will be presented in D3.5.

1.1 e-Science

1.1.1 Property tools

1.1.1.1 The Abel-Noble EOS to calculate CGH2 mass in a volume at particular pressure and temperature (UU)

1.1.1.1.1 Introduction

Note: Model description should appear upon pressing the appropriate button on the home screen of the tool.

The ideal gas equation is not applicable to hydrogen storage pressures above 10 MPa when effects of non-ideal gas are essential. Whenever it comes to the calculation of the density of the gas or the volume or the tank at certain pressure and mass the Abel-Noble equation of state for real hydrogen gas can be applied instead.

Use of the ideal gas law equation instead of the real gas equation has an important safety implications. The ideal gas law if applied for calculation of the mass stored at high pressure would give overestimated results for the mechanical energy and total mass as can be seen in Figure 1.

This model allows to calculate the density, mass of the stored hydrogen, and volume of the tank

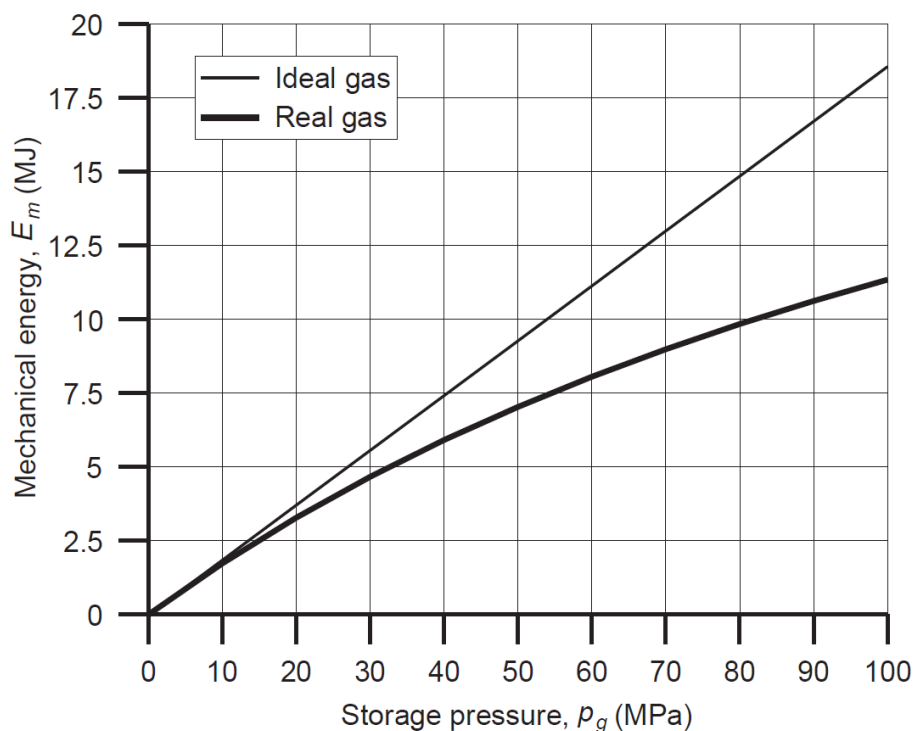


Figure 1 – Mechanical energy as a function of storage pressures in a tank of 72.4 L capacity: thin line e ideal gas, bold line - real gas (Molkov and Kashkarov, 2015).

1.1.1.1.2 Nomenclature

Parameter	Symbol	Unit
Universal gas constant	R	J/(kmol K)
Molecular mass	$M=2.016$	kg/kmol
Hydrogen specific gas constant	R_{H_2}	J/ (kg K)
Hydrogen co-volume constant	$b=0.007691$	m^3/kg
Pressure in reservoir	p_1	Pa
H ₂ density in reservoir	ρ_1	kg/m^3
Temperature in reservoir	T_1	K
Volume of reservoir	V	m^3
Hydrogen mass in reservoir	m_{H_2}	kg

1.1.1.1.3 Choice of the model

When the tool is selected the screen with the choice should appear prompting to select the option.

Please choose the option you want to calculate:

- 1. Calculate density and mass of hydrogen in the tank for the given volume and pressure
- 2. Calculate volume of the tank for the given mass and pressure

Note: Example of the model choice is the Option (radio) Button. When checked the screen with appropriate input parameters should appear below, together with button to initiate calculation (choice of RUN, CALCULATE, START etc. to be uniform across the e-Laboratory).

1.1.1.1.4 Option 1: Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Hydrogen pressure in reservoir	p_1	20500000	Pa	101325-100000000	20500000
Hydrogen temperature in reservoir	T_1	288	K	230-330	288
Volume of reservoir	V	0.0724	m ³	0.0001-10	0.0724

1.1.1.1.5 Option 1: Calculation procedure

Initial conditions			
1	Hydrogen pressure in reservoir	p_1 - user input	Pa
2	Hydrogen temperature in reservoir	T_1 - user input	K
3	Volume of reservoir	V - user input	m
Calculation			
4	Universal gas constant	$R=8314.47$	J/K/kmol
5	H2 molar mass	$M_{H2}=2.016$	kg/kmol
6	Hydrogen specific gas constant	$R_{H2}=R/M_{H2}$	J/ (kg K)
7	H2 co-volume constant	$b= 0.007691$	m ³ /kg
8	H ₂ density in reservoir	$\rho_1 = \frac{p_1}{(p_1 b + R_{H2} T_1)}$	kg/m ³
9	H ₂ mass in reservoir	$m_{H2}=\rho_1 V$	kg

1.1.1.1.6 Option 1: Output values

Parameter name	Symbol	Output value	Unit
Density in the reservoir,	ρ_1	15.237	kg/m ³
Hydrogen mass in reservoir	m_{H2}	1.1031	kg

1.1.1.1.7 Option 2: Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Hydrogen pressure in reservoir	p_1	20500000	Pa	101325-100000000	20500000
Hydrogen temperature in reservoir	T_1	288	K	230-330	288
Hydrogen mass in reservoir	m_{H2}	1.1031	kg		

1.1.1.1.8 Option 2: Calculation procedure



Initial conditions			
1	Hydrogen pressure in reservoir	p_1 - user input	Pa
2	Hydrogen temperature in reservoir	T_1 - user input	K
3	Hydrogen mass in reservoir	m_{H_2} - user input	kg
Calculation			
4	Universal gas constant	$R=8314.47$	J/K/kmol
5	H2 molar mass	$M_{H_2}=2.016$	kg/kmol
6	Hydrogen specific gas constant	$R_{H_2}=R/M_{H_2}$	J/ (kg K)
7	H2 co-volume constant	$b=0.007691$	m ³ /kg
8	H ₂ density in reservoir	$\rho_1 = \frac{p_1}{(p_1 b + R_{H_2} T_1)}$	kg/m ³
9	Volume of reservoir	$V = m_{H_2} / \rho_1$	m ³

1.1.1.1.9 Option 2: Output values

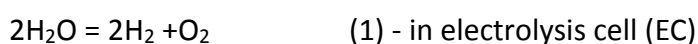
Parameter name	Symbol	Output value	Unit
Density in the reservoir,	ρ_1	15.237	kg/m ³
Volume of reservoir	V	0.0724	m ³

1.1.1.1.10 References

Molkov, V., Kashkarov, S., 2015. Blast wave from a high-pressure gas tank rupture in a fire: Stand-alone and under-vehicle hydrogen tanks. Int. J. Hydrog. Energy 40, 12581–12603. <https://doi.org/10.1016/j.ijhydene.2015.07.001>

1.1.2 Electrochemistry tools

The energy conversion in the water electrolysis cells (electrical to chemical) and in hydrogen fuel cells (chemical to electrical) is based on reversible electrochemical reactions:



The understanding of the working principal and performance efficiency of these hydrogen energy systems requires basic knowledge on fundamental electrochemistry.

1.1.2.1 Faraday laws of electrolysis (IEES)

1.1.2.1.1 Introduction



In 19th century Michael Faraday discovered the electrolysis and found empirically relationship between the mass of the reactant, its chemical nature, and the electric charge, required for proceeding of electrochemical transformation (oxidation/reduction reaction). This relationship was quantified in the Faraday's law of the electrolysis, broadly used in electrogravimetry (to calculate the amount of substance deposited at an electrode), coulometry (to find the total amount of electricity required for complete electrolysis of a compound), and numerous other applications for instance, to determine the number of electrons participating in an electrolytic process.

1.1.2.1.2 Nomenclature

Parameter	Symbol	Unit
Time of electrolysis	Δt	s
Applied current	I_a	A
Total electric charge passed	Q	C
Mass of the substance reacted on the electrode	m	g
Molar mass of substance	M	g/mol
Number of electrons involved in the reaction	n	dimensionless
Faraday constant	F	96485.33289 C/mol

1.1.2.1.3 Model description

$$m = \frac{M}{nF} Q$$

$$m = \frac{M}{nF} I \Delta t \quad - \text{constant current}$$

$$m = \frac{M}{nF} \int_0^t I dt \quad - \text{time dependent current – see Appendix}$$

1.1.2.1.4 Input values

Parameter	Symbol	Input value	Unit	Limits (min-max)	Defaults
Time of electrolysis	Δt	Independent variable	s	$[0, +\infty)$	
Applied current	I_a	1	A	$(0, +\infty)$	
Molar mass of substance	M	<i>link to the periodic table of the elements</i>	g/mol		
Number of electrones involved in the reaction	n	1	dimensionless	$[1;2;3]$	

1.1.2.1.5 Calculation procedure

Standard calculation F(x), where $\Delta x \leq 0.001$;

m(t)



1.1.2.1.6 Output values

Plots which the user can chose:

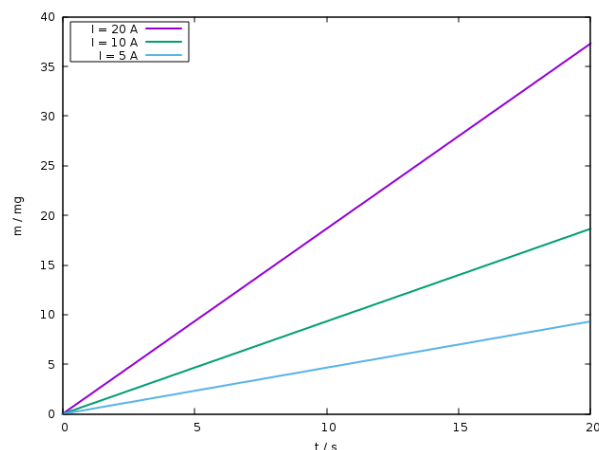
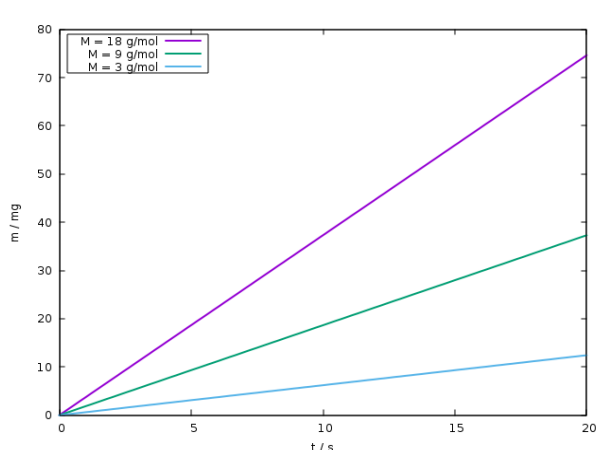
$m(t)$ – option for multiple plots on the same graph

Parameter name	Symbol	Output value	Unit
mass	m	plot	g, mg, kg

1.1.2.1.7 Conversion of input and output units

Standard units for calculation and storage in database (all values would be stored and processed in these units)

Parameter name	Standard unit name	Symbol	Unit
Time of electrolysis	<i>second</i>	Δt	s
Applied current	<i>ampere</i>	I_a	A
Total electric charge passed	<i>coulomb</i>	Q	C
Mass of the substance deposited on the electrode	<i>gram</i>	m	g
Molar mass of substance	<i>gram per mol</i>	M	g/mol
Number of electrons involved in the reaction	<i>integer</i>	n	dimensionless
Faraday constant	<i>Coulomb per mol</i>	F	96485.33289 C/mol

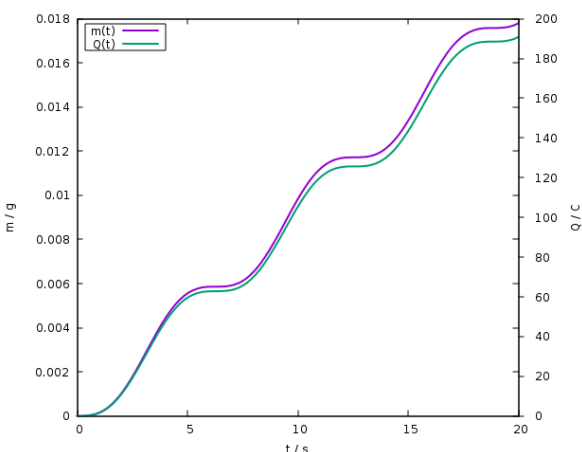
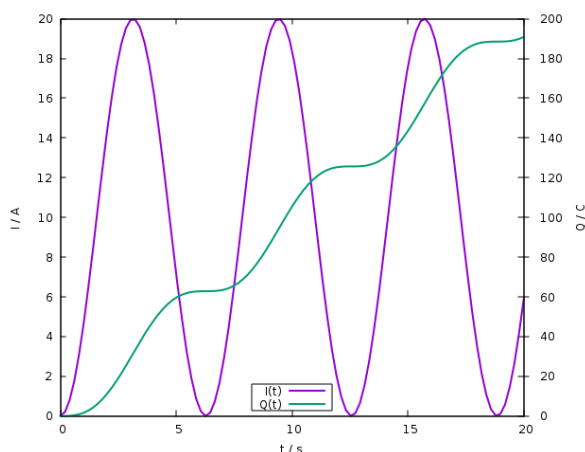


1.1.2.1.8 Appendix

$I_a(t) = \frac{1}{2}(I_0 - I_0 \cos(t))$ - time dependent current, where I_0 is the maximum current

$Q(t) = \int_0^t I_a(t) dt = \frac{1}{2}(I_0 t - I_0 \sin(t))$ - total charge for given time

$m(t) = \frac{M}{nF} Q(t) = \frac{M}{nF} \frac{1}{2}(I_0 t - I_0 \sin(t))$ - total mass for given time



1.1.2.2 Electrolytic (molar) conductivity (Kohlrausch's Law) (IEES)

1.1.2.2.1 Introduction

According to the nomenclature introduced by Faraday the electrolytes are second class conductors in which the charge carriers are ions. In contrast to the conductivity of the metals (first class conductors), the molar (ionic) conductivity is smaller, increases with the increase of temperature, and is not a material constant but depends on the concentration. In dilute electrolytes it is a linear function of the concentration obeying the Kohlrausch empirical equation, while in strong electrolytes it decreases with the increasing concentration due to an increase of the ion-ion interactions.

1.1.2.2.2 Nomenclature

Parameter	Symbol	Unit
Molar conductivity	Λ_m	$\text{S.m}^2.\text{mol}^{-1}$
Molar conductivity at infinite dilution	Λ_0	$\text{S.m}^2.\text{mol}^{-1}$
Empirical constant	K	dimensionless
Molar concentration	C	mol/L

1.1.2.2.3 Model description

$$\Lambda_m = \Lambda_0 - K\sqrt{C}$$

1.1.2.2.4 Input values

Parameter	Symbol	Input value	Unit	Limits (min-max)	Defaults
Molar conductivity at infinite dilution	Λ_0	0.02	$\text{S.m}^2.\text{mol}^{-1}$	[0.001, 0.04]	
Empirical constant	K	0.05	dimensionless	[0.001, 0.1]	
Molar concentration	C	independent variable	mol/L	(0, 0.1]	

1.1.2.2.5 Calculation procedure



Standard calculation $F(x)$, where $\Delta x \leq 0.001$

1.1.2.2.6 Output values

Plots which the user can choose:

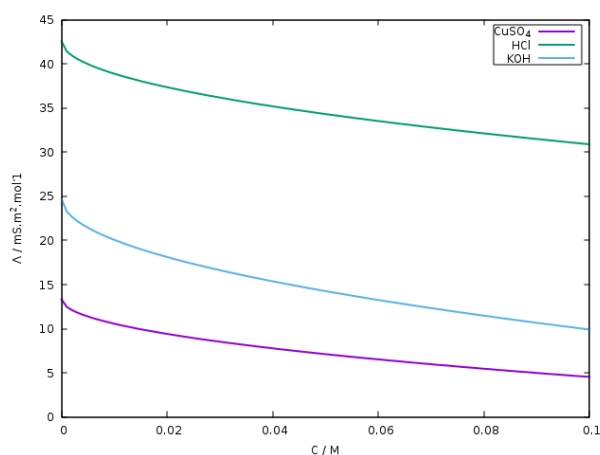
Λ_m - with different values for Λ_0 and K

Parameter name	Symbol	Output value	Unit
Molar conductivity	Λ_m	plot	$S.m^2.mol^{-1}$, $mS.m^2.mol^{-1}$

1.1.2.2.7 Conversion of input and output units

Standard units for calculation and storage in database (all values would be stored and processed in these units)

Parameter name	Standard unit name	Symbol	Unit
Molar conductivity	<i>siemens square meter per mol</i>	Λ_m	$S.m^2.mol^{-1}$
Molar conductivity at infinite dilution	<i>siemens square meter per mol</i>	Λ_0	$S.m^2.mol^{-1}$
Empirical constant	<i>dimensionless</i>	K	dimensionless
Molar concentration	<i>mol per liter</i>	C	mol/L



1.1.2.3 Electrochemical potential (IEES)

1.1.2.3.1 Introduction

The free Gibbs energy is a thermodynamic function that determines unambiguously the macroscopic state of a system. It depends on the pressure and temperature and when normalized to one mol of substance, is called molar Gibbs energy or chemical potential. For a system containing electrically charged species, the Gibbs free energy depends also on the electrical potential and when normalized to one mol, it is called electrochemical potential. In other words, the electrochemical potential is a thermodynamic measure of the chemical potential that takes also into account the energy contribution of the electrostatics. The electrochemical potential of a given phase represents the work needed for transferring of one mol charged particles from a given reference state into his phase overcoming both chemical bonding forces and electrical forces.



1.1.2.3.2 Nomenclature

Parameter	Symbol	Unit
Electrochemical potential of species i	μ_i	J/mol
Chemical potential of species i	μ_i	J/mol
Charge of ion of type i	Z_i	dimensionless(integer)
Electric potential at given point	ϕ	V
Faraday constant	F	96485.33289 C/mol

1.1.2.3.3 Model description

$$\bar{\mu}_i = \mu_i + z_i F \phi$$

$\phi = \phi_0/x$ - this dependence of the potential is for simplicity and should be used only for calculation, should not be shown to the user

1.1.2.3.4 Input values

Parameter	Symbol	Input value	Unit	Limits (min-max)	Defaults
Chemical potential of species i	μ_i	-10000	J/mol	[-100000, 100000]	
Charge of ion of type i	Z_i	1	integer	[-4,4] integers	
Electric potential at zero point	ϕ_0	2	V	[-100, 100]	

1.1.2.3.5 Calculation procedure

Standard calculation $F(g(x))$, where $\Delta x \approx 0.001$

1.1.2.3.6 Output values

Plots which the user can choose:

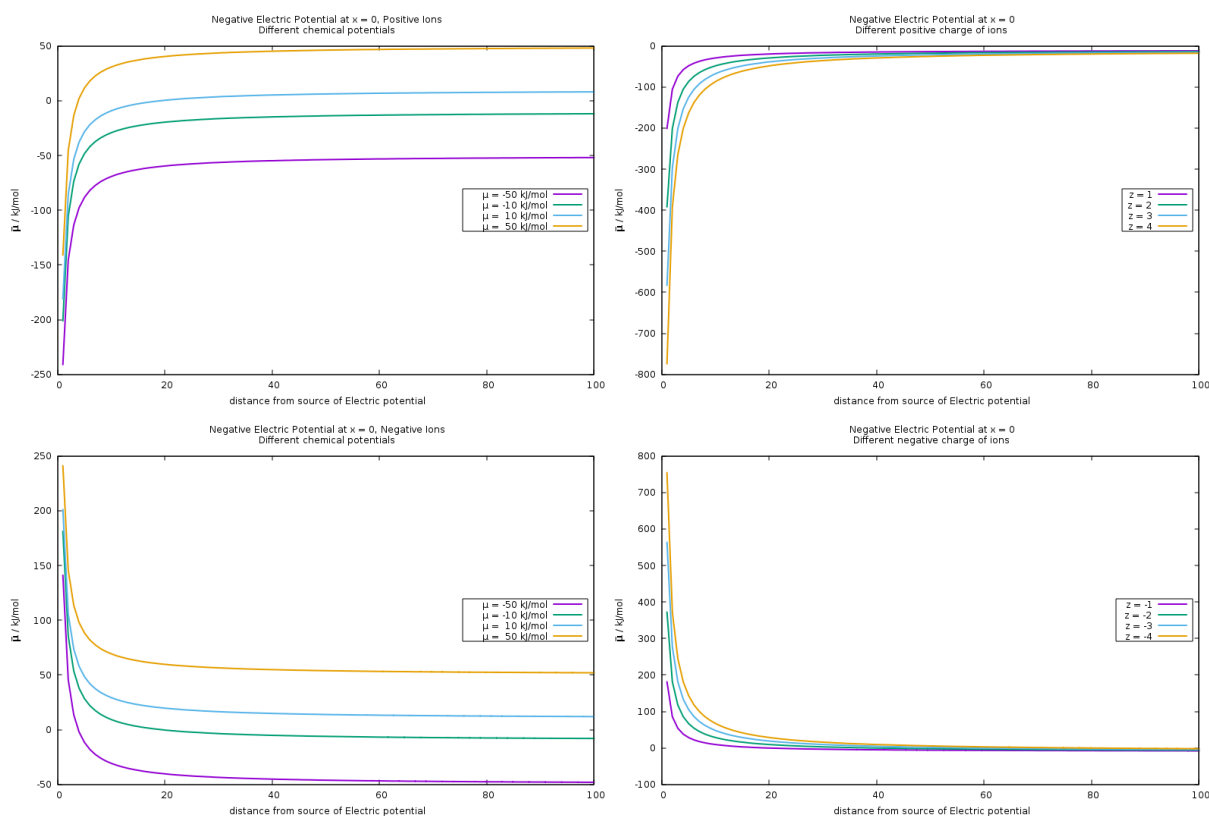
- effect of charge of ions
- effect of chemical potential
- effect of electric potential at zero point

Parameter name	Symbol	Output value	Unit
Electrochemical potential	μ_i	plot	J/mol, kJ/mol, MJ/mol

1.1.2.3.7 Conversion of input and output units

Standard units for calculation and storage in database (all values would be stored and processed in these units)

Parameter name	Standard unit name	Symbol	Unit
Electrochemical potential of species i	joul per mol	μ_i	J/mol
Chemical potential of species i	joul per mol	μ_i	J/mol
Charge of ion of type i	dimensionless	Z_i	integer
Electric potential at given point	volt	ϕ	V
Faraday Constant	coulomb per mol	F	96485.33289 C/mol



1.1.2.4 Nernst equation (IEES)

1.1.2.4.1 Introduction

The Nernst equation relates the redox potential of an electrochemical reaction (half-cell or full cell reaction) to the standard electrode potential, temperature, and activities (often approximated by concentrations) of the chemical species undergoing reduction or/and oxidation. In other words it shows how the reaction species in terms of chemical activity (concentration) and the reaction temperature influence the electrode potential.

If a system follows the Nernst equation or an equation derived from it, the electrode reaction is considered thermodynamically or electrochemically reversible (Nernstian reaction).

1.1.2.4.2 Nomenclature

Parameter	Symbol	Unit
Electrode potential	E	V
Equilibrium potential	E_{eq}	V
Absolute temperature	T	K
Universal gas constant	R	8.31447 J/K/mol
Number of electrons involved in the electrochemical reaction	n	dimensionless
Faraday constant	F	96485.33289 C/mol
Chemical activity of the reduced form	a_{Red}	mol/m ³
Chemical activity of the oxidized form	a_{Ox}	mol/m ³

1.1.2.4.3 Model description



$$E = E_{eq} - \frac{RT}{nF} \ln \frac{a_{Ox}}{a_{Red}}$$

1.1.2.4.4 Input values

Parameter	Symbol	Input value	Unit	Limits (min-max)	Defaults
Equilibrium potential	E_{eq}	1.23	V	[-2, 2]	1.23
Absolute temperature*	T	298	K	[100,1200]	298
Number of electrons involved in the electrode reaction	n	1	dimensionless	[1;2;3]	1
Chemical activity of reduced form	a_{Red}		mol/m ³	[0.0001, 0.1]	0.001
Chemical activity of oxidized form	a_{Ox}		mol/m ³	[0.0001, 0.1]	0.001

1.1.2.4.5 Calculation procedure

Standard calculation $F(x)$, where $\Delta x \leq 0.001$

Different independent variables:

$$E(T), \ln(a_{Ox}/a_{Red}) = \text{const},$$

$$E(\ln(a_{Ox}/a_{Red})), T = \text{const}$$

1.1.2.4.6 Output values

Plots which the user can choose :

$$E(T), \ln(a_{Ox}/a_{Red}) - \text{with different values, plot on one graph}$$

$$E(\ln(a_{Ox}/a_{Red})), T - \text{with different values, plot on one graph}$$

Parameter name	Symbol	Output value	Unit
Electrode potential	E	plot	V, mV

1.1.2.4.7 Conversion of input and output units

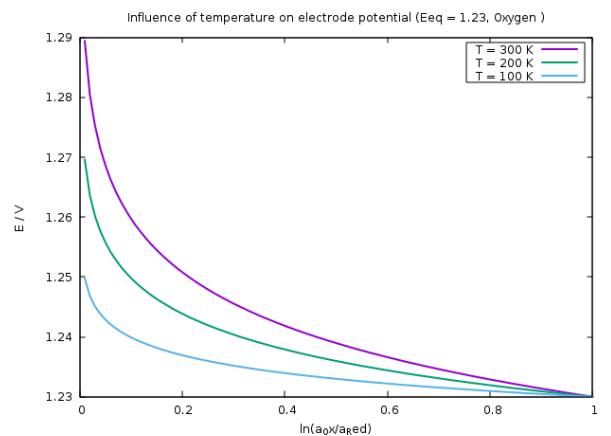
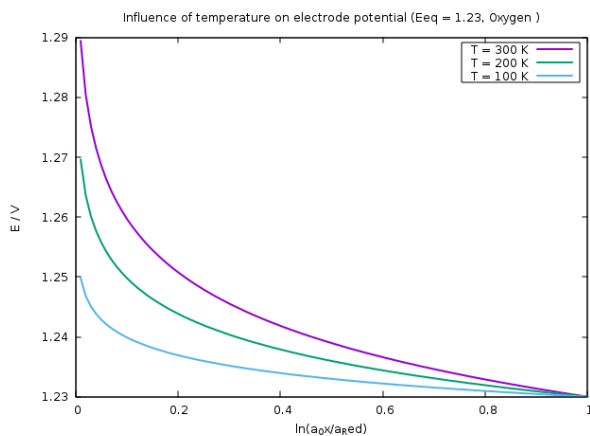
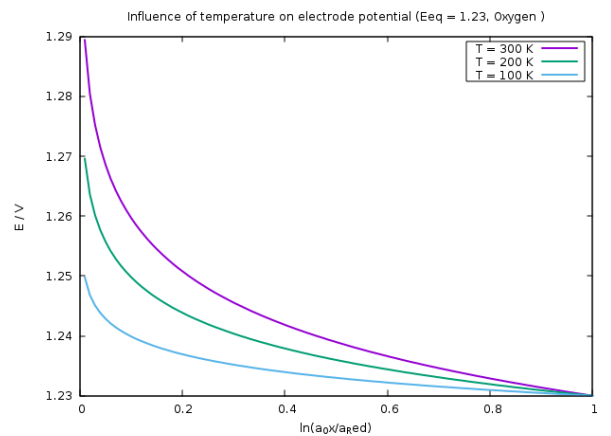
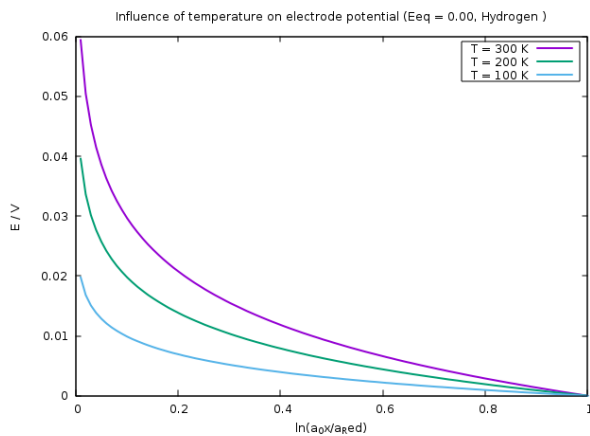
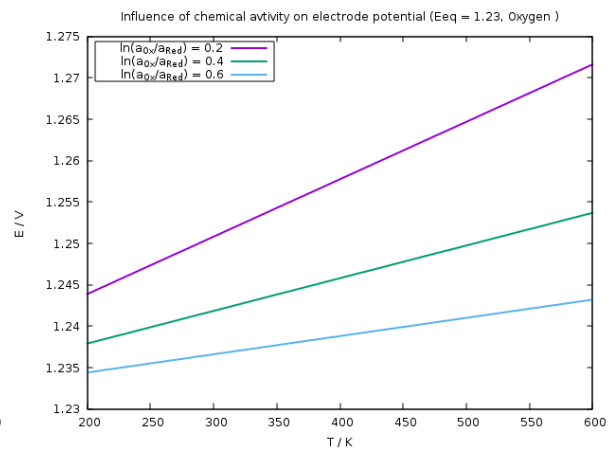
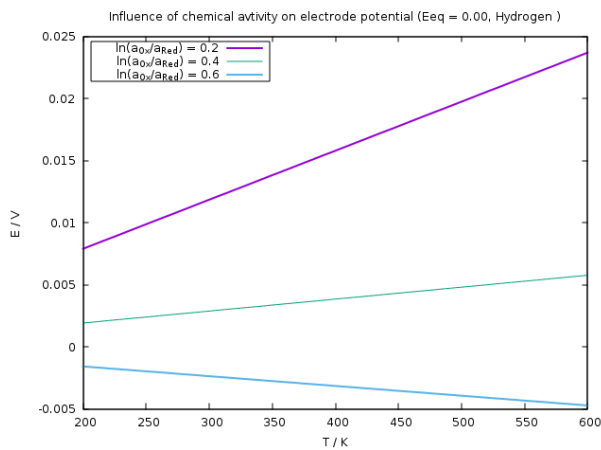
Standard units for calculation and storage in database (all values would be stored and processed in these units).

Parameter name	Standard unit name	Symbol	Unit
Temperature	kelvin	T	K
Faraday Constant	Coulomb per mol	F	96485.33289 C/mol
Universal gas constant	joule per kelvin per mol	R	8.31447 J/K/mol
Electrode Potential	volt	E	V
Equilibrium Potential	volt	E_{eq}	V
Chemical activity of reduced form	mol per cubic meter	a_{red}	mol/m ³
Chemical activity of oxidized form	mol per cubic meter	a_{ox}	mol/m ³



Alternative units for user inputs and outputs

Parameter name	Unit name	Symbol	Unit	Conversion from standard unit	Conversion to standard unit
Temperature	degree Celsius	T	C	$T(K) - 273.15$	$T(C) + 273.15$
Temperature	degree Fahrenheit	T	F	$T(K) * 9/5 - 459.67$	$(T(F) + 459.67) * 5/9$





1.1.2.5 Butler-Volmer equation (IEES)

1.1.2.5.1 Introduction

The electrochemical reactions are heterogeneous surface reactions proceeding on the phase boundary electrode (first class conductor) / electrolyte (second class conductor). Their rate is proportional to the density of the electric current passing through this phase boundary. In similarity to the chemical reactions, the rate of an electrochemical reaction (respectively, the current density) depends on the reactant concentration and the temperature. A unique characteristic of the electrochemical reactions is the dependence of the rate on the electrode potential. Each electrochemical reaction proceeds through several steps as the most important are the transfer of electric charges through the phase boundary and the mass transfer of the reactants to/from the electrode. The slowest reaction step limits the rate of the whole reaction. If the slowest step proceeds under kinetic/activation control (the charge transfer is the limiting step), the relationship between the current density and the electrode potential is quantified by the Butler-Volmer equation which is the basis of the electrochemical kinetics. It shows that the measured current density of an electrode reaction is a function of electrode over potential, exchange current density and anodic/ cathodic transfer coefficients.

1.1.2.5.2 Nomenclature

Parameter	Symbol	Unit
Total current density	j	A/m ²
Anodic current density	j_a	A/m ²
Cathodic current density	j_c	A/m ²
Exchange current density	j_0	A/m ²
Electrode potential	E	V
Equilibrium potential	E_{eq}	V
Absolute temperature	T	K
Universal gas constant	R	8.31447 J/K/mol
Number of electrones involved in the electrode reaction	n	dimensionless
Transfer coefficient	α	dimensionless
Faraday constant	F	96485.33289 C/mol
Overpotential	η	V

1.1.2.5.3 Model description

$$j_a = j_0 * e^{\frac{(1-\alpha)nF}{RT}\eta}$$

$$j_c = -j_0 * e^{\frac{-\alpha nF}{RT}\eta}$$

$$j = j_a + j_c$$

$$\eta = E - E_{eq}$$

1.1.2.5.4 Input values

Parameter	Symbol	Input value	Unit	Limits (min-max)	Defaults
Exchange current density	j_0	5	A/m ²	(0, 10]	5
Electrode potential	E	independent var.	V	[-2, 2]	
Equilibrium potential	E_{eq}	1.23	V	[-2, 2]	1.23
Absolute temperature*	T	298	K	Constant	298
Number of electrons involved in the electrode reaction	n	2	dimensionless	[1;2]	2
Transfer coefficient	α	0.5	dimensionless	(0,1)	0.5

1.1.2.5.5 Calculation procedure

Standard calculation $F(x) = F1(x)+F2(x)$, where $\Delta x \approx 0.001$

$$j(\eta) = j_a(\eta)+j_c(\eta)$$

1.1.2.5.6 Output values

Plots which the user can choose:

$j(\eta)$, $j_a(\eta)$, $j_c(\eta)$ – option for multiple plots on the same graph

$j(\eta)/j_0$, $j_a(\eta)/j_0$, $j_c(\eta)/j_0$ – option for multiple plots on the same graph

Parameter name	Symbol	Output value	Unit
Total current density	j	plot	A/m ² , A/cm ² , mA/cm ²
Anodic current density	j_a	plot	A/m ² , A/cm ² , mA/cm ²
Cathodic current density	j_c	plot	A/m ² , A/cm ² , mA/cm ²

1.1.2.5.7 Conversion of input and output units

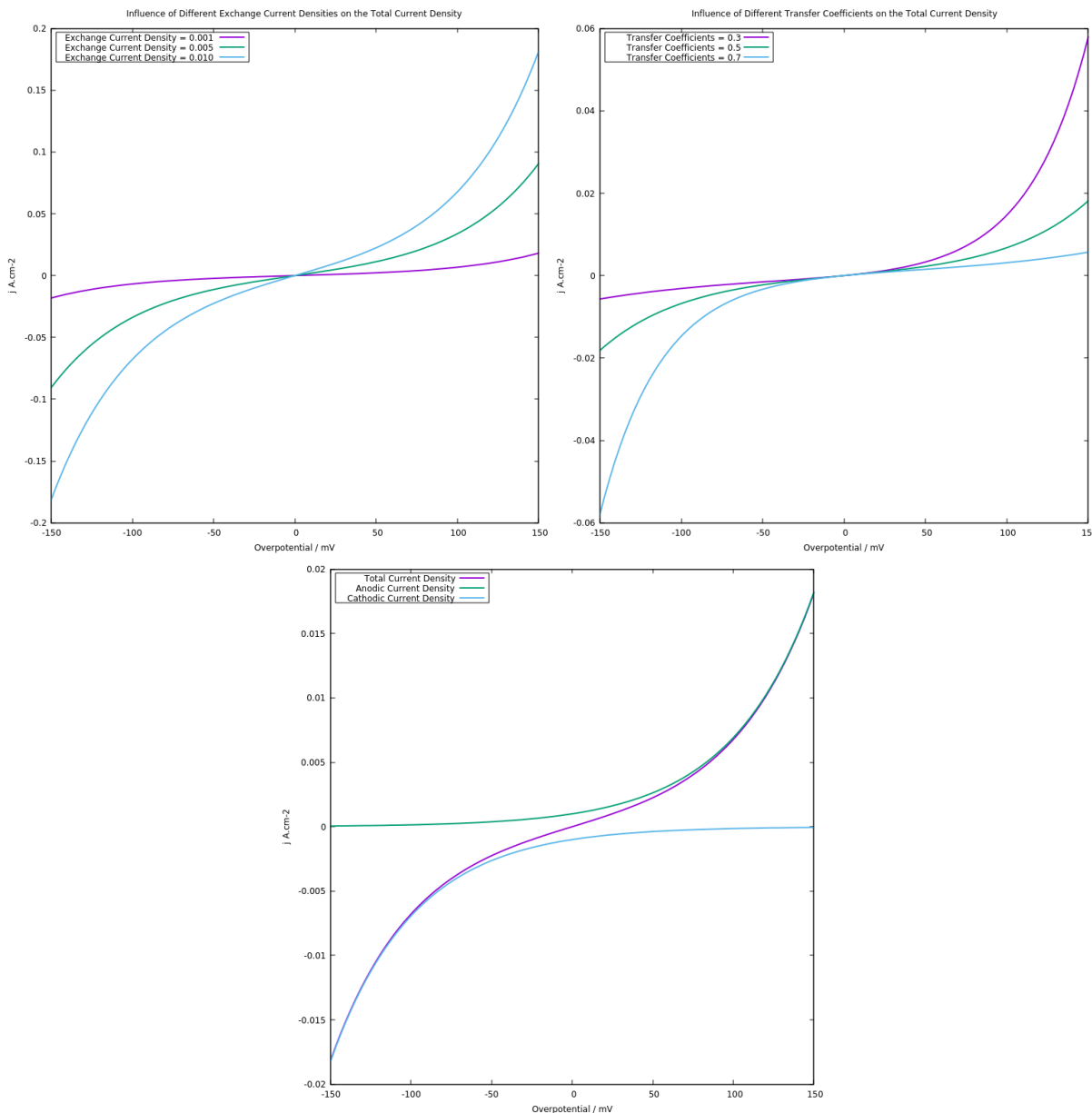
Standard units for calculation and storage in database (all values would be stored and processed in these units)

Parameter name	Standard unit name	Symbol	Unit
Temperature	kelvin	T	K
Current Density	ampere per square meter	j	A/m ²
Anodic current density	ampere per square meter	j_a	A/m ²
Cathodic current density	ampere per square meter	j_c	A/m ²
Exchange current density	ampere per square meter	j_0	A/m ²
Faraday Constant	Coulomb per mol	F	96485.33289 C/mol
Universal gas constant	joul per kelvin per mol	R	8.31447 J/K/mol
Electrode Potential	volt	E	V
Equilibrium Potential	volt	E_{eq}	V
Overpotential	volt	η	V

Alternative units for user inputs and outputs



Parameter name	Unit name	Symbol	Unit	Conversion from standard unit	Conversion to standard unit
Temperature	degree Celsius	T	C	$T(K) - 273.15$	$T(C) + 273.15$
Temperature	degree Fahrenheit	T	F	$T(K) * 9/5 - 459.67$	$(T(F) + 459.67) * 5/9$



1.1.2.6 Tafel equation (IEES)

1.1.2.6.1 Introduction

The Tafel equation can be derived from the Butler-Folmer equation for cases when the electrode overpotential is far from equilibrium. It quantifies the dependence of current density on the electrode potential for a highly polarised (anodically or cathodically) electrode. The plot of the overpotential against the decadic logarithm of the absolute value of the current density yields the so called "Tafel plot" from which the Tafel constants (**a** and **b**) can be determined. These constants are further used to



calculate the kinetic parameters exchange current density, j_0 , and transfer coefficient, α , which characterise the charge transfer reaction under study.

1.1.2.6.2 Nomenclature

Parameter	Symbol	Unit
Applied current density	j_a	mA/cm ²
First Tafel Constant (Tafel intercept)	a	mV
Second Tafel Constant (Tafel slope)	b	mV.cm ² /mA mV/dec – log scale
Overpotential	η	mV

1.1.2.6.3 Model description

$$\eta = a + b * \lg(|j_a|)$$

For anodic reactions:

$$a = \frac{-RT}{(1-\alpha)F} \lg i_0 b = \frac{(1-\alpha)F}{2.3RT}$$

For cathodic reactions:

$$a = \frac{RT}{\alpha F} \lg i_0 b = \frac{-\alpha F}{2.3RT}$$

1.1.2.6.4 Input values

Parameter	Symbol	Input value	Unit	Limits (min-max)	Defaults
Applied current density	j_a	independent var.	mA/cm ²	[1, 500]	
Tafel intercept	a	-100	mV	[-300, 300]	100
Tafel slope	b	100	mV.cm ² /mA	[-300, 300]	100

1.1.2.6.5 Calculation procedure

Standard calculation F(x), where $\Delta x \approx 0.001$

$$\eta(j_a)$$

$$\eta(\lg(j_a))$$

$$\eta(j_c)$$

$$\eta(\lg(j_c))$$

1.1.2.6.6 Output values

Plots which the user can choose:

$$\eta(j_a) \text{ with different values for } \mathbf{a} \text{ and } \mathbf{b}$$

$$\eta(\lg(j_a)) \text{ with different values for } \mathbf{a} \text{ and } \mathbf{b}$$

$$\eta(j_c) \text{ with different values for } \mathbf{a} \text{ and } \mathbf{b}$$

$$\eta(\lg(j_c)) \text{ with different values for } \mathbf{a} \text{ and } \mathbf{b}$$

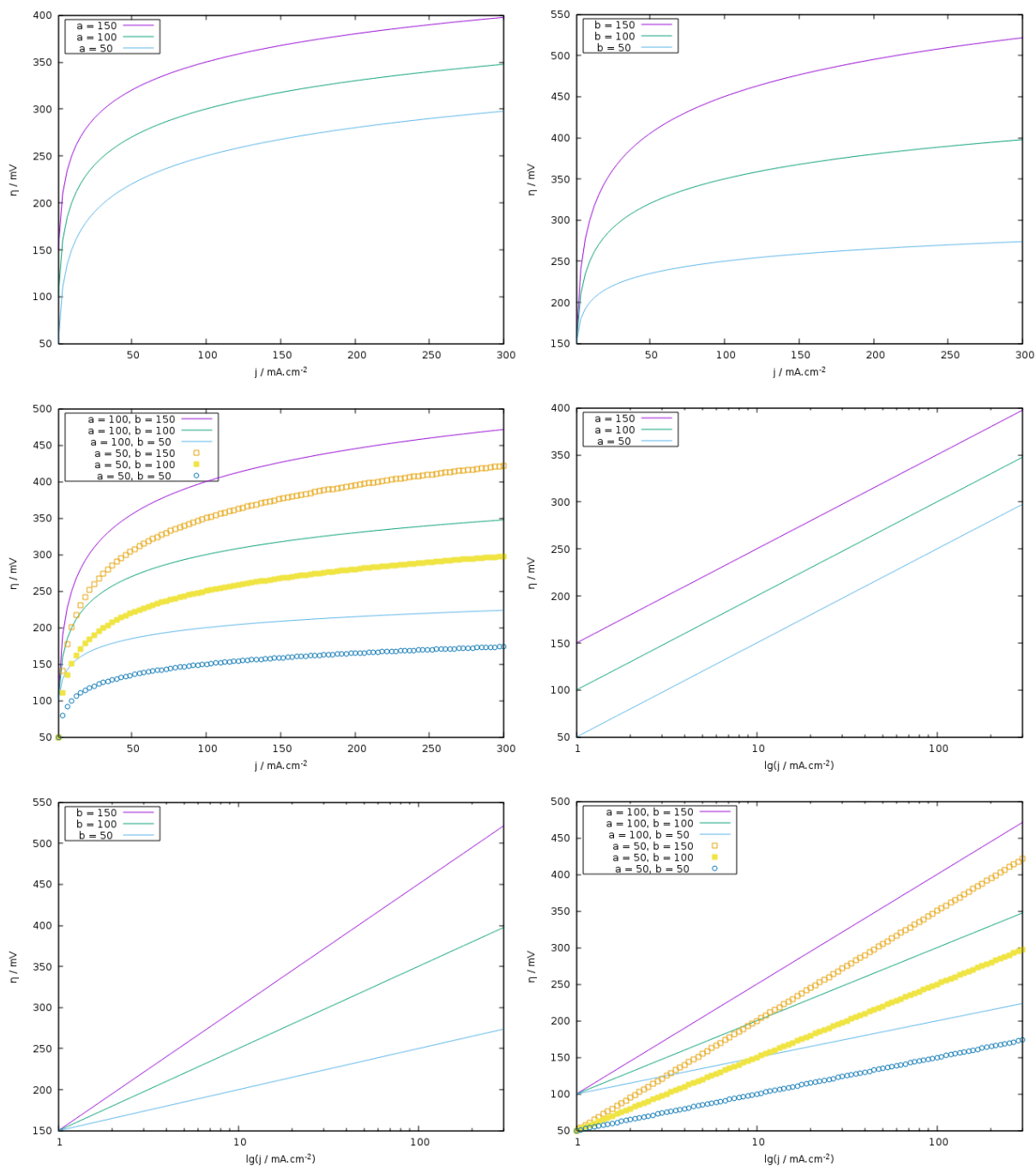


Parameter name	Symbol	Output value	Unit
Overpotential	η	plot	mV

1.1.2.6.7 Conversion of input and output units

Standard units for calculation and storage in database (all values would be stored and processed in these units)

Parameter name	Standard unit name	Symbol	Unit
Applied Current Density	ampere per square meter	j	mA/cm ²
First Tafel Constant (Tafel intercept)	millivolts	a	mV
Second Tafel Constant (Tafel slope)	millivolts per milliamperes	b	mV.cm ² /mA
Overpotential	millivolt	η	mV



1.1.2.7 Levich equation (IEES)

1.1.2.7.1 Introduction

The electrochemical reactions proceed with transfer of charges through the electrode/electrolyte interface and transfer of substance (reactants and reaction products) to and from the electrode. If the mass transport is the slowest reaction step, the electrode reaction proceeds under mass transport control and the reaction rate depends on the concentration gradient. In such cases the mathematical treatment of the electrode reaction involves relationships between the concentrations, their gradients, and the current densities (respectively, the rate of the processes occurring at the electrode/electrolyte interface). The mass transport in an electrolyte can occur by three different mechanisms: molecular



diffusion (the driving force is the concentration gradient or the gradient of chemical potential of the electrolyte species); migration (the driving force is the gradient of electric field resulting from movement of charged species and the arising ohmic drop), and convection (transport of species in a flux).

The Levich equation refers to electrode reactions occurring under conditions of convection. The convection assists the transport of the reactants to the electrode surface but in the vicinity of the electrode the governing mass transport mechanism is the diffusion. Using a rotating disk electrode Levich succeeds to quantify the dependence of the current density on the concentration of the reactants. He introduces the quantity limiting current density, which is proportional to the square root of the angular rate of the rotating electrode.

The rotating disk electrode has numerous applications in the analytical chemistry and electrochemistry such as quantitative analysis of different ions, determination of the diffusion coefficients of substances, evaluation of the number of electrons participating in the electrode reaction, etc. Levich theory is a powerful electrochemical tool for investigation of the mechanism of electrochemical reactions and determination of the limiting reaction step.

1.1.2.7.2 Nomenclature

Parameter	Symbol	Unit
Levich current	I_L	A
Electrode surface	A	cm ²
Diffusion coefficient	D	cm ² /s
Angular rotation rate of the electrode	ω	rad/s
Kinematic viscosity	ν	cm ² /s
Molar concentration	C	mol/cm ³
Number of electrons involved in the electrode reaction	n	dimensionless
Faraday constant	F	96485.33289 C/mol

1.1.2.7.3 Model description

$$I_d = zFAD \frac{C_0 - C_s}{1.61D^{2/3}\nu^{1/6}\omega^{1/2}}$$

When an electrode reaction is governed only by mass transfer, the concentration of the electroactive ion at the surface of the electrode is zero $C_s=0$, and the equation leads to the Levich equation of limiting current:

$$I_l = 0.620nFAD^{2/3}\nu^{-1/6}C\omega^{1/2}$$

1.1.2.7.4 Input values

Parameter	Symbol	Input value	Unit	Limits (min-max)	Defaults
Electrode surface	A	1	cm ²	[0.5, 5]	



Diffusion coefficient	D	1.e-5	cm ² /s	[0.01e-5, 9.00e-5]	
Angular rotation rate of the electrode	ω	independent variable	rad/s	[0, 200]	
Kinematic viscosity	ν	0.8925e-3	cm ² /s	[0.3e-3, 2.0e-3]	
Molar concentration	C	0.0001	mol/cm ³	[]	
Number of electrones involved in the electrode reaction	n	1	dimensionless	[1;2]	

1.1.2.7.5 Calculation procedure

Standard calculation $F(x)$, where $\Delta x \leq 0.001$

I_L

1.1.2.7.6 Output values

Plots wich the user can choose :

$I_L(\omega)$ - option for multiple plots on the same graph, with different values of parameters

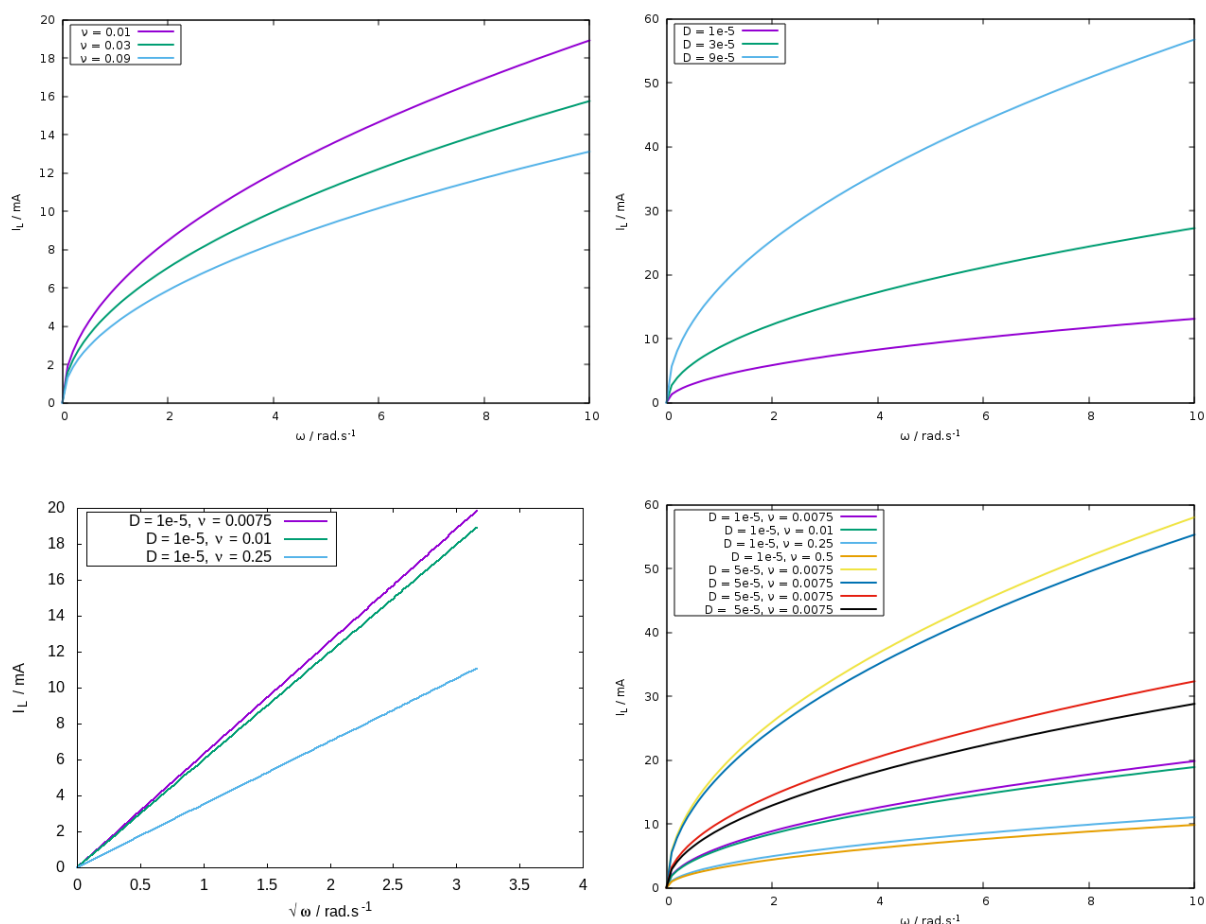
$I_L(\sqrt{\omega})$ - option for multiple plots on the same graph, with different values of parameters

Parameter name	Symbol	Output value	Unit
Levich current	I_L	plot	A, mA

1.1.2.7.7 Conversion of input and output units

Standard units for calculation and storage in database (all values would be stored and processed in these units)

Parameter name	Standard unit name	Symbol	Unit
Levich current	<i>ampere</i>	I_L	A
Electrode surface	<i>square centimeter</i>	A	cm ²
Diffusion coefficient	<i>square centimeter per second</i>	D	cm ² /s
Angular rotation rate of the electrode	radian per second	ω	rad/s
Kinematic viscosity	centimeter per second	ν	cm ² /s
Molar concentration	<i>mol per cubic centimeter</i>	C	mol/cm ³
Number of electrones involved in the electrode reaction	-	n	dimensionless
Faraday constant	Coloumb per mol	F	96485.33289 C/mol



1.1.2.8 Ionic conductivity (IEES)

1.1.2.9 References

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A. J. Bard, L. R. Faulkner, *Electrochemical Methods: Fundamentals and Applications*, 2nd ed., Wiley: New York, 2001

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David R. Lide, ed., *CRC Handbook of Chemistry and Physics*, CRC Press, Boca Raton, FL, 2005.

1.1.3 Storage tools

1.1.3.1 Comsol Multiphysics for simulation of hydrogen production and FCH technologies (NCSR)

This tool involves modeling transport phenomena and reaction kinetics for H₂ related technologies with Comsol Multiphysics v5.3 (build 316). It includes two separate tools: a) the methane steam reformer and b) the Solid Oxide Fuel Cell (SOFC). *The second tool is an **addition** to the toolbox that was not included in the initial planning and structure of e-Laboratory.* According to the feedback



gained by the Experts Workshop organized on the 19th -20th of March 2018, the simulation of SOFC was considered a useful addition in the e-Laboratory platform and its implementation was recommended by NCSR and accepted by all partners. The description of the two storage tools and their implementation in the platform is provided next.

This tool is standalone tool using third party software. Upon selection of one of the “Comsol Multiphysics for simulation of hydrogen production and FCH technologies” tools a link to download the respective tutorial and any relevant case file should be available. The user will perform the simulations in their personal computer outside the platform using the Comsol Multiphysics software.

1.1.3.1.1 Introduction

The tool provides an exemplary, complete and step-by-step guided simulation activity of a Methane Steam Reformer and a solid oxide fuel cell. For the Steam reformer three case studies are included.

A. Base case study

B. Parametric Study varying the Inlet Heating Tubes Temperature $600K \leq T_{(int_ht)} \leq 900K$

C. Bed Pressure parameter $165Pa \leq dp \leq 400Pa$

When the Storage tools are selected, the screen with the followings should appear:

- Storage tools
 - Comsol Multiphysics for simulation of hydrogen production and FCH technologies
 - A) Methane steam reformer
 - B) Solid Oxide Fuel Cell (SOFC)

Upon selection of the *Methane steam reformer* the following should appear:

- Storage tools
 - Comsol Multiphysics for simulation of hydrogen production and FCH technologies
 - A) Methane steam reformer
 - B) Solid Oxide Fuel Cell (SOFC)

Please download the tutorial for three case studies for simulation of hydrogen production (Steam Reformer) using the COMSOL Multiphysics software here:

Download the Tutorial

When the user clicks on “**Download the Tutorial**” the download of the Tutorial-Methane reformer.zip file will get started. This compressed folder contains the tutorial, the parameters and the variables that can be implemented in Comsol, the results and the mph file (Comsol file) with the entire case built.

Upon selection of the *Solid Oxide Fuel Cell* the following should appear:

- Storage tools
 - Comsol Multiphysics for simulation of hydrogen production and FCH technologies
 - A) Methane steam reformer
 - B) Solid Oxide Fuel Cell (SOFC)

Please download the tutorial for the SOFC using the COMSOL Multiphysics software here:

Download the Tutorial

When the user clicks on “**Download the Tutorial**” the download of the Tutorial-SOFC.zip file will get started. This compressed folder contains the tutorial, the mph files and the results.

1.1.3.1.2 Methane Steam Reformer

The objective of this tool is to provide a tutorial case for methane steam reforming for H₂ production using the Comsol Multiphysics code (CFD code). Steam reforming is one of the predominant ways for the production of hydrogen and is both a valuable current technology pillar as well as an indispensable intermediate step towards the transition towards hydrogen economy, with reforming done either externally or internally in devices like fuel cells. Hydrogen is used heavily in the oil industry and for the production of ammonia, while it is the cleanest of all fuel.

The tutorial demonstrates how to build a typical steam reformer model for the production of hydrogen. Briefly, the model consists of a perforated cylinder by heating tubes (Figure 2). The reformation chemistry occurs in the cylindrical porous catalytic bed where energy is supplied through the heating tubes to drive the system of overall endothermic reaction. The reactor is enclosed in an insulating jacket. The chosen kinetics are accounting for the endothermic conversion of methane to hydrogen and the gas-shift reaction. The model also includes the coupled mass and momentum transport in porous media, i.e. convection-diffusion-reaction and Navier-Stokes equations. Furthermore, the energy transport is considered through proper form for the heat convected and conducted throughout the device. Finally, the model introduces the inter-dependence of the material properties with the chemical composition and the thermal distribution of the flow.

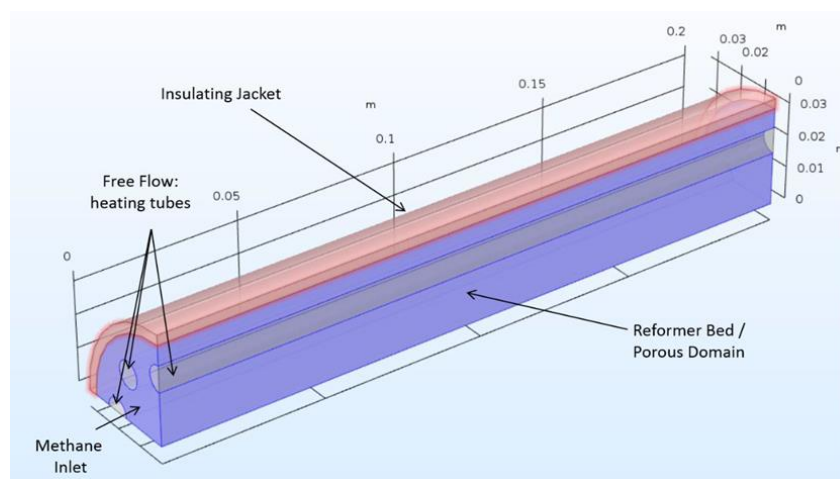


Figure 2. Axisymmetric reactor components.

Apart from the base case, parametric analysis for the bed temperature and pressure are also performed and presented. The tutorial will include the following topics:

1. *Introduction on the state of the art of Steam Methane Reforming*
2. *Theoretical summary describing the model, its assumptions, strengths, limitations and room for improvement*

3. A step-by-step description for building the model from scratch
4. Emphasis will be given on the solving process for the highly-non-linear problem
5. Model Post-processing sequence for getting results
6. Brief discussion of main results
7. Short reference to extension of the work at hand.

The user would be able to download through the platform:

1. The tutorial
2. The files with input parameters and variables
3. The mph file (comsol file) with the built case

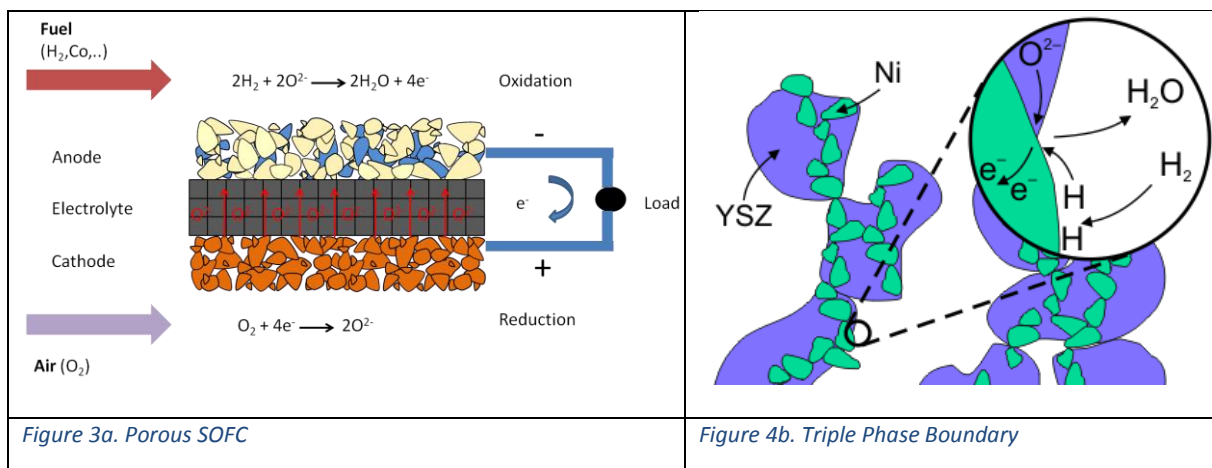
1.1.3.1.3 Solid Oxide Fuel

The objective of this tool is to provide a tutorial for a simple show case of Solid Oxide Fuel Cell (SOFC) simulation using the Comsol software. The model of the SOFC shown in this work is a typical, state-of-the-art fuel cell for the electro-chemical conversion of hydrogen to energy. It includes the following physics:

1. Electronic and ionic conduction
2. Electro-chemical reactions
3. Fluid flow through porous media

The above physics combined with the appropriate boundary conditions are solved over a typical planar fuel cell geometry.

The Interconnect of a Solid Oxide Fuel Cell SOFC is of vital importance for the functionality and the performance of the cell. The basic functions of a SOFC are depicted in Figure 3.



It serves the purposes of electron conduction between the anode of the one cell with the cathode of the next one in a stack of cells. In the same time, it allows the inflow of fuel gas, hydrogen or other, and the outflow of not reacted fuel and reaction's products on the anode side. On the cathode side the interconnect is responsible for the inflow of oxygen/air and its outflow. This flow of air or oxygen also contributes to the cell's cooling. The cell's efficiency is greatly affected by not only the choice of interconnect material, but also from its actual design. In this study it is shown how cylindrical metallic



pillars, dispersed in a hexagonal pattern inside the interconnect affect the energetic aspects of the cell.

The user would be able to download through the platform:

4. The tutorial
5. The files with input parameters and variables
6. The mph file (comsol file) with the built case

1.1.3.1.4 References

1. Xu J., Froment G.F., 1989, Methane Steam Reforming, Methanation and Water-Gas Shift: I. Intrinsic Kinetics, AIChE Journal, 35, (1), 88-96.
2. Panagakos G., Stamatakis E., Stubos G., Panopoulos K., Stubos A., 2016 A 2D axisymmetric Modelling Investigation of Membrane Methane Steam Reformers, ACS Annual Meeting, ENFL 230.
3. Todd B., Young J.B, Thermodynamic and transport properties of gases for use in solid oxide fuel cell modelling. Journal of Power Sources 110 (2002) 186–200
4. Yakabe H., Hishinuma M., Uratani M., Matsuzaki Y., Yasuda I. Evaluation and modeling of performance of anode-supported solid oxide fuel cell, Journal of Power Sources 86 2000. 423–431
5. Transport Phenomena, Bird, Stewart, Lightfoot. Wiley, 2nd Edition

1.1.4 FC tools

1.1.4.1 Modelling of transport processes in electrodes and electrolytes (DTU)

Due by (M34) in 2nd version of e-Science toolbox D3.5

1.1.5 HyFOAM

1.1.5.1 Release and dispersion of horizontal under-expanded hydrogen jet - HSL experiment (UU)

Due by (M34) in 2nd version of e-Science toolbox D3.5

1.1.5.2 Large scale deflagration in the open atmosphere - Fraunhofer ICT experiment (UU)

Due by (M34) in 2nd version of e-Science toolbox D3.5

1.1.5.3 Blast wave and fireball from high-pressure tank rupture in a fire -Weyandt experiment (UU)

Due by (M34) in 2nd version of e-Science toolbox D3.5

1.1.5.4 Hydrogen/helium dispersion in vented enclosures - CEA experiment (NCSR)

Due by (M34) in 2nd version of e-Science toolbox D3.5

1.1.5.5 Vented deflagration - FM Global experiment (NCSR)

Due by (M34) in 2nd version of e-Science toolbox D3.5