



# Novel Education and Training Tools based on digital Applications related to Hydrogen and Fuel Cell Technology

Karlsruhe Institute of Technology

Institute of Nuclear- and Energy Technologies (IKET)

**Olaf Jedicke**; Giovanni Cinti<sup>(1)</sup>, Evelina Slavcheva<sup>(2)</sup>

[EFC 2017; Naples 12<sup>th</sup> – 15<sup>th</sup> December 2017]

<sup>(1)</sup> University of Perugia (Italy)

<sup>(2)</sup> Bulgarian Academy of Science (Bulgaria)

- ✦ General Target and Aim
- ✦ General Objectives (overview of structure)
- ✦ e-Laboratory (e-engineering, e-science)
- ✦ Explicit Examples
- ✦ e-Learning (LMS)
- ✦ e-Learning (more specifics)
- ✦ Collaboration
- ✦ e-infrastructure (implementation)
- ✦ Conclusion



# Education

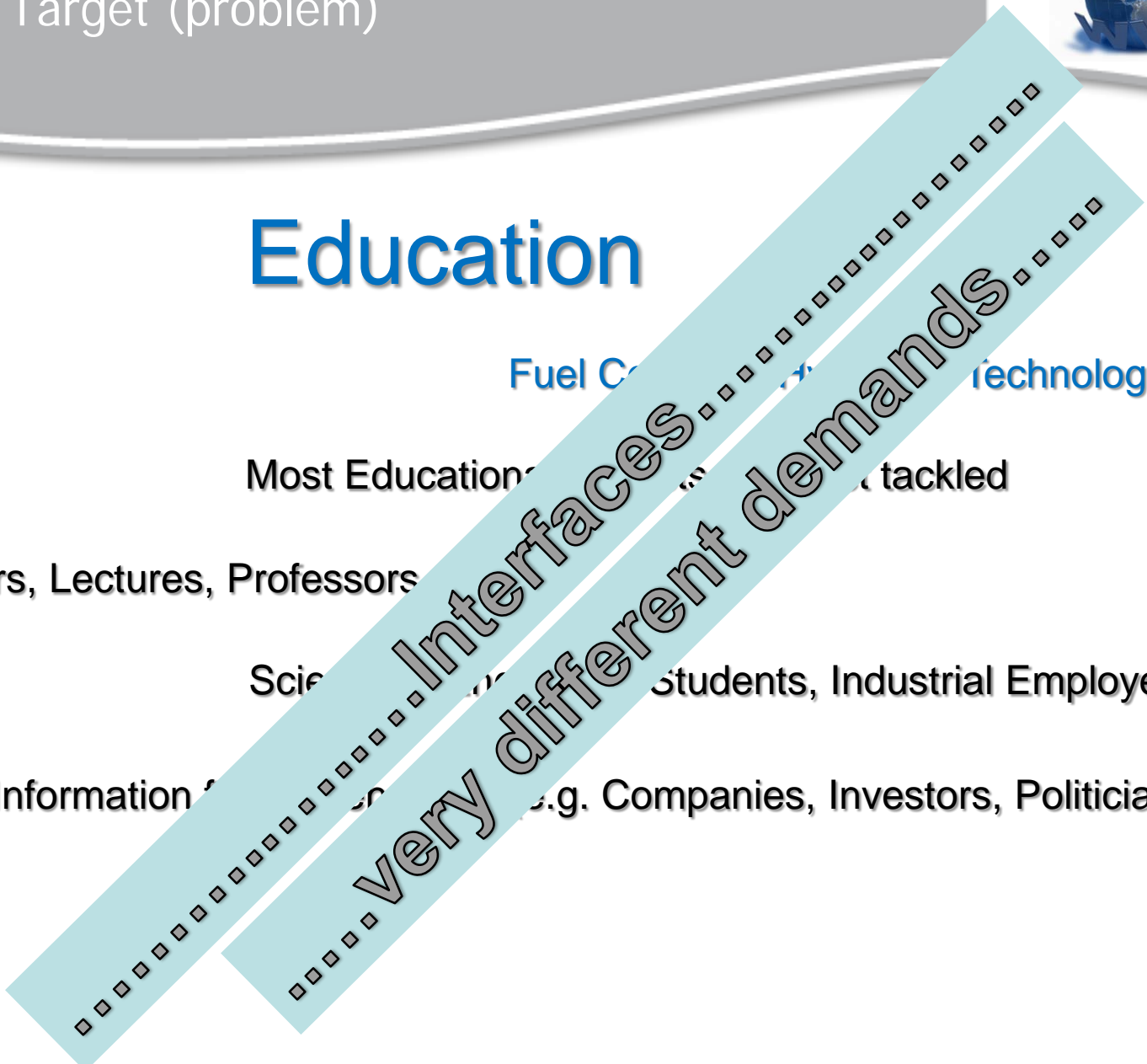
Fuel Cells, Fuel Cells technologies

Most Educational institutions are not tackled

Trainers, Lectures, Professors

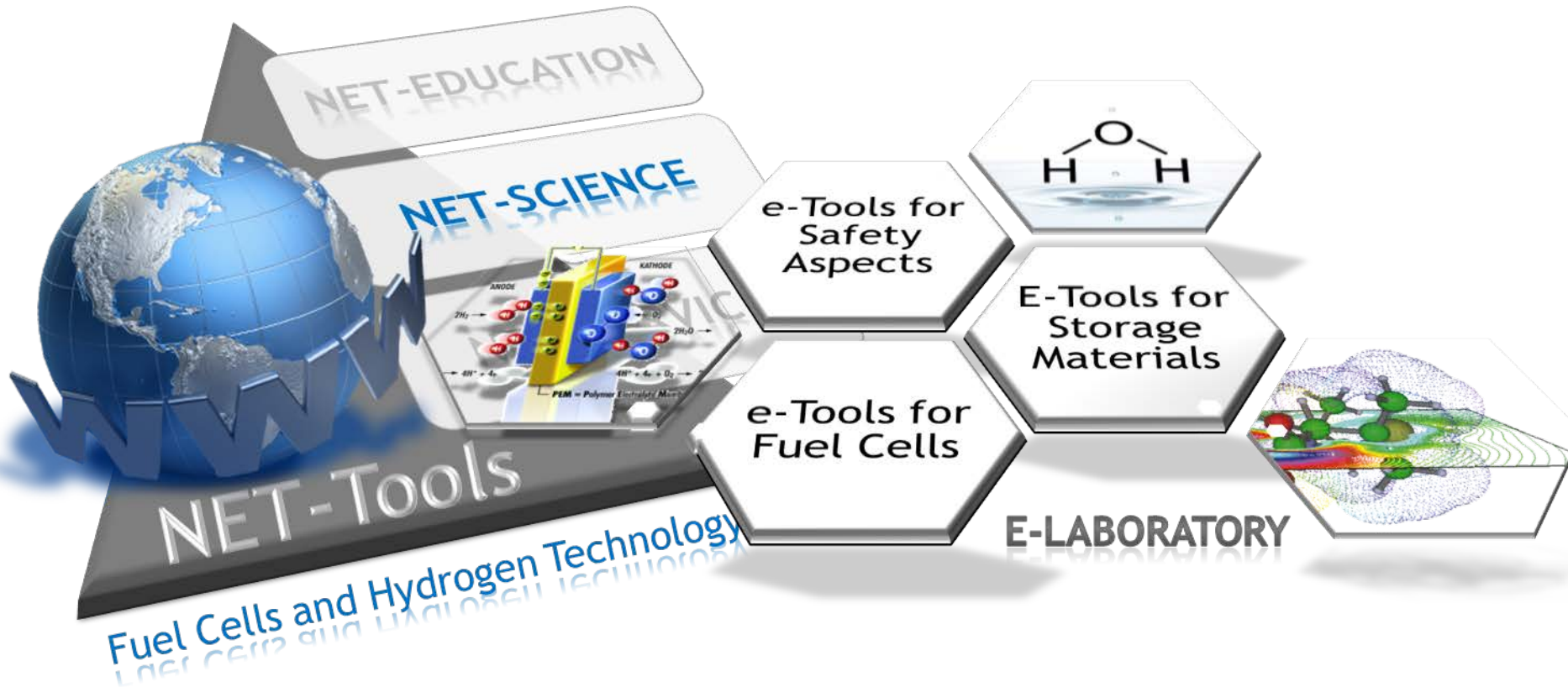
Scientists, Students, Industrial Employees

Information providers (e.g. Companies, Investors, Politicians)

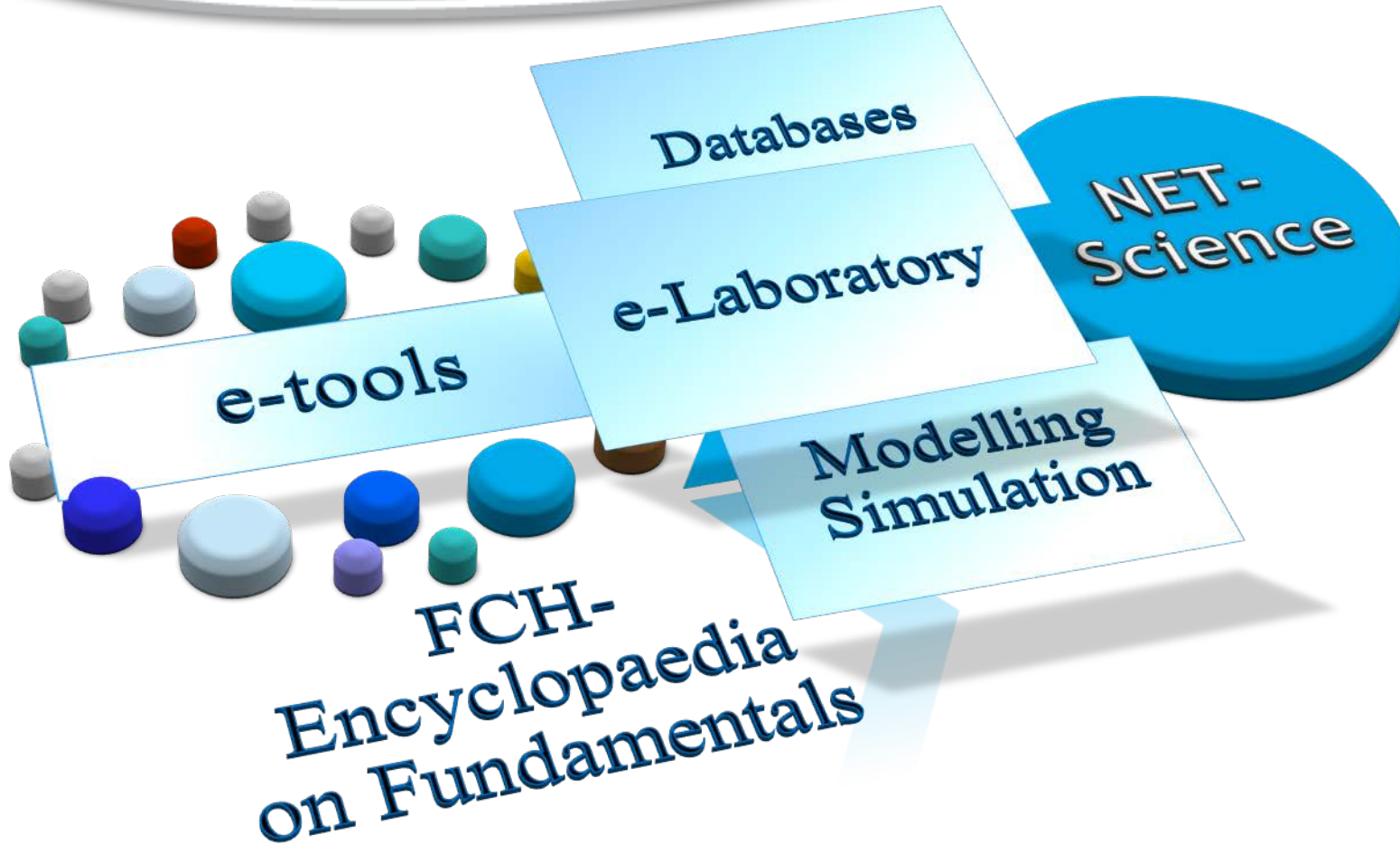


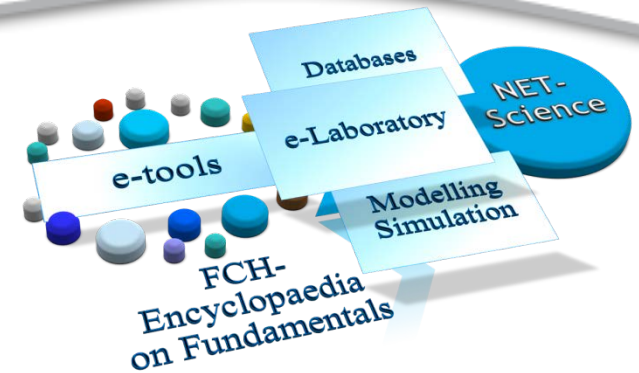
# General Aim (graphical overview)

To develop, realize, promote and provide a common e-platform



# General Aim (structural overview)





- ✦ Development of an e-Laboratory Platform  
subdivided into:
  - ✦ e-Engineering Toolbox
    - Modelling and simulation of FCH related technical aspects
    - Guidelines and brief handbooks of e-tools
  - ✦ e-Science Toolbox
    - Modelling and simulation of FCH relevant phenomena
    - Database of results received from done experiments
    - Database related CFD programming (validation and verification of codes)
    - Guidelines
  - ✦ Database
    - Repository of done experiments and results
    - Guidelines and handbooks

# e-Engineering (samples of tools)

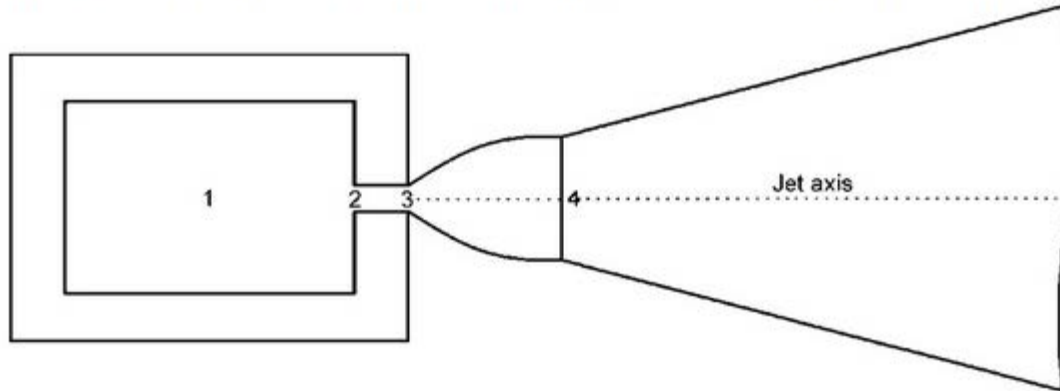


e-Engineering	Renewable energy system (RES) tools	1. Design and optimization of hybrid RES-hydrogen systems	Simulation of SOFC based on natural gas as fuel
	Fuel cells (FC) tools	1. Simulation of SOFC based on natural gas as fuel	
		2. Energy balances and hydrogen costs for various electrolysis techniques	
		3. Cell and stack models for both fuel cells and electrolysis	Cell and stack models for both fuel cells and electrolysis
		4. Thermo-mechanical models to predict lifetime of high temperature FCs and electrolysis	
	Storage tools	1. Storage material properties	
		2. gProms thermal design of storage tanks optimization ( <a href="http://www.psenterprise.com/gproms.html">http://www.psenterprise.com/gproms.html</a> ).	
	FC integrated into CHP tools	1. Simulation of FC system integrated into mCHP application, including electrolyser operation	
		1. Under-expanded jet parameters model	Forced ventilation system parameters
	Safety engineering tools	2. Adiabatic and isothermal model of blowdown of storage tank dynamics	Adiabatic and isothermal model blowdown of storage tank dynamics
		3. Flame length correlation and three hazard distances for jet fires	
		4. Continuity law for concentration dependent hydrogen expanded and under-expanded jets and vented jet based distances	
		6. Passive ventilation in an enclosure with one vent: uniform hydrogen concentration	
		7. Mitigation of uniform mixture deflagration by venting technique	
		8. Forced ventilation	Calculation of upper limits of hydrogen inventory in closed space
		9. Blast	
		10. Effect of buoyancy on decrease of hazard distance for unignited releases	
11. Pressure peaking phenomenon for ignited releases			
12. Upper limit of hydrogen inventory in closed space			
13. Mitigation of localised non-uniform deflagration by venting			
14. Blowdown time as a function of storage pressure, volume, and TPRD diameter			
15. Radiation from hydrogen fireball after high-pressure hydrogen tank rupture in a fire			
16. Effect of buoyancy on hazard distances for jet fires			
17. Calculation of choked flow for stagnation conditions in vapor, liquid or supercritical regimes.			

## Cyber Laboratory

### Underexpanded jet parameters

The model describes parameters in an underexpanded jet through characteristic stages of its development - in reservoir (1), orifice (2), and effective nozzle diameter (4). The model is based on Abel-Noble equation of state for hydrogen; conservation equations for mass and energy; assumption that at state (4) (so called "effective nozzle diameter") pressure is equal to the ambient one and velocity is equal to the local sound speed. The model does not account pressure losses in the nozzle (between states (2) and (3)).



### Reference:

- Free eBook: V. Molokov "Fundamentals of Hydrogen Safety Engineering", www.BookBoon.com, October, 2012

### INPUT VALUES

Units for pressure input:

[bar] ▾

Pressure in tank:

700 [bar]

Temperature in tank:

240 [K]

Orifice diameter:

2 [m]

Ambient pressure:

650 [bar]

RUN





## Result - Underexpanded jet parameters

### INPUT VALUES

Pressure in tank:	700.0	[bar]
Hydrogen temperature in reservoir:	240.0	[K]
Orifice diameter:	2.0	[m]
Ambient pressure:	650.0	[bar]

### OUTPUT VALUES

Density in the tank:	45,80589 [kg/m <sup>3</sup> ]
Density at the orifice:	27,68593 [kg/m <sup>3</sup> ]
Pressure in orifice:	26240224,60627 [Pa]
Velocity in orifice:	1300,72777 [m/s]
Temperature at the orifice:	180,87414 [K]
Diameter of effective nozzle exit:	1,69233 [m]
Density in effective nozzle exit:	49,12897 [kg/m <sup>3</sup> ]
Velocity in effective nozzle exit:	1023,76062 [m/s]
Temperature in effective nozzle exit:	199,5842 [K]
Mass flow rate:	113134,56842 [kg/s]

The calculation can last for a few seconds. If you want to start a calculation, click twice on the update button for it.

Temperature of the environment [K]  288.4000000000000

pressure of the environment [Pa]  101325.00000000000

jet exit diameter [m]  0.12000000000000000

```

#####
# INCLUDE PARAMETERS OF ENVIRONMENT
# T = temperature of the environment / K
#T = 288.40
T=ind
# p = pressure of the environment / Pa
#p = 101325.0
p=ind
# rho = density of environment / kg/m3
rho = Rho(p,R_0air,T)
#####
# INCLUDE JET PARAMETERS
# d_j = jet exit diameter / m
#d_j = 0.12
d_j=ind
#####
# SET GAS TO HYDROGEN
# c_p = c_p_H2
Tmax = Tmax_H2
Mpc0 = Mpc0_H2
alpha = alpha_H2
# mu = mu_H2
# mu_0 = mu_0_H2
# mu_0 = 1.224e-05
rho_j = 0.084
alpha_j = 24.40

Fr_j = rho_j * c_p**0.5 / (rho_j / rho)**0.25 / ((Tmax/T - 1.0) * g * d_j)**0.5
#print "Fr_j = ", Fr_j

# L_star = 0.1
L_star = 10.0 * Fr_j**0.4 / (1.0 + 0.07 * Fr_j**2)**0.2
d_star =
L_star = 20
#print "L_star = ", L_star

L_star = L_star * d_j * sqrt(rho_j / rho) / Es
#print "L_star = ", L_star, " m"
                    
```

# e-Engineering (flame length and separation distance for jet fires)

If you want to start a calculation, click twice on the update button for it.

Hydrogen pressure in reservoir  $p_1$  [Pa]

Hydrogen temperature in reservoir  $T_1$  [K]

Orifice diameter  $D_0$  [m]

Ambient temperature  $T_{amb}$  [K]

Close and the pressure [Pa]

Update

please insert data and press update

Parameter	Symbol	Unit	Range (min/max)
Hydrogen pressure in reservoir	$p_1$	Pa	100000-10000000
Hydrogen temperature in reservoir	$T_1$	K	>0
Orifice diameter	$D_0$	m	0.0001-0.0017
Ambient temperature	$T_{amb}$	K	200-3000

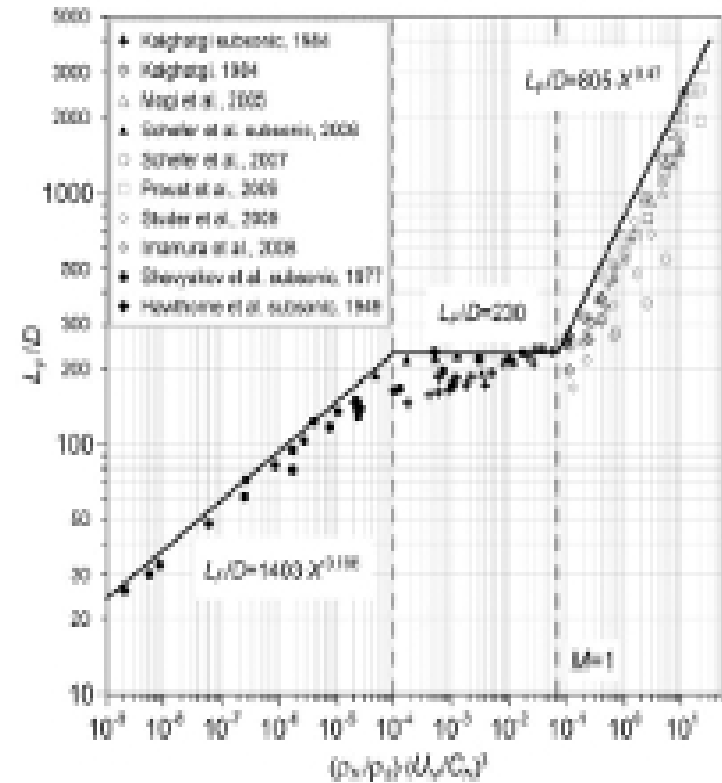


Figure 1 – Dimensionless (conservative) correlation for hydrogen jet fires (in form also shown in figure “X” denotes the similarity group  $(p_1/p_1) \cdot (U_0/C_0)^2$  (Malikov & Buffers, 2010)

## MODEL DESCRIPTION FOR STEADY-STATE HYDROGEN UNIFORM CONCENTRATION

The neutral plane (NP) is a horizontal plane where pressure inside and outside an enclosure are equal. In general case of passive ventilation of the enclosure with release of gas lighter than air, the neutral plane is located at or below the half height of the vent for steady-state conditions. Below NP air enters the enclosure and above NP lighter hydrogen-air mixture exits the enclosure (Fig. 1, left).

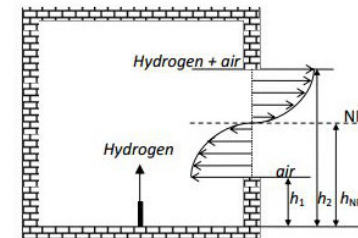


Figure 1. Flow velocity through the vent for a case when neutral plane is between the lower edge and half height of the vent.

### 1. STEADY-STATE HYDROGEN UNIFORM CONCENTRATION FOR THE GIVEN RELEASE RATE AND VENT SIZE

You can calculate the mass flow rate by using the [hydrogen jet parameters model](#).

If you want to start a calculation, click twice on the update button for it.

Hydrogen mass flow rate $\dot{m}$ [kg/s]	<input type="text" value="0"/>
Ambient pressure $p_2$ [choose]	<input type="text" value="0"/>
Ambient temperature $T_2$ [K]	<input type="text" value="0"/>
Vent height $H$ [m]	<input type="text" value="0"/>
Vent width $W$ [m]	<input type="text" value="0"/>
Discharge coefficient $CD$ [-]	<input type="text" value="0.600000000"/>
Choose unit for pressure	<input type="text" value="Pa"/> ▼
<input type="button" value="Update"/>	
<p>please insert data</p>	

# e-Engineering (computing mass balances at the anode & cathode of an operating PEM fuel cell)

If you want to start calculations, click twice on the update button for it.

Cell surface area (m <sup>2</sup> )	<input type="text"/>
Number of cells (N)	<input type="text"/>
Circuit density I (A/m <sup>2</sup> )	<input type="text"/>
Stack temperature T (K)	<input type="text"/>
Anodic ratio to stoichiometry (R <sub>A</sub> ) (%)	<input type="text"/>
Cathodic ratio to stoichiometry (R <sub>C</sub> ) (%)	<input type="text"/>
Anodic pressure (inlet) (Pa)	<input type="text"/>
Cathodic pressure (inlet) (Pa)	<input type="text"/>
Anodic pressure drop (Pa)	<input type="text"/>
Cathodic pressure drop (Pa)	<input type="text"/>
Anodic relative humidity (RH <sub>A</sub> ) (%)	<input type="text"/>
Cathodic relative humidity (RH <sub>C</sub> ) (%)	<input type="text"/>
Fraction of produced water that crosses the membrane (x)	<input type="text"/>

please insert some data

Parameter	Symbol	Unit	Range (min./max.)
Cell surface area	S	m <sup>2</sup>	0*10 <sup>-4</sup> / 200*10 <sup>-4</sup>
Number of cells	n	NO	1 / 1000
Circuit density	I	A/m <sup>2</sup>	1 / 0*10 <sup>-4</sup>
Stack temperature	T	K	290.15 / 440.15
Anodic ratio to stoichiometry	R <sub>A</sub>	NO	1-10 / 10
Cathodic ratio to stoichiometry	R <sub>C</sub>	NO	1-2 / 10
Anodic pressure (inlet)	P <sub>A</sub>	Pa	10 <sup>5</sup> / 4*10 <sup>5</sup>
Cathodic pressure (inlet)	P <sub>C</sub>	Pa	10 <sup>5</sup> / 4*10 <sup>5</sup>
Anodic pressure drop	ΔP <sub>A</sub>	Pa	0 / 0.8*10 <sup>5</sup>
Cathodic pressure drop	ΔP <sub>C</sub>	Pa	0 / 0.8*10 <sup>5</sup>
Anodic relative humidity	RH <sub>A</sub>	%	0 / 100
Cathodic relative humidity	RH <sub>C</sub>	%	0 / 100
Fraction of produced water that crosses the membrane	x	NO	-1 / 1

## Simple tool for computing mass balances at the anode & the cathode of an operating PEM fuel cell (CEA)

### Introduction / description

From user data about the cell or stack operating conditions (for instance stoichiometric ratios, relative humidity), the model computes the input data that is needed for designing a fuel cell system or test bench (for instance mass flows for the different species, requirements for gases hydration).

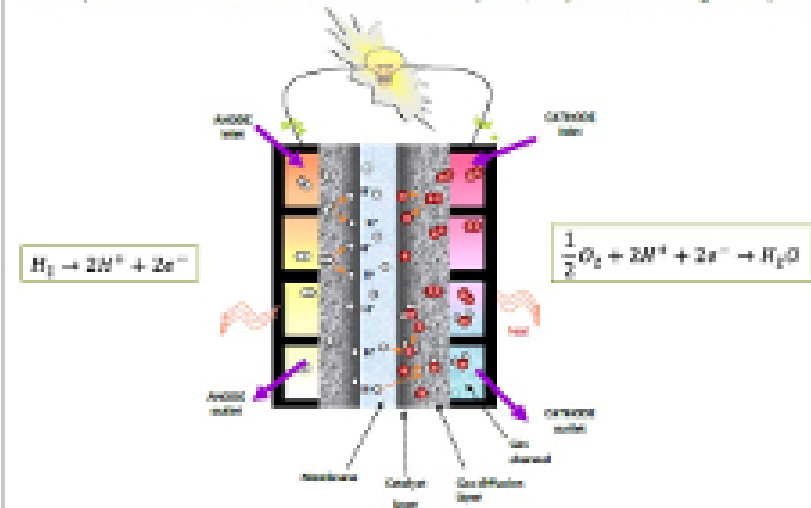
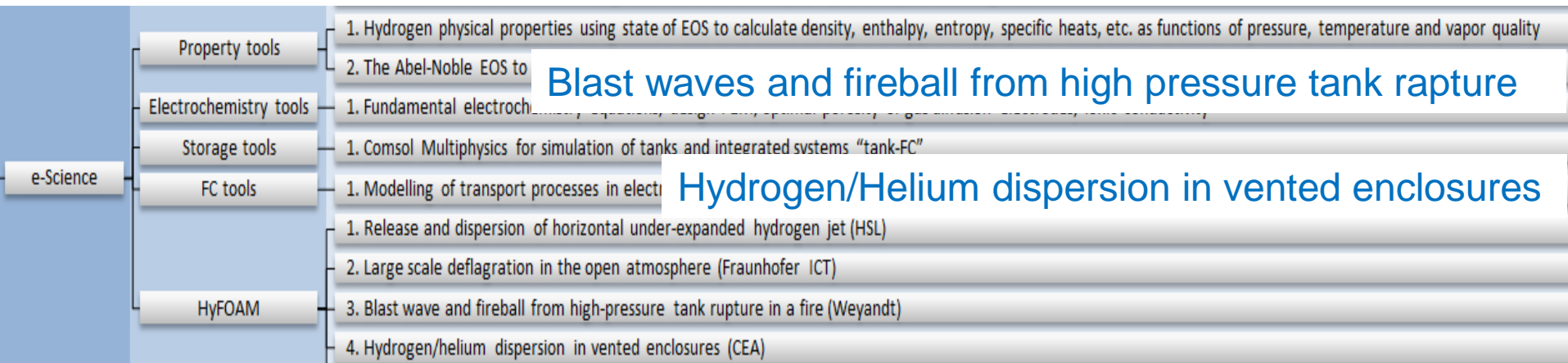


Figure 1 - Simple schematic of a fuel cell

## Thermo-physical properties of Hydrogen

## Release and dispersion phenomena



- ✦ Normal thermo-physical properties of hydrogen using the NIST-EoS, (Helmholtz free energy based)
- ✦ Obtain properties in the gas-liquid-supercritical range as function of  $P$ ,  $T$
- ✦ Level of complexity high
- ✦ Code built in Java, by NCSRD
  
- ✦ **J. W. Leachman, R. T. Jacobsen, S. G. Penoncello, and E. W. Lemmon, "Fundamental Equations of State for Parahydrogen, Normal Hydrogen, and Orthohydrogen," J. Phys. Chem. Ref. Data, vol. 38, no. 3, p. 721, 2009**

## Description

$$\alpha(\tau, \delta) = \alpha^0(\tau, \delta) + \alpha^r(\tau, \delta) \quad \tau = \frac{T_c}{T} \quad \delta = \frac{\rho}{\rho_c}$$

$$\alpha^0 = \ln \delta + 1.5 \ln \tau + a_1 + a_2 \tau + \sum_{k=3}^N a_k \ln[1 - \exp(b_k \tau)]$$

$$\alpha^r(\tau, \delta) = \sum_{i=1}^l N_i \delta^{d_i} \tau^{t_i} + \sum_{i=l+1}^m N_i \delta^{d_i} \tau^{t_i} \exp(-\delta^{p_i})$$

$$+ \sum_{i=m+1}^n N_i \delta^{d_i} \tau^{t_i} \exp[\varphi_i(\delta - D_i)^2 + \beta_i(\tau - \gamma_i)^2]$$

$$P(T, \rho) = \rho RT \left[ 1 + \delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_{\tau} \right] \quad Z(T, \rho) = \frac{P}{\rho RT} = 1 + \delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_{\tau}$$

**Complexity: Iterations required to find  $\rho$  from  $P$ ,  $T$ .**



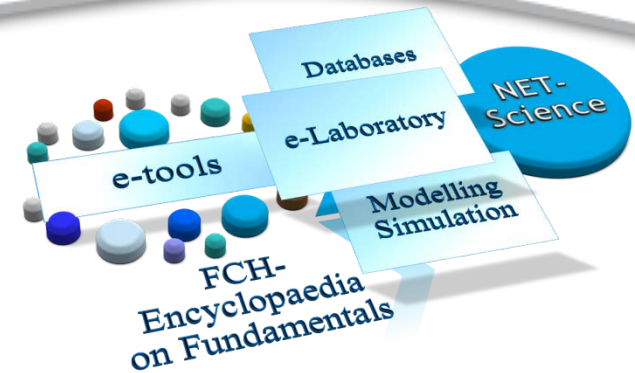
## Description (continued)

$$h(T, \rho) = RT \left\{ \tau \left[ \left( \frac{\partial \alpha^0}{\partial \tau} \right)_\delta + \left( \frac{\partial \alpha^r}{\partial \tau} \right)_\delta \right] + \delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_\tau + 1 \right\}$$

$$s(T, \rho) = R \left\{ \tau \left[ \left( \frac{\partial \alpha^0}{\partial \tau} \right)_\delta + \left( \frac{\partial \alpha^r}{\partial \tau} \right)_\delta \right] - \alpha^0 - \alpha^r \right\}$$

$$c_p(T, \rho) = c_v + R \frac{\left[ 1 + \delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_\tau - \delta \tau \left( \frac{\partial^2 \alpha^r}{\partial \delta \partial \tau} \right) \right]^2}{\left[ 1 + 2\delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_\tau + \delta^2 \left( \frac{\partial^2 \alpha^r}{\partial \delta^2} \right)_\tau \right]}$$


$$\omega(T, \rho) = \sqrt{\frac{RT}{M} \left[ 1 + 2\delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_\tau + \delta^2 \left( \frac{\partial^2 \alpha^r}{\partial \delta^2} \right)_\tau \frac{\left[ 1 + \delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_\tau - \delta \tau \left( \frac{\partial^2 \alpha^r}{\partial \delta \partial \tau} \right) \right]^2}{\tau^2 \left[ \left( \frac{\partial^2 \alpha^0}{\partial \tau^2} \right)_\delta + \left( \frac{\partial^2 \alpha^r}{\partial \tau^2} \right)_\delta \right]} \right]}$$

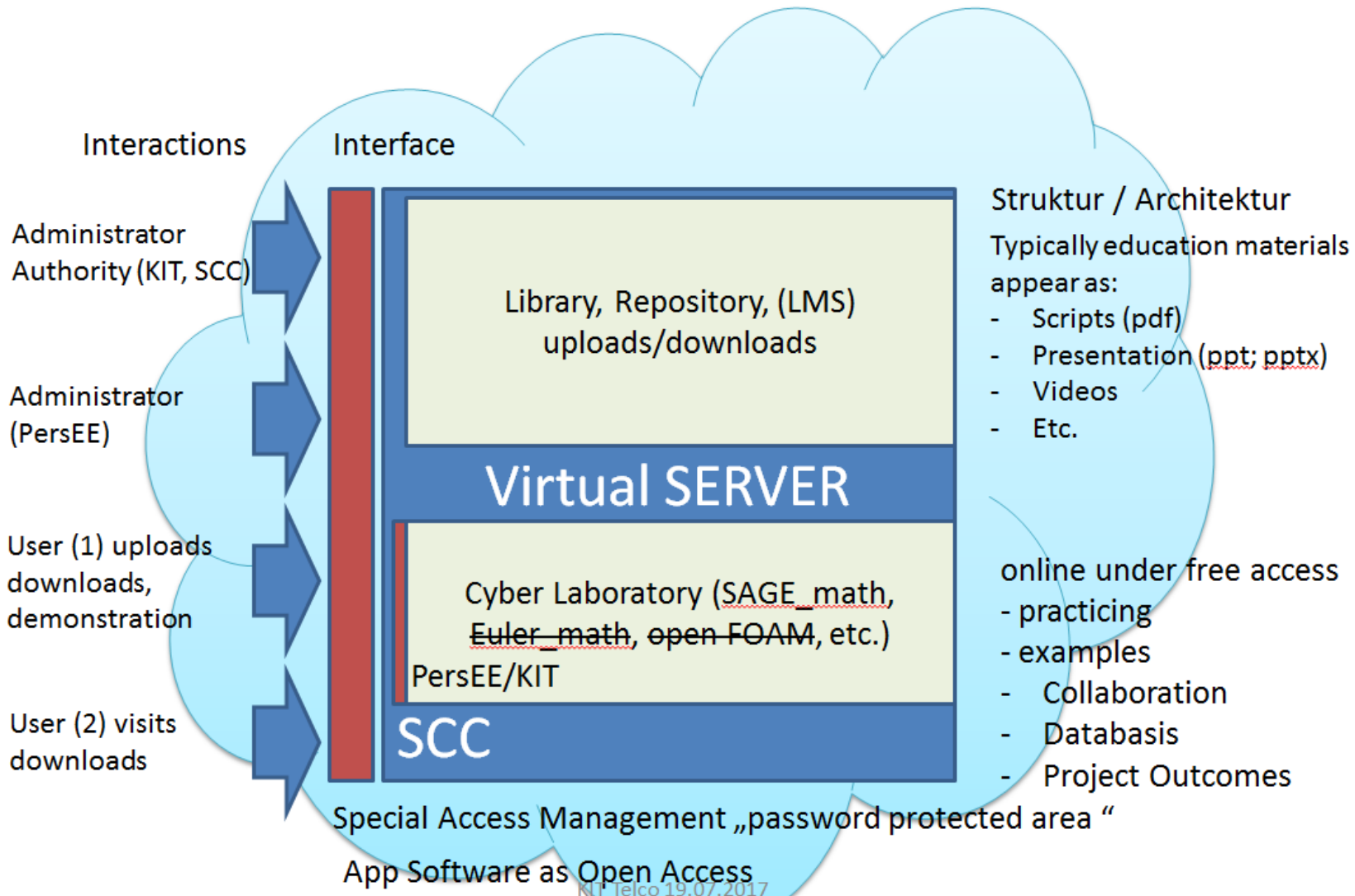


- ✪ Development of an e-Educational Platform  
subdivided into:
  - ✪ e-Learning
    - Conventional Learning Management System (LMS)
    - Technical features to support users concerning communication, planning, exchange of documents, etc.
    - Quality assurance (probably review)
    - Guidelines
  - ✪ e-Repository of FCH relevant information
    - Database
    - Documentations
    - e-books ?
    - Guidelines

- Educational materials
  - Course materials
  - Survey of existing course materials
  
- Specific Courses (Master Courses) in collaboration with **TeachHy**
  - Course Curricula (University level)
  - Content descriptions (based on modules)
  - Specific educational course materials
  - List of European Universities providing the master course (faculties, professors, lectures, etc.)
  - Access for students and teachers (lectures)
  
- e-Learning for Industrial Use
  - Typical industrial demands
  - Industrial level (technicians and engineers)
  - Facing industrial problems

- ✪ Provide a **comprehensive platform for online courses (MOOCs)** for teaching on technologies on various levels (from vocational to academic education) with innovative features compared to existing online education platforms
- ✪ Provide an **overview and incorporate existing educational materials** and important players in the field of fuel cells and hydrogen, industry and academia
- ✪ Provide **online courses as first examples in relevant areas** for the sector and analyze their impact. Suggested areas are (subject to Advisory Board discussion):
  - ➔ Basis to hydrogen (physical (also thermodynamically) and chemical behavior, economic and ecological aspects)
  - ➔ Basic processes of hydrogen production and technologies
  - ➔ Transportation, storage and handling of hydrogen as an energy carrier
  - ➔ Complete Fuel Cell technology, systems and applications
- ✪ **Start compiling/hosting online courses/digital** from other education and training institutions beyond the NET-Tools consortium
- ✪ Develop **tools and guidelines for acceptance and certification** of online/digital education

Technical Realisation	Implementation	Exploitation
<p><b>WP2</b> Specification and Development of NET-Tools digital Infrastructure</p> 	<p><b>WP3</b> e-Laboratory</p> <p><b>WP4</b> e-Learning and Education Materials</p>	<p><b>WP5</b> Networking</p> <p>Dissemination Knowledge Experience</p> <ul style="list-style-type: none"> <li>• Expert Workshop</li> <li>• Educational Schools</li> <li>• Flying Teachers</li> <li>• International Collaboration</li> </ul>
<p><b>WP1</b> Consortium Management, Project Monitoring, Business Strategy</p>		



# Direct Collaboration and Inputs



H<sub>2</sub>FC

EUROPEAN RESEARCH INFRASTRUCTURE



- HySafe (Network of Excellence)
- HyFOAM
- H2FC (Research Infrastructure Project)
- SUSANA Project (FCH-Joint Undertaking)
- TeachHy (FCH-Joint Undertaking)
- International Institutions (e.g. DOE, Japan)
- Hydrogen Europe (industry grouping)
- Hydrogen Europe Research (research grouping)
- others





H2FC  
EUROPEAN RESEARCH INFRASTRUCTURE

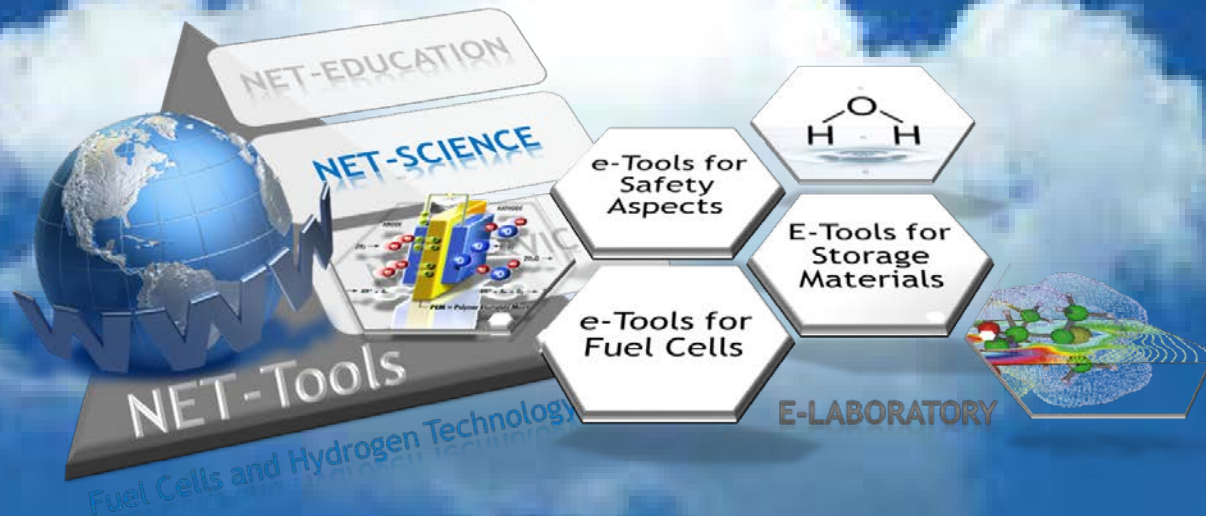


- ✦ Expert Workshop (2018)
  - Stakeholders from Industry
  - Stakeholders from Academia
  - Advisory Board Members
  - Others
- ✦ Two Educational Schools (2018 and 2019)
  - To enrol and test NET-Tools e-platform on practical level (in operando)
  - Feedback for further improvement and development
- ✦ Flying Teachers
  - To enrol and test the acceptance of new teaching strategy in combination with NET-Tools
  - H2FC (Research Infrastructure Project)
- ✦ Newsletter

















# NET-Tools Conclusions

- Development and compilation of specific e-tools
- Development of e-Laboratory (scientific and engineering basis)
- Development of e-Education (repository and LMS)
- Development of e-Platform (cloud based) to provide e-Laboratory and e-Education under free access



TO PROVIDE an EUROPEAN DIGITAL PLATFORM to the FCH Community

Acronym	KIT coordinator leader WP 1	Membership
	Karlsruher Institute of Technology GERMANY (KIT) Research Organisation	
<b>Acronym</b>	<b>PersEE leader WP 2</b>	
	PersEE FRANCE Small and Medium Enterprise (SME)	
<b>Acronym</b>	<b>NCSR</b>	
	National Center For Scientific Research DEMOKRITOS GREECE University (Higher Education)	
<b>Acronym</b>	<b>UU leader WP 3</b>	
	University of Ulster UNITED KINGDOM University (Higher Education)	
<b>Acronym</b>	<b>DTU leader WP 4</b>	
	Danmarks Tekniske Univeritet DENMARK University (Higher Education)	
<b>Acronym</b>	<b>IEES leader WP 5</b>	
	Bulgarian Academy of Science BULGARIA Institute of Electrochemistry and Energy Systems University (Higher Education)	
<b>Acronym</b>	<b>UNIPG</b>	
	Università Delgi Studi di Perugia ITALY University (Higher Education)	
<b>Acronym</b>	<b>EE leader industrial advisory board</b>	

- Grant agreement No: **736648**
- Action acronym: **NET-Tools**
- Action full title: **Novel Education and Training Tools based on digital applications related to Hydrogen and Fuel Cell Technology**
- Topic: **Novel education and training tools**
- Type of action: **Coordination & support action**
- Granting authority: **Fuel Cells and Hydrogen 2**
- Action duration (in months): **36**
- Starting Date of Action: **1 March 2017**
- **NET-Tools gets funding from**



**FUEL CELLS AND HYDROGEN**  
JOINT UNDERTAKING



# NET-TOOLS

e-tools for  
education in  
modern

FCH-technology

Created by Olaf Jedicke

