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**Safety of Hydrogen as an Energy Carrier**

**Draft for Development of an International Curriculum on  
Hydrogen Safety Engineering**

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**1 INTRODUCTION**

The onset and further development of the hydrogen economy are known to be constrained by safety barriers, as well as by the level of public acceptance of new applications. Educational and training programmes in hydrogen safety, which are currently absent in Europe, are considered to be a key instrument in lifting these limitations and to ensure

the safe introduction of hydrogen as an energy carrier. Therefore, the European Network of Excellence Safety of Hydrogen as an Energy Carrier (NoE HySafe) embarked on the establishment of the e-Academy of Hydrogen Safety. This work is led by the University of Ulster and carried out in cooperation with international partners from five other universities (Universidad Politecnica de Madrid, Spain; University of Pisa, Italy; Warsaw University of Technology, Poland; Instituto Superior Technico, Portugal; University of Calgary, Canada), two research institutions (Forschungszentrum Karlsruhe and Forschungszentrum Juelich, Germany), and one enterprise (GexCon, Norway). The development of an International Curriculum on Hydrogen Safety Engineering aided by world-class experts from within and outside NoE HySafe, is of central importance to the establishment of the e-Academy of Hydrogen Safety. Experts who have contributed to the curriculum development up to now are listed in Table 1. Despite its key role in identifying the knowledge framework of the subject matter, and its role in aiding educators with the development of teaching programmes on hydrogen safety, no such curriculum appears to have been developed previously. The current structure of the International Curriculum on Hydrogen Safety Engineering, and the motivation behind it, are described in this report. Future steps in the development of a system of hydrogen safety education and training in Europe are briefly described.

Table 1: List of contributors to the curriculum.

Baraldi, D.	The European Commission's Joint Research Center	The Netherlands
Bauwens, L.	University of Calgary	Canada
Bjerkedvedt, D.	Telemark	Denmark
Crespo, A.	Universidad Polytecnicade Madrid	Spain
Dahoe, A.E.	University of Ulster	United Kingdom
Donze, M.	Delft University of Technology	The Netherlands
Dorofeev, S.B.	FM Global	United States of America
Engebo, A.	Det Norske Veritas	Norway
Faudou, J.-Y.	Air Liquide	France
Gallego, E.	Universidad Polytecnicade Madrid	Spain
Garcia, J.	Universidad Polytecnicade Madrid	Spain
Hansen, O.	GexCon	Norway
Jordan, T.	Forschungszentrum Karlsruhe	Germany
Kirillov, I.	Kurchatov Institute	Russia
Makarov, D.V.	University of Ulster	United Kingdom
Marangon, A.	University of Pisa	Italy
Martinfuertes, F.	Universidad Polytecnicade Madrid	Spain

Migoya, E.	Universidad Polytechnica de Madrid	Spain
Molkov, V.V.	University of Ulster	United Kingdom
Nilsen, S.	Norsk Hydro	Norway
Palliere, H.	Commissariat a l Energie Atomique	France
Pasman, H.J.	Delft University of Technology	The Netherlands
Reinecke, E.	Forschungszentrum Juelich	Germany
Roekaerts, D.J.E.M.	Delft University of Technology	The Netherlands
Schneider, H.	Fraunhofer Institut Chemische Technologie	Germany
Teodorczyk, A.	Warsaw University of Technology	Poland
Tsuruda, T.	NRIFD	Japan

Hydrogen is known to have some properties that make its behaviour during accidents different from that of most other combustible gases. When no use is made from hydrogen's greatest safety asset, buoyancy, it can become more dangerous than conventional fuels such as gasoline, LPG and natural gas. When mixed with air, hydrogen's lower flammability limit is higher than that of LPG or gasoline, but its flammable range is very large (4-75% hydrogen in air). In the concentration range of 15-45%, the ignition energy of hydrogen is one-tenth of that of gasoline. The quenching gap, i.e. the smallest spacing through which a flame can propagate - is considerably smaller for hydrogen than for today's fossil fuels. This implies that requirements for mitigation, such as flame arrestors and similar equipment, must be more stringent. It is a strong reducing agent and contact with metal oxides (rust) leads to an exothermic reaction. It can cause material embrittlement and diffuses more easily through many conventional materials used for pipelines and vessels, and through gaps that are normally small enough to seal other gases safely. The safety and combustion literature indicates that releases of hydrogen are more likely to cause explosions than releases of today's fossil fuels do. Many countries' building codes require garages to have ventilation openings near the ground to remove gasoline vapour, but high-level ventilation is not always addressed. As a result, accidental releases of hydrogen in such buildings will inevitably lead to the formation of an explosive mixture at the ceiling-level. Moreover, combustion insights have revealed that burning behaviour becomes far less benign when the limiting reactant is also the more mobile constituent of a combustible mixture. Owing to the extreme lightness of the molecule, this is particularly true with hydrogen.

For many decades, hydrogen has been used extensively in the process industries (e.g. refineries and ammonia synthesis) and experience has shown that hydrogen can be handled safely in industrial applications as long as appropriate standards, regulations and best practices are being followed. This is particularly true for the nuclear industry, where the high safety standards have resulted in the development of sophisticated hydrogen mitigation technologies (IAEA-TECDOC-1196 (2001) [1]). Interestingly, these technologies rely on the same anomalous properties, such as the large diffusivity and extreme lightness

that make hydrogen more dangerous than conventional fuels. For example, these properties are used to preclude the formation of flammable mixtures after accidental hydrogen releases, and to prevent further development towards more dangerous concentrations, once the flammability limit is exceeded (hydrogen removal by buoyancy, application of catalytic re-combiners, or benign burns, dilution by mixing with an inert gas, e.g. steam).

This experience, however, is very specific and can not easily be transferred to the daily use of new hydrogen technologies by the general public. Firstly, because new technologies involve the use of hydrogen under circumstances that are not yet addressed by research or taken into account by existing codes and recommended practices. For example, virtually all vehicle demonstration projects by manufacturers involve the use of hydrogen as a compressed gas at extremely high pressures (over 350 bar). There is no precedent for the safe handling of hydrogen at such conditions and current codes and standards for hydrogen were not written with vehicle fuelling in mind. Secondly, in industries, hydrogen is handled by people who received specific training at a professional level, and, installations involving hydrogen are subject to professional safety management and inspection. The hydrogen economy, on the other hand, involves the use of hydrogen technologies by general consumers. Since a similar dedication to safety, e.g. training general consumers to a professional level, would become impractical, hydrogen safety education should target professionals engaged in the conception or creation of new knowledge, products, processes, methods, systems, regulations and project management in the hydrogen economy. Between this community of scientific and engineering professionals, including entrepreneurs developing hydrogen technologies, and general consumers of hydrogen applications, there is another group of vital importance to the successful introduction of hydrogen into our social infrastructure. A group that must be targeted as well by hydrogen safety education. These are the educators, local regulators, insurers, rescue personnel, investors, and public service officials. Their involvement is essential to the acceptance and use of the new technology by the general public. Without the establishment of a consolidated consumer market there will be no transition from our present fossil-fuel economy into a sustainable one based on hydrogen. This process depends entirely on the public acceptance and use of hydrogen technologies.

Sufficient and well-developed human resources in hydrogen safety and related key areas are of vital importance to the emerging hydrogen economy. With our present fossil-fuel based economy increasingly being replaced by a hydrogen economy, a shortfall in such knowledge capacity will hamper Europe's innovative strength and productivity growth. A lack of professionals with expert knowledge in hydrogen safety and related key areas will impose a serious setback on innovative developments required to propel this transition, and, ongoing efforts to achieve public acceptance of the new technology might be thwarted. Recently, the European Commission identified a shortage (COM (2003) 226 final [2], SEC (2003) 489 of 30.4.2003 [3], COM (2005) 576 final [4]) of experts in the key disciplines (natural sciences, engineering, technology) relevant to hydrogen safety. The workforce in R&D is presently relatively low, as researchers account for only 5.1 in every thousand of the workforce in Europe, against 7.4 in the US and 8.9 in Japan (COM (2001) 331 final [5]). An even larger discrepancy is observed if one considers only the number of corporate researchers employed in industry: 2.5 in every thousand in Europe, against 7.0 in the US and 6.3 in Japan. Moreover, the number of young people attracted to careers in science and research appears to be decreasing. In the EU, 23% of the people aged between 20 and 29 years are in higher education, compared to 39% in the USA. Knowing that research is a powerful driving force for economic growth, and a continuous supply of



a skilled workforce is of paramount importance to the emerging hydrogen economy, this situation calls for drastic improvement.

To explore possibilities for improvement it would be helpful to consider what might have caused this situation in the first place. Firstly, there are the quality and attractiveness of Europe for investments in research and development in relation to that of other competing knowledge economies. The quality of research, and the number of young people embarking on higher education in natural sciences, engineering, and technology, depend primarily on investments made in R&D-activities. Presently, this amounts to 1.96% of GDP in Europe, against 2.59% in the United States, 3.12% in Japan and 2.91% in Korea. The gap between the United States and Europe, in particular, is currently about 120 billion a year, with 80% of it due to the difference in business expenditure in R&D. At this point it is important to notice that the quality of the European research base will not improve, unless larger investments are made in R&D. It has been diagnosed (COM (2002) 499 final [6]) that multinational companies accounting for the greater share of business R&D expenditure, increasingly tend to invest on the basis of a global analysis of possible locations. This results in a growing concentration of trans-national R&D expenditure in the United States. Moreover, there appears to be a decline in the global attractiveness of Europe as a location for investment R&D as compared to the United States. This alarming development could be reversed by improving the quality of the European research base, such that corporate investments in R&D are increased to 3% of GDP in Europe (COM (2002) 499 final [6]).

Secondly, there is the problem of a retiring science and technology workforce that needs to be succeeded by a younger generation of experts. The identified lack of experts in natural sciences, engineering, and technology creates an unstable situation for investment in R&D. This is particularly true if one considers that innovative developments take place over a time-span of several years. No investor will commission research projects to a retiring workforce without a prospect of succession by a capable younger generation.

Thirdly, there is the problem of changes in the skill-set sought by employers and investors. The purpose of science and engineering education is to provide the graduate with sufficient skills to meet the requirements of the early stages of the professional career, and a broad enough basis to acquire additional skills as needed in the later stages. Because of the transitional nature of the hydrogen economy, and the consequential development and implementation of new technologies, the skill-set sought by employers is expected to change more rapidly than ever before. This phenomenon has already manifested itself in the information technology sector, and is anticipated to occur in the hydrogen economy as well. Science and engineering education related to the hydrogen economy must therefore be broad and robust enough, such, that when todays expert-skills have become obsolete, graduates possess the ability to acquire tomorrows expert-skills.

The International Curriculum on Hydrogen Safety Engineering, discussed further in this report, aims at tackling these three causes of detriment to Europes research base and innovation strength. It is important to be aware of the fact that Europe is the worlds greatest knowledge centre because it has over 500 universities with about one million students. The reasons why this competitive potential is not yet fully exploited on the world market of knowledge is fragmentation caused by language barriers, the enclosure of the educational systems within national borders. The establishment of an International Curriculum on Hydrogen Safety Engineering, one that will be used as a blueprint for the development of educational and training programmers at universities throughout Europe, will stimulate the mobility of students and faculty, international

collaboration at all levels, and efforts related to the unification of resources in the area of science and further education. This mobilisation of human capital and resources with an emphasis on hydrogen safety and related key areas will increase Europe's competitive strength as a knowledge economy and enable Europe to fulfil a leading role in achieving global understanding of, and agreement on dealing with hydrogen safety matters.

The European Commission has launched a number of measures (SEC (2003) 905 [7], COM (2000) 318 final [8]) to co-ordinate e-learning activities with the aim to propel Europe towards becoming the most competitive and dynamic knowledge-based economy in the world. Universities are using e-learning as a source of added value for their students, and for providing off-campus, flexible, virtual learning through web-based resources. Some universities are entering into strategic partnerships and adopting new business models to serve the changing education market and to face the challenges posed by global competition. From an employer point of view, greater emphasis is being placed on cost savings and on flexible, just-in-time education and training, to provide employees with the necessary skills and competence that match changing business needs. Owing to the transitional nature of the hydrogen economy, the continual introduction of new technologies, and the consequential rapid diversification of the skill-set sought by employers, e-learning is expected to become important in providing education and training in hydrogen safety. Because e-learning does not confine trainees to a specific campus location, employees are given maximal opportunity to acquire new skills and competencies while continuing in full-time employment, and to maintain family and domestic commitments. Moreover, e-learning makes it possible for experts working at the forefront of hydrogen safety to deliver teaching on the state-of-the-art in the field, while continuing their research of endeavour.

While the e-learning market in Europe is estimated at 12 billion euro per year, and is experiencing rapid growth, the lack of good quality e-learning content remains a matter of concern. The development of the International Curriculum on Hydrogen Safety Engineering, as described in the previous section, will improve this situation because the mechanism of extracting the state-of-the-art in hydrogen safety from the HySafe network, and the coherent coupling of this knowledge into existing engineering curricula is the best guarantee for quality. Moreover, the deployment of this curriculum in conjunction with e-learning for the delivery of hydrogen safety education, with the latter being unrestricted in terms of catchment area, will enable Europe to fulfil a leading role in exporting knowledge on hydrogen safety to the world.

## 2 DESCRIPTION OF THE MODULES

Developing an International Curriculum on Hydrogen Safety Engineering entails identifying and demarcating the knowledge framework of the subject matter. The process results in a definition of Hydrogen Safety Engineering as a basis for development of new educational programmes, and it determines its relationship with other branches of engineering (see Figure 1). This, to avoid duplication of educational efforts, but also to achieve cross-fertilisation with existing engineering programmes through the introduction of topics with an emphasis on hydrogen safety. Because graduates in hydrogen safety will be involved in all aspects of the hydrogen economy to ensure safety, it is important that the following issues are taken into account during the development of the curriculum:

- what kind of organisations will employ graduates in hydrogen safety (industry,

engineering consultancies, research institutions, teaching institutions, rescue brigades, fire brigades, legislative bodies, insurance companies, governmental bodies, etc),

- at what level will graduates in hydrogen safety operate within the organisation (design, construction, operation, manufacture, teaching, research, development of standards and guidelines, etc), and,
- which mode of education is the most appropriate to match the skill-set sought at the various levels of engagement within these organisations (undergraduate education, postgraduate degree, continuous professional development).

The emerging hydrogen economy will require both undergraduates and professionals with a post-graduate degree dedicated to hydrogen safety. The undergraduate programme should be well-rounded in the engineering science core in Figure 1, but also supplemented by topics and additional courses with an emphasis on hydrogen safety. An International Curriculum on Hydrogen Safety Engineering, proposed as the basis of educational and training programmes at universities throughout Europe, will therefore not only cover the nodes in the HySafe activity matrix shown in Figure 2, but also provide a mechanism to introduce hydrogen safety topics at all levels. Furthermore, because the topics connected to the nodes in Figure 2 are subject to continuous change as the hydrogen economy evolves, the curriculum needs to be comprehensive enough to absorb these changes and new knowledge generated along the way. To comply with these requirements, the International Curriculum on Hydrogen Safety Engineering is designed to consist of basic modules, fundamental modules, and applied modules. This approach was inspired by Magnusson et al. (1995) [9], who adopted a similar approach for the development of a model curriculum for Fire Safety Engineering. The current modular structure is summarised in Table 3, and the detailed topical content of the curriculum may be viewed at the e-Academy page of the HySafe consortium (<http://www.hysafe.org>).

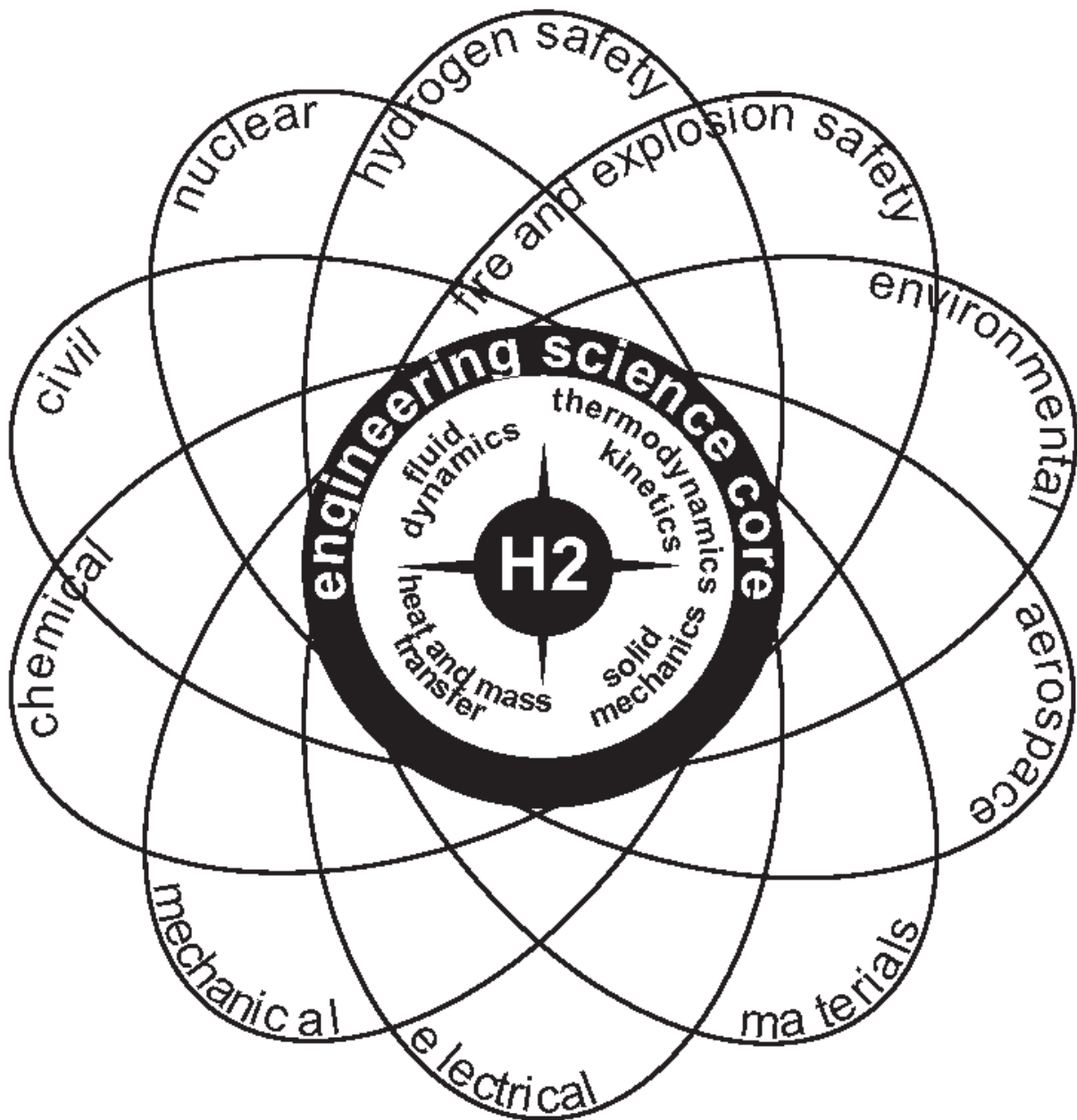


Figure 1: Hydrogen safety in relation to other branches of engineering.

The four basic modules, i.e. thermodynamics; fluid dynamics; heat and mass transfer; solid mechanics, are mainly intended for undergraduate instruction mainly (although these modules contain topics belonging to the postgraduate level). They are similar to any other undergraduate course in the respective subject areas, but comprehensive enough to provide a broad basis for dealing with hydrogen safety issues involving hydrogen embrittlement, unscheduled releases of liquefied and gaseous hydrogen, and accidental ignition and combustion of hydrogen, etc. The purpose of these modules is twofold. Firstly, to enable the coupling of knowledge relevant to hydrogen safety into existing engineering curricula, and secondly, to provide support to the knowledge framework contained in the fundamental and applied modules.

The six fundamental modules, i.e. introduction to hydrogen as an energy carrier; fundamentals of hydrogen safety; release, mixing and distribution; hydrogen ignition; hy-

drogen fires; deflagrations and detonations, define the fundamental knowledge framework that form the backbone of hydrogen safety. While these modules, except for the first one, are intended for instruction at the postgraduate level, their topical content may also be used to develop teaching materials for undergraduate instruction to supplement existing engineering curricula with courses dedicated to hydrogen safety. The topical content of these modules is relevant to the nodes in the HySafe-activity matrix (Figure 2). These topics are initially based on the existing literature, and updated continuously as new knowledge becomes available, particularly from the HySafe network. Obviously, the fundamental modules play a pivotal role in the curriculum development as the hydrogen economy evolves. New knowledge enters the curriculum through the fundamental modules, and this information is subsequently used to tune the basic and applied modules.

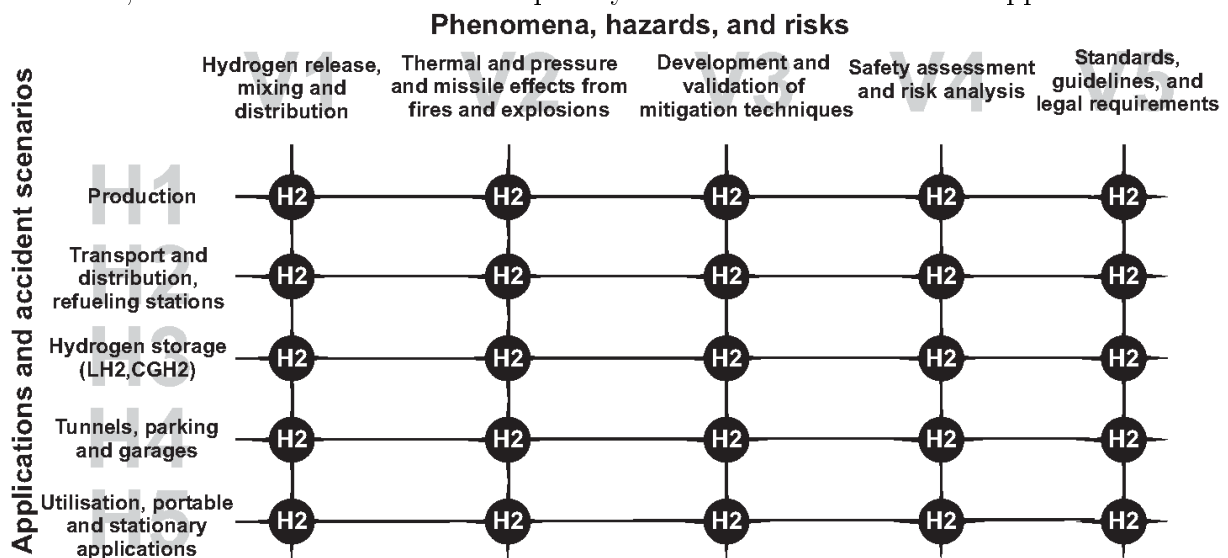


Figure 2: The Hysafe activity matrix.

The four applied modules, i.e. fire and explosion effects on people, structures, and the environment; accident prevention and mitigation; computational hydrogen safety engineering; risk assessment, are intended to provide graduates with the skill-set needed to tackle hydrogen safety problems. These are postgraduate modules, but their topical content may also be used to develop undergraduate courses on hydrogen safety to complement existing undergraduate engineering curricula. The topics covered by these modules also coincide with the nodes in the HySafe-activity matrix (Figure 2). Like the fundamental modules, the role of these modules is also pivotal in the development of the curriculum. Methodologies and front-line techniques to deal with hydrogen safety problems are extracted from the HySafe network and incorporated into these modules. Modifications to these modules due to new information are followed by tuning of the topical content of the basic and fundamental modules to preserve coherence throughout the entire curriculum.

The development of a curriculum in any branch of engineering would obviously be meaningless without a market of trainees. Since the level of interest in hydrogen safety education primarily depends on the number of people involved in hydrogen related activities, the e-Academy of Hydrogen Safety maintains a database of organisations working in the hydrogen industry (this may be viewed at the e-Academy page of the HySafe consortium (<http://www.hysafe.org>)). As an exercise (see deliverable D17), it was attempted

to use this database to assess the market of potential trainees in hydrogen safety. A questionnaire was sent to 600 companies and institutions contained in the database. There were 28 respondents and an analysis of their replies indicates that 119 potential trainees would be interested in hydrogen safety education on an annual basis. This implies that a projected market of 5000 companies and institutions would yield 1000 trainees on an annual basis. As a result, it will be necessary to deploy educational/training resources at a number of universities throughout Europe to meet this demand for hydrogen safety education. Further analysis of the replies indicates that the relative interest in the various modes of hydrogen safety education is as follows: postgraduate certificate (PGC): 10.7%, postgraduate diploma (PGD): 1.5%, master of science (MSc): 29.3%, short course (SC): 42.2%, and continuous professional development (CPD): 16.3%. It was also attempted to resolve the employment pattern, and hence the skill-set sought by employers. Within these 28 companies and institutions the employment pattern appears to be: 1.3% in design, 13.0% in manufacture, 0.9% in legislation, 0.4% in maintenance, 1.1% in installation, 19.0% in research and 19.0% in teaching (notice that these percentages do not sum up to 100%; this is due to the limited set defining the pattern). Given the small size of the catchment population, these outcomes must be considered preliminary. The process of arriving at these results nevertheless illustrates the mechanism of how the market of trainees in hydrogen safety could be assessed, and how the employment pattern of people working in hydrogen related areas, and the skill-set sought by employers might be resolved.

Table 3: Structure of International Curriculum on Hydrogen Safety Engineering.

Basic modules
Module thermodynamics
Module fluid dynamics
Module heat and mass transfer
Module solid mechanics
Fundamental modules
Module introduction to hydrogen as an energy carrier
Module fundamentals of hydrogen safety
Module release, mixing and distribution
Module hydrogen ignition
Module hydrogen fires
Module explosions: deflagrations and detonations
Applied modules
Module fire and explosion effects on people, structure, and the environment
Module accident prevention and mitigation
Module computational hydrogen safety engineering
Module risk assessment

## 3 BASIC MODULES

### 3.1 MODULE THERMODYNAMICS

#### 3.1.1 INTRODUCTORY STATEMENT

This is a background module in classical thermodynamics and intended for undergraduate instruction only. It is similar to any other undergraduate engineering thermodynamics course, but comprehensive enough to provide a broad basis for dealing with hydrogen safety issues involving hydrogen embrittlement, unscheduled releases of liquefied and gaseous hydrogen, and accidental ignition and combustion of hydrogen. The topics covered by this module are based on the texts by Abbott & Van Ness (1972) [10], Moran & Shapiro (2000) [11], Smith, Van Ness & Abbott (2001) [12], and Sonntag, Borgnakke & Van Wylen (2003) [13].

#### 3.1.2 PREREQUISITE MATTER

Calculus up to ordinary differential equations, classical mechanics.

#### 3.1.3 CONTENTS OF THE MODULE

##### 3.1.3.1 States of matter (U: 4 hrs)

Contents States of matter: solid, liquid, gas. Thermodynamic properties. Thermodynamic property tables. Macroscopic versus microscopic. Kinetic gas theory. Avogadro's hypothesis. Ideal gas law and van der Waals equations of state. Critical points. Critical constants for van der Waals gas. Compressibility. Viscosity. Newtonian and non-Newtonian fluids. Mixtures of gases. Definition of mole and mass fractions.

##### 3.1.3.2 First law of thermodynamics (U: 6 hrs)

Contents Work. Energy. Reversible and irreversible processes. Specific heat. Internal energy, enthalpy, and their relation. Joule expansion. Adiabatic expansion. Adiabatic work. Joule-Thompson expansion. Polytropic processes. Making and breaking chemical bonds. Ions in solution. Relation to fuel cells.

##### 3.1.3.3 Second law of thermodynamics (U: 6 hrs)

Contents The equation itself. What does entropy measure? Heat cycles and heat pumps: Carnot cycle, Joule cycle, Otto cycle, Diesel cycle. Definition of equilibrium. Heat and refrigeration engines. Entropy change calculations. Entropy of mixing. Helmholtz energy. Gibbs energy. Maxwell's Equations. Gibbs-Helmholtz equation.

##### 3.1.3.4 Chemical thermodynamics (U: 6 hrs)

Contents Third law of thermodynamics: entropy changes in chemical reactions. Simple combustion process and stoichiometric reactions. Enthalpy of formation. Heat of reaction. Heat of combustion. The adiabatic flame temperature. Comment on non-equilibrium concentration of species in a flame. Partial molar properties. Chemical potential. Fugacity. Gibbs-Duhem equation.

### **3.1.3.5 Phase equilibrium (U: 6 hrs)**

Contents One-component phase diagrams. Clapeyron equation. Clausius-Clapeyron equation. Vapour pressure. Saturation. Partial molar quantities. Equality of fugacity as a criterion for phase equilibrium. Activity coefficient. Vapour pressure diagrams. Henry's law. Boiling diagrams. Colligative properties. Gibbs phase rule. Two-component phase-diagrams: cooling curves, bubble point, dew point. Dewdrop pressure. Capillarity. Ionic strength.

### **3.1.3.6 Thermodynamics and electrochemistry (U: 4 hrs)**

Contents Electrical work. Open cell potential and its relation with Gibbs energy. Faraday number. Electrochemical cells. Half-cells. Reduction potentials. Electrode potentials. Volt-ampere characteristics. Polarization. Cells with no salt bridge. Cell from reaction.

## **3.2 MODULE FLUID DYNAMICS**

### **3.2.1 INTRODUCTORY STATEMENT**

This module serves as a first introduction to fluid dynamics at the undergraduate level, and extends to cover more advanced topics at the graduate level. This, to aid the understanding of fluid dynamical problems related to hydrogen safety engineering. The topics in this module are based on the texts by Hughes & Brighton (1999) [14], Massey & Ward-Smith (1998) [15], Prasuhn (1980) [16], and White (2003) [17]. Additional references are given along with the topics.

### **3.2.2 PREREQUISITE MATTER**

Calculus, classical mechanics, thermodynamics.

### **3.2.3 CONTENTS OF THE MODULE**

#### **3.2.3.1 Definitions (U: 2 hrs)**

Contents Pressure. Viscosity. Friction and ideal flow. Laminar flow and turbulent flow. Surface tension. Compressible and incompressible flow. Subsonic and supersonic flow. Steady flow. Physical classifications and types of flow.

#### **3.2.3.2 Fluid statics (U: 2 hrs)**

Contents Pascals law. Differential equations of fluid statics. Manometry. Fluid forces on submerged bodies. Buoyancy. Archimedes principle. Accelerating fluids in the absence of shear stresses.

#### **3.2.3.3 Mathematical models of fluid motion (U: 6 hrs; G: 4 hrs)**

Contents Integral equations: conservation of mass, momentum, angular momentum, energy, and second law of thermodynamics. Differential equations: continuity equation, momentum equation, momentum equation for frictionless flow,



stress-strain rate relationships in fluids, Euler equations, Navier-Stokes equations. Energy equation, second law of thermodynamics and entropy production. Special forms of integral equations. Brief introduction to numerical schemes. Brief overview of numerical methods for the simulation of fluid flow.

### **3.2.3.4 Dimensional analysis and similitude (U: 6 hrs; G: 4 hrs)**

Contents Dimensions in fluid mechanics. Dynamic, geometric and kinematic similarities. Similitude in fluid dynamics. Parameters of incompressible flow. Parameters of compressible flow. Additional parameters involved in free convective heat transfer in fluids. Buckingham pi theorem. Repeating variable method. Methodology of differential equations. Alternative formulation of pi parameters. Dimensionless parameters: Reynolds, Froude, Mach, Weber, Nusselt, Richardson, Peclet, Stanton, etc. Limitations of scaling.

### **3.2.3.5 Incompressible potential flow (U: 6 hrs; G: 4 hrs)**

Contents Potential flow theory. Bernoulli theorem. Kelvin vortex theorem and vortex motion. Velocity potential and stream function. Streamlines and pathlines. Simple flow patterns: uniform flow, sources and sinks, potential vortex, superposition, the method of images. The complex potential: complex velocity, conformal mapping. Complex potential for simple flows: uniform flow field, sources and sinks, potential vortex, dipole or doublet, streaming motion past a cylinder. Circulation and the Kutta-Joukowski theorem.

### **3.2.3.6 Boundary layer concepts (U: 6 hrs; G: 4 hrs)**

Contents What is a boundary layer? Prandtl's hypothesis and consequences. Boundary layer thickness. Atmospheric boundary layer. Wall shear stress. External flows. Flow over a flat plate and the drag law. Von Karman momentum-integral equation. Prandtl boundary layer equations. Blasius solution. Turbulent boundary layers. Internal flow: entrance flow, fully developed flows.

### **3.2.3.7 Incompressible turbulent flow (G: 4 hrs)**

Contents Equations of mean velocity. Statistical approach. Turbulent velocities and Reynolds averaging. Equations of motion for turbulent flow. Phenomenological theories. Eddy viscosity or turbulent viscosity. Prandtl momentum mixing length. Other phenomenological theories. Turbulence correlations. Isotropic turbulence. Wall turbulence: boundary layer flow along a flat plate, fully developed turbulent flow in a pipe. Free turbulence: wake flows, jet flows.

### **3.2.3.8 One-dimensional compressible flow (U: 6 hrs; G: 4 hrs)**

Contents Ideal gas approximation. Speed of sound. Propagation of an infinitesimal disturbance. The Mach cone. Isentropic flow. Shock wave. Normal shocks. Adiabatic constant area flow (Fanno line). Frictionless constant area flow with heating and cooling. Isothermal flow with friction. Incompressible flow for low Mach numbers. The shock tube.

### **3.2.3.9 Two-dimensional compressible flow Gasdynamics (U: 6 hrs; G: 4 hrs)**

Contents Equations of frictionless compressible flow. Isentropic nozzle flow. Shock-expansion theory. Oblique shock. Supersonic expansion and the Prandtl-Meyer function. Combined oblique shocks and expansions. Simple and non-simple regions. Thin airfoil theory. Small perturbations and the linearised theory. Boundary conditions. Supersonic thin airfoil theory. The method of characteristics. Under-expanded jet: contact discontinuity, Prandtl-Meyer expansion, barrel shock, Mach disk.

### **3.2.3.10 Compressible turbulent flow (G: 4 hrs)**

Contents Favre averaging. Compressible turbulent boundary layers. Compressible law of the wall. Equations of compressible turbulent flow and merits of the Favre-averaged form. Overview of current research on turbulent compressible flows. References: Van Driest (1951) [18], Favre (1965) [19], Lele (1994) [20], Gatski, Hussaini & Lumley (1996) [21].

## **3.3 MODULE HEAT AND MASS TRANSFER**

### **3.3.1 INTRODUCTORY STATEMENT**

This module is similar to any other heat transfer course and intended for instruction at the undergraduate and graduate level. The topics in the module are covered by Holman (1997) [22], and Incropera & De Witt (2002) [23], and Pitts & Sissom (1977) [24], Kaviany (2002) [25], Welty, Wicks, Wilson & Rorrer (2001) [26]. Additional references are given along with the topics.

### **3.3.2 PREREQUISITE MATTER**

Calculus up to ordinary differential equations, thermodynamics and fluid dynamics, Laplace transforms.

### **3.3.3 CONTENTS OF THE MODULE**

#### **3.3.3.1 Basic modes of heat transfer and particular laws (U: 4 hrs)**

Contents Conduction heat transfer. Convection heat transfer. Radiation heat transfer. Continuous radiation. Selective radiation. Combined modes of heat transfer. Analogy between heat transfer and the flow of electric current. Material properties: thermal conductivity, thermal diffusivity, specific heat of gases, liquids and solids.

#### **3.3.3.2 One-dimensional steady state conduction (U: 4 hrs)**

Contents General conductive energy equation. Conduction heat transfer in a flat plate: differential formulation, solution, boundary conditions, short method of solution. Conduction heat transfer in radial systems: critical radius. Variable thermal conductivity. Internal energy sources. Convective boundary conditions. Extended surfaces: fin resistance, fin efficiency.

### **3.3.3.3 Multidimensional steady-state conduction (U: 4 hrs)**

Contents Analytical solution techniques. Conductive shape factor.

### **3.3.3.4 Unsteady conduction (U: 6 hrs; G: 4 hrs)**

Contents Definition and significance of Biot and Fourier numbers. Lumped analysis. Analytical solution techniques. Numerical approach. Analogy approach. Graphical approach. One-dimensional systems. Thermally thick and thermally thin solids.

### **3.3.3.5 Forced convection: laminar flow (U: 3 hrs; G: 2 hrs)**

Contents Thermal boundary layer: flat plate; Pohlhausen solution. Isothermal pipe flow. Heat transfer in pipe flow.

### **3.3.3.6 Forced convection: equations of motion (U: 3 hrs; G: 2 hrs)**

Contents Heat transfer and skin friction: Reynolds analogy. Flow over a flat plate. Flow in pipes. External flow over submerged bodies. Heat transfer to liquid metals.

### **3.3.3.7 Natural convection (U: 3 hrs; G: 2 hrs)**

Contents Dimensionless groups: Grashoff, Prandtl and Nusselt numbers. Vertical flat plate. Empirical correlations: isothermal surfaces, free convection in enclosed spaces, mixed free and forced convection.

### **3.3.3.8 Boiling and condensation (U: 3 hrs; G: 2 hrs)**

Contents Boiling phenomena. Pool boiling. Flow (convection) boiling. Crisis of boiling. Film boiling. Leidenfrost point. Nucleate boiling. Condensation. Latent heat of condensation. Example: effect of air condensation in accidents with LH<sub>2</sub>. References: Collier & Thome (1996) [27].

### **3.3.3.9 Heat exchangers (U: 3 hrs; G: 2 hrs)**

Contents Types of heat exchangers. Heat transfer calculations. Heat exchanger effectiveness (NTU method). Fouling factors.

### **3.3.3.10 Radiation heat transfer (U: 6 hrs; G: 4 hrs)**

Contents Basic definitions and laws of thermal radiation. Blackbody radiation. Radiative properties of real and gray surfaces. Radiative exchange: black surfaces, gray surfaces. Radiation shielding. Radiative properties of molecular gases. Radiative properties of particulate media (soot). Lambert-Beers law. Mean beam length. Heat exchange between gas volume and surfaces. Spectral and angular dependence of radiosity. References: Modest (2003) [28].

### **3.3.3.11 Isothermal mass transfer (U: 3 hrs; G: 2 hrs)**

Contents Ficks law. Diffusion coefficient. Diffusion in gases. Mass transfer coefficient. Non-dimensional parameters (Schmidt and Lewis numbers). Stefans law of mass transfer and droplet evaporation.

### **3.3.3.12 Simultaneous heat and mass transfer (U: 4 hrs; G: 2 hrs)**

Contents Formulation of governing equations. Thermo-diffusion. Droplet evaporation. Lewis number. Stagnant boundary layer formation. B-number. Wet-bulb temperature.

## **3.4 MODULE SOLID MECHANICS**

### **3.4.1 INTRODUCTORY STATEMENT**

The topics in this module are for undergraduate instruction only. They identify the subject matter of solid mechanics and provide a broad enough basis to develop an understanding of hydrogen safety problems. The particular texts used to select the material contained in this module are: Beer & Johnston (1981) [29], Beer & Johnston (1992) [30], Fitzgerald (1982) [31], Higdon, Ohlsen, Stiles, Weese & Riley (1985) [32], Mase (1970) [33], and Nash (1998) [34].

### **3.4.2 PREREQUISITE MATTER**

Analysis, linear algebra, vector analysis, differential and integral calculus.

### **3.4.3 CONTENTS OF THE MODULE**

#### **3.4.3.1 Analysis of stress (U: 6 hrs)**

Contents Continuum concept. Homogeneity. Isotropy. Mass-density. Body forces. Surface forces. Cauchys stress principle. The stress vector. State of stress in a point. Stress tensor. Stress tensor stress vector relationship. Force and moment. Equilibrium. Stress tensor symmetry. Stress transformation laws. Stress quadric of Cauchy. Principal stresses. Stress invariants. Stress ellipsoid. Maximum and minimum shear stress values. Mohrs circles for stress. Plane stress. Deviator and spherical stress tensors.

#### **3.4.3.2 Deformation and strain (U: 6 hrs)**

Contents Particles and points. Continuum configuration. Deformation and flow concepts. Position vector. Displacement vector. Lagrangian and Eulerian description. Deformation gradients. Displacement gradients. Deformation tensors. Finite strain tensors. Small deformation theory. Infinitesimal strain tensors. Relative displacements. Linear rotation tensor. Rotation vector. Linear strain tensors. Stretch ratio. Finite strain interpretation. Stretch tensors. Rotation tensor. Transformation properties of principal strain. Strain invariants. Cubical dilatation. Spherical and deviator strain tensors. Plane strain. Mohrs circles for strain. Compatibility equations for linear strains.

### **3.4.3.3 Tension and compression (U: 6 hrs)**

Contents Internal effects of forces (axially loaded bar, normal stress, normal strain, stress-strain curve, ductile and brittle materials, Hookes law, modulus of elasticity). Mechanical properties of materials (proportional limit, elastic limit, elastic and plastic ranges, yield point, ultimate strength or tensile strength, breaking strength, modulus of resilience, modulus of toughness, percentage reduction in area, percentage elongation, working stress, strain hardening, yield strength, tangent modulus, coefficient of linear expansion, Poissons ratio, general form of Hookes law, specific strength, specific modulus). Dynamic effects. Elastic vs. plastic analysis.

### **3.4.3.4 Statically indeterminate force systems (U: 4 hrs)**

Contents Definition determinate and indeterminate force system. Method of elastic analysis. Analysis for ultimate strength.

### **3.4.3.5 Thin walled pressure vessels (U: 2 hrs)**

Contents Nature of stresses. Limitations. Applications.

### **3.4.3.6 Direct shear stresses (U: 4 hrs)**

Contents Definition of shear force and shear stress. Comparison of shear and normal stresses. Applications. Deformation due to shear stresses. Shear strain. Modulus of elasticity in shear. Welded joints (electron beam welding, laser beam welding).

### **3.4.3.7 Torsion (U: 4 hrs)**

Contents Definition of torsion. Twisting moment. Polar moment of inertia. Torsional shearing stress. Shearing strain. Modulus of elasticity in shear. Angle of twist. Plastic torsion of circular bars.

### **3.4.3.8 Shearing force and bending moment (U: 4 hrs)**

Contents Definition of a beam. Cantilever beams. Simple beams. Overhanging beams. Statically determinate beams. Statically indeterminate beams. Types of loading. Internal forces and moments in beams. Resisting moment. Resisting shear. Bending moment. Shearing force. Sign conventions. Shear and moment equations. Shearing force and bending moment diagrams. Relations between load intensity. Shearing force and bending moment, singularity functions.

### **3.4.3.9 Centroids, moments of inertia, and products of inertia of plane areas (U: 4 hrs)**

Contents First moment of an element area. First moment of a finite area. Centroid of an area. Second moment or moment of inertia of a finite area. Parallel-axis theorem for moment of inertia of a finite area. Radius of gyration. Product of inertia of an element of area. Product of inertia of a finite area. Parallel-axis theorem for product of inertia of a finite area. Principal moments of inertia. Principal axes. Information from statics.

#### **3.4.3.10 Stresses in beams (U: 4 hrs)**

Contents Types of loads acting on beams. Effects of loads. Types of bending. Nature of beam action. Neutral surface. Neutral axis. Bending moment. Elastic bending of beams (normal stresses in beams, location of the neutral axis, section modulus, shearing force, shearing stresses in beams). Plastic bending of beams (elasto-plastic action, fully plastic action, location of neutral axis, fully plastic moment).

#### **3.4.3.11 Elastic deflection of beams: double integration method (U: 4 hrs)**

Contents Definition of deflection of a beam. Importance of beam deflections. Methods of determining beam deflection. Double-integration method. The integration procedure. Sign conventions. Assumptions and limitations. Method of singularity functions.

#### **3.4.3.12 Statically indeterminate elastic beams (U: 4 hrs)**

Contents Statically determinate beams. Statically indeterminate beams. Types of statically indeterminate beams.

#### **3.4.3.13 Special topics in elastic beam theory (U: 4 hrs)**

Contents Shear center. Unsymmetric bending. Curved beams.

#### **3.4.3.14 Plastic deformation of beams (U: 4 hrs)**

Contents Plastic hinge. Fully plastic moment. Location of plastic hinges. Collapse mechanism. Limit load.

#### **3.4.3.15 Columns (U: 4 hrs)**

Contents Definition of a column. Type of failure of a column. Definition of the critical load of a column. Slenderness ratio of a column. Critical load of a long slender column. Influence of end conditions-effective length. Design of eccentrically loaded columns. Inelastic column buckling. Design formulas for columns having intermediate slenderness ratios. Beam columns. Buckling of rigid spring-supported bars.

#### **3.4.3.16 Strain energy methods (U: 4 hrs)**

Contents Internal strain energy. Sign conventions. Castiglianos theorem. Application to statically determinate beams. Application statically indeterminate problem. Assumptions and limitations.

### **3.4.3.17 Combined stresses (U: 4 hrs)**

Contents General case of two-dimensional stress. Sign convention. Stresses on an inclined plane. Principal stresses. Directions of principal stress. Principal planes. Shearing stresses on principal planes. Maximum shearing stresses. Directions of maximum shearing stress. Mohrs circle. Sign conventions used with Mohrs circle. Determination of principal stresses by means of Mohrs circle. Determination of stresses on an arbitrary plane by means of Mohrs circle.

### **3.4.3.18 Members subject to combined loadings (U: 4 hrs)**

Contents Axially loaded members subject to eccentric loads. Cylindrical shells subject to combined internal pressure and axial tension. Cylindrical shells subject to combined torsion and axial tension/compression. Circular shaft subject to combined axial tension and torsion, and combined bending and torsion.

## **4 FUNDAMENTAL MODULES**

### **4.1 MODULE INTRODUCTION TO HYDROGEN AS AN ENERGY CARRIER**

#### **4.1.1 INTRODUCTORY STATEMENT**

This module may be used for instruction at the undergraduate and the graduate level. Its purpose is to provide a brief overview of the use of hydrogen as an energy carrier and safety issues connected to it. Appropriate references are cited along with the topics.

#### **4.1.2 PREREQUISITE MATTER**

Undergraduate programme in Mechanical Engineering, Chemical Engineering or Applied Physics.

#### **4.1.3 CONTENTS OF THE MODULE**

##### **4.1.3.1 Hydrogen as an energy carrier (U: 2 hrs; G: 2 hrs)**

Contents Overview of hydrogen programmes in Europe, USA, Japan and other countries. Environmental, societal and safety aspects of the hydrogen economy: reduction of greenhouse gases, renewable energy, sustainable energy supply, etc.

##### **4.1.3.2 Introduction to hydrogen applications and case studies (U: 5 hrs; G: 5 hrs)**

Contents Production: centralised and decentralised hydrogen production (hydrogen production via reforming, hydrogen production via electrolysis, hydrogen production via thermolysis, photo-electrolysis, biophotolysis and fermentation,

hydrogen as an industrial byproduct, plasma reforming, hydrogen liquefaction, hydrogen production via conversion, small-scale photo-electrolysis), Accidental hydrogen production. Storage and distribution: hydrogen transmission to stationary systems (pipelines, liquid supply and/or gaseous supply, stationary storage), hydrogen supply for transport systems (re-fuelling stations, on-board storage), hydrogen supply for portable systems (cylinders and cartridges, refilling and recycling centres), garages and repair workshops, etc. Case studies.

#### **4.1.3.3 Equipment for hydrogen applications (U: 5 hrs; G: 5 hrs)**

Contents Main components of hydrogen equipment: compressor, gates, check valves, piping, pipelines, storage, liquefier/evaporator, fuel cells, internal combustion engines. Sensors for hydrogen detection. Equipment for passive and active mitigation, etc.

#### **4.1.3.4 Possible accident scenarios (U: 2 hrs; G: 2 hrs)**

Contents Accident scenarios in production, storage distribution, and utilisation. Case studies. Accident scenarios in the chemical process industries: gas to liquid conversion (methane to methanol), fertiliser production (ammonia process), chlorine production plants (hydrogen-chlorine hazard). Accident scenarios in the petrochemical industries. Accident scenarios in the power grid: transformer explosions, batteries, power turbines (coolant).

#### **4.1.3.5 Definitions and overview of phenomena and methodologies related to hydrogen safety (U: 3 hrs; G: 3 hrs)**

Contents Release, leaks, mixing, dispersion, distribution. Permeation. Boil-off. Ignition and auto-ignition. Jet and pool fires. Explosions: deflagrations, detonations, and transitional phenomena. Hydrogen prevention and mitigation technologies, good practices. Selected scenarios. Choice of possible risk assessment methodologies. Legal issues and standards.

## **4.2 MODULE FUNDAMENTALS OF HYDROGEN SAFETY**

### **4.2.1 INTRODUCTORY STATEMENT**

This is a postgraduate module. Its purpose is to provide a basis for the knowledge framework covered by related fundamental modules (i.e. modules release, mixing and distribution; hydrogen ignition; hydrogen fires; explosions: deflagrations and detonations), and the applied modules (i.e. fire and explosion effects on people, structures, and the environment; accident prevention and mitigation; risk assessment; computational hydrogen safety engineering). Appropriate references are cited along with the topics. References covering a wide range of topics in combustion are: Barnard and Bradley (1985) [35], Drysdale (1999) [36], Glassman (1996) [37], Griffiths & Barnard (1995) [38], Kanury (1977) [39], Kuo (1986) [40], Lewis and von Elbe (1987) [41], Poinot & Veynante (2001) [42], Toong (1983) [43], Turns (2000) [44], Warnatz, Maas & Dibble (2005) [45] and Williams (1985) [46]. Other references are cited along with the topics.



## 4.2.2 PREREQUISITE MATTER

Modules on thermodynamics, fluid dynamics, heat and mass transfer, and solid mechanics, and knowledge of basic chemistry.

## 4.2.3 CONTENTS OF THE MODULE

### 4.2.3.1 Hydrogen properties (U: 10 hrs; G: 6 hrs)

Contents Atomic structure: isotopes, ortho-hydrogen, para-hydrogen. Aggregation states. Molecular mass and density. Expansion ratio. Specific heats. Boiling point. Melting point. Thermal conductivity. Diffusion coefficient. Viscosity. Electrostatic properties. Optical properties. Radiation absorption. Temperature dependence of vapour pressure. Gaseous (GH<sub>2</sub>), liquefied (LH<sub>2</sub>) and slush (SLH<sub>2</sub>) forms of hydrogen. Gaseous hydrogen: Boyles law, Charles law, ideal gas law, critical properties, Joule-Thompson inversion temperature, vapour pressure, compressibility factor: the virial equation of state, Pitzer correlations for the compressibility factor, Pitzer correlation for the second virial coefficient; cubic equations of state: van der Waals equation of state, generic cubic equation of state; buoyancy. Liquefied hydrogen: Racketts equation, Lydersen, Greenkorn & Hougens equation. Slush hydrogen. Phase equilibrium: dew point, bubble point; Raoult's law; Henry's law; K-value correlations. Comparison with properties of hydrocarbon fuels. Physiological hazards of hydrogen: asphyxiation, cryogenic burn, jet cutting. Fire and explosion indexes of hydrogen: flash point, fire point, auto-ignition temperature, minimum ignition energy, flammability limits, detonability limits, limiting oxygen index, maximum explosion pressure, burning velocity, minimum diluents concentration, maximum experimental safe gap (and their dependence on pressure, temperature, and mixture composition). Flash points and their relationship to flammability limits. Dependence of burning velocity and flammability limits on pressure and temperature. Dependence of auto-ignition temperature and detonability limits on problem scale. References: College of the Desert (2001) [47], Smith, Van Ness & Abbott (2001) [12] and Sonntag, Borgnakke & Van Wylen (2003) [13].

### 4.2.3.2 Influence of hydrogen on equipment (U: 6 hrs; G: 6 hrs)

Contents Low-temperature influence. Material embrittlement. Stress-strain corrosion mechanism. Hydrogen attack.

### 4.2.3.3 Hydrogen thermo-chemistry (G: 6 hrs)

Contents Combustion reaction of hydrogen in air: stoichiometry, equivalence ratio, global reaction vs. elementary reactions, free radical reactions, rates of reactions, molecularity and order, reaction mechanisms, homogeneous (gas phase), volatile (gas/liquid) and heterogeneous (gas/solid) reactions. Heat of combustion. Adiabatic flame temperature. Combustion kinetics: using the H<sub>2</sub>/O<sub>2</sub> reaction as an example, and difference with H<sub>2</sub>/air reaction. Ignition of gas mixtures containing hydrogen. Thermal explosion in adiabatic and non-adiabatic conditions. Chain reactions - linear and branched. Auto ignition

and its measurement. Water-shift reaction. Inertisation with steam. Catalysis and inhibition. Flame emissivity. References: Atkins & de Paula (2002) [48], Benson (1982) [49], Frank-Kamenetzky (1967) [50] and Moore (1983) [51].

#### **4.2.3.4 Governing equations of multi-component reacting flows (G: 6 hrs)**

Contents Deterministic governing equations for conservation of mass, momentum, species and energy. Non-dimensional form. Dimensionless groups. Shvab-Zeldovich equation. Concept of conserved scalar.

#### **4.2.3.5 Premixed flames (G: 6 hrs)**

Contents Air to fuel ratio. Equivalence ratio. Combustion waves: deflagration and detonation. Analysis of the structure of the reaction zone. Flame temperature. Laminar burning velocity. Laminar flame thickness. Zeldovich theory. Effect of equivalence ratio, pressure and temperature on laminar burning velocity. Flame stretch. Markstein lengths. Flame wrinkling. Flames and flame induced flow in confined and unconfined space, and around obstacles. Flame instabilities. Turbulence generated by the flame front itself. Critical ignition kernel. Theory of flame spread: Semenov and Frank-Kamenetskii theory. Relevance to deflagration and detonation. References: Barnard and Bradley (1985) [35], Clavin (1985) [52], Drysdale (1999) [36], Glassman (1996) [37], Griffiths & Barnard (1995) [38], Kanury (1977) [39], Karlovitz, Denniston & Wells (1951) [53], Kuo (1986) [40], Lewis & von Elbe (1987) [41], Poinot & Veynante (2001) [42], and Williams (1985) [46].

#### **4.2.3.6 Diffusion flames (G: 6 hrs)**

Contents Mixture fraction. State relationships. The Burke-Schumann flame structure. Structure of the reaction zone (laminar flame) in the mixture fraction space. Relevance to accidental combustion of hydrogen. Irreversible infinitely fast chemistry, reversible infinitely fast chemistry, and frozen chemistry, momentum jet flames - laminar and turbulent. Relationship between flame height and fuel flow rate. Hottel and Hawthorne's equation. Buoyant diffusion flames: structure of the fire plume using McCaffrey's correlations of temperature and velocity with height and heat output. Concept of flame height. Correlation of flame heights with rate of heat release. References: Kanury (1977) [39], Hottel & Hawthorne (1949) [14] and McCaffrey (1979) [54].

#### **4.2.3.7 Partially premixed flames (G: 2 hr)**

Contents Non-uniform mixtures: triple flames. Insight into diffusion flame stabilisation on the burner. Application of mixture fraction concept to non-uniform mixtures.

#### **4.2.4 Turbulent premixed combustion (G: 6 hrs)**

Contents Turbulence scales. Reynolds and Favre average. Closure problem. Turbulent burning velocity. Turbulent flame thickness. Combustion regimes (Borghi-diagram). Gibson scale. Gradient and counter-gradient transport. Flamelet models and Flame Surface Density models (Bray-Moss-Libby (BML) model, Cant, Pope, Bray (CPB) model, Mantel and Borghi model, Cheng and Diringer model, Yakhot model). G-equation model. Relevance to confined, unconfined and vented deflagrations. Flame extinction by turbulence. References: Borghi (1988) [55], Clavin (1985) [52], Makarov & Molkov (2004) [56], Peters (1991) [57], Peters (2000) [58] and Yakhot (1988) [59].

#### **4.2.5 Turbulent non-premixed combustion (G: 6 hrs)**

Contents Turbulent diffusion jet flame: flame structure, specific features. Scales and combustion regimes in turbulent non-premixed combustion. Relationship between flame geometry and fuel flow rate. Stable lifted flames and blow-out phenomenon. Stability curves (dependence of blow-out pressure ratio on nozzle diameter: subsonic and highly under-expanded branches, critical diameter). Dependence of flame length and shape on jet direction: upward, downward, horizontal free jets, horizontal jets along boundary (ground). Jet fires in congested environment, effect of delayed ignition. Flamelet and PDF models. References: Peters (2000) [58] and Turns (2000) [44].

##### **4.2.5.1 Ignition and burning of liquids and solids (G: 8 hrs)**

Contents Application of the B-number to the evaporation and burning of fuel droplets. Boundary layer, with and without combustion. Relevance to the burning of liquid pools in air. Blinov and Khudiakov's data and Hottel's interpretation. Simple thermal model for the steady burning of liquids and solids. Heats of gasification. Measurement of the rate of heat release using oxygen depletion calorimetry. Combustion efficiency. Flash points and their relationship to flammability limits. The wick effect and its relevance to the ignition of high flashpoint liquid pools. Application of the concepts of flash point and fire point to the ignition of solids. Rasbash's fire point equation and the use of the B-number. Effect of the physical form of the fuel on ignitability and flame spread. Flame spread over liquids. Flame spread over solids: rate of flame spread, effect of surface orientation and direction of propagation. References: Babrauskas (1995) [60], Drysdale (1999) [36], Kanury (1977) [39], McCaffrey (1995) [61], Spalding (1955) [62] and Tewarson (1995) [63].

##### **4.2.5.2 Fire through porous media (G: 2 hrs)**

Contents Spontaneous ignition in bulk solids. Smouldering combustion. Application of the Frank-Kamenetskii model. Flame propagation in porous media. References: Drysdale (1999) [36].

## **4.3 MODULE RELEASE, MIXING AND DISTRIBUTION**

### **4.3.1 INTRODUCTORY STATEMENT**

This is a postgraduate module on release and mixing phenomena that are specific to the safe handling of hydrogen as an energy carrier. Its purpose is to provide the student with the technical background needed for the applied modules (i.e. fire and explosion effects on people, structures, and the environment; accident prevention and mitigation; risk assessment; computational hydrogen safety engineering). Appropriate references are cited along with the topics.

### **4.3.2 PREREQUISITE MATTER**

Modules on thermodynamics, fluid dynamics, heat and mass transfer and solid mechanics.

### **4.3.3 CONTENTS OF THE MODULE**

#### **4.3.3.1 Fundamentals of hydrogen release and mixing (G: 4 hrs)**

Contents Permeation induced flows. sub-sonic, transonic, and supersonic flows. Mixing phenomena and jets: molecular mixing, diffusion, mixing due to density differences (temperature gradients, concentration gradients), turbulent mixing, Langevin equation, Fokker-Planck equation, gradient hypothesis, plane jet, round jet, impinging jets. Non-combusting underexpanded supersonic jets. Mixing in the atmospheric boundary layer. Two-phase flows. Characterisation of different types of releases: release of GH<sub>2</sub> in open atmosphere, release of GH<sub>2</sub> in confined space, release of GH<sub>2</sub> in congested area, release of LH<sub>2</sub> in open atmosphere, release of LH<sub>2</sub> in confined space, release of LH<sub>2</sub> in congested area. Effect of air condensation. References: Pope (2000) [64], and Witcofski & Chirivella (1984) [65].

#### **4.3.3.2 Handling hydrogen releases (G: 6 hrs)**

Contents Types of scheduled (purgings, permeation) and unscheduled releases: leaks and subsonic gaseous releases, high-momentum gaseous releases, cryogenic hydrogen spills, two-phase releases and explosive evaporation, catastrophic failures. Boil off and state-of-the-art technological solutions. Permeability and materials for hydrogen handling. Hydrogen detection and hydrogen sensors. Hydrogen removal: the use of hydrogens greatest safety asset, i.e. a dominant buoyancy effect. Ventilation. Passive and active mitigation. Thermal recombiners. Autocatalytic recombiners (effect of geometric and operational constraints, influence of convection, quantitative assessment of effectiveness with regard to hydrogen dilution to non-flammable or less sensitive mixtures). Case studies and analysis of experimental data on liquefied and gaseous hydrogen releases.

## **4.4 MODULE HYDROGEN IGNITION**

### **4.4.1 INTRODUCTORY STATEMENT**

This is a postgraduate module. Its purpose is to provide the student with the technical background needed for the applied modules (fire and explosion effects on people,

structures, and the environment; accident prevention and mitigation; risk assessment; computational hydrogen safety engineering). Appropriate references are cited along with the topics.

#### **4.4.2 PREREQUISITE MATTER**

Modules on thermodynamics, fluid dynamics, heat and mass transfer, solid mechanics.

#### **4.4.3 CONTENTS OF THE MODULE**

##### **4.4.3.1 Hydrogen ignition properties and ignition sources (G: 3 hrs)**

Contents Flammability diagram and theory of hydrogen flammability limits. Minimum ignition energy: effect of mixture composition, pressure and temperature. Comparison with flammability ranges of other fuels. Standard auto-ignition temperature and ignition by hot surfaces at real conditions. Minimum ignition temperature. Critical ignition kernel. Relationship with flame propagation parameters. Effect of flow properties. Spontaneous ignition delay for hydrogen-air mixtures under constant volume conditions: effect of temperature, pressure and diluent concentration. Comparison between hydrogen and other fuels ignition properties. Ignition sources: electrostatic electricity, capacitive and inductive sparks in electrical circuits, friction sparks, hot surfaces, impact, shock wave, hot jet ignition, explosives, lightning, self-ignition, pyrophoric substances, open fire, external explosion, laser, etc. References: Bach, Knystautas & Lee (1969) [66], Bull, Elsworth & Hooper (1978) [67], Clarke, Kassoy & Riley (1986) [68], Clarke, Kassoy, Meharzi, Riley, & Vasantha (1990) [69], Dold & Kapila (1991) [70], Eckett, Quirk & Shepherd (2000) [71], Glassman (1996) [37], Fickett & Davis (2001) [72], He & Clavin (1994) [73], He & Lee (1995) [74], He (1996) [75], Kuo (1986) [40], Lee (1977) [76], Lee & Moen (1980) [77], Lee & Higgins (1999) [78], Nettleton (1987) [79], Nettleton (2002) [80], Turns (2000) [44] and Williams (1985) [46].

##### **4.4.3.2 Prevention of hydrogen ignition (G: 3 hrs)**

Contents Electrical circuits and the use of EX-rated equipment. Control of static electricity. Critical conditions for ignition by shock waves. Permissive approach to maintenance work, including the use of welding and open fire. Ignition by hot gas jet and water screens. Ignition by hot surfaces and standard auto-ignition temperature. Limitations of spark-proof mechanical tools. Problems involving other ignition sources: explosives, exothermic reaction, pyrophoric substances, lightning. Preventive ignition of unscheduled releases: glow plug igniters, spark igniters, catalytic igniters. Case studies and analysis of experimental data on hydrogen ignition.

## **4.5 MODULE HYDROGEN FIRES**

### **4.5.1 INTRODUCTORY STATEMENT**

This is a postgraduate module on fires and thermal effects arising from accidental combustion involving hydrogen. Its purpose is to provide the student with the technical background needed for the applied modules (fire and explosion effects on people, structures,

and the environment; accident prevention and mitigation; risk assessment; computational hydrogen safety engineering). Appropriate references are cited along with the topics.

#### **4.5.2 PREREQUISITE MATTER**

Modules on thermodynamics, fluid dynamics, heat and mass transfer and solid mechanics.

#### **4.5.3 CONTENTS OF THE MODULE**

##### **4.5.3.1 Fundamentals of hydrogen fires (G: 4 hrs)**

Contents Jet fires and pool fires. Heat load from fires. Radiation from fires. Radiation transfer in real atmosphere: role of admixtures. Stable lifted flames and blow-out phenomenon; stability curves (dependence of blow-out pressure ratio on nozzle diameter: subsonic and highly underexpanded branches, critical diameter). Dependence of flame length and shape on jet direction: upward, downward, horizontal free jets, horizontal jets along boundary (ground). Jet fires in congested environment, effect of delayed ignition. Liquified hydrogen pool fires: boundary layer with and without combustion. Blinov and Khudiakov' s data and Hottel' s interpretation.

### **4.6 MODULE DEFLAGRATIONS AND DETONATIONS**

#### **4.6.1 INTRODUCTORY STATEMENT**

This is a postgraduate module on explosion with an emphasis on hydrogen safety. Its purpose is to provide a basis for the module explosion effects, and the applied modules (accident prevention and mitigation, risk assessment, and computational hydrogen safety). Appropriate references are cited along with the topics.

#### **4.6.2 PREREQUISITE MATTER**

Modules on thermodynamics, fluid dynamics, heat and mass transfer and solid mechanics.

#### **4.6.3 CONTENTS OF THE MODULE**

##### **4.6.3.1 Deflagrations (G: 6 hrs)**

Contents Definition of deflagration. Flame speed in products. Explosion severity parameters: relationship between explosion severity parameters and flame propagation parameters, pressure and temperature dependence of explosion severity parameters. Mache effect. Integral balance models. Comprehensive models. Deflagrations in open atmosphere: flame induced flow, flame instabilities and wrinkling, accelerated flame propagation, predictions of deflagration dynamics. Confined deflagrations: dynamics of flame propagation flame acceleration and pressure build up in closed space; Vented deflagrations: multi-peak structure of pressure transients and underlying physical phenomena, turbulence generated by venting process, coherent deflagrations in a system enclosure-atmosphere and the role of external explosions. The Le Chatelier-Brown principle analogue for vented deflagrations. Effect of obstacles on flame

propagation, flame acceleration and pressure build up. Slow and fast deflagrations. Dependence of deflagration pressure wave amplitude on flame propagation velocity and acceleration. References: Baker, Cox, Westine, Kulesz & Strehlow (1983) [81], Bartknecht (1981) [82], Bradley & Mitcheson (1976) [83], Dahoe & de Goeij (2003) [84], Dorofeev, Kuznetsov, Alekseev, Efimenko & Breitung (2001) [85], Dorofeev (2002) [86], Eckhoff (2003) [87], Eckhoff (2005) [88], Kuznetsov, Matsukov & Dorofeev (2002) [89], Kuznetsov, Alekseev, Yankin & Dorofeev (2002) [90], Molkov & Nekrasov (1982) [91], Makarov & Molkov (2002) [91], and Tamanini (1993) [92].

#### **4.6.3.2 Detonation (G: 6 hrs)**

**Contents** Hugoniot curve. Chapman-Jouget velocity. Detonation limits. One-dimensional wave structure. Multi-dimensional wave structure. Deflagration to detonation transition. Direct versus mild initiation of detonation. Zeldovich-von Neumann-Doering model; steady detonation; non-steady solution; structure of the detonation front. Detonation cell size. Unconfined and confined detonations. References: Dorofeev, Efimenko, Kochurko & Chaivanov (1995) [93], Dorofeev, Bezmelnitsin & Sidorov (1995) [94], Fickett & Davis (2001) [72], Gavrikov (2000) [95], Kuo (1986) [40], Lee (1977) [76], Lee (1984) [96], Nettleton (1987) [79], Nettleton (2002) [80], Williams (1985) [46] and Zeldovich (1960) [97].

#### **4.6.3.3 Transitional hydrogen explosion phenomena (G: 6 hrs)**

**Contents** Flame acceleration (FA) and Deflagration to detonation transition (DDT): phenomenology of flame acceleration and deflagration to detonation transition. Criteria for spontaneous flame acceleration to supersonic flame speed. Run-up distances. The SWACER mechanism. Zeldovich's spontaneous flame, induced by gradient of induction time. Criteria for onset of detonations. Effects of chemical composition, pressure, temperature, geometry, and physical size of the system. DDT during venting of hydrogen deflagrations. Modeling and validations of CFD models of transitional phenomena of hydrogen combustion. References: Alekseev, Kuznetsov, Yankin & Dorofeev (2001) [98], Dorofeev, Bezmelnitsin & Sidorov (1995) [94], Dorofeev, Sidorov, Kuznetsov, Matsukov & Alekseev (2000) [99], Dorofeev, Kuznetsov, Alekseev, Efimenko & Breitung (2001) [85], Dorofeev (2002) [86], Kuznetsov, Matsukov & Dorofeev (2002) [89], Kuznetsov, Alekseev & Yankin (2002) [90], Molkov, Makarov & Puttock (2004) [56], Whitehouse, Greig & Koroll (1996) [100].

## **5 APPLIED MODULES**

### **5.1 MODULE FIRE AND EXPLOSION EFFECTS ON PEOPLE, STRUCTURES AND THE ENVIRONMENT**

#### **5.1.1 INTRODUCTORY STATEMENT**

This is a postgraduate module on fire and explosion effects of hydrogen. Appropriate references are cited along with the topics.

## 5.1.2 PREREQUISITE MATTER

The basic modules (thermodynamics, fluid dynamics, heat and mass transfer, solid mechanics) and the fundamental modules (introduction to hydrogen as an energy carrier, fundamentals of hydrogen safety, hydrogen release, mixing and distribution, hydrogen ignition, hydrogen fires, deflagrations and detonations).

## 5.1.3 CONTENTS OF THE MODULE

### 5.1.3.1 Thermal effects of hydrogen combustion (G: 4 hrs)

Contents Prediction of jet fire parameters: temperature, visibility, flame length and shape, radiation. Pool fire characteristics. Fireball characteristics. Thermal effects on people and construction elements: tolerance limits, fire resistance rating. Damage criteria for buildings, vehicles and people. Safety distances for hydrogen fires. Case studies and analysis of experimental data on thermal effects of hydrogen fires and explosions. Kuznetsov, Alekseev & Yankin (2002) [90].

### 5.1.3.2 Blast waves (G: 4 hrs)

Contents Blast parameters: overpressure, positive and negative impulse; difference with high explosives. Scaling of overpressures, positive and negative impulses with the use of the Sachs variables: unconfined detonations, confined detonations, fuel-rich clouds, atmospheric and ground effects. Comparison between consequences of gaseous and heterogeneous detonations. Shortcomings of the TNT-equivalence concept for the estimation of pressure effects of gaseous explosions. Multi-energy methods for estimation of gaseous explosions. Reflection of shock waves: normal and oblique incidence. Diffracted loadings. Bursting spheres. Vented chambers. Unconfined vapor cloud explosions. Physical explosions. Pressure vessel failure for flash-evaporating liquids. References: Baker, Cox, Westine, Kulesz & Strehlow (1983) [81], Dorofeev (1996) [101], Dorofeev & Sidorov (1996) [102], and the Yellow Book (1997) [103].

### 5.1.3.3 Calculation of pressure effects of explosions (G: 4 hrs)

Contents Calculation of overpressure in pressure waves from unconfined hydrogen deflagrations with different velocities and acceleration of flame front propagation in open atmosphere. Overview of experimental results on hydrogen explosion pressures above standard detonation pressure. Prediction of blast effects from hydrogen explosions: the use of the Sachs variables, atmospheric and ground effects. Blast effects from bursting spheres. Physical explosions. Safety distances for hydrogen explosions. Case studies and analysis of experimental data on pressure effects of hydrogen explosions. References: Baker, Cox, Westine, Kulesz & Strehlow (1983) [81], Dorofeev (1996) [101], Dorofeev & Sidorov (1996) [102] and Groethe, Colton, Chiba & Sato (2004) [104].

### 5.1.3.4 Structural response, fragmentation and missile effects (G: 4 hrs)



Contents Structural response to explosion loadings: amplification factors for sinusoidal and blast loadings. P-I diagrams for ideal blast sources and nonideal explosions. Energy solutions. Dimensionless P-I diagrams. Structural response times for plates. Response of structural elements to fires: fire resistance. Materials for hydrogen services. Example problems. Fragmentation and missile effects: primary and secondary fragments, drag-type and lifting-type fragments, impact effects, trajectories and impact conditions. Jet effect on fragment surface and missile propulsion. Example problems. References: Baker, Cox, Westine, Kulesz & Strehlow (1983) [81] and Molkov, Eber, Grigorash, Tamanini & Dobashi (2003) [105].

### **5.1.3.5 Fracture mechanics (U: 4 hrs)**

Contents Theories of failure. Maximum normal stress theory. Maximum shearing stress theory. Huber-Von Mises-Henckey (Maximum Energy of Distortion) theory. Damage theory (CDM). Size effect in failure. Ill-posedness. Localisation. Material models with intrinsic length scale. Strain-rate effects. Micro-cracking. Macro-cracking (steel/concrete). Grain structures.

## **5.2 MODULE ACCIDENT PREVENTION AND MITIGATION**

### **5.2.1 INTRODUCTORY STATEMENT**

This is a postgraduate module on mitigation techniques relevant to the safe storage, distribution and handling of hydrogen.

### **5.2.2 PREREQUISITE MATTER**

The basic modules (thermodynamics, fluid dynamics, heat and mass transfer, solid mechanics), the fundamental modules (introduction to hydrogen as an energy carrier; fundamentals of hydrogen safety; release, mixing and distribution; hydrogen ignition; hydrogen fires; deflagrations and detonations) and the applied module fire and explosion effects. This module may be taught simultaneously with the fundamental modules and the applied module on explosion effects on people, structures and the environment.

### **5.2.3 CONTENTS OF THE MODULE**

#### **5.2.3.1 Prevention, protection and mitigation (G: 4 hrs)**

Contents Use of inherent safety features and controls. Hydrogen detection. Overpressure protection of storage vessels and piping systems, safety valves, odorisation. Passive mitigation systems: inherently safe design, mechanical reinforcement, stopping walls, compartmentalization, natural convection, catalytic recombiners, etc. Active mitigation systems: detection (sensors), combustion suppression, preventive ignition, pressurisation of safety zones, thermal recombiners, forced convection, etc. Case studies and analysis of experimental data on hydrogen mitigation techniques.

### **5.2.3.2 Basic phenomena underpinning mitigation technologies (G: 4 hrs)**

Contents Flame quenching and quenching diameter. Maximum experimental safe gap: effect of mixture composition, pressure and temperature; application to flame arresters; flame propagation in porous media. Deflagrations in a system of connected vessels and their mitigation. Venting of deflagrations with inertial vent covers and the role of the vent cover jet effect. The jet effect and missile projections. Dilution of hydrogen-air mixtures. Effect of water sprays on combustion dynamics. Catalytic combustion of hydrogen.

### **5.2.3.3 Standards, regulations and good practices related to hydrogen safety (G: 4 hrs)**

Contents Safety philosophy. Design and layout of plant. Plan of emergency response. Key performance of safety barriers. How to match safety performances and needs. Built-in safety principles. Maintenance. Prevention measures: safety procedures and training, automatic system shut down, decoupling of installations. Detection measures: detection of hazardous conditions (explosive atmospheres, ignition sources), detector layout, maintenance of detectors. Standardization activities: UN ECE WP.29 GRPE; ISO TC 197 Hydrogen technologies, IEC TC 105 Fuel Cells, IEC 60079-10, ISO TC 58 and CEN TC 23 Pressure vessels, ISO TC 22 Road vehicles; ISO TC 21 Equipment for fire protection and fire fighting, CEN TC 197 Road tankers, CEN TC 305 Potentially explosive atmospheres explosion prevention and protection, ISO TC 92 Fire safety, European Integrated Hydrogen Project, NFPA 68, NFPA 50A and 50B, CENELEC mandate (M/349) Feasibility study in the area of Hydrogen and Fuel Cells, etc. Performance-based approach to fire safety engineering (BS 7974). Design philosophy. Guidelines: NASA safety standard for hydrogen and hydrogen systems Guidelines for Hydrogen System Design, Materials Selection, Operations, Storage, and Transportation (1997); US DoE Guidelines for Safety Aspects of Proposed Hydrogen Properties, etc. Concepts of prevention and mitigation.

### **5.2.3.4 Inertisation (G: 4 hrs)**

Contents Hydrogen removal: thermal recombiners; passive autocatalytic recombiners (effect of geometric and operational constraints, influence of convection, quantitative assessment of effectiveness with regard to hydrogen dilution to non-flammable or less sensitive mixtures); preventive ignition: igniters (glow plug igniters, spark igniters, catalytic igniters), the role of high quality flow simulation in optimizing the location of igniters (avoid DDT), hydrogen dilution (by steam, nitrogen, carbon dioxide): post-accident inertisation by injection of an inert gas (effect on limiting pressure buildup; preclusion of flame acceleration); regulations, codes and standards.

### **5.2.3.5 Containment (G: 4 hrs)**

Contents Compartmentalisation, regulations, codes and standards.

### **5.2.3.6 Explosion venting (G: 4 hrs)**

Contents Standards and guidelines on venting of deflagrations. Overview of guidelines for venting of deflagrations with inertial vent covers. The problem of DDT during venting of hydrogen deflagrations. Case studies and analysis of experimental data on vented explosions. References: Bartknecht (1981) [82], Molkov, Dobashi, Suzuki & Hirano (1999) [106], NFPA 68 (2002) [107], Molkov (2001) [108], Molkov (2002) [109], Grigorash, Eber & Molkov (2004) [110].

### **5.2.3.7 Flame arresters and detonation arresters (G: 4 hrs)**

Contents Applications of flame arresters and detonation arresters; principles of operation of flame arresters and detonation arresters; installation in process systems, maintenance, regulations, codes and standards. References: Korzhavin, Klimenko & Babkin (2004) [111].

## **5.3 MODULE COMPUTATIONAL HYDROGEN SAFETY ENGINEERING**

### **5.3.1 INTRODUCTORY STATEMENT**

This module concerns the computational modeling of hydrogen release, mixing, distribution and accidental combustion at different scenarios. It is a postgraduate module intended to provide a general understanding of the computational methods, tools and models applied to hydrogen safety engineering. The references used to compile this module include: Cox (1995) [112], Cox & Kumar (2002) [113], Ferziger & Peric (2002) [114], Patankar (1980) [115], Poinsoot & Veynante (2001) [42], Pope (2000) [64], Roy, Frolov & Givi (1997) [116] and Warsi (1999) [117]. Specific references are given along with the topics.

### **5.3.2 PREREQUISITE MATTER**

Calculus, the basic modules (thermodynamics, fluid dynamics, heat transfer), differential analysis, and partial differential equations.

### **5.3.3 CONTENTS OF THE MODULE**

#### **5.3.3.1 Introduction to CFD (G: 4 hrs)**

Contents Basic concept of numerical methods. CFD as one of the methods for solution of fluid dynamics and heat- and mass-transfer problems. Advantages and limitations of numerical methods in fluid dynamics and heat- and mass-transfer. Problem formulation for numerical solution: mathematical model, discretisation method (numerical grid, differential approximations), linear equation system, numerical solution. Solution method: solution consistency, stability, grid and time step convergence, conservation, boundedness.

### **5.3.3.2 Introduction to thermodynamic and kinetic modeling (G: 6 hrs)**

Contents Basic numerical notions and methods for chemical thermodynamics and kinetics simulations: stiff ODE systems, polynomial representation of thermodynamic properties, detailed / skeletal / reduced kinetic scheme, mechanism, sensitivity analysis, kinetic model reduction (ILD, CSP, etc.). Integrated software systems for kinetic and thermodynamic calculations (Chemkin library, Chemical WorkBench environment). The references used to compile these topics include: Chernyi (2003).

### **5.3.3.3 Mathematical models in fluid dynamics (G: 6 hrs)**

Contents Conservation equations for mass, momentum, energy, species. Characteristic forms of conservation equations steady-state and transient conservation equations; compressible, weakly compressible, incompressible flows; inviscid flow; boundary layer approximation; corresponding mathematical classification (elliptic, hyperbolic, parabolic differential equations) and characteristic flow behaviour. Generic convection-diffusion transport equation for conserved scalar: transient, convection, diffusion and source terms.

### **5.3.3.4 Finite Difference Method (G: 6 hrs)**

Contents Approximation of first and second order derivatives, mixed derivatives. Forward, backward, central difference schemes, higher order schemes. Discretisation error and use of Taylor series expansion for analysis of truncation error. Approximation schemes for convective terms (upwind, power-law, 2nd order upwind, quadratic interpolation, tridiagonal matrix algorithm (TDMA)). Numerical diffusion. Finite volume based finite difference method. Interpolation of surface and volume integrals. Finite volume method.

### **5.3.3.5 Solution of the generic transport equation (G: 6 hrs)**

Contents Steady-state transport equation: finite difference analogue of the equation, linear equation system, arising from it, symmetric and not symmetric matrices. Direct methods for solution of linear equation systems: Gauss elimination, TDMA, cyclic reduction, LU decomposition. Transient transport equation: finite difference analogue of the equation. Explicit and implicit schemes. Numerical stability for transient diffusion problem, convection problem. Time-marching algorithms: Runge-Kutta method, predictor-corrector method. Iterative methods for solution of linear equation systems: conjugate gradient method, strongly implicit procedure (incomplete LU decomposition), other iterative methods. Concept of relaxation coefficient. Verification and validation of CFD-models and numerical simulations. References: AIAA G-077-1998 (1998) [118] and Cox & Kumar (2002) [113].

### **5.3.3.6 Solution of weakly compressible Navier-Stokes equations (G: 6 hrs)**

Contents Navier-Stokes equations as generic transport equations: finite-difference analogue of the momentum equations, pressure field problem. Arrangement of

variables on the grid: staggered grid, collocated grid, representation of the pressure gradient term, representation of the mass conservation equation. SIMPLE-similar algorithms for pressure-velocity coupling (SIMPLE, SIMPLER, PISO): pressure and velocity corrections, pressure correction equation, implementation of the boundary conditions. Relative nature of pressure for incompressible and weakly compressible flows.

### **5.3.3.7 Solution of compressible Navier-Stokes equations (G: 6 hrs)**

Contents Overview of methods for compressible flows, pressure-correction methods for arbitrary Mach number, pressure-velocity-density coupling, implementation of the boundary conditions, non-reflecting boundary condition.

### **5.3.3.8 Turbulent flow modeling (G: 6 hrs)**

Contents Phenomenological description of turbulence: variety of turbulent flows, random nature of turbulence, generation and decay of turbulence, scales of turbulent flows, turbulent energy distribution spectra, isotropic and anisotropic turbulence, vorticity. Reynolds-averaged Navier-Stokes equations (RANS): Boussinesq hypothesis, averaged and fluctuation velocity/scalar components, Reynolds equations, Reynolds stresses. Overview of algebraic models for turbulent viscosity: mean turbulent viscosity, mixing-length models. Overview of one-equation models for turbulent viscosity transport: Spalart-Allmaras model. Overview of two-equation models: standard and renormalization group (RNG) k-epsilon models, effect of buoyancy on turbulence mixing and buoyancy correction for k-epsilon model, wall functions. Overview of Reynolds-stress models. Large-eddy simulations (LES): concept of filter, filtered and residual (subgrid scale, SGS) velocity/scalar components, filtered conservation equations. SGS viscosity models: Smagorinsky and RNG models, Germano dynamic model. Requirements for LES resolution. Boundary conditions, near-wall treatment, detached-eddy simulation (DES). Very-large eddy simulation (VLES). Overview of direct numerical simulations (DNS).

### **5.3.3.9 Combustion modeling (G: 6 hrs)**

Contents Turbulent diffusion combustion: phenomenological description, interaction between flame and turbulence, combustion regimes, flame structure (jet and fire). Overview of models for 1 step irreversible, infinitely fast chemistry: mixture fraction concept, Burke-Schumann model, eddy-dissipation concept (EDC) for mean reaction rate. Models with finite rate chemistry: flamelet and PDF models. Premixed combustion: laminar, quasi-laminar, turbulent combustion, flame wrinkling, premixed combustion diagram; models based on the turbulent burning velocity correlations, gradient method, eddy-break-up model (EBU), Bray-Moss-Libby model (BML), flame surface density models, interplay between the models. Overview of approaches to non-uniform mixture combustion. References: Veynante & Vervisch (2002) [119].

### **5.3.3.10 Multiphase flows (G: 6 hrs)**

Contents Multi-phase flows and free-surface flows. Overview of models based on Euler-Lagrange approach and Euler-Euler approach: discrete phase modeling, particle tracking, volume of fluid methods.

### **5.3.3.11 Special topics (G: 6 hrs)**

Contents Rules of good practice, improvement of efficiency and accuracy, complex geometries, moving boundaries, unstructured and adaptive grids. Fluid-structure interaction. CFD for detonation modeling. CFD for hydrogen risk mitigation. Multi-processor computing, computer clustering. Practical exercises with CFD-codes (deflagration, detonation, dispersion, mitigation). References: Abdo, Magnaud, Paillere, Studer & Bachelierie (2003) [120], Becantini & Pailhories (2002) [121] and Bielert et al (2001) [122].

## **5.4 MODULE RISK ASSESSMENT**

### **5.4.1 INTRODUCTORY STATEMENT**

This is a postgraduate module on risk assessment in Hydrogen Safety Engineering. Its structure is derived from the document Guidance for Safety Aspects of Proposed Hydrogen Projects by the US Department of Energy (2004) [123].

### **5.4.2 PREREQUISITE MATTER**

The basic modules (thermodynamics, fluid dynamics, heat and mass transfer, solid mechanics), the fundamental modules (introduction to hydrogen as an energy carrier; fundamentals of hydrogen safety; release, mixing and distribution; hydrogen ignition; hydrogen fires; deflagrations and detonations) and the applied modules fire and explosion effects on people, structures, and the environment, and, accident prevention and mitigation. This module may be taught simultaneously with the fundamental modules and the applied modules. General background on the nature of explosion and fire hazards and the methodology of Risk Assessment can be obtained from the standard work by Lees (1996) [124, 125, 126]. More information on hydrogen specific hazards will be extracted from the International Conference on Hydrogen Safety in Pisa, Italy (8-10 September 2005), organised by M. Carcassi.

### **5.4.3 CONTENTS OF THE MODULE**

#### **5.4.3.1 Effect analysis of hydrogen accidents (G: 6 hrs)**

Contents Effect on people and tolerance limits: jet impact from high-momentum releases, damage by low temperature releases, asphyxiation by hydrogen, thermal effects from fires, pressure effects from explosions [124, 125, 126], materials for hydrogen services [127]. Environmental effects of hydrogen accidents. References: Lees (1996) [124, 125, 126] and Perry & Green (1997) [127].

#### **5.4.3.2 Risk assessment methodologies (G: 6 hrs)**

Contents Deterministic risk analysis: assessment of effects of unscheduled releases, ignition, pressure and thermal effects in detailed, reasonable-worst-case, credible scenarios. Probabilistic risk analysis [128, 129]: event tree analysis, frequency analysis, consequence analysis, frequency analysis, system analysis, statistical interference, uncertainty. Comparative risk analysis of hydrogen and hydrocarbon fuels at different levels of abstraction: Component, subsystem/installation, overall system level. Relation with workers' safety, public safety and spatial planning. Effectiveness of different mitigation techniques and procedures. Safety Management System [130]. Precursor analysis [131]. Risk perception and acceptance [132]. Examples of risk assessment of hydrogen applications. References: AIChE (1989) [128, 130], Bedford & Cooke (2001) [129], Pasman & Vrijling (2003) [133], and Pasman, Körvers & Sonnemans (2004) [131].

#### **5.4.3.3 Hazard identification and scenario development (G: 4 hrs)**

Contents Index methods. Checklist analysis. FMEA. HAZOP [132]. What-if analysis (threats to or impact on: personnel, equipment, business interruption, environment) [124, 125, 126]. Event tree analysis (and its role as the central part of quantitative risk analysis). EU ATEX directives [134, 135]. IEC Standard 61511 (2001). Layers of protection analysis [136, 137]. References: AIChE (2001) [136], Crawley & Preston (2000) [132], EU ATEX 100 (1994) [134], EU ATEX 137 (1999) [135], Lees (1996) [124, 125, 126], and Pasman, Schupp & Lemkowitz (2003) [137].

#### **5.4.3.4 Vulnerability analysis (G: 4 hrs)**

Contents Preliminary failure mode analysis. What-if analysis. Comprehensive identification and classification hazard analysis. Damage models. Probits for various types of damage [138]. Fault tree analysis [139, 140]. Data bases. Probabilistic assessment [129]. Appropriate equivalent methodology. Bedford & Cooke (2001) [129], Green Book (1989) [138], Hauptmanns (2004) [139], and Khan & Abbasi (2000) [140].

#### **5.4.3.5 Application of hazard identification in the basic processes of the hydrogen economy (G: 5 hrs)**

Contents Application of hazard identification techniques and layers of protection analysis to production, storage and distribution installations in a selection of the detailed topical content given under Introduction to hydrogen applications of module Introduction to hydrogen as an energy carrier. Case studies and European hydrogen incident/accident database.

#### **5.4.3.6 Application of vulnerability analysis to mitigation technologies in the hydrogen economy (G: 5 hrs)**

Contents Application of vulnerability analysis to the potential of an initial incident to inhibit or destroy mitigation technologies in Production, Storage and Distribution in a selection the detailed topical content given under Introduction to hydrogen applications of module Introduction to hydrogen as an energy carrier. Case studies and European hydrogen incident/accident database.

## 6 CONCLUSIONS

Despite the growing hydrogen economy and the consequential demand for knowledge and codes in the field of hydrogen safety, there are practically no hydrogen safety training and educational programmes in Europe. The establishment of the e-Academy of Hydrogen Safety by the NoE HySafe is a first step in overcoming this deficiency. The initial stage of the development of an International Curriculum on Hydrogen Safety Engineering as the backbone of the e-Academy of Hydrogen Safety is presented, and, its need in relation to Europe's innovative and competitive strength at the onset of the hydrogen economy is described. Because of the wide spectrum of the hydrogen economy, and its transient nature involving the continual introduction of new technologies, the curriculum is designed to extract knowledge on hydrogen safety as it becomes available, and to couple it with existing science and engineering curricula. A modular structure, consisting of basic modules, fundamental modules, and applied modules appears to be the most appropriate for this purpose. The current version of the curriculum may be viewed on the e-Academy page of HySafe (<http://www.hysafe.org>) and further development of the curriculum will mainly consist of further enrichment of these modules.

Since the development of an International Curriculum on Hydrogen Safety Engineering would make no sense without a market of trainees, it was attempted to probe its existence by means of a questionnaire (see deliverable D17). Although these results must be considered preliminary because of the small catchment population, there appears to be a potential market of 1000 trainees on an annual basis. To meet this demand for hydrogen safety education it will be necessary to deploy educational/training programmes at a number of universities throughout Europe. The e-learning mode of education and training is seen as the most appropriate in the initial stage to overcome limitations in teaching resources and mobility restrictions of trainees. To propel this development further, the Marie Curie actions (<http://www.cordis.lu/mariecurie-actions/scf/home.html>) will be used and efforts are underway to create a European Summer School on Hydrogen Safety.



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