



SIXTH FRAMEWORK PROGRAMME
Sustainable Energy Systems

NETWORK OF EXCELLENCE



Contract No SES6-CT-2004-502630

Safety of Hydrogen as an Energy Carrier

International Curriculum on Hydrogen Safety Engineering

Author: A.E. Dahoe
Knowledge Center for Explosion and Hydrogen Safety
<http://www.explosionsolutions.org/kcehs/>

Partners: UU, UNIPI, UPM, WUT, UC, FZK, FZJ, BRE, GexCon, DNV, KI
Dissemination Level: PU (Public),
Document Version: Updated and corrected on **01.02.2016**
Date of submission: 31.07.2008 (WP15 Deliverable D30)
Due date of delivery: **31.07.2008**

CONTENTS

1	INTRODUCTION	6
1.1	The safety of hydrogen	6
1.2	Educational and training programmes in hydrogen safety	8
1.3	The role of hydrogen safety education in the transition towards a hydrogen economy	12
1.4	The International Curriculum on Hydrogen Safety Engineering	13
1.5	Assessment of the need for hydrogen safety education and formation of a market of potential trainees	16
1.6	e-Learning, the European Summer School on Hydrogen Safety, the Joint European Summer School on Fuel Cell and Hydrogen Technology, and, the Master of Science in Hydrogen Safety Engineering	17
2	BASIC MODULES	19
2.1	MODULE THERMODYNAMICS	19
2.1.1	INTRODUCTORY STATEMENT	19
2.1.2	PREREQUISITE MATTER	19
2.1.3	CONTENTS OF THE MODULE	19
2.1.3.1	Fundamental concepts and first principles (U: 6 hrs)	19
2.1.3.2	Volumetric properties of a pure substance (U: 6 hrs)	21
2.1.3.3	The first law of thermodynamics (U: 6 hrs)	21
2.1.3.4	The first law of thermodynamics and flow processes (U: 6 hrs)	22
2.1.3.5	The second law of thermodynamics (U: 6 hrs)	22
2.1.3.6	The second law of thermodynamics and flow processes (U: 6 hrs)	22
2.1.3.7	The first and second law of thermodynamics, and chemically reacting systems (U: 6 hrs)	23
2.1.3.8	Phase equilibrium (U: 6 hrs)	23
2.1.3.9	Thermodynamics and electrochemistry (U: 4 hrs)	23
2.2	MODULE CHEMICAL KINETICS	23
2.2.1	INTRODUCTORY STATEMENT	23
2.2.2	PREREQUISITE MATTER	24
2.2.3	CONTENTS OF THE MODULE	24
2.2.3.1	The rates of chemical reactions (U: 6 hrs; G: 4 hrs)	24
2.2.3.2	The kinetics of complex reactions (U: 6 hrs; G: 4 hrs)	24
2.2.3.3	Surface reactions (U: 6hrs; G: 4 hrs)	25
2.2.3.4	Application of sensitivity analysis to reaction mechanisms (G: 6hrs)	25

2.2.3.5	Reduction of complex reaction systems to simpler reaction mechanisms (G: 6hrs)	25
2.2.3.6	Chemical kinetics and the detonation of combustible mixtures (G: 5hrs)	26
2.3	MODULE FLUID DYNAMICS	26
2.3.1	INTRODUCTORY STATEMENT	26
2.3.2	PREREQUISITE MATTER	26
2.3.3	CONTENTS OF THE MODULE	26
2.3.3.1	Fluid statics (U: 4 hrs)	27
2.3.3.2	Kinematics of the flow field (U: 6 hrs)	27
2.3.3.3	Kinematics of incompressible potential flow (U: 8 hrs)	28
2.3.3.4	Kinematics of compressible flow (U: 8 hrs)	30
2.3.3.5	Incompressible laminar viscous flow (U: 8 hrs)	30
2.3.3.6	Mathematical models of fluid motion (U: 8 hrs; G: 6 hrs)	32
2.3.3.7	Dimensional analysis and similitude (U: 4 hrs; G: 3 hrs)	33
2.3.3.8	Incompressible turbulent flow (U: 12 hrs, G: 9 hrs)	33
2.3.3.9	Waves in fluids and the stability of fluid flow (U: 8 hrs, G: 6 hrs)	35
2.3.3.10	Compressible turbulent flow (G: 8 hrs)	35
2.4	MODULE HEAT AND MASS TRANSFER	35
2.4.1	INTRODUCTORY STATEMENT	35
2.4.2	PREREQUISITE MATTER	35
2.4.3	CONTENTS OF THE MODULE	35
2.4.3.1	Basic modes of heat transfer and particular laws (U: 5 hrs)	36
2.4.3.2	Isothermal mass transfer (U: 5 hrs)	36
2.4.3.3	Heat conduction (U: 12 hrs; G: 9 hrs)	37
2.4.3.4	Convection heat transfer (U: 8 hrs; G: 6 hrs)	38
2.4.3.5	Forced convection (U: 8 hrs; G: 6 hrs)	38
2.4.3.6	Natural convection (U: 8 hrs; G: 6 hrs)	39
2.4.3.7	Heat Transfer with Phase Change (U: 8 hrs; G: 6 hrs)	39
2.4.3.8	Radiation heat transfer (U: 12 hrs; G: 9 hrs)	40
2.4.3.9	Simultaneous heat and mass transfer (U: 8 hrs; G: 6 hrs)	41
2.5	MODULE SOLID MECHANICS	41
2.5.1	INTRODUCTORY STATEMENT	42
2.5.2	PREREQUISITE MATTER	42
2.5.3	CONTENTS OF THE MODULE	42
2.5.3.1	Analysis of stress (U: 6 hrs)	42
2.5.3.2	Deformation and strain (U: 6 hrs)	42
2.5.3.3	Tension and compression (U: 6 hrs)	42
2.5.3.4	Statically indeterminate force systems (U: 4 hrs)	43
2.5.3.5	Thin walled pressure vessels (U: 2 hrs)	43
2.5.3.6	Direct shear stresses (U: 4 hrs)	43
2.5.3.7	Torsion (U: 4 hrs)	43
2.5.3.8	Shearing force and bending moment (U: 4 hrs)	43
2.5.3.9	Centroids, moments of inertia, and products of inertia of plane areas (U: 4 hrs)	43
2.5.3.10	Stresses in beams (U: 4 hrs)	44

2.5.3.11	Elastic deflection of beams: double integration method (U: 4 hrs)	44
2.5.3.12	Statically indeterminate elastic beams (U: 4 hrs)	44
2.5.3.13	Special topics in elastic beam theory (U: 4 hrs)	44
2.5.3.14	Plastic deformation of beams (U: 4 hrs)	44
2.5.3.15	Columns (U: 4 hrs)	44
2.5.3.16	Strain energy methods (U: 4 hrs)	44
2.5.3.17	Combined stresses (U: 4 hrs)	45
2.5.3.18	Members subject to combined loadings (U: 4 hrs)	45
3	FUNDAMENTAL MODULES	46
3.1	MODULE HYDROGEN AS AN ENERGY CARRIER	46
3.1.1	INTRODUCTORY STATEMENT	46
3.1.2	PREREQUISITE MATTER	46
3.1.3	CONTENTS OF THE MODULE	46
3.1.3.1	Introduction to hydrogen as an energy carrier (U: 2 hrs; G: 2 hrs)	46
3.1.3.2	Introduction to hydrogen applications and case studies (U: 5 hrs; G: 5 hrs)	47
3.1.3.3	Equipment for hydrogen applications (U: 5 hrs; G: 5 hrs)	47
3.1.3.4	Possible accident scenarios (U: 2 hrs; G: 2 hrs)	48
3.1.3.5	Definitions and overview of phenomena and methodologies related to hydrogen safety (U: 3 hrs; G: 3 hrs)	48
3.2	MODULE FUNDAMENTALS OF HYDROGEN SAFETY	48
3.2.1	INTRODUCTORY STATEMENT	48
3.2.2	PREREQUISITE MATTER	48
3.2.3	CONTENTS OF THE MODULE	48
3.2.3.1	Hydrogen properties (U: 10 hrs; G: 6 hrs)	49
3.2.3.2	Compatibility of metallic materials with hydrogen (U: 6 hrs; G: 6 hrs)	49
3.2.3.3	Hydrogen thermo-chemistry (G: 6 hrs)	50
3.2.3.4	Governing equations of multi-component reacting flows (G: 6 hrs)	51
3.2.3.5	Premixed flames (G: 6 hrs)	51
3.2.3.6	Diffusion flames (G: 6 hrs)	52
3.2.3.7	Partially premixed flames (G: 2 hr)	52
3.2.3.8	Turbulent premixed combustion (G: 6 hrs)	52
3.2.3.9	Turbulent non-premixed combustion (G: 6 hrs)	52
3.2.3.10	Ignition and burning of liquids and solids (G: 8 hrs)	53
3.2.3.11	Fire through porous media (G: 2 hrs)	53
3.3	MODULE RELEASES, MIXING AND DISPERSION	53
3.3.1	INTRODUCTORY STATEMENT	53
3.3.2	PREREQUISITE MATTER	53
3.3.3	CONTENTS OF THE MODULE	53
3.3.3.1	Fundamentals of hydrogen release and mixing (G: 4 hrs)	54
3.3.3.2	Handling hydrogen releases (G: 6 hrs)	54
3.4	MODULE HYDROGEN IGNITION	54
3.4.1	INTRODUCTORY STATEMENT	54

3.4.2	PREREQUISITE MATTER	54
3.4.3	CONTENTS OF THE MODULE	54
	3.4.3.1 Hydrogen ignition properties and ignition sources (G: 3 hrs)	55
	3.4.3.2 Prevention of hydrogen ignition (G: 3 hrs)	55
3.5	MODULE HYDROGEN FIRES	55
3.5.1	INTRODUCTORY STATEMENT	55
3.5.2	PREREQUISITE MATTER	56
3.5.3	CONTENTS OF THE MODULE	56
	3.5.3.1 Fundamentals of hydrogen fires (G: 4 hrs)	56
3.6	MODULE EXPLOSIONS: DEFLAGRATIONS AND DETONATIONS .	56
3.6.1	INTRODUCTORY STATEMENT	56
3.6.2	PREREQUISITE MATTER	56
3.6.3	CONTENTS OF THE MODULE	56
	3.6.3.1 Deflagrations (G: 6 hrs)	56
	3.6.3.2 Detonations (G: 6 hrs)	57
	3.6.3.3 Transitional hydrogen explosion phenomena (G: 6 hrs) .	57
4	APPLIED MODULES	59
4.1	MODULE FIRE AND EXPLOSION EFFECTS ON PEOPLE, STRUC- TURES AND THE ENVIRONMENT	59
4.1.1	INTRODUCTORY STATEMENT	59
4.1.2	PREREQUISITE MATTER	59
4.1.3	CONTENTS OF THE MODULE	59
	4.1.3.1 Thermal effects of hydrogen combustion (G: 4 hrs) . . .	59
	4.1.3.2 Blast waves (G: 4 hrs)	59
	4.1.3.3 Calculation of pressure effects of explosions (G: 4 hrs) .	60
	4.1.3.4 Structural response, fragmentation and missile effects (G: 4 hrs)	60
	4.1.3.5 Fracture mechanics (U: 4 hrs)	60
4.2	MODULE ACCIDENT PREVENTION AND MITIGATION	60
4.2.1	INTRODUCTORY STATEMENT	61
4.2.2	PREREQUISITE MATTER	61
4.2.3	CONTENTS OF THE MODULE	61
	4.2.3.1 Prevention, protection and mitigation (G: 4 hrs)	61
	4.2.3.2 Basic phenomena underpinning mitigation technologies (G: 4 hrs)	61
	4.2.3.3 Standards, regulations and good practices related to hy- drogen safety (G: 4 hrs)	61
	4.2.3.4 Inertisation (G: 4 hrs)	62
	4.2.3.5 Containment (G: 4 hrs)	62
	4.2.3.6 Explosion venting (G: 4 hrs)	62
	4.2.3.7 Flame arresters and detonation arresters (G: 4 hrs) . . .	62
4.3	MODULE COMPUTATIONAL HYDROGEN SAFETY ENGINEERING	63
4.3.1	INTRODUCTORY STATEMENT	63
4.3.2	PREREQUISITE MATTER	63
4.3.3	CONTENTS OF THE MODULE	63
	4.3.3.1 Introduction to CFD (G: 4 hrs)	63

4.3.3.2	Introduction to thermodynamic and kinetic modeling (G: 6 hrs)	63
4.3.3.3	Mathematical models in fluid dynamics (G: 6 hrs)	63
4.3.3.4	Finite Difference Method (G: 6 hrs)	64
4.3.3.5	Solution of the generic transport equation (G: 6 hrs)	64
4.3.3.6	Solution of weakly compressible Navier-Stokes equations (G: 6 hrs)	64
4.3.3.7	Solution of compressible Navier-Stokes equations (G: 6 hrs)	64
4.3.3.8	Turbulent flow modeling (G: 6 hrs)	65
4.3.3.9	Combustion modeling (G: 6 hrs)	65
4.3.3.10	High speed reactive flows	65
4.3.3.11	Modeling of hydrogen-air diffusion flames and turbulence-radiation interactions	66
4.3.3.12	Modeling of liquid hydrogen pool fires	66
4.3.3.13	Multiphase flows (G: 6 hrs)	66
4.3.3.14	Special topics (G: 6 hrs)	66
4.4	MODULE RISK ASSESSMENT	66
4.4.1	INTRODUCTORY STATEMENT	67
4.4.2	PREREQUISITE MATTER	67
4.4.3	CONTENTS OF THE MODULE	67
4.4.3.1	General risk assessment and protective measures for hazardous materials processing and handling (G: 6 hrs)	67
4.4.3.2	Regulations, codes and standards (G: 4 hrs)	67
4.4.3.3	Risk assessment methodologies (G: 4 hrs)	68
4.4.3.4	Hazard identification and scenario development (G: 6 hrs)	69
4.4.3.5	Effect analysis of hydrogen accidents (G: 6 hrs)	69
4.4.3.6	Vulnerability analysis (G: 4 hrs)	70
4.4.3.7	Risk reduction and control in the hydrogen economy (G: 6 hrs)	70
	5 CONCLUDING REMARKS	71
	BIBLIOGRAPHY	97

1 INTRODUCTION

1.1 The safety of hydrogen

The safety of hydrogen is known to be of vital importance to the onset and further development of the hydrogen economy. The development and introduction of hydrogen technologies, as well as the level of public acceptance of hydrogen applications, are presently being constrained by safety barriers. Hydrogen is perceived to be dangerous because it has some properties that make its behaviour during accidents different from that of most other combustible gases. It may cause material embrittlement and diffuses more easily through many conventional materials used for pipelines and vessels. Gaps that are normally small enough to seal other gases safely are found to leak hydrogen profusely. Unlike other combustible gases, it has a Joule-Thompson inversion temperature (i.e. the temperature above which the Joule-Thompson coefficient becomes negative and expansion leads to warming instead of cooling) which is well below that of many applications involving gaseous hydrogen. This makes hydrogen more susceptible to ignition after sudden releases from high pressure containment. When hydrogen's greatest safety asset, buoyancy, is not properly taken into account in the design of infrastructures and technologies for production, storage, transportation and utilisation, it becomes more dangerous than conventional fuels such as gasoline, LPG and natural gas. Many countries' building codes, for example, require garages to have ventilation openings near the ground to remove gasoline vapour, but high-level ventilation is not always addressed. As a result, even very slow releases of hydrogen in such buildings will inevitably lead to the formation of an explosive mixture, initially at the ceiling-level. The safety and combustion literature indicates that releases of hydrogen are more likely to cause explosions than releases of today's fossil fuels do. 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 [1]. Owing to the extreme lightness of the molecule, this is particularly true with hydrogen. A mixture of hydrogen with air has a lower flammability limit which is higher than that of LPG (1.7% [2]) or gasoline (1.0% [2]), but the flammable range is very wide (4-75%) [2]. In the concentration range of 15-45%, the ignition energy of hydrogen is one-tenth of that of gasoline and the quenching gap, i.e. the smallest spacing through which a flame can propagate, is considerably smaller for hydrogen (0.61 mm [3]) than for today's fossil fuels (2.0 mm for methane, 1.8 mm for ethane and propane [3]). This implies that requirements for mitigation, such as flame arrestors and similar equipment, must be more stringent.

For many decades, hydrogen has been used extensively in the process industries (e.g. refineries and ammonia synthesis) and experience has shown that it 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 [4]. Interestingly, these technologies rely on the same anomalous properties, such as the large diffusivity and extreme lightness that make hydrogen so different compared to 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 cannot 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, vehicle demonstration projects by manufacturers involve the use of hydrogen as a compressed gas at extremely high pressures (over 350 bar), or, in liquefied form at an extremely low temperature (-253 °C). There is no precedent for the safe handling of hydrogen by the general public at such conditions and current codes and standards for hydrogen were not written with vehicle fueling 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 and a similar dedication to safety, e.g. training general consumers to a professional level, would become impractical. The safety of hydrogen technologies and applications must therefore be ensured before entering the consumer market.

Presently, public acceptance and understanding of the safety of hydrogen is such that accidents with hydrogen not only cause resistance to its use. Accidents also cause people to disregard social, economic, political and environmental improvements that may result from a hydrogen economy. Hydrogen is currently being produced from fossil fuels, particularly from natural gas by steam reforming. But it can also be produced from a variety of other sources (e.g. nuclear, geothermal, solar, wind, hydroelectric plants, biomass, etc.), some of which can operate at large and small scale in areas that are currently suffering fuel poverty (i.e. areas where the cost of energy consumes more than 10% of the household budget). The replacement of fossil fuels by hydrogen from alternative sources will not only benefit people in fuel poverty areas by reducing their dependency on the diminishing resource of imported fossil fuels – it might also enable fossil fuel importing economies to become leading exporters of hydrogen [5]. The consequential demand for ever increasing quantities of hydrogen, and the possibility of producing hydrogen in fuel poverty areas will lead to social improvement by employment opportunities [5]. The replacement of fossil fuels by hydrogen also contributes to averting disastrous effects from pollutant emissions and global warming. It is well-known that combustion products from fossil fuels cause health problems and acid rain due to emissions of particulates, carbon monoxide, sulfur and nitrogen oxides, and other local air pollutants. Continued fossil fuel consumption will not only increase the number of pollution related deaths in cities like Delhi, Beijing and Mexico City [5], but also the magnitude of problems involving reduced agricultural productivity and the loss of biodiversity [5]. There is also an increasing scientific community which has come to the belief that the use of fossil fuels is causing the world's climate to change because of carbon dioxide emissions [5]. Hydrogen is a clean fuel with no carbon dioxide emissions and can be produced by carbon-free or

carbon-neutral processes. When utilised in combustion processes, it produces water only, and reduced amounts of nitrogen oxides.

1.2 Educational and training programmes in hydrogen safety

Educational and training programmes in hydrogen safety are considered to be a key instrument in lifting barriers imposed by the safety of hydrogen. Owing to the impracticality of training general consumers to a professional level in hydrogen safety, such training programmes should primarily 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 that needs to be targeted as well. These are the educators, local regulators, insurers, fire brigades and rescue personnel, investors, and public service officials. Their involvement is indispensable to the acceptance and use of the new technology by the general public, and hence a consolidated consumer market as the principal driving force behind the hydrogen economy. Without their involvement there will be no transition from our present fossil-fuel economy into a sustainable one based on hydrogen. With this in mind, the European Network of Excellence ‘Safety of Hydrogen as an Energy Carrier’ (NoE HySafe) has begun to establish the e-Academy of Hydrogen Safety.

The e-Academy of Hydrogen Safety is part of the dissemination cluster of the NoE HySafe, whose objectives are [6, 7]: (i) to achieve common understanding and common approaches for addressing hydrogen safety issues; (ii) to integrate experience and knowledge within industrial organisations familiar with hydrogen processing technology and research organisations with facilities for experimental research and exploitation of results from numerical prediction tools; (iii) to integrate and harmonise the fragmented research base; (iv) to provide contributions based on safety and risk studies to EU-legal requirements, standards, codes of practice and guidelines; (v) to support education and training in hydrogen safety to achieve an improved technical culture for the safe handling of hydrogen as an energy carrier. To establish the e-Academy of Hydrogen Safety, the following activities were employed: (i) development of an international curriculum on hydrogen safety engineering; (ii) coherent implementation of teaching/learning on hydrogen safety into existing courses and modules; (iii) development of new courses and modules, including optional modules for existing safety courses; (iv) joint training exploiting different modes of education: short courses, summer schools, block-releases, continuous professional development courses, etc.; (v) creation of a pool of specialists from both academic and non-academic institutions able to deliver teaching on hydrogen safety engineering at the highest level by introduction of latest research results into the educational process; (vi) promotion of academic mobility programmes, e.g. by integration of regional academic programmes into a common European course on hydrogen safety engineering with the possibility to distribute course modules in different countries; (vii) joint supervision of research (PhD) students; (viii) creation of a database of organisations working in hydrogen industry to form a market of potential trainees and to disseminate the results from mutual activities of the network; (ix) and the introduction of joint distance

teaching/learning courses in hydrogen safety on the international market.

Due to the absence of a curriculum on the subject, a substantial effort is being devoted to the development of an International Curriculum on Hydrogen Safety Engineering as a first step in the establishment of the e-Academy of Hydrogen Safety. The development of the International Curriculum on Hydrogen Safety Engineering is led by the University of Ulster and carried out in cooperation with international partners from four other universities (Universidad Politecnica de Madrid, Spain; University of Pisa, Italy; Warsaw University of Technology, Poland; University of Calgary, Canada), three research institutions (Karlsruhe Institute of Technology and Forschungszentrum Juelich, Germany; Building Research Establishment, United Kingdom), one enterprise (GexCon, Norway) and one foundation (Det Norske Veritas, Norway). This development is also aided by experts from within the NoE HySafe and external experts from all over the world (see Table 1), representing educational institutions, research organisations, industrial corporations and governmental bodies. This report exposes the current structure of the International Curriculum on Hydrogen Safety Engineering, the motivation behind it, and further steps in the development of a system of hydrogen safety education and training are described.

Table 1: List of contributors to the International Curriculum on Hydrogen Safety Engineering.

Adams, P.	Volvo Technology	Sweden
Amyotte, P.R.	Dalhousie University	Canada
Baraldi, D.	The European Commission's Joint Research Center	The Netherlands
Barthelemy, H.	Air Liquide	France
Bauwens, L.	University of Calgary	Canada
Bell, J.B.	Lawrence Berkeley National Laboratories	United States of America
Bengaouer, A.	Commissariat a l Energie Atomique	France
Bjerketvedt, D.	Telemark University	Norway
Bradley, D.	University of Leeds	United Kingdom
van den Braken - van Leersum, A.M.	Akzo-Nobel Safety Services	The Netherlands
Breitung, W.	Institut fur Kern- und Energietechnik, Karlsruhe Institute of Technology	Germany
Calhoun, D.	Commissariat a l Energie Atomique	France
Cant, R.S.	University of Cambridge	United Kingdom
Carcassi, M.	University of Pisa	Italy
Ciccarelli G.	Queens University	Canada
Crespo, A.	Universidad Polytecnica de Madrid	Spain
Dahoe, A.E.	University of Ulster	United Kingdom
Dhanasekaran, P.C.	University of Cambridge	United Kingdom
Djukic, M.	University of Belgrade	Serbia
Donze, M.	Delft University of Technology	The Netherlands
Dorofeev, S.B.	FM Global	United States of America
Eckhoff, R.K.	University of Bergen	Norway
Engebo, A.	Det Norske Veritas	Norway

Fairweather, M.	University of Leeds	United Kingdom
Faudou, J.-Y.	Air Liquide	France
Gallego, E.	Universidad Polytecnica de Madrid	Spain
Garcia, J.	Universidad Polytecnica de Madrid	Spain
Glowacki, B.A.	University of Cambridge	United Kingdom
Goodwin, D.G.	California Institute of Technology	United States of America
Groethe, M.	Stanford Research Institute	United States of America
Hanjalic, K.	Delft University of Technology	The Netherlands
Hansen, O.	GexCon	Norway
Haugom, G.-P.	Det Norske Veritas	Norway
Hawksworth, S.	Health and Safety Laboratory	United Kingdom
Hayashi, K.	Aoyama Gakuin University	Japan
Hirano, T.	Chiba Institute of Science	Japan
Hochgreb, S.	University of Cambridge	United Kingdom
Huston, D.R.	University of Vermont	United States of America
Irvine, J.T.S.	University of St Andrews	United Kingdom
Jordan, T.	Institut fur Kern- und Energietechnik, Karlsruhe Institute of Technology	Germany
Keller, J.O.	Sandia National Laboratory	United States of America
Kirillov, I.	Kurchatov Institute	Russia
Komen, E.	Nuclear Research and Consultancy Group (NRG)	The Netherlands
Kotchourko A.	Institut fur Kern- und Energietechnik, Karlsruhe Institute of Technology	Germany
Kuhl, A.L.	Lawrence Livermore National Laboratories	United States of America
Kumar, S.	Building Research Establishment	United Kingdom
LaChance, J.	Sandia National Laboratories	United States of America
Law, C.K.	Princeton University	United States of America
Ledin, H.S.	Health and Safety Laboratory	United Kingdom
Lee, J.H.S.	McGill University	Canada
Lelyakin, A.	Institut fur Kern- und Energietechnik, Karlsruhe Institute of Technology	Germany
Lemkowitz, S.M.	Delft University of Technology	The Netherlands
Linderoth, S.	Technical University of Denmark	Denmark
Lipatnikov, A.N.	Chalmers University of Technology	Sweden
Makarov, D.V.	University of Ulster	United Kingdom
Makhviladze, G.	University of Central Lancashire	United Kingdom
Marangon, A.	University of Pisa	Italy
Martinfuertes, F.	Universidad Polytecnica de Madrid	Spain
Migoya, E.	Universidad Polytecnica de Madrid	Spain
Molkov, V.V.	University of Ulster	United Kingdom
Moretto, P.	The European Commission's Joint Research Center	The Netherlands
Newsholme, G.	Health and Safety Executive	United Kingdom
Nilsen, S.	Statoil	Norway

Ooms G.	Delft University of Technology	The Netherlands
Oran, E.S.	Naval Research Laboratory	United States of America
Palliere, H.	Commissariat a l Energie Atomique	France
Pasman, H.J.	Delft University of Technology	The Netherlands
	Texas A & M University	United States of America
Picken, S.J.	Delft University of Technology	The Netherlands
Pegg, M.J.	Dalhousie University	Canada
Quadackers, W.J.	Forschungszentrum Juelich	Germany
Quintiere, J.G.	University of Maryland	United States of America
Reinecke, E.-A.	Forschungszentrum Juelich	Germany
Reiners S.	Heliocentris Energy Solutions	Germany
Roekaerts, D.J.E.M.	Delft University of Technology	The Netherlands
Ruiz, A.	US Department of Energy	United States of America
Sanderson, W.E.	Amgen Inc.	United States of America
Schitter, C.	Bayerische Motoren Werke (BMW)	Germany
Schmidtchen, U.	Bundesanstalt für Materialforschung und -prüfung	Germany
Schneider, H.	Fraunhofer Institut für Chemische Technologie	Germany
Serre-Combe, P.	Commissariat a l Energie Atomique	France
Shebeko, Yu. N.	All-Russian Scientific Research Institute for Fire Protection	Russia
Sheffield, J.W.	Missouri University of Science and Technology	United States of America
Shepherd, J.E.	California Institute of Technology	United States of America
Shirvill, L.	Shell Global Solutions	United Kingdom
Simmie, J.M.	National University of Ireland	Ireland
Skjold, T.	University of Bergen	Norway
	GexCon	Norway
Somerday, B.	Sandia National Laboratories	United States of America
Steen, M.	The European Commission's Joint Research Center	The Netherlands
Steinberger-Wilckens, R.	University of Birmingham	United Kingdom
Stoecklin, M.	Bayerische Motoren Werke (BMW)	Germany
Sunderland, P.	University of Maryland	United States of America
Tam, V.Y.H.	British Petroleum	United Kingdom
Tchouvelev, A.V.	Tchouvelev & Associates	Canada
Teodorczyk, A.	Warsaw University of Technology	Poland
Tomov, R.I.	University of Cambridge	United Kingdom
Tsuruda, T.	NRIFD	Japan
Venetsanos, A.G.	National Centre for Scientific Research Demokritos	Greece
Verfondern, K.	Forschungszentrum Juelich	Germany
Wen, J.X.	Kingston University London	United Kingdom

Westbrook, C.K.	Lawrence Livermore National Laboratories	United States of America
Williams, F.A.	University of California, San Diego	United States of America
Woods, S.S.	NASA Johnson Space Center White Sands Test Facility	United States of America
Woudstra T.	Delft University of Technology	The Netherlands
Wurster R.	L-B-Systemtechnik	Germany
Zalosh R.G.	Worcester Polytechnic Institute	United States of America

1.3 The role of hydrogen safety education in the transition towards a hydrogen economy

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 not only impose a serious setback on innovative developments required to propel this transition, but also thwart ongoing efforts to achieve public acceptance of the new technology. Recently, the European Commission identified a shortage of experts in the key disciplines (natural sciences, engineering, technology [8–10] 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 [10,11]. 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 [9]. 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 [12]. 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 of America, 3.12% in Japan and 2.91% in Korea. The gap between the United States of America and Europe, in particular, is more than 120 billion euro a year [8], 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 [13] 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 transnational R&D expenditure in the United States of America. Moreover, there appears to be a decline in the global attractiveness of Europe as a location for investment R&D as com-

pared to the United States of America. 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 [13]. 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 timespan 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 professional career, and a broad enough basis to acquire additional skills as needed. 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 today's expert-skills have become obsolete, graduates possess the ability to acquire tomorrow's expert-skills. The International Curriculum on Hydrogen Safety Engineering, aims at tackling these three causes of detriment to Europe's research base and innovation strength by extracting the state-of-the-art in hydrogen safety and related key areas, and by the rapid dissemination of this knowledge at all levels in higher and further education and training. According to the Strategic Research Agenda [14], which acts as a guide for defining a comprehensive research programme that will mobilise stakeholders and ensure that European competences are at the forefront of science and technology worldwide, education will continue to play a pivotal role in spreading hydrogen applications to the broader public until 2050. In the short term outlook from 2005 to 2015, training and education efforts are needed to build the necessary human resources to lead research and to allow a steady stream of trained scientists and technicians to develop the area. The Workgroup on Cross Cutting Issues [15], dealing primarily with the non-technical barriers to the successful implementation of the deployment strategy for hydrogen and fuel cells in Europe, indicates that educational and training efforts are needed during this period to avoid any dissonances that might hinder the building of consumer and non-technical executive confidence. The Workgroup on Cross Cutting Issues [15] has estimated that during the framework 7 period (2007-2013), the educated staff needed may amount to 500 new graduates from postgraduate studies on an annual basis in all of Europe.

1.4 The International Curriculum on Hydrogen Safety Engineering

The hydrogen economy requires professionals with a postgraduate degree dedicated to hydrogen safety, which is a subset of the aforementioned 500 new graduates. A preliminary study (see Section 1.5) indicates that this subset amounts to 119 graduates on an annual basis. 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 by the curriculum:

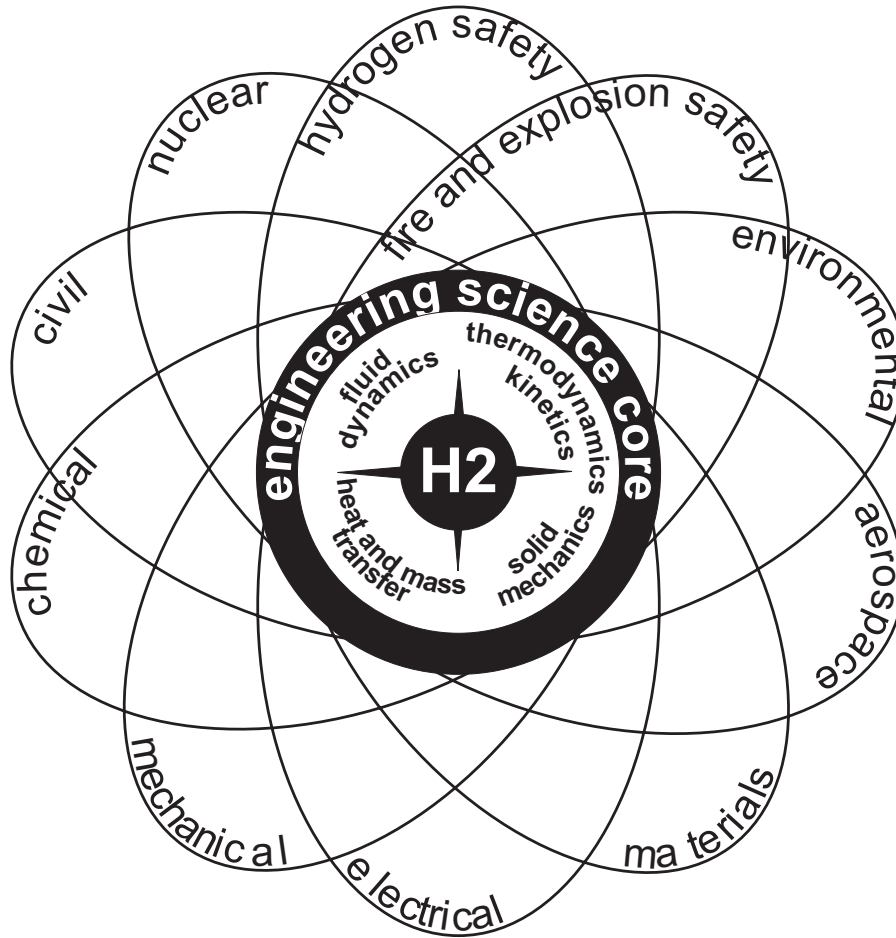


Figure 1: Hydrogen safety in relation to other branches of engineering science.

- what kind of organisations will employ graduates in hydrogen safety (process industry, energy industry, civil works, aerospace industry, automotive industry, transport and distribution, fire and rescue brigades, insurance, teaching institutions, research institutions, legislative bodies, etc.),
- at what level will graduates in hydrogen safety operate within the organisation (consulting, manufacture, design, teaching, research, operation, construction, legislation, 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, continuing professional development, short courses, etc.).

Moreover, the undergraduate programme should be well-rounded in the engineering science core (see Figure 1) and supplemented by topics and additional courses with an emphasis on hydrogen safety. Duplication of educational efforts may be avoided by defining hydrogen safety engineering in relation to other branches of engineering, and cross-fertilisation with existing engineering programmes may be achieved by the introduction of topics relevant to hydrogen safety into the engineering science core. The postgraduate programme consists of specialised courses covering the nodes of the HySafe activity matrix shown in Figure 2. Because the topics connected to the nodes in Figure 2 are subject to continuous development as the hydrogen economy evolves, the curriculum needs to be

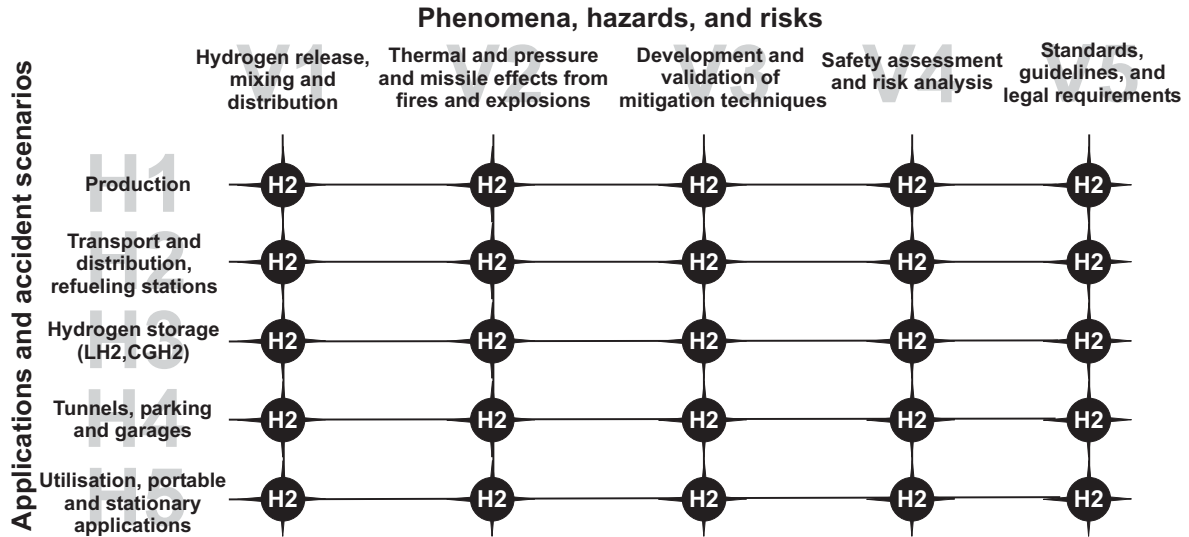


Figure 2: The Hysafe activity matrix.

comprehensive enough to absorb these changes as new knowledge becomes available.

To comply with the aforementioned 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. [16], who adopted a similar approach for the development of a model curriculum for fire safety engineering. The current modular structure is summarised in Table 2, and the current detailed topical content of the International Curriculum on Hydrogen Safety Engineering is given in subsequent sections.

The five basic modules, i.e. Modules Thermodynamics; Chemical Kinetics; Fluid Dynamics; Heat and Mass Transfer; and Solid Mechanics, are intended for undergraduate instruction (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, 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 support the knowledge framework contained in the fundamental and applied modules.

The six fundamental modules, i.e. Modules Hydrogen as an Energy Carrier; Fundamentals of Hydrogen Safety; Releases, Mixing and Dispersion; Hydrogen Ignition; Hydrogen Fires; and Explosions: Deflagrations and Detonations, 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 connected to the nodes in the HySafe activity matrix. These topics are initially based on the existing literature, and updated continuously as new knowledge becomes available, particularly from the NoE HySafe.

Obviously, the fundamental modules play a pivotal role in the curriculum development as the hydrogen economy evolves: new knowledge enters the curriculum through the

Table 2: Structure of the International Curriculum on Hydrogen Safety Engineering.

Basic Modules
Module Thermodynamics
Module Chemical Kinetics
Module Fluid Dynamics
Module Heat and Mass Transfer
Module Solid Mechanics
Fundamental Modules
Module Hydrogen as an Energy Carrier
Module Fundamentals of Hydrogen Safety
Module Releases, Mixing and Dispersion
Module Hydrogen Ignition
Module Hydrogen Fires
Module Explosions: Deflagrations and Detonations
Applied Modules
Module Fire and Explosion effects on People, Structures, and the Environment
Module Accident Prevention and Mitigation
Module Computational Hydrogen Safety Engineering
Module Risk Assessment

fundamental modules, and this information is subsequently used to tune the basic and applied modules. Together, these six fundamental modules form the hydrogen safety engineering science core to support the applied modules.

The four applied modules, i.e. Modules Fire and Explosion Effects on People, Structures, and the Environment; Accident Prevention and Mitigation; Computational Hydrogen Safety Engineering; and Risk Assessment, are intended to provide graduates with the skill-set needed to solve 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. Like the fundamental modules, the role of these modules is also pivotal in the development of the curriculum. Methodologies and front-line techniques for dealing with hydrogen safety problems are extracted from the HySafe-network and incorporated into these modules. Modification of these modules due to new information is followed by the tuning and refinement of the topical content of the basic and fundamental modules to preserve coherence throughout the entire curriculum.

1.5 Assessment of the need for hydrogen safety education and formation of a market of potential trainees

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 has developed, and maintains a database of organisations working in the hydrogen industry. A first attempt to use this database to assess the market of potential trainees in hydrogen safety was made by sending a questionnaire to 600 companies and institutions 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 continuing 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 (these percentages do not sum up to 100% because of 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.

1.6 e-Learning, the European Summer School on Hydrogen Safety, the Joint European Summer School on Fuel Cell and Hydrogen Technology, and, the Master of Science in Hydrogen Safety Engineering

The European Commission has launched a number of measures [17,18] 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 scientific endeavour. This is in line with the University of

Ulster's aim to promote the further development and expansion of e-learning and blended learning programmes.

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. This is true for well-established subject areas, and even more so for hydrogen safety. To cope with this situation, the European Commission has funded a series of annual European Summer Schools on Hydrogen Safety (HyCourse, contract MSCF-CT-2005-029822, 2006-2010) The University of Ulster coordinated four annual four annual summer schools (2006, 2007, 2008, 2008, see: www.hysafe.org/SummerSchool) During each event at least 12 leading experts from all over the world delivered keynote lectures to an international audience of at least 60 researchers. The topics taught included: hydrogen releases, mixing, and dispersion; mechanisms of hydrogen ignition; hydrogen fires; deflagration, detonation and transitional phenomena; computational modelling in hydrogen safety; thermal, pressure and missile effects from fires and explosions; development and validation of mitigation techniques; safety assessment and risk analysis; and standards, guidelines and legal requirements. The nodal points of the HySafe activity matrix were covered from fundamentals to applications following the topical content of the International Curriculum on Hydrogen Safety Engineering. Junior researchers were given the opportunity to benefit from the experience of leading world-class experts.

Following the successful summer schools under the HyCourse-project, the European Commission continued its support to this work. Co-funding was provided to organise the Joint European Summer School on Fuel Cell and Hydrogen Technology (TrainHy, Call FCH-JU-2009-1, Project ID 256703, 2011-2013) via the Fuel Cell and Hydrogen Joint Undertaking (FCH JU) which is a joint agency of the European Commission, and, European Industry and Research Groups. In 2011 and 2012 the University of Birmingham and the Forschungszentrum Juelich, in cooperation with the University of Ulster, the Technical University of Denmark and Heliocentris GmbH organised two summer school events (see: www.hysafe.org/TrainHyProf).

With hydrogen safety being a novel area, and therefore lacking the prerequisites to prepare a skilled workforce for the technological challenges to come, this approach is considered to be the way forward to create the next generation of researchers and educators in this subject area, and to preserve the life-blood of research. The lecture notes and presentations of the keynote lectures at the European Summer School on Hydrogen Safety and the Joint European Summer School on Fuel Cell and Hydrogen Technology are implemented into the distance learning modules of the Master of Science in Hydrogen Safety Engineering offered by the University of Ulster (see: www.hysafe.org/MScHSE). The module provision of the MSc-programme consists of six modules: Module *Principles of Hydrogen Safety*, Module *Hydrogen Safety Technologies*, Module *Regulations, Codes and Standards*, Module *Hydrogen Powered Transport and Infrastructure Safety*, Module *Progress in Fuel Cell and Hydrogen Technologies*, and, a *Dissertation* Module. Since the first delivery of this course in January 2007 it was attended by an international group of learners from several countries including Finland, France, Germany, Iceland, Ireland, Italy, the Netherlands, Poland, Russia, Spain, the United Kingdom and the United States of America.

2 BASIC MODULES

2.1 MODULE THERMODYNAMICS

2.1.1 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) [19], Atkins & de Paula (2006) [20], Metz (1976) [21], Moran & Shapiro (2000) [22], Smith, Van Ness & Abbott (2007) [23], and Sonntag, Borgnakke & Van Wylen (2003) [24]. Specific references are given along with the topics.

2.1.2 PREREQUISITE MATTER

Calculus (including linear algebra, complex functions, complex analysis, Laplace transforms, Fourier analysis), ordinary differential equations, partial differential equations, vector analysis, tensor analysis, classical mechanics, continuum mechanics, elementary fluid dynamics statistical mechanics.

2.1.3 CONTENTS OF THE MODULE

2.1.3.1 Fundamental concepts and first principles (U: 6 hrs)

Contents The three primitive gas laws [20]: Boyle's law (Boyle-Mariotte law), Charles's law or Gay-Lussac's law, combinend gas law (Boyle-Gay-Lussac's law). Avogrado's hypothesis [20] (equal volumes of ideal or perfect gases, at the same temperature and pressure, contain the same number of particles, or molecules). Ideal gas law (adding Avogrado's hypothesis to the combined gas law) [20]. Dalton's law (the pressure exerted by mixtures of gases is the sum of the partial pressures of its constituents) and mixtures of gases [20]. Macroscopic and microscopic point of view. Kinetic theory of gases [20] (postulates: constant random motion, elastic collision, volume occupied by molecules,

attraction forces between molecules; definition of ideal gas in the light of postulates; definition of real gas in the light of postulates (molecular interactions affect the equation of state [20]); Maxwell's distribution for the speed of molecules [20, 25], calculation of the root-mean-square velocity of molecules [20]; definition of pressure; mechanical equilibrium (the condition of equality of pressure on either side of a movable wall [20]); definition of absolute temperature and Boltzmann's constant; diathermic boundary (a boundary that permits the passage of energy as heat [20]); adiabatic boundary (a boundary that prevents the passage of energy as heat [20]); thermal equilibrium (the condition in which no change of state occurs when two objects are brought in contact through a diathermic boundary [20]); relationship between Boltzmann's constant, universal gas constant and Avogadro's number (Carnot's law [26]); collision frequency [20]; mean free path [20]. Thermodynamic properties: intensive properties (density, pressure, temperature, internal energy, entropy, chemical potential of a species, mole fraction of a species, mass fraction of a species) and extensive properties (volume, mass, kinetic energy, potential energy, internal energy (Joule's law [27]: in a perfect gas the internal energy is a function of the absolute temperature alone), entropy, enthalpy, Helmholtz energy, Gibbs energy). Thermodynamic property tables. State functions. Exact and inexact differentials. Statement of the thermodynamic laws: Zeroth law of thermodynamics (if A is in thermal equilibrium with B, and B is in thermal equilibrium with C, then C is also in thermal equilibrium with A [20]), First law of thermodynamics (the internal energy of an isolated system is constant [20]; energy defined as the capacity to do work), Second law of thermodynamics (Kelvin's statement: no process is possible in which the sole result is the absorption of heat from a reservoir and its complete conversion into work [20], statement in terms of entropy: the entropy of an isolated system increases in the course of spontaneous change [20]; entropy as an indicator of the direction of spontaneous change [20], thermodynamic definition of entropy (concept of irreversibility, concept of availability), relation between entropy and the distribution and dispersal of energy, Boltzmann's definition of entropy, examples of spontaneous change (expansion of gas into a vacuum, conversion of diamond into graphite, the helix-coil transitions in polypeptides, models of origins (propagation of genetic properties, evolution of biological species)), the widespread misinterpretation that the second law of thermodynamics does not permit order to spontaneously arise from disorder (counter-example: the spontaneous formation of snowflakes with six-sided crystalline symmetric structure from randomly moving water vapour molecules; reversibility of the transition between water and ice at the melting point; irreversibility of the transition of water to ice below the melting point; irreversibility of the transition of ice to water above the melting point)), Third law of thermodynamics (the entropy of all crystalline substances is zero at zero absolute temperature [20]). Zeroth law of thermodynamics (existence of temperature as an intensive property; existence of an equation of state between temperature, pressure, volume and amount of substance). First law of thermodynamics (existence of total energy as an extensive property consisting of internal energy, potential energy and kinetic energy; isolated systems (systems with a boundary through which neither matter nor energy can be transferred), closed systems (systems with a boundary through which energy can be transferred but matter cannot) and open systems (systems with a boundary through which both energy and matter can be transferred)). Second law of thermodynamics (existence of an absolute scale for temperature; existence of an extensive property called entropy; inequality of Clausius [24]: reversibility and irreversibility). Third law of thermodynamics (existence of a zero entropy reference offset for evaluating entropies of pure substances [23, 24]; zero entropy of a perfect crystal at the absolute

zero of temperature [24]; entropy from the microscopic point of view: Boltzmann's definition of entropy in terms of disorder [23, 24]). Thermodynamic equilibrium (mechanical equilibrium, thermal equilibrium, chemical equilibrium). Le Chatelier - Braun principle (if a chemical system at equilibrium experiences a change in concentration, temperature, volume, or partial pressure, then the equilibrium shifts to counteract the imposed change and a new equilibrium is established). **References:** Batchelor (1994) [26], Feynman, Leighton & Sands (1989) [25], and Milne-Thomson (1968) [27].

2.1.3.2 Volumetric properties of a pure substance (U: 6 hrs)

Contents States of matter: solid, liquid, gas. Stability of phases [20]: phase transition, stable phase, metastable phase, allotropy, transition temperature. Phase boundaries: boiling point, melting point, vapour pressure, sublimation vapour pressure, fusion curve, sublimation curve, vaporisation curve, triple point, critical point, critical properties. Phase diagrams. The PT-diagram of a pure substance (solid region, liquid region, vapour region, gas region, fluid region) [23]. The PV-diagram of a pure substance (solid region, liquid region, liquid-vapour region, vapour region, gas region, super-heated vapor, sub-cooled liquid) [23]. The compressibility factor. The virial equations of state [19, 23]. Extended virial equation of state: the Benedict-Webb-Rubin equation [23]. Cubic equations of state: the van der Waals equation of state [19, 23, 24], relation between the van der Waals constants and critical properties of a pure substance [19, 24], the Redlich-Kwong equation of state [19, 24], the Beattie-Bridgeman equation of state [24]. Corresponding-states correlations for gases: the two-parameter theorem of corresponding states, the acentric factor, the three-parameter theorem of corresponding states, the Pitzer correlations for the compressibility factor [23], the Pitzer correlations for the second virial coefficient [23], the Lee-Kesler equation, the Soave-Redlich-Kwong equation, the Peng-Robinson equation. Generalised correlations for liquids: Rackett's correlation [23], the Lydersen-Greenkorn-Hougen correlation [23].

2.1.3.3 The first law of thermodynamics (U: 6 hrs)

Contents Work, heat and energy: when is work done?, what is the energy of a system?, what is the relationship between energy of a system and heat?, diathermic and adiabatic boundaries, exothermic and endothermic processes. The First Law: internal energy as an extensive property, internal energy as a state function, the conservation of energy, the mechanical definition of heat. Work and heat: expansion work, the general expression for work, free expansion, expansion against constant pressure, reversible expansion, isothermal reversible expansion. Heat transactions: heat capacity, the molar heat capacity at constant volume, the specific heat capacity at constant volume. Enthalpy: its definition, relating enthalpy and internal energy, the variation of enthalpy with temperature, the specific heat at constant pressure, the relation between the constant pressure specific heat capacity and the constant volume specific heat capacity, specific heat ratio. Temperature dependence of the specific heat capacity. The work of adiabatic change: isotherms and adiabats in the PVT-diagram. The isentropic adiabatic compression laws. Polytropic process. Enthalpies of physical change (latent heats of pure substances): standard heat of vaporisation, standard heat of fusion. Temperature dependence of the heat

of vaporisation: the Clapeyron equation, the Riedel equation for the prediction of the effect of temperature on heat of vaporisation.

2.1.3.4 The first law of thermodynamics and flow processes (U: 6 hrs)

Contents The first law of thermodynamics as a rate equation. Conservation of mass and the control volume. The first law of thermodynamics for a control volume. Energy equations for closed systems. The uniform-state, uniform flow process. The steady-state flow process. Energy equations for steady-state flow processes. General energy equations.

2.1.3.5 The second law of thermodynamics (U: 6 hrs)

Contents Entropy and the direction of spontaneous change. The inequality of Clausius. Reversibility and irreversibility. Entropy as an extensive property. The thermodynamic definition of entropy. Example: entropy change for the adiabatic free expansion of an ideal gas into an evacuated space (Joule expansion). Entropy as a state function. Entropy as a system property. Entropy of a pure substance. Thermodynamic diagrams: temperature-entropy diagram, pressure-enthalpy diagram (Mollier diagram). Efficiency of the heat cycle (conversion of heat into work) of heat. Example: the Carnot cycle. The first and second proposition regarding the efficiency of the Carnot engine. The absolute thermodynamic temperature scale. Entropy change of a reversible process. Thermodynamic relationships between entropy, enthalpy and internal energy. Factors that render a process irreversible: friction, unrestrained expansion, heat transfer through a finite temperature difference, hysteresis, I^2R loss in electrical circuits, mixing of two different substances. Impossibility of the perpetuum mobile. Entropy change of an irreversible process. Lost work. Entropy change of an ideal gas. The reversible polytropic process for an ideal gas. Principle of the increase of entropy. Entropy calculations [21]: isothermal expansions, phase transitions, temperature changes, adiabatic processes, isothermal mixing. Heat pumps and power cycles: the Rankine cycle (effect of pressure and temperature on efficiency), the reheat cycle, the regenerative cycle, deviation of actual power cycles from ideal cycles (friction losses, turbine losses, pump losses, condenser losses), the Carnot cycle (revisited), the Joule cycle, the Otto cycle, the Diesel cycle, the Ericsson cycle, the Stirling cycle, the Brayton cycle. Refrigeration cycles: vapor compression refrigeration cycles, the ammonia absorption refrigeration cycle, the air standard refrigeration cycle.

2.1.3.6 The second law of thermodynamics and flow processes (U: 6 hrs)

Contents The second law of thermodynamics for a control volume. The steady-state, steady-flow process and the uniform-state, uniform-flow process. The steam turbine. The reversible steady-state steady-flow process, the idealised simple steam power plant. Principle of the increase of entropy for a control volume. Irreversibility and availability. Duct flow of compressible fluids [23]: pipe flow, nozzles (efficiency of a nozzle, converging nozzle, diverging nozzle, converging-diverging nozzle, relation between velocity and pressure in an isentropic nozzle), throttling process (isenthalpic process, flashing of droplets during throttling to a lower pressure, Joule-Thompson inversion temperature, Joule-Thompson coefficient [28], Joule-Thompson inversion curve, reduced Joule-Thompson

inversion curve). Expansion process (turbines, enthalpy-entropy diagram, efficiency of a turbine). Compression process (compressors, enthalpy-entropy diagram, efficiency of an adiabatic compressor, efficiency of a cooled compressor). **References:** Hirschfelder, Curtiss & Bird [28].

2.1.3.7 The first and second law of thermodynamics, and chemically reacting systems (U: 6 hrs)

Contents Chemical reaction. Chemical reaction stoichiometry. Stoichiometric coefficients. Reaction coordinates. Enthalpies of chemical change: standard heat of reaction, Hess's law, standard enthalpies of formation, heat of reaction in terms of standard enthalpies of formation, the temperature dependence of the heat of reaction (Kirchhoff's law). Property changes of reaction: the Gibbs function change of reaction. The Gibbs energy. The Helmholtz energy. Maxwell's Equations. The Gibbs-Helmholtz equation. 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. Non-equilibrium concentration of species in a flame. Partial molar properties. Chemical potential. Fugacity. Gibbs-Duhem equation.

2.1.3.8 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.

2.1.3.9 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.

2.2 MODULE CHEMICAL KINETICS

2.2.1 INTRODUCTORY STATEMENT

This is a background module in chemical kinetics for instruction at the undergraduate and the graduate level. Its purpose is to provide a basis for dealing with hydrogen safety issues involving hydrogen embrittlement, and accidental ignition and combustion of hydrogen. The topics covered by this module are based on the texts by Atkins & de

Paula (2002) [20], Kuo (2005) [29] and Turns (2000) [3]. Additional references are given along with the topics.

2.2.2 PREREQUISITE MATTER

Calculus (including ordinary differential equations, linear algebra), statistical mechanics, thermodynamics.

2.2.3 CONTENTS OF THE MODULE

2.2.3.1 The rates of chemical reactions (U: 6 hrs; G: 4 hrs)

Contents The stoichiometric equation. Definition of the rate of reaction via concentrations of reactants/products in batch reactors. Relationship between reaction rate and chemical species concentration, the Rate Law. Rate constants and half-lives. Order of a reaction. Consecutive and parallel reactions. Rate-determining steps. Reversible/opposing reactions. Classification of the speed of reactions: relatively slow (non-explosive reactions), very fast explosive reactions. Global versus elementary reactions. Molecularity. Elementary reactions and their Rate Laws from the Law of Mass Action. Molecularity. Third bodies/chaperons. Rate constants. Total collision frequency. Temperature dependence of reaction rates. The Arrhenius Equation. A-factors and activation energies. Simple theories of reaction rates: simple and modified collision theory. Reactions at equilibrium. Fundamental relationship between kinetics (forward & reverse rate constants) and thermodynamics (equilibrium constant). Re-definition of reaction rate using stoichiometric coefficients. Kinetics in plug and continuously-stirred flow reactors. Complex versus elementary reactions. One-step chemical reactions of various orders: first-order reactions, second-order reactions, third-order reactions. Consecutive reactions: formation of intermediates, the steady-state approximation, pre-equilibria. Unimolecular reactions: isomerisation, decomposition, dissociation, the Lindeman-Hinselwood mechanism. The fall-off reaction rate: the Lindemann fall-off rate constant, the Stewart fall-off rate constant, the Troe fall-off rate constant. Termolecular reactions: recombination reactions involving a third body. The activation energy of a composite reaction. Competitive reactions. Opposing reactions: first-order reaction opposed by a first-order reaction. First-order reaction opposed by a second-order reaction. Second-order reaction opposed by a second-order reaction.

2.2.3.2 The kinetics of complex reactions (U: 6 hrs; G: 4 hrs)

Contents Intermediates in complex reactions. Chain reactions. Chain carriers. Radicals. Classification of reaction steps: initiation (thermolysis, photolysis), propagation (the branching step), termination. Branching chain reactions. The structure of chain reactions. The rate laws of chain reactions. Steady-state analysis of simple chain reactions. Activation energy of a chain reaction. Complex reactions: the hydrogen-bromine reaction. Chain-branching explosions. Photochemical reactions: quantum yield, photochemical rate laws, photosensitisation, quenching. Catalysis: homogeneous catalysis, autocatalysis. Oscillating reactions: the Lotka-Volterra mechanism, the brusselator, the

oregonator, bistability. Chemical chaos. Departures from Arrhenius behaviour. Explosions: autocatalytic, thermal & branched-chain reactions. Hydrogen-oxygen explosion diagram in static reactor. First, second and third limits. Dependence explosion limits of hydrogen-oxygen systems on containment shape, nature of surface, added inert gases. Comprehensive reaction mechanisms of hydrogen-oxygen systems: the Dougherty & Rabitz mechanism, the Miller mechanism, the Marinov, Westbrook & Pitz mechanism, the O’Conaire, Curran, Simmie, Pitz & Westbrook mechanism [30], the Saxena & Williams mechanism [31]. Validation of kinetic mechanisms from critically-reviewed experiments including stretch-free laminar burning velocities, flow reactor species profiles, ignition delay times in shock tubes [32], etc. Importance of thermodynamic and transport data in a detailed mechanism [33,34]. Software tools for analysing detailed chemical kinetic mechanisms.

2.2.3.3 Surface reactions (U: 6hrs; G: 4 hrs)

Contents Surface adsorption processes: relation to catalysis, improvement of the miners’ safety lamp due to Henry in 1824 by the addition of platinum powder to the reacting surface, Faraday’s view on the role of adsorption to the surface in catalysis, physisorption, van der Waals adsorption, chemisorption, Langmuir’s concept of the unimolecular layer, Langmuir’s adsorption isotherm, monolayer adsorption, multi-layer adsorption, adsorption with dissociation, competitive adsorption. Surface reaction processes: reaction mechanism, the Langmuir-Hinselwood mechanism, the Langmuir-Rideal-Eley mechanism, the precursor mechanism, Unimolecular surface reactions. Bimolecular surface reactions. Desorption. Kinetic model of hydrogen-oxygen reaction on the platinum surface. Kinetic rates of hydrogen-oxygen reaction on the platinum surface.

2.2.3.4 Application of sensitivity analysis to reaction mechanisms (G: 6hrs)

Contents Role of sensitivity analysis in chemical kinetics: reduce number of reactions, identify rate limiting steps in reaction mechanism, resolve relative importance of reactions in a mechanism. Sensitivity coefficients. First-order sensitivity matrix. Sensitivity matrices of higher order. Deterministic sensitivity analysis: the direct method, the Green’s function method, the Taylor series expansion method. Stochastic sensitivity analysis: the FAST method, Monte Carlo methods, pattern methods. Local sensitivity analysis: effect of a small change in one parameter on the first-order sensitivity coefficients. Application of local sensitivity analysis: time-dependent zero-dimensional problems, steady-state one-dimensional problems, time-dependent one-dimensional problems, one-dimensional flame fronts. Global sensitivity analysis: average effect of simultaneous parameter variations of arbitrary magnitudes.

2.2.3.5 Reduction of complex reaction systems to simpler reaction mechanisms (G: 6hrs)

Contents Quasi-Steady-State Assumption (QSSA). Partial equilibrium assumption. The method of Intrinsic Low-Dimensional Manifolds (ILDM) [35], Computational Singular Perturbation (CSP) methods for stiff equations [36]. Example: a four-step reduced

mechanism for hydrogen-air mixtures using CSP [37]. **References:** Lam & Goussis (1994) [36], Maas & Pope (1992) [35] and Lu, Ju & Law (2001) [37].

2.2.3.6 Chemical kinetics and the detonation of combustible mixtures (G: 5hrs)

Contents Initial conditions for self-sustained detonation: mixture composition, thermodynamic state, fluid mechanical state, ignition source properties. Boundary conditions for self-sustained detonation: size and geometry of combustible mixture. Application of chemical kinetics to predict detonation limits of hydrogen-air and hydrogen-oxygen mixtures [29, 38]. Detonability criteria, detonation cell size and chemical kinetics [29]. Chemical kinetics of detonation in hydrogen-air-diluent mixtures [29, 39]. Application of chemical kinetics to detonability criteria through induction times measured in shock tubes [29]. The onset of detonation by the gradient field of induction times (due to concentration-temperature nonuniformity) through the mechanism of shock wave amplification by coherent energy release (the SWACER mechanism) [40–43]. Photochemical initiation of detonation in hydrogen-oxygen and hydrogen-chlorine mixtures with nonuniform concentration. **References:** Belles (1959) [38], Knystautas, Lee, Moen & Wagner (1979) [42], Lee, Knystautas & Yoshikawa (1978) [44], Lee & Moen (1980) [43] and Shepherd (1986) [39].

2.3 MODULE FLUID DYNAMICS

2.3.1 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 Batchelor (1994) [26], Bird, Stewart & Lightfoot (2002) [45], Drazin & Reid (1981) [46] Hughes & Brighton (1999) [47], Kundu & Cohen [48], Lighthill [49], Massey & Ward-Smith (1998) [50], Milne-Thomson (1968) [27], Prasuhn (1980) [51], Schlichting (1968) [52], and White (2003) [53]. Additional references are given along with the topics.

2.3.2 PREREQUISITE MATTER

Calculus (including linear algebra, complex functions, complex analysis, Laplace transforms, Fourier analysis), ordinary differential equations, partial differential equations, thermodynamics, vector analysis, tensor analysis, classical mechanics, continuum mechanics, statistical mechanics, wave mechanics.

2.3.3 CONTENTS OF THE MODULE

2.3.3.1 Fluid statics (U: 4 hrs)

Contents The usefulness of fluid statics: examples of immediate application to engineering problems without becoming involved in complex notions. The two kinds of forces to be considered in fluid statics: body forces (forces acting on the fluid particles at a distance: gravity, magnetic field, etc.) and surface forces (forces due to direct contact with other fluid particles or solid walls: pressure, shear stress, surface tension, etc.). Mechanical equilibrium of a fluid: a state in which each fluid particle is either at rest or has no relative motion with respect to other particles. Representation of surface forces by the stress tensor [26]: normal stresses, tangential stresses, principal axes of the stress tensor, principal stresses). The stress tensor in a fluid: decomposition into a symmetric part (isotropic part) and an anti-symmetric part (departure of the stress tensor from the isotropic form, also known as the deviatoric stress tensor [26,47]). Definition of the *static fluid pressure* [26]: the stress tensor in a fluid at rest [26], zero deviatoric stress tensor, definition of the static fluid pressure as the magnitude of the normal components in the isotropic part of the stress tensor in a fluid at rest, consequences of this definition (independence of direction, acting equally in all directions). Conditions for mechanical equilibrium in a fluid [26]: balance between body force and static fluid pressure gradient, a body floating in fluid at rest (Archimedes' theorem), fluids at rest under gravity (linear decrease of pressure with elevation in incompressible fluids (Pascal's law) [26,47]; exponential decrease of pressure with elevation in a compressible fluid e.g. Earth's atmosphere [47], pressure distribution in a self-gravitating star [26]). Manometry: determination of pressure differences using Pascal's law, the U-tube manometer [47], the two-fluid manometer [47]. Fluid forces on submerged bodies: application Archimedes' theorem for determining the force on submerged bodies [26,47], horizontal plane surface [47], inclined plane surface [47], curved surface [47], buoyancy and Archimedes' principle (the upward force equals the weight of the fluid displaced) [47]. Accelerating fluids in the absence of shear stress: fluids moving as a rigid body (each fluid particle has no motion relative to its immediate neighbour), accelerating container of fluid [47], rotating container of fluid [47]. Surface tension.

2.3.3.2 Kinematics of the flow field (U: 6 hrs)

Contents Specification of the flow field [26]: Eulerian type and Lagrangian type, the Eulerian fluid element and the material fluid element. Streamline [27]: its definition as a line drawn in the fluid so that its tangent is in the direction of the fluid velocity, it alters from instant to instant because it depends on position and time, the aggregate of all streamlines at a given instant constitutes the flow pattern at that instant, set of differential equations of which the solution at a given time is the family of streamlines [26]. Differentiation following the motion of the fluid [26]: the notion of material volumes, surfaces and lines consisting always of the same fluid particles and moving with them, acceleration of a fluid element, material derivative (time derivative following the motion of the fluid). Particle path [27]: its definition as the path described by a fluid particle during its motion, tangency of fluid particle motion to the particle path, tangency between the particle path and the streamline which passes through the instantaneous position of the fluid particle, concept of a streak line [26]. Connection between streamlines and particle paths [27]: streamlines show how each particle is moving at a given instant, particle

paths show how a given particle is moving at each instant, particle paths coincide with streamlines when the motion is steady. Virtual mass and added mass (hydrodynamic mass) [27, 49, 54–56]: the presence of the fluid effectively increases the mass of a moving rigid body, the added mass is equal to that of the liquid displaced by the Darwin drift (the net displacement of fluid particles due to the passage of rigid bodies), added mass of a cylinder [49], added mass of a sphere [49], trajectory of the particle path due to the passage of a rigid body (net displacement between the undisturbed initial and final position of a fluid particle in the direction of the moving body, tangents at the beginning and end point of the particle path are parallel to the direction of motion of the body) [27]. Stream tube: its definition as a collection of stream lines through each point of a closed curve. Stream filament [27]: its definition as a stream tube whose cross-section is a curve of infinitesimal dimensions, constancy of the product between the speed and cross-sectional area along a stream filament of a fluid in steady motion. Conservation of mass: general condition of mass conservation (Gauss’ divergence theorem) [26], general condition of mass conservation in the form of a differential equation (continuity equation) [26], rate of expansion (rate of dilatation) [26], solenoidal flow fields [26] (incompressible fluids, compressible fluids in the incompressible limit), use of a stream function to satisfy mass conservation (exact differential relating velocity components to a differential change in the stream function [26], stream function as an equation defining stream lines [26], relation between the stream function and the volume flux between two points [26], existence of the stream function as a mere consequence of the continuity and incompressibility of the fluid [27]). The relative motion near a point: stress-strain rate relationships [26, 47], the velocity gradient tensor [26, 47], decomposition of the velocity gradient into a rate-of-strain tensor (symmetric part, deformation motion (dilatation, shear strain)) and a rotation tensor (anti-symmetric part, rigid body motion (translation, rotation)) [26, 47], angular velocity vector and vorticity [26, 47], example of irrotational flow in a sink vortex [47], example of rotational flow in a curved pipe [47], the velocity vector becoming the gradient of a scalar function of position called the velocity potential when the motion is irrotational [27]. Flow fields with a specified rate of expansion and vorticity: velocity distributions (concept of a point source [26], concept of a source doublet (dipole) [26]), vorticity distributions (vortex-line [26], vortex-tube [26], concept of circulation and the strength of the vortex tube [26], line vortices [26], sheet vortices [26]). Flow fields with a zero rate of expansion and vorticity: incompressible potential flow (solenoidal irrotational flow [26, 45]). **References:** Darwin (1953) [54], Lighthill (1956) [55], and Rankine [56].

2.3.3.3 Kinematics of incompressible potential flow (U: 8 hrs)

Contents Incompressible potential flow: its definition as a flow for which the velocity is derivable from the velocity potential [47]. Further considerations that make incompressible potential flow distinct [26, 27, 45, 47]: the velocity potential becomes harmonic (under conditions of incompressibility, substitution of the velocity in terms of the velocity potential into the continuity equation results in Laplace’s equation), the stream function becomes harmonic (substitution of the velocity in terms of the stream function into the condition of irrotationality results in Laplace’s equation), velocity potential and stream function satisfy the Cauchy-Riemann equations, solutions of different flows (e.g. source, sinks, potential vortex, uniform flow) may be superposed to represent new ones, Rankine’s method for constructing a new streamline pattern from two existing ones [27]),

values of the velocity potential and stream function at every point in space may be added directly to obtain new values of the velocity potential and stream function, determination of the velocity components from the equipotential lines and streamlines using the Cauchy-Riemann equations and determination of the pressure field from the equation of motion of an ideal fluid once the velocity components are known [45]. Deducing the equations of the streamlines for some simple flow patterns: uniform flow [47], sources and sinks [47], the potential vortex [47]. Examples of superposition of two or more potential flows: flow over a Rankine oval [47], reflection about a solid boundary by the method of images from a source near the wall [47]. The complex potential and the complex velocity [26,27,45]: any analytic function of a complex variable can be regarded as the complex potential of a certain flow field, the use of complex variable theory and conformal transformations (examples: Mercator projection as a conformal mapping of the Earth onto a flat surface, the Joukowski transformation for mapping concentric circles into confocal ellipses [27], mapping a uniform flow into the flow in a corner [47]), definition of a holomorphic function [27], Cauchy-Riemann equations arising from differentiation of a holomorphic function [27], conjugate functions of a holomorphic function [27], two systems of orthogonal curves (i.e. equipotential lines and streamlines) arising from equating conjugate functions to constants [27], any holomorphic function satisfying Laplace's equation [27], the Area theorem [27], Cauchy's integral theorem [27], Morera's theorem [27], obtaining the complex velocity directly from the complex potential by differentiation [27]. Deducing the complex potential for some simple flow patterns: uniform flow [47], sources and sinks [47], the potential vortex [47], the dipole flow [47], streaming motion past a circular cylinder [47]. The complex potential of more complicated flow patterns: circular cylinder held in a stream of uniform velocity [26], flow past an elliptic cylinder [27], flow past a plate (degenerate elliptic cylinder) [27], flow over a ditch or mound [27], flow past a cylindrical log [27], impinging jets [27], direct impact of two equal jets [27], direct impact of two unequal jets [27], flow through an aperture [27]. Stokes' stream function for axisymmetrical flows [26, 27]: its advantage to deal with motion in three dimensions where the complex potential can no longer be used, simple source, submarine explosion, uniform stream, source in a uniform stream, finite line source, airship forms, Rankine's solids, Butler's sphere theorem (analogue of the Circle theorem), sphere in a stream, moving sphere, venturi tube. Bernoulli's theorem [26,27,47]: the sum of the pressure divided by the density and the energy per mass unit has the same value at every point of the same streamline in the steady motion of an inviscid fluid. The constant in Bernoulli's theorem [27]: when the flow is irrotational the sum of the pressure divided by the density and the energy per mass unit has the same value at every point of the fluid. Dynamic fluid pressure [27]: the pressure in Bernoulli's theorem is the sum of the static fluid pressure and a dynamic fluid pressure, the dynamic pressure is the greatest where the speed is least, and its greatest value occurs at points of zero velocity. The Pitot tube [27]: determination of the velocity using Bernoulli's theorem. The Venturi tube [27]: determination of the velocity using Bernoulli's theorem. The flow through an aperture [27]: the vena contracta, Torricelli's theorem, coefficient of contraction, Borda's mouthpiece, rounded nozzle projecting outwards. Euler's momentum theorem [27]. d'Alembert's paradox [26, 27]: the fluid offer no resistance (zero force) to steady translational motion of a rigid body as the result of Euler's momentum theorem and Bernoulli's theorem. Development of a form drag force to circumvent d'Alembert's paradox (e.g. Newton's drag force on a sphere, development of the von Karman vortex street [52]) [27]. Circulation [26,27,47]: circulation about a circular cylinder, circulation about an elliptic cylinder, the Circle theorem [26, 27], the

Blasius theorem [26, 27, 47], the theorem of Kutta and Joukowski [26, 27, 47], Kelvin's vortex theorem [27]: constancy of circulation in a closed circuit (i.e. always consisting of the same fluid particles) moving with the fluid, circulation about an airfoil.

2.3.3.4 Kinematics of compressible flow (U: 8 hrs)

Contents Definition of a homentropic flow [47]: frictionless, irrotational and isentropic throughout the flow field. The equations of change for homentropic flow [47]: continuity, momentum, isentropic relationship (involving the equation of state e.g. ideal gas law). Breakdown of the equations of motion of homentropic flow whenever shock waves occur: the flow is not isentropic through shock waves. The isentropic relationship resulting from the ideal gas law [47]. Propagation of an infinitesimal disturbance: sonic velocity in an ideal gas [47], sonic velocity in dense gases and liquids [47, 49], the Mach number, the Mach cone. Classification of compressible flows: subsonic flow when the mach number is less than unity (behaviour as an incompressible flow when the Mach number is less than 0.3), sonic flow when the Mach number equals unity, supersonic flow when the Mach number exceeds unity (occurrence of transonic flow when the stream over a body is partly subsonic and partly supersonic, hypersonic flow when the Mach number becomes larger than six and assumptions made for ordinary supersonic flow become invalid). Compressible potential flow: its definition as an extension of incompressible potential flow where Poisson's equation for the velocity potential reduces to Laplace's equation as the sonic velocity tends towards infinity [47]. Examples of homentropic flow: effect of area change [47], converging nozzle flow [47], converging diverging nozzle [47], isentropic equations for one-dimensional steady flow of an ideal gas [47]. Shock waves: normal shocks [47], the equilibrium states of the Fanno line and the Rayleigh line (only the states where these lines intersect in the enthalpy-entropy diagram are allowed, lower portion of the curves is supersonic, upper part of the curves is subsonic, discontinuity in intensive and extensive properties when a shift in the flow conditions occurs between the two states) [47], choking effects [47], the piston generated shock [47]. Shock-expansion theory [47]: oblique shock, supersonic expansion (on a convex surface: around a curve, around a sharp corner, formation of a slipstream), supersonic compression (on a concave surface), the Prandtl-Meyer function, the Prandtl-Meyer expansion fan, combined oblique shocks and expansions (obtaining the flow pattern over complex shapes by patching together the oblique shock and isentropic expansion flow solutions, the wave drag). Thin airfoil theory. The plug nozzle (application in the supersonic jet engine e.g. SR-71 Blackbird).

2.3.3.5 Incompressible laminar viscous flow (U: 8 hrs)

Contents Molecular transport of momentum in a fluid: the hypothesis of a linear relationship between the momentum flux vector and the local velocity gradient (Newton's momentum law) [26], the proportionality constant (i.e. the dynamic viscosity) in Newton's momentum law as a measure of the internal friction opposing deformation of the fluid [26], positivity of the dynamic viscosity as a result of the momentum flux vector pointing in such a direction as to tend to eliminate the non-uniformity of the fluid velocity [26], the application of Newton's momentum law as an empirical expression for the tangential stresses (i.e. the off-diagonal components of the deviatoric stress tensor) in a

fluid [26]. The kinematic viscosity (i.e. dynamic viscosity divided by the density) as a measure of the internal friction per mass unit of fluid [26]. The coefficient of bulk viscosity in the pure expansion of a fluid: distinction and independence between the shear viscosity and the bulk (dilatational) viscosity [28, 45]. The concept of a Newtonian fluid [26]: the relation between the deviatoric stress and the rate-of-strain, the absence of a way to deduce the dependence of the deviatoric stress tensor and the velocity gradient tensor, adoption of the hypothesis that the deviatoric stress tensor is a linear function of the various components of the velocity gradient for sufficiently small magnitudes of the latter, the linear proportionality between the the deviatoric stress tensor and the velocity gradient tensor is a fourth order tensor coefficient, the fourth order tensor coefficient takes a simple form when the molecular structure of the fluid is statistically isotropic and the deviatoric stresses generated in a fluid element by a given velocity gradient is independent of the orientation of the element. Examples of viscosities of gases, liquids, and liquid metals [45]. Non-Newtonian fluids [26, 45, 47]: directional dependence of the deviatoric stresses generated in a fluid element by a given velocity gradient due to alignment of molecules, time independent non-Newtonian fluids (Bingham plastics, pseudoplastic fluids, dilatant fluids), time dependent non-Newtonian fluids (thixotropic fluids, rheopectic fluids), viscoelastic fluids (Maxwell liquids). Empirical models for the viscosity of non-Newtonian fluids: the Bingham model [45], the Ostwald-de Waele model [45], the Eyring model [45], the Ellis model [45], the Reinier-Philippoff model [45]. The equation of motion for a Newtonian viscous fluid [27, 57]: the Navier-Stokes equations, linear system of equations for flows where the convective acceleration vanishes, nonlinear system where the convective acceleration does not vanish, equation of motion satisfied by the stream function [27], the equation of compatibility [27], equation of motion satisfied by the stream function in axisymmetrical motion (the Stokes stream function) [27]. Example of the application of the stream function to a viscous fluid [26, 27, 45, 57]: reduction of the equation for the stream function to the biharmonic form when inertia becomes negligible, the drag force (Stokes' law) due to creeping flow around a sphere obtained from Stokes' stream function and the stress tensor at the surface, friction contributing two-thirds and pressure contributing one-third of the drag force. Circulation in a viscous fluid [27]: circulation in a fluid originally at rest can only arise by the diffusion of vorticity inwards from the boundary, dependence of the sense of rotation of water running out of the bath on the temperature rather than the location of Northern and Southern hemispheres (opposite vorticities are acquired as the bath is filled with the hot or the cold tap when the water moves near the boundary). Dimensionless groups in viscous flows (including heat and mass transfer): Reynolds number, Rossby number, Prandtl number, Eckert number, Grashof number, Nusselt number, Sherwood number, Peclet number, Knudsen number, specific heat ratio, cavitation number, Weber number. Solutions of the Newtonian viscous flow equations: Couette shear flows (steady flow between two parallel plates [57], flow between rotating concentric cylinders [57]), steady flow of a falling film [45], adjacent flow of two immiscible fluids [45], steady duct flows (Hagen-Poiseuille flow [57], ducts with a non-circular cross-section (concept of the hydraulic diameter [45, 57], rectangle [57], ellipse [57], concentric annulus [57], circular sector [57], eccentric annulus [57], equilateral triangle) [57], flow near a wall suddenly set in motion (Stokes's first problem) [45], unsteady duct flows: starting flow in a circular pipe [45, 57], flow due to oscillating pressure gradient [57]). **References:** Hirschfelder, Curtiss & Bird [28] and White (1974) [57].

2.3.3.6 Mathematical models of fluid motion (U: 8 hrs; G: 6 hrs)

Contents The four basic laws describing fluid motion: conservation of mass, Newton's second law of motion, conservation of energy (the first law of thermodynamics), and, the second law of thermodynamics [47]. Classification of the equations of change according to approaches to solving problems [47]: integral (control volume) equations - gross effects, differential equations - distribution of quantities and properties. Classification of the equations of change according to working form [47]: system equations (time rate of change of mass, linear momentum equation (Newton's second law), angular momentum equation, first law of thermodynamics, inequality of Clausius), integral equations (control volume form of the continuity equation, control volume form of the momentum equation, the angular momentum equation, control volume form of the energy equation, control volume form of the inequality of Clausius), and, differential equations (continuity equation, momentum equation, energy equation, control volume form of the inequality of Clausius). The linear advection equation [58]: the solution to the linear advection equation, propagation of initial conditions as left-running and right-running waves, wave fronts (characteristics, propagation of wave information, wave speeds and characteristic speeds, wave diagrams), specification of boundary conditions (well-posedness, ill-posedness due to over-specification of boundary conditions, ill-posedness due to under-specification, inconsistency when two wavefronts meet (illustration of this inconsistency in the wave diagram, occurrence of a shock wave due to this inconsistency, interpretation a shock wave as the 'black hole' of waves, the jump discontinuity in the solution due to shock waves and the use of jump relations to overcome inconsistency, the shock condition, the contact condition and contact discontinuity). Scalar conservation laws [58]: convex and nonconvex scalar conservation laws, jump discontinuity in the initial condition of a convex scalar conservation law (valid for an ideal gas; solution contains at most one shock, one contact discontinuity, one centered expansion fan), jump discontinuity in the initial condition of a nonconvex scalar conservation law (valid for a real gas; solution contains multiple shocks, multiple contact discontinuities, multiple expansion fans; general implicit solution of the Riemann problem for a nonconvex scalar conservation law). Example [59]: under-expanded jet with barrel shock and Mach disk, slip line, barrel length. The non-linear form of the advection equation [58]: the inviscid Burgers equation (convex scalar conservation law; the Riemann problem i.e. solution for constant initial values except for a single jump condition, analytical solution of the Riemann problem), the Bucky-Leverett equation (nonconvex scalar conservation law; shock condition must be supplemented by the Oleinik entropy condition). The Euler equations [58]: conservation form of the Euler equations, quasi-linear form of the Euler equations, primitive form of the Euler equations, the Riemann problem for the Euler equations (exact solution). Boundary conditions for the Euler equations [60,61]: solid wall, subsonic inflow (reflecting and non-reflecting), subsonic outflow (reflecting and non-reflecting), supersonic inflow, supersonic outflow. The Navier-Stokes equations: control volume form, differential form, equation for the stream function corresponding with the Navier-Stokes equations, application of Enskog's perturbation method to the Boltzmann equation [28] (first order perturbation leading to the Navier-Stokes equations, second order perturbation leading to the Burnett equations), the compressible Navier-Stokes equations (control-volume form, differential form). Boundary conditions for the incompressible Navier-Stokes equations: second order velocity derivatives require two boundary conditions at a solid wall [57] (no-slip condition: specification

of tangential velocity, normal velocity), impossibility of potential flows to satisfy the no-slip condition [57] (specification of normal velocity, no restriction on tangential velocity), constant pressure boundary, inlet, outlet, periodic, symmetry. Boundary conditions for the compressible Navier-Stokes equations [62]: solid walls, fluid boundaries (stress continuity), subsonic inflow (reflecting and non-reflecting), subsonic outflow (reflecting and non-reflecting), supersonic inflow, supersonic outflow. Similarity solutions for the full Navier-Stokes equations: reduction of a system of partial differential equations to ordinary differential equations by a similarity transformation, the Blasius solution for flat plate flow [57], the Hiemenz solution for stagnation flow [52, 57], the Falkner-Skan solutions for wedge flows [57], the flow near an infinite rotating disk [57], the Jeffery-Hamel flow in a wedge shaped region [57], the two-dimensional laminar jet [57], creeping flow around a sphere [26, 27, 45, 57] (also treated in Section 2.3.3.5). **References:** Hirschfelder, Curtiss & Bird (1967) [28], Laney (1998) [58], Poinot & Lele (1992) [62], White (1974) [57], and Thompson (1987, 1990) [60, 61].

2.3.3.7 Dimensional analysis and similitude (U: 4 hrs; G: 3 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.

2.3.3.8 Incompressible turbulent flow (U: 12 hrs, G: 9 hrs)

Contents Fluid turbulence: the greatest challenge of classical physics and applied mathematics, Leonardo da Vinci as the first to recognise the cascading of large vortical motions into smaller ones and to postulate the Reynolds decomposition in 1510 ("...thus the water has eddying motions, one part of which is due to the principal current, the other to the random and reverse motion.") [63, 64], the ultimate goal of turbulence research [65] (unification of the von Karman-Prandtl universal logarithmic law in the wall region and the Kolmogorov-Obukhov scaling laws for the local structure of fully developed turbulent flow into a future complete theory of turbulence). The boundary layer concept: a thin layer near the wall where the velocity increases from zero (no-slip at the wall) to its full value corresponding to external frictionless flow (the Prandtl hypothesis) [52], definition of the boundary layer thickness (displacement thickness, momentum thickness) [47, 52], wall shear stress [52], separation from the wall and vortex formation [52], the von Karman vortex street [52], the frequency of vortex shedding in the von Karman vortex street [52]. Velocity profile in the boundary layer [47, 52]: law of the wall (linear layer, logarithmic layer), velocity defect law, definition of the point of separation (limit between forward and reverse flow in the immediate neighbourhood of the wall). The boundary layer equations [52]. Transformation of the boundary layer equations into the diffusion equation [52]: the von Mises transformation. The momentum integral equation for the boundary layer (von Karman's integral equation) [52]: displacement thickness, momentum thickness. The energy-integral equation for the boundary layer [52]: energy thickness. Exact solutions

to the boundary layer equations (similarity solutions): the flow over a flat plate (Blasius solution, local skin friction, average skin friction) [66], the flow past a wedge [52], the flow in a convergent channel [52], the suddenly accelerated plane wall (Stokes's first problem, also treated in Section 2.3.3.5) [52], the flow near an oscillating flat plate (Stokes's second problem), [52]. Skin friction: external flows (drag coefficients [45,47]: flat plate (tangential), flat plate (normal), circular disk (normal), sphere, hollow sphere (convex, concave), solid sphere (convex, concave), circular cylinder, square cylinder), internal flows (Fanning friction factor [45,47]: flow in tubes (Blasius formula for the friction factor), flow through packed beds (friction factors in the Blake-Kozeny equation, and the Burke-Plummer equation; limiting cases of the Ergun equation)). The scales of turbulent motion: the energy cascade and Kolmogorov's hypotheses [67] (definition of local homogeneity [67], definition of local isotropy [67], hypothesis of local isotropy [67], Kolmogorov's first similarity hypothesis [67], Kolmogorov's second similarity hypothesis [67]), autocorrelation function [67,68] (Kolmogorov time scale, integral time scale), structure functions [67], the second order velocity structure function [67], longitudinal and transverse structure functions [67], two-point velocity correlation functions [67] (longitudinal autocorrelation function, transverse autocorrelation function), the longitudinal integral length scale [67], the transverse integral length scale [67], the longitudinal Taylor microscale [67], the transverse Taylor microscale [67], relationship between the Taylor and Kolmogorov scales [67], the von Karman-Howarth equation [45,67], solution of the von Karman-Howarth equation for the decay of turbulence behind a grid [45,67,69], the Kolmogorov $-4/5$ -law [67], the velocity-spectrum tensor [67] (Fourier transform pair of the two-point velocity correlation function), the energy spectrum function [67], Taylor's hypothesis [67] (frozen turbulence approximation), power law energy spectra [67], Kolmogorov spectra [67] (energy containing range, universal equilibrium range (inertial subrange, dissipation range)). Turbulence modeling: Reynolds decomposition, Reynolds' rules for averages [47], the Reynolds averaged Navier-Stokes equations [67], Reynolds stresses [67], Reynolds stress tensor [67], the closure problem [67], closure hypotheses (the eddy viscosity hypothesis (Boussinesq's eddy viscosity [45], Prandtl's mixing length hypothesis [45], von Karman's similarity hypothesis [45], the k-epsilon model [67], the Renormalisation Group k-epsilon model, the k-omega model, the Spallart-Allmaras model), the gradient diffusion hypothesis [67], Reynolds-stress models (algebraic stress models [67], return-to-isotropy models [67], rapid-distortion equations [67], pressure-rate-of-strain models [67], elliptic relaxation models [67])). Large Eddy Simulation: Leonard's decomposition [70], filtering and scale separation [70] (properties of the filter (conservation of constants, linearity, commutation with differentiation), temporal filtering [70] (time low-pass filter, elliptic filter, parabolic filter, convective and Lagrangian filters), spatial filters [70] (box or top hat filter, Gaussian filter, spectral filter, second order commuting filter, high order commuting filters)), differences between rules for obtaining filtered averages and Reynolds' rules for averages, the filtered Navier-Stokes equations [70], the subgrid stress tensor (consisting of the sum of the cross-stress tensor and the Reynolds subgrid tensor) [70], Leonard's triple decomposition: further decomposition of the Reynolds subgrid tensor to obtain the Leonard stress tensor [70], subgrid viscosity closure models for the forward energy cascade process (spectral models (Chollet-Lesieur model, constant effective viscosity model, dynamic spectral model, Lesieur-Rogallo model), physical space models (Smagorinsky model, structure function model, Yoshizawa model, mixed scale model, Germano-Lilly model)), subgrid viscosity closure models for the backward energy cascade process [70] (Chasnov's spectral model, Bertoglio model, Mason-Thomson model,

Schumann model), differential subgrid stress models [70]: Deardorff model. **References:** Barenblatt (2003) [65], Kreith & Bohn (2001) [66], Lesieur (1987) [68], Pope (2000) [67] and Sagaut & Germano [70].

2.3.3.9 Waves in fluids and the stability of fluid flow (U: 8 hrs, G: 6 hrs)

Contents The wave equation [49]. Sound waves [47, 49]. The speed of sound [49]. The phasor representation of traveling sound waves [47]. Acoustic energy [49]. Acoustic intensity [49]. Dissipation of acoustic energy [49]. Gravity waves [47]. Capillary waves [47]. Stability theory [46, 47]. Transition to turbulence in a pipe as observed by Reynolds [46]. Stability of a liquid jet [46, 47]. Kelvin-Helmholtz instability [46]. Rayleigh-Taylor instability [46]. Schlichting-Tolmien waves [46].

2.3.3.10 Compressible turbulent flow (G: 8 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) [71], Favre (1965) [72], Gatski, Hussaini & Lumley (1996) [73], and Lele (1994) [74].

2.4 MODULE HEAT AND MASS TRANSFER

2.4.1 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) [75], Hottel & Sarofim (1967) [76], Incropera, De Witt, Bergman & Lavine (2006) [77], Kaviany (2002) [78], Kreith & Bohn (2001) [66], Pitts & Sissom (1977) [79], and Welty, Wicks, Wilson & Rorrer (2001) [80]. Additional references are given along with the topics.

2.4.2 PREREQUISITE MATTER

Calculus (including linear algebra, complex functions, complex analysis, Laplace transforms, Fourier analysis), ordinary differential equations, partial differential equations, thermodynamics, vector analysis, tensor analysis, classical mechanics, optics, continuum mechanics, statistical mechanics, fluid dynamics, wave mechanics, elementary quantum mechanics.

2.4.3 CONTENTS OF THE MODULE

2.4.3.1 Basic modes of heat transfer and particular laws (U: 5 hrs)

Contents The relation of heat transfer to thermodynamics [66, 77]: limitations of classical thermodynamics, engineering heat transfer (conservation of energy for a control volume, the surface energy balance). The three distinct modes of heat transfer [66, 77]: conduction, radiation and convection. Conduction heat transfer [66, 77, 81]: Fourier's law, thermal conductivity (examples of thermal conductivities of some metals, alloys, nonmetallic solids, liquids, gases [66, 77]), the heat flux (heat transfer per unit area) and the heat rate by conduction [77], thermal resistance, analogy between thermal resistance and electrical circuits, plane walls in series and parallel [66], variation of thermal conductivity for gases and liquids [66], thermal contact resistance (temperature drop through contact resistance [66], effect of surface roughness [66], thermal contact resistance for metallic interfaces under vacuum conditions [66, 82], effect of contact pressure on thermal contact resistance [66, 82], effect of different interfacial fluids on thermal contact resistance [66, 82], example: application of high conductivity pastes to mount electronic components to heat sinks). Convection heat transfer: Newton's cooling law, convection heat transfer coefficient, dependence of the convection heat transfer coefficient on fluid density, viscosity, and velocity [66]. Radiation heat transfer [66, 77]: difference between conduction or convection heat transfer and radiation heat transfer (conduction or convection requires a material medium, radiation does not), the concept of an ideal radiator or blackbody, the surface emissive power (radiant heat emission rate), the Stefan-Boltzmann law for the upper limit of the emissive power, the Stefan-Boltzmann constant, independence of the surface emissive power from the conditions of the surroundings, the concept of the gray surface to represent real surfaces, emissivity (efficiency of energy emission by a radiating surface relative to a blackbody, representative values for metals, nonmetallic substances, etc. [77]), modification of the Stefan-Boltzmann law to describe the emissive power of real surfaces, incident radiation on a surface from its surroundings, irradiation (rate of incident radiation per unit area), absorptivity (opaque surfaces, semitransparent surfaces), equality of absorptivity and emissivity (gray surface), the net rate of radiation heat transfer from the surface (the balance equation for the thermal energy released due to radiation and that which is gained due to radiation absorption, modification to the balance equation to include the geometric shape factor), the radiation heat transfer coefficient, continuous radiation, selective radiation. Combined modes of heat transfer: convection and conduction in series [66], convection and radiation in parallel [66], overall heat transfer coefficient. **References:** Fried (1969) [82], Maas, Warnatz & Dibble (2005) [81].

2.4.3.2 Isothermal mass transfer (U: 5 hrs)

Contents Mixture composition. Species mass density. Molar concentration. Mass fraction. Mole fraction. Fick's law of diffusion [77, 81]. Binary diffusion coefficient (mass diffusivity). Ordinary diffusion (motion of species due to concentration gradient). Other modes of diffusion [28, 45]: pressure diffusion (motion of species due to pressure gradient), thermal diffusion (motion of species due to temperature gradient), forced diffusion (motion of species due to external force). Diffusion velocity [45]: definition with respect to mass average velocity, definition with respect to molar average velocity. Pressure and temperature dependence of mass diffusivity [28, 45, 77]. Conservation of species in a control

volume: the species diffusion equation, the species convection-diffusion equation. Multi-component mixtures: the Stefan-Maxwell equations [45], the effective binary diffusivity of a species in a multi-component mixture [45], equation of continuity for each species in a multi-component mixture [45]. **References:** Bird, Stewart & Lightfoot (2002) [45], Hirschfelder, Curtiss & Bird [28] Maas, Warnatz & Dibble (2005) [81].

2.4.3.3 Heat conduction (U: 12 hrs; G: 9 hrs)

Contents The conduction rate equation (Fourier's law) [66, 77]: it is the cornerstone of conduction heat transfer, it is a generalisation of experimental observations, it is not an expression derived from first principles, it defines the thermal conductivity as a material property, it applies to all matter regardless of its state (solid, liquid, gas). The sign convention for conduction heat flow [66, 77]. The heat flux as a vector perpendicular to isotherms [77]. The conduction rate equation as a relationship between the heat flux across a surface and the temperature gradient in a direction perpendicular to the surface [77]. Independence of the value of the thermal conductivity of coordinate direction in isotropic media [77]. The thermal conductivity [77]: the solid state (conduction heat transfer as the sum of two additive processes: the migration of free electrons and lattice vibrational waves, the thermal conductivity as the sum of an electronic component and a lattice component, inverse proportionality of the electronic component to the electrical resistivity), the fluid state (proportionality to the number of particles per unit volume, the root-mean-square velocity, and the mean free path, the Chapman-Enskog formula for the thermal conductivity of monoatomic gases [45], the Eucken formula for the thermal conductivity of polyatomic gases [45], Bridgman's equation for the thermal conductivity of liquids [45], difficulties with physical mechanisms for explaining the thermal conductivity [83]). Concept of the effective thermal conductivity in insulation materials consisting of finely dispersed solid material (fiber-, powder-, flake-like insulations). The heat diffusion equation (the conduction equation) [66, 77]. The thermal diffusivity. Heat diffusion equation in cartesian, cylindrical and spherical coordinates [66, 77]. Boundary conditions for the heat diffusion equation at the surface [77]: constant surface temperature, constant surface heat flux (finite heat flux, adiabatic or insulated heat flux), convection surface condition. Non-dimensional form of the heat diffusion equation [66]. Dimensionless groups in the non-dimensional form of the heat diffusion equation [66]: the Fourier number and the dimensionless heat generation number. Consequences of prevailing and vanishing Fourier numbers. Steady heat conduction in simple geometries [66]: plane wall with and without heat generation, cylindrical and spherical shapes without heat generation (critical radius), long solid cylinder with heat generation. Extended surfaces [66, 77]: examples of different types of fins [66] (longitudinal fin of rectangular profile, cylindrical tube with fins of rectangular profile, longitudinal fin of trapezoidal profile, longitudinal fin of parabolic profile, cylindrical tube with radial fin of rectangular profile, cylindrical tube with radial fin of truncated conical profile, cylindrical pin fin, truncated conical spine, parabolic spine), examples of typical finned-tube heat exchangers [77], analysis of temperature distribution and heat transfer of fins of uniform cross section [66, 77], fin performance [66, 77] (fin effectiveness, fin resistance, fin efficiency (common fin shapes [77], non uniform cross-sectional area [77]), overall fin efficiency). Multidimensional steady conduction [66, 77]: the method of separation of variables, the graphical method (method of constructing a flux plot, determination of the heat transfer rate, the conduction shape

factor). Transient heat conduction: the lumped capacitance method [77] (validity of the method: the Biot number, spatial effects: the Fourier number, examples: the plane wall with convection, radial systems with convection, the semi-infinite solid). **References:** Bird, Stewart & Lightfoot (2002) [45].

2.4.3.4 Convection heat transfer (U: 8 hrs; G: 6 hrs)

Contents The convection heat transfer problem [66, 77]: relationship between the convection of heat and the flow of the fluid, the local heat flux, the local convection heat transfer coefficient, the total heat flux over an entire surface, the average convection heat transfer coefficient for an entire surface, relationship between the average heat convection transfer coefficient for an entire surface and the the local convection heat transfer coefficient (example: average heat convection transfer coefficient in case of flow over a flat plate, dependence on distance from the leading edge), dependence of convection heat transfer coefficients on surface geometry and flow conditions, the influence of boundary layers that develop on the surface. Convection boundary layers [66, 77]: the velocity boundary layer, the thermal boundary layer, the concentration boundary layer. Conservation of energy in a control volume: the heat diffusion equation, the heat convection-diffusion equation. Boundary layer similarity [66, 77]. The convection transfer equations [66, 77]: the conservation equations for mass, momentum, and energy for laminar flow over a flat plate. The boundary layer approximations. The boundary layer equations. Non-dimensional boundary layer equations. Boundary layer similarity parameters: Reynolds number, Prandtl number, Schmidt number. Functional form of solutions to the boundary layer equations: existence of a universal relationship between momentum, mass, and heat transfer coefficients, and, boundary layer similarity parameters. Friction coefficient. Nusselt number. Sherwood number. Relationship for the local convection heat transfer coefficient in a laminar boundary layer over a flat plate based on the Nusselt number [66]. Pohlhausen solution for the thermal boundary layer [79] (temperature profile, solution for the local heat transfer coefficient, analogy with Blasius solution). Application of the von Karman integral technique to the thermal boundary layer (integral energy equation, comparison with integral momentum equation, solution for the local heat transfer coefficient, approximate solution due to polynomial assumption for the temperature profile (in contrast with exact Pohlhausen solution)). The heat and mass transfer analogy. The Reynolds analogy (analogy between heat transfer and skin friction). The Stanton number. Correlations for the local convection heat transfer coefficient based on the Stanton number (laminar boundary layer [66], turbulent boundary layer [66], high speed flows [66]).

2.4.3.5 Forced convection (U: 8 hrs; G: 6 hrs)

Contents Forced convection inside tubes and ducts [66, 77]: Nusselt number based on the hydraulic diameter, reference fluid temperature and the convection heat transfer coefficient (average fluid bulk temperature, mixing-cup temperature, difficulties imposed by variations in the bulk temperature in the flow direction), effect of Reynolds number on heat transfer, effect of pressure drop on heat transfer, effect of Prandtl number on heat transfer, entrance effects (growth of boundary layers, variation of velocity distribution, variation of temperature distribution), variation of physical properties, concept of the

average film temperature to account for variation of physical properties, thermal boundary conditions, compressibility effects for high Mach number flows. Analysis of laminar forced convection in a long tube [66]: momentum analysis and velocity distribution, energy analysis (uniform heat flux, uniform surface temperature). Correlations for laminar forced convection [66, 77]: short circular and rectangular ducts, ducts of non-circular cross section, effect of property variations (Dittus-Boelter equation, Sieder and Tate equation, Kays-London correlation, Pethuklov-Popov correlation, Sleicher-Rouse correlation), effect of natural convection (forced, natural, and mixed convection regimes), coiled tubes (primary and secondary flows, the Dean number, negligible secondary flow inertia forces (heat transfer correlation between the peripherally averaged Nusselt number and the Dean number), secondary flow inertia forces balancing viscous forces (heat transfer correlation), prevailing secondary flow inertia forces (heat transfer correlation)), cylinder in cross-flow. sphere. Empirical correlations for turbulent forced convection: circular ducts and tubes, ducts of non-circular shape and coiled tubes, cylinder in cross flow, sphere, banks of tubes (aligned, staggered), impinging jets (single round jet, single slot jet, in-line array of round jets, staggered array of round jets, array of slot jets), packed beds (bed of spheres, effect of particle shape, effect of void fraction). Heat exchangers [66, 77]: basic types of heat exchangers (recuperators, regenerators, direct contact heat exchangers), concentric tube heat exchanger (parallel flow, counterflow), shell and tube heat exchanger (shell passes, tube passes), baffles used in shell and tube heat exchanger (orifice baffle, disk-and-doughnut baffle, segmental baffle), cross-flow heat exchanger (finned, unfinned). Overall heat transfer coefficient. Fouling factors. Log mean temperature difference. Heat exchanger effectiveness (NTU-method, NTU-relations).

2.4.3.6 Natural convection (U: 8 hrs; G: 6 hrs)

Contents Natural convection (free convection) [66, 77]: existence of convection currents in the absence of external forcing, existence of convection currents due to the combined presence of a fluid density gradient and a body force (gravitational force, centrifugal force, Coriolis force) that is proportional to density. Free boundary flows (plume, buoyant jet) and surface bounded flows (boundary layer development along a heated vertical plate). The governing equations of natural convection currents. The Boussinesq approximation: assumption of the fluid to be incompressible while accounting for the effect of variable density in the buoyancy force. The volumetric thermal expansion coefficient. Non-dimensional form of the equations of natural convection currents and similarity considerations. Grashof number. Rayleigh number. Heat transfer relations (correlations) between the Nusselt number and the Grashof number: laminar free convection along a vertical surface (transition to turbulence), empirical correlations (vertical plate, inclined planes, horizontal planes (upper surface hot or lower surface cool, upper surface cool or lower surface hot), the long horizontal cylinder, cylinders, spheres, cones, enclosed spaces (parallel plate channels, vertical channels, inclined channels, concentric cylinders, concentric spheres), rotating cylinders, rotating disks, rotating spheres). Combined free and forced convection: criteria for prevalence of free or forced convection, assisting flow, opposing flow, transverse flow.

2.4.3.7 Heat Transfer with Phase Change (U: 8 hrs; G: 6 hrs)

Contents Dimensionless groups in boiling and condensation [66, 77]: the Jakob number, the Bond number, and a nameless parameter bearing strong resemblance to the Grashof number. Crisis of boiling. The Leidenfrost phenomenon [84–95] (Leidenfrost point, maximum residence time of a droplet on a heated surface, firewalking). Boiling modes [66, 77]: pool boiling, forced convection boiling, subcooled boiling, saturated boiling. Pool boiling [66, 77]: excess temperature, boiling curve (heat flux versus excess temperature), critical heat flux, critical excess temperature, extrema and inflection points of the boiling curve as boundaries between different modes of pool boiling, modes of pool boiling (free convection boiling, nucleate pool boiling (individual bubble regime, slugs and columns regime, bubble growth mechanisms, inertia controlled bubble growth for large values of the Jakob number multiplied by the liquid-to-vapour density ratio, heat transfer controlled bubble growth for small values of the Jakob number multiplied by the liquid-to-vapour density ratio, evaporation microlayer, relaxation microlayer), transition boiling, stable film boiling), pool boiling correlations (nucleate pool boiling heat transfer coefficient defined as the ratio between the heat flux and the excess temperature, Rohsenow correlation for the heat flux for nucleate pool boiling, Kutateladze-Zuber correlation for the critical heat flux for nucleate pool boiling, Zuber correlation for the minimum heat flux at the boundary between the transition boiling regime and the stable film boiling regime, Bromley correlations for the heat transfer coefficient in the stable film boiling regime). Boiling in forced convection [66, 77]: bubble flow regime, slug flow regime, annular flow regime, mist flow regime. Nucleate forced convection boiling: application of the pool boiling heat flux correlation to forced convection boiling. Boiling with net vapour production: the Chen correlation for the heat transfer coefficient. Condensation [66, 77]: physical mechanisms, latent heat of vaporisation. Modes of condensation: film condensation, dropwise condensation on a surface, homogeneous condensation or fog formation, direct contact condensation. Classical approach by Nusselt to obtain theoretical relations for calculating heat transfer coefficients and film thickness of filmwise condensation (Nusselt’s film theory) [66]. Laminar film condensation on a vertical plate. Deviations from Nusselt’s film theory when condensate flow becomes turbulent or the vapour velocity is very large. Turbulent film condensation: effect of film turbulence (correlation by Colburn for the local heat transfer coefficient), effect of high vapour velocity (Carpenter-Colburn correlation for the local heat transfer coefficient). Film condensation on radial systems: sphere, single horizontal tube, vertical tier of horizontal tubes with a continuous condensate sheet, vertical tier of horizontal tubes with dripping condensate. Example: effect of air condensation in accidents with LH2. Freezing and melting [66]. **References:** Agrawal & Menon (1994) [84], Bent [85], Collier & Thome (1996) [96], Curzon [86] Gottfried, Lee & Bell [87], Hall, Board, Clare, Duffey, Playle & Poole [88], Leidenfrost [89], Leikind & McCarthy [90], Leikind & McCarthy [91], Taylor [92], Thimbleby [93], Walker [94], and Zhang & Gogos [95].

2.4.3.8 Radiation heat transfer (U: 12 hrs; G: 9 hrs)

Contents Fundamental concepts [66, 77, 97]. The spectrum of electromagnetic radiation: relationship between the distribution of electromagnetic radiation and changes in the electronic, vibrational, and rotational states of atoms and molecules. Classification of the spectrum of electromagnetic radiation: cosmic rays, gamma rays, X-rays, thermal radiation (ultraviolet, visible, near infrared, far infrared), Hertzian waves. Concept of the

photon. Concept of colour in the visible range. Planck's constant. The blackbody as an ideal surface: absorbing all radiation regardless of wavelength and direction, no surface can emit more energy than a blackbody for a given temperature and wavelength, diffuse emitter (emitted radiation is independent of direction). Planck's distribution law. Wien's displacement law. The Stefan-Boltzmann law. Absorption and emission at solid surfaces. Band emission. Absorptivity and emissivity. Kirchhoff's law for radiation equilibrium with any solid surface. Poynting vector (magnitude and direction of electromagnetic energy transfer). Validity of Kirchhoff's law for each wavelength separately. Emissive power: (spectral emissive power, total emissive power). Radiation intensity: (spectral intensity, total intensity). Relation between radiation intensity and emissive power. Radiation flux. Irradiation. Radiosity. Reflection. Transmission. Radiation pressure. Polarisation (state of polarisation, linear polarisation, circular polarisation, elliptic polarisation, parallel and perpendicular polarisation components, Stokes' parameters of a wave train, degree of polarisation, dependence of reflective behaviour of a surface on the polarisation of incoming radiation, tendency of a surface to alter the state of polarisation). Gray bodies [66,77,97]: grey body assumption for engineering analysis of real surfaces, limitations of grey body assumption. Real surface characteristics [66,77,97]: radiative properties of metals, radiative properties of nonconductors, effects of surface roughness, effects of surface damage and oxide films, radiative properties of semi-transparent sheets, special surfaces. Radiation exchange between surfaces [66,77,97]. Definition of view factors. View factors for two- and three-dimensional geometries. Methods for the evaluation of view factors: the view factor integral, view factor algebra, crossed-strings method, inside-sphere method, unit sphere method, Radiation exchange between black surfaces. Radiation exchange between grey, diffuse surfaces (electrical network analogy). Radiation exchange between partially-specular gray surfaces (specular reflectors, electrical network analogy, radiation shields, semi-transparent sheets, reradiating surface). Radiation exchange between nonideal surfaces (nongray surfaces, band approximation, directionally nonideal surfaces). Radiative properties of molecular gases (emission and absorption probabilities, atomic and molecular spectra (rotational transitions, vibrational transitions), line radiation, spectral models for radiative transfer (line-by-line method, narrow band models, wide band models)). Radiative properties of particulate media (absorption and scattering from a single sphere, small sphere (Rayleigh scattering, Rayleigh-Gans scattering), large sphere (diffraction, specular reflection, diffuse reflection) radiative properties of a particle cloud, clouds of uniform particle size, clouds of non-uniform particle size, radiation properties of combustion particles (pulverised coal, fly ash dispersions, soot)). **References:** Modest (2003) [97] and Siegel & Howell (1993) [98].

2.4.3.9 Simultaneous heat and mass transfer (U: 8 hrs; G: 6 hrs)

Contents Formulation of governing equations. Thermo-diffusion. Droplet evaporation. Stefan's law of mass transfer and droplet evaporation. Lewis number. Stagnant boundary layer formation. B-number. Wet-bulb temperature.

2.5 MODULE SOLID MECHANICS

2.5.1 INTRODUCTORY STATEMENT

The topics in this module are for undergraduate instruction only. They cover 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) [99], Beer & Johnston (1992) [100], Fitzgerald (1982) [101], Higdon, Ohlsen, Stiles, Weese & Riley (1985) [102], Mase (1970) [103], and Nash (1998) [104].

2.5.2 PREREQUISITE MATTER

Calculus (including linear algebra, complex functions, complex analysis, Laplace transforms, Fourier analysis), ordinary differential equations, partial differential equations, thermodynamics, vector analysis, tensor analysis, classical mechanics, continuum mechanics, wave mechanics.

2.5.3 CONTENTS OF THE MODULE

2.5.3.1 Analysis of stress (U: 6 hrs)

Contents Continuum concept. Homogeneity. Isotropy. Mass-density. Body forces. Surface forces. Cauchy's 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. Mohr's circles for stress. Plane stress. Deviator and spherical stress tensors.

2.5.3.2 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. Mohr's circles for strain. Compatibility equations for linear strains.

2.5.3.3 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, Hooke's 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, Poisson's ratio, general form of Hooke's law, specific strength, specific modulus). Dynamic effects. Elastic vs. plastic analysis.

2.5.3.4 Statically indeterminate force systems (U: 4 hrs)

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

2.5.3.5 Thin walled pressure vessels (U: 2 hrs)

Contents Nature of stresses. Limitations. Applications.

2.5.3.6 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).

2.5.3.7 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.

2.5.3.8 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.

2.5.3.9 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.

2.5.3.10 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).

2.5.3.11 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.

2.5.3.12 Statically indeterminate elastic beams (U: 4 hrs)

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

2.5.3.13 Special topics in elastic beam theory (U: 4 hrs)

Contents Shear center. Unsymmetric bending. Curved beams.

2.5.3.14 Plastic deformation of beams (U: 4 hrs)

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

2.5.3.15 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.

2.5.3.16 Strain energy methods (U: 4 hrs)

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

2.5.3.17 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. Mohr's circle. Sign conventions used with Mohr's circle. Determination of principal stresses by means of Mohr's circle. Determination of stresses on an arbitrary plane by means of Mohr's circle.

2.5.3.18 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.

3 FUNDAMENTAL MODULES

3.1 MODULE HYDROGEN AS AN ENERGY CARRIER

3.1.1 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.

3.1.2 PREREQUISITE MATTER

Modules Thermodynamics, Chemical Kinetics, Fluid Dynamics, Heat and Mass Transfer, and, Solid Mechanics.

3.1.3 CONTENTS OF THE MODULE

3.1.3.1 Introduction to hydrogen as an energy carrier (U: 2 hrs; G: 2 hrs)

Contents Overview of hydrogen programmes in Europe, USA, Japan and other countries. Global energy consumption (global energy systems transition in the period from 1850 to 2150, transition from non-sustainable economic growth to sustainable economic growth), energy security (depletion of fossil fuel resources, imbalance between annual world oil reserves additions and annual consumption, Hubbert's curve and peak oil production, forecasts of peak oil production and peak natural gas production, sectorwise impact of peak oil production (e.g. transportation, industrial, electric power, residential), economic impact of peak oil production (developed nations, developing countries), practical mitigation of the problems associated with world oil peaking (conservation, improved oil recovery, heavy oil and oil sands, gas-to-liquids, liquid fuels from coal, liquid fuels from oil shale, liquid fuels from biomass, fuel switching to electricity, fuel switching to natural gas, hydrogen), hydrogen as an energy carrier, provision of energy services demanded by civilisation by the synergy and shared characteristics of hydrogen and electricity, interchangeability between hydrogen and electricity versus non-interchangeability between fossil fuel energy carriers and electricity). Environmental impact (effect of continued

rises in fossil fuel use on global warming, effect on altering the balance of incoming and outgoing energy in the Earth-atmosphere system, effect on atmospheric concentrations of nitrous oxides and anthropogenic sulphur oxides). Averting economical and environmental consequences arising from continued fossil fuel use by switching to hydrogen. The Hydrogen economy: timing of the hydrogen transition, hydrogen as an energy carrier: today's industrial hydrogen system, production (hydrogen production from hydrocarbons, fossil hydrogen and CO₂ sequestration, hydrogen production via electrolysis, advanced hydrogen production methods using renewable or nuclear energy), usage (hydrogen use in transportation, hydrogen for heat and power in buildings, early niche applications), storage (storage as a compressed gas, storage as a cryogenic liquid, criteria automobile hydrogen storage system), distribution and infrastructure (delivery of liquid hydrogen by truck or rail, compressed gas hydrogen pipelines, refuelling stations), hydrogen safety and regulatory issues (safety issues, comparison between safety relevant properties of hydrogen and those of other conventional fuels, public acceptance and safety, safety becoming a barrier to the introduction of hydrogen if not appropriately considered (e.g. resistance from insurers), transnational nature of safety regulations, codes and standards; approval of new hydrogen technologies by regulations, codes and standards (example of hydrogen road vehicles [105], the case of hydrogen refuelling stations [105])).

References: Cadwallader & Herring [106], Dunn (2002) [5], European Commission, RTD Info (2003) [107], European Commission, RTD Info (2006) [108], Hirsch, Bezdek R. & Wendling [109], Hubbert (1956) [110], Hydrogen Now [111], Intergovernmental Panel on Climate Change, Working Group I (2001) [112], Jordan (2006) [113], Maugeri (2004) [114], Ogden (2004) [115], Sperling & Cannon (2004) [116], Wikipedia Encyclopedia (The Hindenburg Disaster), [117], Wikipedia Encyclopedia (Peak Oil), [118], and Wurster (2006) [105].

3.1.3.2 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 [119, 120], 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.

References: Janssen, Bringmann, Emonts & Schroeder (2004) [119].

3.1.3.3 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.

3.1.3.4 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).

3.1.3.5 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.

3.2 MODULE FUNDAMENTALS OF HYDROGEN SAFETY

3.2.1 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 Releases, Mixing and Dispersion; 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 & Bradley (1985) [121], Drysdale (1999) [122], Glassman (1996) [123], Griffiths & Barnard (1995) [124], Kanury (1977) [125], Kuo (2005) [29], Lewis and von Elbe (1987) [126], Poinot & Veynante (2001) [127], Toong (1983) [128], Turns (2000) [3], Warnatz, Maas & Dibble (2005) [81], and Williams (1985) [129]. Other references are cited along with the topics.

3.2.2 PREREQUISITE MATTER

Modules Thermodynamics, Chemical Kinetics, Fluid Dynamics, Heat and Mass Transfer, and, Solid Mechanics.

3.2.3 CONTENTS OF THE MODULE

3.2.3.1 Hydrogen properties (U: 10 hrs; G: 6 hrs)

Contents Atomic structure of a hydrogen molecule and safety related consequences: spin of the atomic nucleus, ortho-hydrogen, para-hydrogen, equilibrium between ortho-hydrogen and para-hydrogen (temperature dependence of the equilibrium, normal hydrogen), the release of heat accompanying ortho- to para-conversion, rate of the non-catalytic ortho- to para-hydrogen conversion. Safety issues connected to the storage of unconverted liquefied hydrogen (evaporation due to conversion heat release, possible hazard due to naturally occurring deuterium). Comparison between safety-related physical and thermo-physical properties of normal- and para-hydrogen. States of matter (gaseous hydrogen, liquid hydrogen, solid hydrogen and other states of matter). Gaseous (GH2), liquefied (LH2) and slush (SLH2) forms of hydrogen. Phase diagram of hydrogen (PT-diagram): comparison with the general phase diagram of a pure substance, phase boundaries (boiling point (safety issues connected to the low boiling point of hydrogen), melting point, vapour pressure, sublimation vapour pressure, fusion curve, sublimation curve, vaporisation curve (the Clausius-Clapeyron equation), triple point, critical point, critical properties), composition of the PT-diagram (solid region, liquid region, vapour region, gas region, fluid region). Temperature dependence of vapour pressure. The density of hydrogen (gaseous hydrogen (the compressibility factor, corresponding states principle, prediction of the density: ideal gas law, van der Waals equation of state, the Noble-Abel equation of state, the Beattie-Bridgeman equation of state), liquid hydrogen (prediction of the density: Rackett's correlation, the Lydersen-Greenkorn-Hougen correlation), safety issues arising from the density of hydrogen), Sonic velocity. Diffusivity (safety problems arising from the diffusivity of hydrogen). Viscosity. Thermal conductivity. Joule-Thompson inversion temperature. Phase equilibrium: dew point, bubble point; Raoult's law; Henry's law; K -value correlations. Properties connected to fire and explosion hazards: phenomenology of fires (diffusion flame, premixed flame, flash fire, jet fire), deflagrations, detonations (deflagration to detonation transition); adiabatic flame temperature, minimum spark ignition energy, flammability limits, flammability range of hydrogen and air, laminar burning velocity, critical charge for detonation initiation, detonation wave structure, detonation limits, detonation cell size (effect of equivalence ratio, comparison between hydrogen and hydrocarbon fuels), relationship between detonation cell width versus critical initiation energy for the onset of detonation, critical tube diameter for the onset of detonation (effect of equivalence ratio, comparison between hydrogen and hydrocarbon fuels). Health hazard properties: gaseous hydrogen (asphyxiant), liquefied hydrogen (cryogenic burns, frostbite, hypothermia, lung damage from inhalation of cold vapour). **References:** Atkins & de Paula (2006) [20], Cadwallader & Herring [106], ISO TR 15916 E (2004) [2], Lanz, Heffel & Messer (2001) [130], NASA NSS 1740.16 (1997) [131], Smith, Van Ness & Abbott (2007) [23], Sonntag, Borgnakke & Van Wylen (2003) [24], and Zabetakis, Furno & Martindill (1961) [132].

3.2.3.2 Compatibility of metallic materials with hydrogen (U: 6 hrs; G: 6 hrs)

Contents An overview of reported accidents and incidents caused by hydrogen embrittlement (hydrogen transport vessel, hydrogen cylinder bursts, hydrogen transport pipes, etc.). Internal hydrogen embrittlement. External hydrogen embrittlement. States of

hydrogen in steels: hydrogen in metallic solution, hydrogen in combined state. Gaseous hydrogen embrittlement: steel deterioration due to hydrogen in metallic solution, mechanism due to transport by dislocations, effect of temperature. Hydrogen attack: steel deterioration due to hydrogen in combined state, mechanism of formation of micro-cavities in the steel because of the induced lack of carbon, effect of diffusional transport, effect of temperature. Influence of hydrogen pressure on crack growth rate. Test methods to investigate hydrogen embrittlement and hydrogen attack. Factors affecting hydrogen embrittlement: hydrogen purity, hydrogen partial pressure, temperature, exposure time, surface condition, nature of the material (critical concentration of hydrogen in the material, microstructure, chemical composition, mechanical properties). Mitigation of hydrogen embrittlement by the addition of vanadium and rare earth elements to ferritic steel, or, Ni, C, and Mn to austenitic stainless steels. Hydrogen embrittlement of other materials: brass and copper alloys, aluminum and aluminum alloys, Cu-Be (used in springs and membranes), Ni and high Ni alloys, Ti and Ti alloys. Mitigation of hydrogen attack: chemical composition (addition of Cr, Mo, Ti, W), heat treatment (stress relief treatment), level of stress (elimination of residual stresses by heat treatment). **References:** Barthelemy (2005) [133], Barthelemy (2006) [134], Rogante, Battistella & Cesari (2006) [135].

3.2.3.3 Hydrogen thermo-chemistry (G: 6 hrs)

Contents Combustion reaction of hydrogen in air: stoichiometric equation, global versus elementary reactions, relationship between reaction rate and chemical species concentration, the three-parameter Arrhenius form to describe the reaction-rate constant (activation energy, temperature exponent, pre-exponential factor), overall reaction rate expression, overall reaction order (effect of equivalence ratio and pressure on overall reaction order), overall activation energy (effect of equivalence ratio and pressure on overall activation energy). Heats of reaction (constant pressure combustion: equality of reactant and product enthalpies; constant volume combustion: equality of reactant and product internal energies). Adiabatic flame temperature: the frozen flame temperature (absence of product dissociation), adiabatic flame temperature with product dissociation (equilibrium constants, chemical affinity and chemical potential, equilibrium as the condition of zero chemical affinity, chemical affinity as the partial molar Gibbs function, criteria for equilibrium (Gibbs free energy for constant pressure processes, Helmholtz free energy for constant volume processes)). Calculation of the adiabatic flame temperature by the element potential method (constant pressure combustion: minimisation of the Gibbs free energy; constant volume combustion: minimisation of the Helmholtz free energy; examples of chemical equilibrium codes CANTERA, STANJAN, GASEQ; limitations imposed by the inclusion of the ideal gas law in chemical equilibrium codes; equations of state for high pressure effects up to 700 MPa: virial equations of state, Becker-Kistiakowsky-Wilson equation of state). Reaction mechanisms: forward elementary reactions, backward elementary reactions, the chemical equilibrium constant as the ratio between the forward and backward elementary reaction rates, detailed schemes (the Dougherty & Rabitz mechanism, the Miller, Mitchell, Smooke & Kee mechanism [136], the Marinov, Westbrook & Pitz mechanism, the O’Conaire, Curran, Simmie, Pitz & Westbrook mechanism [30], the Saxena & Williams mechanism [31]), reduced mechanisms (example: a four-step reduced mechanism for hydrogen-air mixtures by Lu, Ju &

Law [37]). Chain branching: the concept of a chain carrier. Removal of chain carriers by a three-body collision with a third body. The crossover temperature. Falloff. The fall-off reaction rate: the Lindemann fall-off rate constant, the Stewart fall-off rate constant, the Troe fall-off rate constant. Chaperon efficiencies. Software tools for analysing detailed chemical kinetic mechanisms: CANTERA, CHEMKIN, FLAMEMASTER. Validation of kinetic mechanisms from critically-reviewed experiments including stretch-free laminar burning velocities, flow reactor species profiles, ignition delay times in shock tubes, etc. Surface reactions. Surface adsorption processes: relation to catalysis, improvement of the miners' safety lamp due to Henry in 1824 by the addition of platinum powder to the reacting surface, Faraday's view on the role of adsorption to the surface in catalysis, physisorption, van der Waals adsorption, chemisorption, Langmuir's concept of the unimolecular layer, Langmuir's adsorption isotherm, monolayer adsorption, multi-layer adsorption, adsorption with dissociation, competitive adsorption. Surface reaction processes: reaction mechanism, the Langmuir-Hinshelwood mechanism, the Langmuir-Rideal-Eley mechanism, the precursor mechanism, Unimolecular surface reactions. Bimolecular surface reactions. Desorption. Kinetic model of hydrogen-oxygen reaction on the platinum surface. Kinetic rates of hydrogen-oxygen reaction on the platinum surface. Application in hydrogen safety: the three explosion limits in the flammability diagram, dependence explosion limits of hydrogen-oxygen systems on containment shape, nature of surface, added inert gases (inertisation by steam), spontaneous ignition of hydrogen leaks. ignition by hot surfaces, catalytic recombiners, initial conditions for self-sustained detonation, boundary conditions for self-sustained detonation, prediction of detonation limits of hydrogen-air and hydrogen-oxygen mixtures, prevention of hydrogen ignition (electrical circuits, static electricity, hot surface, open fire, shock waves, (hot) gas jet, explosives, exothermic reaction, pyrophoric substances, lightning). Overview of hydrogen ignition mechanisms and relevant prevention techniques: electrical circuits, static electricity, hot surface, open fire, shock waves, (hot) gas jet, explosives, exothermic reaction, pyrophoric substances, lightning, etc. Autoignition and safety in hydrogen powered vehicles. Standard IEC 60079-10 'Electrical apparatus for explosive gas atmospheres - Part 10: Classification of hazardous areas'. **References:** Atkins & de Paula (2006) [20], Benson (1982) [137], Dainton (1956) [138], Frank-Kamenetzky (1967) [139], Moore (1983) [140], Shepherd (1986) [39], Westbrook (1982) [141] and Williams (2006) [142].

3.2.3.4 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.

3.2.3.5 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) [121], Buckmaster & Ludford (1982) [143], Clavin (1985) [144], Drysdale (1999) [122], Glassman (1996) [123], Griffiths & Barnard (1995) [124], Kanury (1977) [125], Karlovitz, Denniston & Wells (1951) [145], Kuo (2005) [29], Lewis & von Elbe (1987) [126], Poinsoot & Veynante (2001) [127], and Williams (1985) [129].

3.2.3.6 Diffusion flames (G: 6 hrs)

Contents Mixture fraction [29]. 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:** Hottel & Hawthorne (1949) [146], Kanury (1977) [125], Kuo (2005) [29], McCaffrey (1979) [147] and Williams (1982) [148].

3.2.3.7 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. **References:** Buckmaster, Clavin, Linan, Matalon, Peters, Sivashinsky & Williams (2005) [149].

3.2.3.8 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 hypothesis. Gradient transport. 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 Deringer model, Yakhot model). G-equation model. Relevance to confined, unconfined and vented deflagrations. Flame extinction by turbulence. Correlations for the turbulent burning velocity [145, 150–180]. **References:** Borghi (1988) [181], Clavin (1985) [144], Makarov & Molkov (2004) [182], Peters (1991 [183], 2000 [184]) and Yakhot (1988) [179].

3.2.3.9 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. PDF form of the beta-function [29]. **References:** Kuo (2005) [29], Peters (2000) [184] and Turns (2000) [3].

3.2.3.10 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 (2002) [185], Drysdale (1999) [122], Kanury (1977) [125], Spalding (1955) [186] and Tewarson (2002) [187].

3.2.3.11 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) [122].

3.3 MODULE RELEASES, MIXING AND DISPERSION

3.3.1 INTRODUCTORY STATEMENT

This is a postgraduate module on releases 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.

3.3.2 PREREQUISITE MATTER

Modules Thermodynamics, Fluid Dynamics, Heat and Mass Transfer, and, Solid Mechanics.

3.3.3 CONTENTS OF THE MODULE

3.3.3.1 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 GH₂ in open atmosphere, release of GH₂ in confined space [188,189], release of GH₂ in congested area, release of LH₂ in open atmosphere, release of LH₂ in confined space, release of LH₂ in congested area. Effect of air condensation. **References:** Chen & Rodi (1980), Pope (2000) [67], Swain & Swain (1996) [188], Swain, Filoso, Grilliot & Swain (2003) [189], and Witcofski & Chirivella (1984) [190].

3.3.3.2 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.

3.4 MODULE HYDROGEN IGNITION

3.4.1 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.

3.4.2 PREREQUISITE MATTER

Modules Thermodynamics, Chemical Kinetics, Fluid Dynamics, Heat and Mass Transfer, and, Solid Mechanics.

3.4.3 CONTENTS OF THE MODULE

3.4.3.1 Hydrogen ignition properties and ignition sources (G: 3 hrs)

Contents Flammability diagram [191]. Theory of hydrogen flammability limits. Effect of temperature [191] and steam concentration [191] on hydrogen flammability limits. Minimum ignition energy: effect of mixture composition, pressure and temperature; minimum spark-ignition energy of hydrogen-air mixtures [126, 191, 192]. Comparison with flammability ranges of other fuels. Auto-ignition temperature of hydrogen-air mixtures [191, 193] and hydrogen-steam-air mixtures [194]. 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 times 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 hydrogen jet ignition [191, 195, 196], explosives, lightning, self-ignition, pyrophoric substances, open fire, external explosion, laser, etc. **References:** Bach, Knystautas & Lee (1969) [197], Bull, Elsworth & Hooper (1978) [198], Clarke, Kassoy & Riley (1986) [199], Clarke, Kassoy, Meharzi, Riley, & Vasantha (1990) [200], Del Alamo, Williams & Sanchez (2004) [201], Dold & Kapila (1991) [202], Drell & Belles (1958) [192], Eckett, Quirk & Shepherd (2000) [123], Glassman (1996) [123], Fickett & Davis (2001) [203], He & Clavin (1994) [204], He & Lee (1995) [205], He (1996) [206], Kaplila (1978) [207], Kuo (2005) [29], Lee (1977) [208], Lee & Moen (1980) [43], Lee & Berman [191], Lee & Higgins (1999) [209], Lewis & von Elbe (1987) [126], Nettleton (1987) [210], Nettleton (2002) [211], Stamps & Berman (1991) [193], Turns (2000) [3] and Williams (1985) [129].

3.4.3.2 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.

3.5 MODULE HYDROGEN FIRES

3.5.1 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.

3.5.2 PREREQUISITE MATTER

Modules Thermodynamics, Chemical Kinetics, Fluid Dynamics, Heat and Mass Transfer, and, Solid Mechanics.

3.5.3 CONTENTS OF THE MODULE

3.5.3.1 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.

3.6 MODULE EXPLOSIONS: DEFLAGRATIONS AND DETONATIONS

3.6.1 INTRODUCTORY STATEMENT

This is a postgraduate module on explosion with an emphasis on hydrogen safety. Its purpose is to provide a basis for the applied modules Accident Prevention and Mitigation, Fire and Explosion Effects on People, Structures and the Environment, Computational Hydrogen Safety Engineering, and, Risk Assessment. Appropriate references are cited along with the topics.

3.6.2 PREREQUISITE MATTER

Modules Thermodynamics, Chemical Kinetics, Fluid Dynamics, Heat and Mass Transfer, and, Solid Mechanics.

3.6.3 CONTENTS OF THE MODULE

3.6.3.1 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-Braun 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) [212], Bartknecht (1981) [213], Bradley & Mitcheson (1976) [214], Dahoe & de Goey (2003) [215], Dorofeev, Kuznetsov, Alekseev, Efimenko & Breitung (2001) [216], Dorofeev (2002) [217], Eckhoff (2003) [218], Eckhoff (2005) [219], Kuznetsov, Matsukov & Dorofeev (2002) [220], Kuznetsov, Alekseev, Yankin & Dorofeev (2002) [221], Molkov & Nekrasov (1982) [222], Makarov & Molkov (2002) [221], and Tamanini (1993) [223].

3.6.3.2 Detonations (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 [39, 191, 224]. Unconfined and confined detonations. **References:** Buckmaster & Ludford (1982) [143], Chapman (1899) [225], Denisov & Troshin (1959) [226], Doering (1943) [227], Dorofeev, Efimenko, Kochurko & Chaivanov (1995) [228], Dorofeev, Bezmelnitsin & Sidorov (1995) [229], Fickett & Davis (2001) [203], Fujiwara & Reddy (1989) [230], Jouget (1906) [231], Gavrikov (2000) [232], Kailasanath, Oran, Boris & Young (1985) [233], Kassoy & Clarke (1985) [234], Kuo (2005) [29], Lee (1977) [208], Lee (1984) [224], Nettleton (1987) [210], Nettleton (2002) [211], Pintgen, Eckert, Austin & Shepherd (2003) [235], Soloukin (1965) [236], Strehlow (1967) [237], 1968 [238], 1969 [239], 1970 [240], 1984 [241]), von Neumann (1942) [242], Williams, Bauwens & Oran (1996) [243, 244], White (1961) [245], Williams (1985) [129], Yao & Scott-Stewart (1996) [246] and Zeldovich (1960) [247].

3.6.3.3 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) [248], Dorofeev, Bezmelnitsin & Sidorov (1995) [229], Dorofeev, Sidorov, Kuznetsov, Matsukov & Alekseev (2000) [249], Dorofeev, Kuznetsov, Alekseev, Efimenko & Breitung (2001) [216], Dorofeev (2002) [217], Kuznetsov, Matsukov & Dorofeev (2002) [222], Kuznetsov, Alekseev & Yankin (2002) [220], Molkov, Makarov & Puttock (2004) [182], Urtiew & Oppenheim, Whitehouse [250], Greig & Koroll (1996) [251] and Zeldovich (1940) [252].

4 APPLIED MODULES

4.1 MODULE FIRE AND EXPLOSION EFFECTS ON PEOPLE, STRUCTURES AND THE ENVIRONMENT

4.1.1 INTRODUCTORY STATEMENT

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

4.1.2 PREREQUISITE MATTER

The basic modules (Thermodynamics, Chemical Kinetics, Fluid dynamics, Heat and Mass Transfer, Solid Mechanics) and the fundamental modules (Hydrogen as an Energy Carrier, Fundamentals of Hydrogen Safety, Hydrogen Releases, Mixing and Distribution, Hydrogen Ignition, Hydrogen Fires, Explosions: Deflagrations and Detonations).

4.1.3 CONTENTS OF THE MODULE

4.1.3.1 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) [220].

4.1.3.2 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) [212], Dorofeev (1996) [253], Dorofeev & Sidorov (1996) [254], Tang & Baker (1999) [255], and the Yellow Book (1997) [256].

4.1.3.3 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) [212], Dorofeev (1996) [253], Dorofeev & Sidorov (1996) [254] and Groethe, Colton, Chiba & Sato (2004) [257].

4.1.3.4 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) [212], Tang & Baker (1999) [255], and Molkov, Eber, Grigorash, Tamanini & Dobashi (2003) [258].

4.1.3.5 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.

4.2 MODULE ACCIDENT PREVENTION AND MITIGATION

4.2.1 INTRODUCTORY STATEMENT

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

4.2.2 PREREQUISITE MATTER

The basic modules (Thermodynamics, Chemical Kinetics, Fluid Dynamics, Heat and Mass Transfer, Solid Mechanics), the fundamental modules (Hydrogen as an Energy carrier; Fundamentals of Hydrogen Safety; Releases, Mixing and Distribution; Hydrogen Ignition; Hydrogen Fires; Explosions: Deflagrations and Detonations). This module may be taught simultaneously with the fundamental modules and the applied module on Fire and Explosion Effects on People, Structures and the Environment.

4.2.3 CONTENTS OF THE MODULE

4.2.3.1 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 safer design [259], 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. **References:** Khan & Amyotte (2003) [259].

4.2.3.2 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.

4.2.3.3 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. **References:** AIAA Standard G-095-2004 (2004) [260] and Kayalam & Hay (1987) [261].

4.2.3.4 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.

4.2.3.5 Containment (G: 4 hrs)

Contents Compartmentalisation, regulations, codes and standards.

4.2.3.6 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) [213], Molkov, Dobashi, Suzuki & Hirano (1999) [262], NFPA 68 (2002) [263], Molkov (2001) [264], Molkov (2002) [265], Grigorash, Eber & Molkov (2004) [266].

4.2.3.7 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) [267].

4.3 MODULE COMPUTATIONAL HYDROGEN SAFETY ENGINEERING

4.3.1 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) [268], Cox & Kumar (2002) [269], Ferziger & Peric (2002) [270], Patankar (1980) [271], Poinsot & Veynante (2001) [127], Pope (2000) [67], Roy, Frolov & Givi (1997) [272] and Warsi (1999) [273]. Specific references are given along with the topics.

4.3.2 PREREQUISITE MATTER

Calculus, the basic modules (Thermodynamics, Chemical Kinetics, Fluid Dynamics, Heat and Mass Transfer, Solid Mechanics), vector analysis, tensor analysis, and partial differential equations.

4.3.3 CONTENTS OF THE MODULE

4.3.3.1 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.

4.3.3.2 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 (ILDM, 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).

4.3.3.3 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.

4.3.3.4 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, tri-diagonal matrix algorithm (TDMA)). Numerical diffusion. Finite volume based finite difference method. Interpolation of surface and volume integrals. Finite volume method.

4.3.3.5 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) [274] and Cox & Kumar (2002) [269].

4.3.3.6 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.

4.3.3.7 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.

4.3.3.8 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: Smagorinskiy 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).

4.3.3.9 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) [275].

4.3.3.10 High speed reactive flows

Contents Methods for solving reactive Euler equations for arbitrary Mach numbers. Conservative schemes. The Godunov theorem. Flux limiting and entropy condition. TVD, FCT, ENO and Godunov schemes. Stiff problems and stiff solvers. Numerical simulation of detonation waves. **References:** Bourlioux & Majda (1992) [276], Oran, Boris, Young, Flanigan, Burks & Picone (1981) [277], Quirek (1994) [278], and Taki & Fujiwara (1978) [279].

4.3.3.11 Modeling of hydrogen-air diffusion flames and turbulence-radiation interactions

Contents Modeling radiation emissions from intermediate radicals and atoms in hydrogen flames and comparison with laser-induced fluorescence (LIF) measurements [280,281]. Turbulent radiation interactions [282]. Modeling of NO formation [283,284]. Radiation emissions from water vapour bands [285–288]. Grey-gas versus narrow-band models for turbulent hydrogen-air turbulent diffusion flames [287]. Effect of additions of solid particles on radiation in hydrogen-air flames [289]. **References:** Choudhuri & Gollahalli (2004) [280], Barlow, Dibble, Chen & Lucht (1990) [281], Cox (1977) [282], Barlow, Smith, Chen & Bilger (1999) [283], Kim, Kim, Yoon & Jung (2002) [284], Chelin & Pina (2002) [285], Iibas (2005) [286], Faeth, Jeng & Gore (1985) [287], Liu, Xu, Chen & Wang (2004) [288], Baek, Kim, Kim & Kang (2002) [289].

4.3.3.12 Modeling of liquid hydrogen pool fires

Contents Structure of pool fires [290] [Hottel (1958)]. Pool fire dynamics [Joulain (1998)]. Data correlations for hydrocarbon and cryogenic pool fires [132]. Thermal radiation from pool fires [291–293]. LES simulation of large pool fires [294]. **References:** Blinov & Khudiakov (1957) [290], Hottel (1958) [missing], Joulain (1998) [missing], Zabetakis & Burgess (1961) [132], Burgess, Strasser & Grumer (1961) [291], Burgess & Hertzberg (1974) [292], McGratten, Baum & Hamins (2000) [293], and Greiner, M. & Suo-Anttila (2004) [294].

4.3.3.13 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.

4.3.3.14 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 hydrogen release and dispersion modeling [295]. CFD for deflagration modeling [182, 221, 295–297]. 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 & Bachellerie (2003) [298], Beccantini & Pailhories (2002) [299], Bielert et al (2001) [300], Makarov & Molkov (2002) [221], 2004 [182]) and Venetsanos, Huld, Adams & Bartzis (2003) [295].

4.4 MODULE RISK ASSESSMENT

4.4.1 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) [301].

4.4.2 PREREQUISITE MATTER

The basic modules (Thermodynamics, Chemical Kinetics, Fluid Dynamics, Heat and Mass Transfer, Solid Mechanics), the fundamental modules (Hydrogen as an Energy Carrier; Fundamentals of Hydrogen Safety; Releases, Mixing and Distribution; Hydrogen Ignition; Hydrogen Fires; Explosions: 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) [302–304].

4.4.3 CONTENTS OF THE MODULE

4.4.3.1 General risk assessment and protective measures for hazardous materials processing and handling (G: 6 hrs)

Contents The Management of risk [305,306]: (Some basic terms and definitions: hazard, danger, accident, consequence, likelihood, risk (How an understanding of these provides a basis for reducing risk and increasing safety; What risk are we considering?, The likelihood of what we are considering?; What consequence are we considering?), risk analysis, process safety, risk assessment). A systemic approach to risk management [305] (the root causes of risk; the hazardous system; a brief overview of a modern structured approach to managing the risk from hydrogen). Risk management and the law [305] (an introduction to risk assessment and the goal-setting basis of modern legislation). Structured risk management for hydrogen projects [305] (avoid the risk; control the risk; mitigate the residual risk). Origins and a brief history of risk analysis and loss prevention [306]: Seveso II and IPPC. Basic factors determining hazard and risk of substances [306]. Steps/stages in a risk assessment [306]. The costs of accidents. The costs of safety: investment and profitability, cost optimisation, loss of life, the law of large numbers, limited scope: selection of alternatives). Human factors. Inherent safer design. ATEX directives [307–311]. **References:** van den Braken (2005) [312], European Commission Directive 94/9/EC (1994 [307], 2000 [308,309]), European Commission Directive 1999/92/EC (2000 [310,311]), Newsholme (2007) [305], and, Pasman (2006) [306].

4.4.3.2 Regulations, codes and standards (G: 4 hrs)

Contents Hydrogen safety and regulatory issues [305]. Public acceptance and safety [305]. Trans-national nature of safety regulations, codes and standards (RCS) [305]. Safety legislation: hierarchy in safety legislation; purpose of safety legislation (imposing

duties, responsibilities and accountabilities on people and organisations); the meaning of codes, standards, guidance and regulations; the origin of codes (developed by industry or trade bodies), standards (developed by engineering or standard bodies), and regulations (issued by the State); the Approved Code of Practice. An overview of the key European safety legislation that applies to hydrogen [313]: EU ATEX Directives (ATEX 100 [307–309, 314] (Product Directive) and ATEX 137 [310, 311] (User Directive)). A detailed examination of the structured approach to safety demanded by the ATEX Directives [313](substitution, preventing the formation of explosive atmospheres, containment, dilution through effective ventilation, preventing the ignition of explosive atmospheres, zone classification, mitigating the effects of an explosion, use of explosion resistant equipment, explosion relief, explosion suppression, prevention of explosion propagation, organisational measures to ensure explosion protection). Compliance of the EU ATEX Directives with the EMC Directive 89/336/EEC [315] (modified by 92/31/EEC [316] and 93/68/EEC [317,318](the CE Marking Directive)), the Machine Directive 98/37/EC [319], and, the Low Voltage Directive 73/23/EEC (modified by 93/68/EEC). IEC Standard 61511 [320–322]: structure (Part 1: Framework, definitions, system, hardware and software requirements [320]; Part 2: Guidelines in the application of IEC 61511-1 [321]; Part 3: Guidance for the determination of the required safety integrity levels [322]), and, harmonisation (adoption of IEC 61511 as EN 61511 [320–322] by the European standards body CENELEC; implication: in each of the member states of the European Union the standard is published as a national standard; IEC 61511 [320–322] is not harmonised under any Directive of the European Commission), purpose (sets out what is good practice in the engineering of systems that ensure the safety of an industrial process through the use of instrumentation), and, scope (defines the functional safety requirements established by IEC 61508 [323–330] using process industry sector terminology; applicable to refineries, petrochemical, chemical, pharmaceutical, pulp and paper, and power plants; covers application of electrical, electronic and programmable electronic equipment; focuses attention on one type of instrumented safety system used within the process sector: the Safety Instrumented System (SIS); covers the design and management requirements for SIS’s from cradle to grave: initial concept, design, implementation, operation, and maintenance through to decommissioning). IEC Standard 61508 [323–330]: structure (the standard has seven parts: parts 1–3 contain the requirements of the standard (normative), while 4–7 are guidelines and examples for development), scope (basic functional safety standard applicable to all kinds of industry), and, paradigm (risk is defined as function of frequency (or likelihood) of the hazardous event and the event consequence severity; zero risk can never be reached, safety must be considered from the beginning, and, non-tolerable risks must be reduced (ALARP)). Examples of how codes, standards and guidance may be used to manage risk and comply with the law. Approval of new hydrogen technologies by RCS (example of hydrogen road vehicles [105], the case of hydrogen refuelling stations [105]). **References:** European Commission Directive 94/9/EC (1994 [307], 2000 [308,309]), European Commission Directive 1999/92/EC (2000 [310,311]), Newsholme (2007) [305,313], and, Wurster (2006) [105].

4.4.3.3 Risk assessment methodologies (G: 4 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 [331,332]: 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, sub-system/installation, overall system level. Relation with workers' safety, public safety and spatial planning. Effectiveness of different mitigation techniques and procedures. Safety Management System [333]. Precursor analysis [334]. Risk perception and acceptance [335]. Examples of risk assessment of hydrogen applications. **References:** AIChE (1989) [331,333], Bedford & Cooke (2001) [332], Pasman & Vrijling (2003) [336], and Pasman, Körvers & Sonnemans (2004) [334].

4.4.3.4 Hazard identification and scenario development (G: 6 hrs)

Contents Hazard identification and analysis methods [306]. Checklist analysis: methods based on lists of questions and points related to safety and environment. Hazard ranking methods (Class 1 methods: Hazard Index Methods that rank solely on the basis of substance properties, the NFPA Material Factor. Class 2 methods: Hazard Ranking Systems that rank on basis of properties of materials and quantities, threshold quantities for licensing. Class 3-4 methods: hazard ranking systems that rank on basis of properties of materials, quantities, process conditions, and (certain) preventive and protective measures, the Dow Fire & Explosion Index). FMEA. Hazard and operability studies (HAZOP) [335]. Incident data banks and other means of identification. What-if analysis (threats to or impact on: personnel, equipment, business interruption, environment) [302–304]. Event tree analysis (and its role as the central part of quantitative risk analysis). Layers of protection analysis [337,338]. **References:** AIChE (2001) [337], Crawley & Preston (2000) [335], EU ATEX 100 (1994) [307–309], EU ATEX 137 (1999) [310,311], Lees (1996) [302–304], Pasman, Schupp & Lemkowitz (2003) [338], and, Pasman (2006) [306].

4.4.3.5 Effect analysis of hydrogen accidents (G: 6 hrs)

Contents Consequence analysis [306]. Source terms/emissions: outflow, release modes, selection of release models, outflow of compressed gases, vapour outflow. Outflow of pressurised liquefied gases: two phase flow, outflow of pressurised liquefied gas through holes, two-phase flow in piping. Outflow of liquids: outflow of liquid through a hole, liquid outflow through a pipe. Evaporation of liquids: phenomenon of pool evaporation, heat balance at evaporation, heat flux to boiling liquids from subsoil, heat flux to boiling liquids from a water surface, evaporation of non-boiling liquids (mass transfer of vapour in the air, pool spreading. Dispersion and transmission models [306]: the structure of the atmosphere and its relation to transmission of pollutants, behaviour of plumes. Dispersion models: critical Richardson number criterion, the Gaussian plume model, dense gas dispersion, the Ooms integral plume model [339–344], dispersion from a free turbulent gas jet, effect intensity calculations as inputs for determination of damage. Effect on people and structures: jet impact from high-momentum releases, damage by low temperature releases, asphyxiation by hydrogen, thermal effects from fires, pressure effects from explosions, blast wave strength from vapour cloud explosion, blast interaction with objects, [302–304], materials for hydrogen services [345]. Environmental effects of hydrogen accidents. **References:** Lees (1996) [302–304], Pasman (2006) [306], and Perry & Green (1997) [345].

4.4.3.6 Vulnerability analysis (G: 4 hrs)

Contents Vulnerability and damage [306]: general response function given intensity of effect and time of exposure; fires and dose-response of heat radiation exposure; damage caused by blast waves, blast effects on people; toxic effects; domino effects. Failure frequency estimation: reliability engineering; reliability function; multiple failure modes/Markov model; mean life; repairs and availability; failure rate data: empirical (from experience), reliability data banks/literature, accelerated ageing tests; Fault Tree Analysis (FTA) [306, 346, 347]: minimum cut sets. Risk presentation, acceptance criteria and perception [306]: individual and group risk, and their application to *external or public safety*; perception of risk: rational or irrational?; a note on legal tolerability criteria for human risk elsewhere; uncertainty in risk assessment; future developments. Preliminary failure mode analysis. What-if analysis. Comprehensive identification and classification hazard analysis. Damage models. Probits for various types of damage [348]. Data bases. Probabilistic assessment [332]. Appropriate equivalent methodology. **References:** Bedford & Cooke (2001) [332], van den Braken (2005) [312], Green Book (1989) [348], Hauptmanns (2004) [346], Khan & Abbasi (2000) [347], and, Pasma (2006) [306].

4.4.3.7 Risk reduction and control in the hydrogen economy (G: 6 hrs)

Contents Risk reduction and control [306]: management systems; history of accident frequency; the crucial role of management and human factor: Safety Management System (SMS); accident investigation. Risk reducing measures [306]: rapid ranking and the risk matrix; Layer of Protection Analysis (LOPA); Safety Instrumented Systems (SIS); other protective measures; maintenance; design methods and design safety reviews. 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* (3.1.3.2) of *Module hydrogen as an Energy carrier* (3.1 Application of vulnerability analysis to the potential of an initial incident to inhibit or destroy mitigation technologies. Case studies and European Hydrogen Incident/Accident Database. **References:** Pasma (2006) [306].

5 CONCLUDING REMARKS

The development of an International Curriculum on hydrogen safety Engineering as the backbone of the e-Academy of Hydrogen Safety is described. To cope with 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 for the development of new teaching programmes. To avoid duplication of educational efforts, this knowledge also needs to be coupled into existing engineering curricula. A modular structure, consisting of basic modules, fundamental modules, and applied modules appears to be the most appropriate for achieving this goal.

Because the development of the International Curriculum on Hydrogen Safety Engineering would make no sense without a market of trainees, it was attempted to probe and quantify its existence by means of a questionnaire. 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 establish educational and training programmes at a number of universities throughout Europe. It was also attempted to resolve the employment pattern to address specific educational and training needs. Further research in this direction will concentrate on determining the distribution of the employment pattern (consulting, manufacture, design, teaching, research, operation, construction, legislation, etc.) and the employer pattern (process industry, energy industry, civil works, aerospace industry, automotive industry, transport and distribution, fire and rescue brigades, insurance, teaching institutions, research institutions, legislative bodies, etc.).

Despite the demand for knowledge in the field of hydrogen safety, there are practically no hydrogen safety training and educational programmes in Europe to address this need. The development of the e-Academy of Hydrogen Safety by the NoE HySafe is a first step in overcoming this deficiency. Moreover, the onset and further development of the hydrogen economy in Europe is being hampered by (i) a shortage of experts in the key disciplines relevant to hydrogen safety; (ii) a decrease in the number of young people attracted to careers in science and research; (iii) a deterioration of Europe's attractiveness for R&D investments; (iv) changes in the skill-set sought by employers; (v) the absence of a skilled-workforce to succeed the retiring S&T workforce; and (vi) the lack of educational resources to prepare tomorrow's researchers and educators for the technological challenges posed by the hydrogen economy. The International Curriculum on Hydrogen Safety Engineering, the development of which is aided by experts working at the forefront of hydrogen safety and related key areas will help to improve this situation and increase Europe's innovative and competitive strength at the onset of the hydrogen economy.

To address the needs of employers (i.e. greater emphasis on cost savings and on flexi-

ble, just-in-time education and training, providing employees with the necessary skills and competence to match changing business needs) and needs of professionals working in hydrogen related areas (i.e. providing the latest knowledge on hydrogen safety, removal of restrictions imposed by confinement to a specific campus location) the delivery of teaching in the e-learning mode appears to be the way forward. To meet specific educational needs on hydrogen safety in terms of relevance and timeliness, the lecture notes and presentations of the keynote lectures at the European Summer School on Hydrogen Safety (HyCourse, contract MSCF-CT- 2005-029822, 2006-2010, see: www.hysafe.org/SummerSchool) and the Joint European Summer School on Fuel Cell and Hydrogen Technology (TrainHy, Call FCH-JU-2009-1, Project ID 256703, 2011-2013, see: www.hysafe.org/TrainHyProf) are implemented into the distance learning modules of the Master of Science in Hydrogen Safety Engineering offered by the University of Ulster (see: www.hysafe.org/MSchSE).

It is important to be aware of the fact that Europe is world's 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 are (i) fragmentation caused by language barriers; (ii) the enclosure of the educational systems within national borders; and (iii) the lack of harmonisation between educational programmes. The International Curriculum on Hydrogen Safety Engineering, one that will be used as a blueprint for the development of educational and training programmes at universities throughout Europe, will assist the harmonisation of educational programmes, stimulate the mobility of students and faculty, promote international collaboration at all levels, and support 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 fulfill a leading role in achieving global understanding of, and agreement on dealing with hydrogen safety matters. 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 fulfill a leading role in exporting knowledge on hydrogen safety to the world.

BIBLIOGRAPHY

- [1] Tse S.D., Zhu D.L., and Law C.K. Morphology and burning rates of expanding spherical flames in H₂/O₂/inert mixtures up to 60 atmospheres. In *Proceedings of the Twenty-Eighth Symposium (International) on Combustion*, pages 1793–1800, Pittsburgh, 2000. The Combustion Institute.
- [2] International Standardization Organization (ISO), ISO TR 15916(E). Basic considerations for the safety of hydrogen systems. First Edition. Reference number ISO TR 15916:2004(E). The International Organization for Standardization, 2004. International Standard, Prepared by Technical Committee ISO/TC 197 *Hydrogen Technologies*.
- [3] Turns S.R. *An introduction to combustion: concepts and applications*. McGraw-Hill, New York, second edition, 2000.
- [4] IAEA-TECDOC-1196. Mitigation of hydrogen hazards in water cooled power reactors. International Atomic Energy Agency, February 1998.
- [5] Dunn S. Hydrogen futures: toward a sustainable energy system. *International Journal of Hydrogen Energy*, 27:235–264, 2002.
- [6] Jordan T. Hysafe – The Network of Excellence for Hydrogen Safety. Paper presented at the Sixteenth World Hydrogen Energy Conference, Lyon, France, 13–16 June 2006. International Association for Hydrogen Energy.
- [7] HySafe – Annex I – Description of Work. Safety of hydrogen as an energy carrier, Proposal 502630 (HySafe), December 2004. A Proposal for a Sixth framework Network of Excellence.
- [8] COM (2003) 226 final 2. Communication from the Commission, investing in research: an action plan for Europe. Commission of the European Communities, Brussels, 2003.
- [9] SEC (2003) 489 of 30.4.2003. Investing in research: an action plan for Europe. Commission of the European Communities, Brussels, 2003. Commission Staff Working Paper.
- [10] COM C(2005) 576 final. Commission Recommendation on the European Charter for Researchers and on a Code of Conduct for the Recruitment of Researchers. Commission of the European Communities, Brussels, 2005.
- [11] COM (2001) 331 final. Communication from the Commission to the Council and the European parliament, A mobility strategy for the European research area. Commission of the European Communities, Brussels, 2001.

- [12] COM (2005) 576 final. Green paper on a european programme for critical infrastructure protection. Commission of the European Communities, Brussels, 2005.
- [13] COM (2003) 499 final. Communication from the Commission, More research for Europe, towards 3% of GDP. Commission of the European Communities, Brussels, 2002.
- [14] European Hydrogen and Fuel Cell Technology Platform. Implementation Panel. Strategic Research Agenda, July 2005.
- [15] Wancura H., Mayo B., Reijalt M., Mertens J.J., Maio P., and Claassen P. Draft implementation report WG5 Cross Cutting Issues (XCI). European Hydrogen and Fuel Cell Technology Platform. Implementation Panel, 2006.
- [16] Magnusson S. E., Drysdale D. D., Fitzgerald R. W., Motevalli V., Mowrer F., Quintiere J., Williamson R.B., and Zalosh R. G. A proposal for a model curriculum in fire safety engineering. *Fire Safety Journal*, 25:1,3–39,41–73,75–83,85,87–88, 1995.
- [17] SEC (2003) 905. e-Learning: Designing Tomorrows Education, A Mid-Term Report as requested by the Council Resolution of 13 July 2001. Commission of the European Communities, Brussels, 2003. Commission Staff Working Paper.
- [18] COM (2000) 318 final. Communication from the Commission, e-Learning – Designing tomorrow’s education. Commission of the European Communities, Brussels, 2000.
- [19] Abbott M.M. and Van Ness H.C. *Theory and problems of thermodynamics*. Schaum’s outline series. McGraw-Hill, New York, 1972.
- [20] Atkins P.W. and de Paula J. *Physical Chemistry*. Oxford University Press, Oxford, eighth edition, 2006.
- [21] Metz C.R. *Theory and problems of Physical Chemistry*. Schaum’s outline series. McGraw-Hill, New York, 1976.
- [22] Moran M.J. and Shapiro H.N. *Fundamentals of Engineering Thermodynamics*. John Wiley & Sons, New York, fourth edition, 2000.
- [23] Smith J.M., Van Ness H.C., and Abbott M.M. *Introduction to Chemical Engineering Thermodynamics*. McGraw-Hill, New York, seventh edition, 2007.
- [24] Sonntag R.E., Borgnakke C., and van Wylen G.J. *Fundamentals of Thermodynamics*. John Wiley & Sons, New York, sixth edition, 2003.
- [25] Feynman R.P., Leighton R.B., and Sands M.L. *The Feynman Lectures on Physics*. Addison-Wesley, Reading, Massachusetts, 1989.
- [26] Batchelor G.K. *An introduction to fluid dynamics*. Cambridge Mathematical Library. Cambridge University Press, Cambridge, 1994.
- [27] Milne-Thomson L.M. *Theoretical Hydrodynamics*. MacMillan Press, New York, fifth edition, 1968.

- [28] Hirschfelder J.O., Curtiss C.F., and Bird R.B. *The molecular theory of gases and liquids*. John Wiley & Sons, New York, fourth edition, 1967.
- [29] Kuo K.K. *Principles of Combustion*. John Wiley & Sons, New York, second edition, 2005.
- [30] O’Conaire M., Curran H.J., Simmie J.M., Pitz W.J., and Westbrook C.K. A comprehensive modeling study of hydrogen oxidation. *International Journal of Chemical Kinetics*, 36:603–622, 2005.
- [31] Saxena P. and Williams F.A. Testing a small detailed chemical-kinetic mechanism for the combustion of hydrogen and carbon monoxide. *Combustion and Flame*, 145:316–323, 2006.
- [32] Lee D and Hochgreb S. Hydrogen autoignition at pressures above the second explosion limit (0.6-4.0 MPa). *International Journal of Chemical Kinetics*, 30:385–406, 1998.
- [33] Rolland S. and Simmie J.M. The comparison of detailed chemical kinetic mechanisms; forward versus reverse rates with CHEMRev. *International Journal of Chemical Kinetics*, 37:119–125, 2005.
- [34] Simmie J.M., Rolland S., and Ryder E. Automatic comparison of thermodynamic data for species in detailed chemical kinetic modelling, (CHEMThermo and structure linking explained). *International Journal of Chemical Kinetics*, 37:341–345, 2005.
- [35] Maas U. and Pope S.B. Simplifying chemical kinetics: intrinsic low-dimensional manifolds in composition space. *Combustion and Flame*, 88:239–264, 1992.
- [36] Lam S.H. and Goussis D.A. The CSP method for simplifying kinetics. *International Journal of Chemical Kinetics*, 26:461–486, 1994.
- [37] Lu T., Ju Y., and Law C.K. Complex CSP for simplifying kinetics. *Combustion and Flame*, 126:445–455, 2001.
- [38] Belles F.E. Detonability and chemical kinetics: Prediction of limits of detonability of hydrogen. In *Proceedings of the Seventh Symposium (International) on Combustion*, pages 745–751, London, 1959. Butterworths.
- [39] Shepherd J. Chemical kinetics of hydrogen-air-diluent detonations. *Progress in Aeronautics and Astronautics*, 106:263–293, 1986.
- [40] Zel’dovich Ya.B. Classification of regimes of exothermic reaction in accordance with initial conditions. *Combustion and Flame*, 39:211–214, 1980.
- [41] Bartenev A.M. and Gelfand B.E. Spontaneous initiation of detonations. *Progress in Energy and Combustion Science*, 26:29–55, 2000.
- [42] Knystautas R., Lee J.H.S., Moen I.O., and Wagner H.Gh. Direct initiation of spherical detonation by a hot turbulent gas jet. In *Proceedings of the Seventeenth Symposium (International) on Combustion*, pages 1235–1245, Pittsburgh, 1979. The Combustion Institute.

- [43] Lee J.H.S. and Moen I. O. The mechanism of transition from deflagration to detonation in vapor cloud explosions. *Progress in Energy Combustion Science*, 6:359–389, 1980.
- [44] Lee J.H.S., Knystautas R., and Yoshikawa N. Photochemical initiation of gaseous detonations. *Acta Astronautica*, 5:971–982, 1978.
- [45] Bird R.B., Stewart W.E., and Lightfoot E.N. *Transport phenomena*. Wiley, New York, second edition, 2002.
- [46] Drazin P.G. and Reid W.H. *Hydrodynamic Stability*. Cambridge Monographs On Mechanics and Applied Mathematics. Cambridge University Press, Cambridge, 1981.
- [47] Hughes W.F. and Brighton J.A. *Theory and problems of Fluid Dynamics*. Schaum’s outline series. McGraw-Hill, New York, 1999.
- [48] Kundu K.P. and Cohen I.M. *Fluid Mechanics*. Elsevier Academic Press, Amsterdam, third edition, 2004.
- [49] Lighthill M.J. *Waves in fluids*. Cambridge University Press, Cambridge, 1978.
- [50] Massey B. and Ward-Smith J. *Mechanics of Fluids*. Stanley Thornes Publishers, Cheltenham, United Kingdom, seventh edition, 1998.
- [51] Prasuhn A.L. *Fundamentals of fluid mechanics*. Prentice-Hall, New Jersey, 1980.
- [52] Schlichting H. *Boundary-layer theory*. McGraw-Hill Series in Mechanical Engineering. McGraw-Hill, New York, sixth edition, 1968. Translated by J. Kestin.
- [53] White F.M. *Fluid mechanics*. McGraw-Hill, New York, fifth edition, 2003.
- [54] Darwin C. Note on hydrodynamics. *Proceedings of the Cambridge Philosophical Society*, 49:342–354, 1953.
- [55] Lighthill M.J. Drift. *Journal of Fluid Mechanics*, 1:31–53, 1956.
- [56] Rankine W.J.M. On plane water lines in two-dimensions. *Philosophical Transactions of the Royal Society of London, Series A: Mathematical and Physical Sciences*, 154:369–391, 1864.
- [57] White F.M. *Viscous fluid flow*. McGraw-Hill, New York, 1974.
- [58] Laney C.B. *Computational Gasdynamics*. Cambridge University Press, Cambridge, 1998.
- [59] Ewan B.C.R. and Moodie K. Structure and velocity measurements in underexpanded jets. *Combustion Science and Technology*, 45:275–288, 1986.
- [60] Thompson K.W. Time-dependent boundary conditions for hyperbolic systems. *Journal of Computational Physics*, 68:1–24, 1987.
- [61] Thompson K.W. Time-dependent boundary conditions for hyperbolic systems II. *Journal of Computational Physics*, 89:439–461, 1990.

- [62] Poinso T.J. and Lele S.K. Boundary conditions for direct simulations of compressible viscous flows. *Journal of Computational Physics*, 101:104–129, 1992.
- [63] Lumley J.L. Some comments on turbulence. *Physics of Fluids A*, 4:203–211, 1992.
- [64] Richter J.P. *The notebooks of Leonardo da Vinci*. Dover, New York, 1970. Two Volumes.
- [65] Barenblatt G.I. *Scaling*. Cambridge texts in applied mathematics. Cambridge University Press, Cambridge, 2003.
- [66] Kreith F. and Bohn M.S. *Principles of heat transfer*. Brooks/Cole Publishers, Pacific Grove, CA, sixth edition, 2001.
- [67] Pope S.B. *Turbulent flows*. Cambridge University Press, Cambridge, United Kingdom, 2000.
- [68] Lesieur M. *Turbulence in fluids: stochastic and numerical modelling*. Mechanics of Fluids and Transport Processes. Kluwer Academic Publishers, Dordrecht, The Netherlands, 1987.
- [69] Batchelor G.K. *The theory of homogeneous turbulence*. Cambridge Science Classics. Cambridge University Press, Cambridge, 1993.
- [70] Sagaut P. and Germano M. *Large Eddy Simulation for Incompressible Flows: An Introduction*. Springer, Berlin, second edition, 2002.
- [71] Van Driest E.R. Turbulent boundary layer in compressible fluids. *Journal of the Aeronautical Sciences*, 18:145–160, 1951.
- [72] Favre A. Equations des gaz turbulents compressibles. *Journal de Mecanique*, 4:361–421, 1965.
- [73] Gatski T.B., Hussaini M.Y., and Lumley J.L. (editors). *Simulation and Modeling of Turbulent Flows*. Oxford University Press, Oxford, 1996.
- [74] Lele S.K. Compressibility effects on turbulence. *Annual Reviews of Fluid Mechanics*, 26:211–254, 1994.
- [75] Holman J.P. *Heat transfer*. McGraw-Hill, New York, eighth edition, 1997.
- [76] Hottel H.C. and Sarofim A.F. *Radiative Transfer*. McGraw-Hill, New York, 1967.
- [77] Incropera F.P., De Witt D.P., Bergman T.L., and Lavine A.S. *Fundamentals of Heat and Mass Transfer*. John Wiley & Sons, New York, sixth edition, 2006.
- [78] Kaviany M. *Principles of Heat Transfer*. John Wiley & Sons, New York, 2002.
- [79] Pitts D.R. and Sissom L.E. *Theory and problems of Heat Transfer*. Schaum's outline series. McGraw-Hill, New York, 1977.
- [80] Welty J. R., Wicks C. E., Wilson R. E., and Rorrer G.L. *Fluid mechanics*. John Wiley & Sons, New York, fourth edition, 2001.

- [81] Warnatz J., Maas U., and Dibble R.W. *Combustion: Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation*. Springer, New York, third edition, 2005.
- [82] Fried E. Thermal conduction contribution to heat transfer at contacts. In R.P. Tye, editor, *Thermal Conductivity*, volume 2 of *Thermal Conductivity*, pages 1–64. Academic Press, London, 1969.
- [83] McLaughlin E. Theory of the thermal conductivity of fluids. In R.P. Tye, editor, *Thermal Conductivity*, volume 2, pages 253–257. Academic Press, London, 1969.
- [84] Agrawal D.C. and Menon V.J. Boiling and the Leidenfrost effect in a gravity-free zone: a speculation. *Physics Education*, 29:39–42, 1994.
- [85] Bent H.A. Droplet on a hot metal spoon. *American Journal of Physics*, 54:967, 1986.
- [86] Curzon F.L. The Leidenfrost phenomenon. *American Journal of Physics*, 46:825–828, 1978.
- [87] Gottfried B.S., Lee C.J., and Bell K.J. The Leidenfrost phenomenon: film boiling of liquid droplets on a flat plate. *International Journal of Heat and Mass Transfer*, 9:1167–1187, 1966. De aquae communis nonullis qualitatibus tractatus-On the fixation of water in diverse fire. A tract about some qualities of common water (translated from Latin into English by C. Wares).
- [88] Hall R.S., Board S.J., Clare A.J., Duffey R.B., Playle T.S., and Poole D.H. Inverse Leidenfrost phenomenon. *Nature*, 224:266–267, 1969.
- [89] Leidenfrost J.G. On the fixation of water in diverse fire. *International Journal of Heat and Mass Transfer*, 9:1153–1166, 1966. De aquae communis nonullis qualitatibus tractatus-On the fixation of water in divers fire. A tract about some qualities of common water (translated from Latin into English by C. Wares).
- [90] Leikind B.J. and McCarthy W.J. An investigation of firewalking. *Skeptical Inquirer*, 10:23–34, 1985.
- [91] Leikind B.J. and McCarthy W.J. Firewalking. *Experientia*, 44:310–315, 1988.
- [92] Taylor J.R. Firewalking: a lesson in physics. *The Physics Teacher*, 27:166–168, 1989.
- [93] Thimbleby H. The Leidenfrost phenomenon. *Physics Education*, 24:300–303, 1989.
- [94] Walker J. The amateur scientist. *Scientific American*, 140:126–131, 1977.
- [95] Zhang S. and Gogos G. Film evaporation of a spherical droplet over a hot surface: fluid mechanics and heat/mass transfer analysis. *Journal of Fluid Mechanics*, 222:543–563, 1991.
- [96] Collier J. G. and Thome J. R. *Convective Boiling and Condensation*. Clarendon Press, Oxford, third edition, 1996.

- [97] Modest M.M. *Radiative Heat Transfer*. Academic Press, London, second edition, 2003.
- [98] Siegel R. and Howell J.R. *Thermal radiation heat transfer*. Hemisphere, New York, third edition, 1993.
- [99] Beer F.P. and Johnston E.R. *Mechanics of Materials*. McGraw-Hill, New York, 1981.
- [100] Beer F.P. and Johnston E.R. *Engineering Mechanics: Statics*. McGraw-Hill, New York, fifth edition, 1992.
- [101] Fitzgerald R.W. *Mechanics of Materials*. Addison-Wesley, Boston, second edition, 1982.
- [102] Higdon A., Ohlsen E.H., Stiles W.B., Weese J.A., and Riley W.F. *Mechanics of materials*. John Wiley & Sons, New York, fourth edition, 1985.
- [103] Mase G.E. *Theory and problems of Continuum Mechanics*. Schaum's outline series. McGraw-Hill, New York, 1970.
- [104] Nash W. *Theory and problems of Strength of Materials*. Schaum's outline series. McGraw-Hill, New York, fourth edition, 1998.
- [105] Wurster R. HyApproval - Handbook for approval of hydrogen refuelling stations - Safe and harmonised implementation of hydrogen refuelling stations on a global scale. A lecture presented at the First European Summer School on Hydrogen Safety, 15–24 August 2006.
- [106] Cadwallader L.C. and Herring J.S. Safety issues with hydrogen as a vehicle fuel. Report prepared for the U.S. Department of Energy Office of Energy Research under DOE Idaho Operations Office Contract DE-AC07-94ID13223 INEEL/EXT-99-00522, Idaho National Engineering and Environmental Laboratory, Lockheed Martin Idaho Technologies Company, Idaho Falls, Idaho 83415-3860, 1999.
- [107] European Commission, Directorate-General for Research, Directorate-General for Energy and Transport. Hydrogen energy and fuel cells, a vision of our future. Final Report of the High Level Group, RTD Info, EUR 20719 EN, Brussels, 2003.
- [108] European Commission, Directorate-General for Research, Sustainable Energy Systems. Introducing hydrogen as an energy carrier: safety, regulatory and public acceptance issues. RTD Info, EUR 22002, Brussels, 2006.
- [109] Hirsch R.L., Bezdek R., and Wendling R. Peaking of world oil production: impacts, mitigation, & risk management. A report prepared for the government of the United States of America, February 2005.
- [110] Hubbert M.K. Nuclear energy and the fossil fuels, presented before the spring meeting of the southern district, division of production, american petroleum institute plaza hotel, san antonio, texas march 7–9, 1956. Publication No. 95, Shell Development Company, Exploration and Production Research Division, Houston, Texas, June 1956.

- [111] Hydrogen Now. <http://www.hydrogennow.org>.
- [112] Intergovernmental Panel on Climate Change, Working Group I. Summary for policymakers: a report of Working Group I of the Intergovernmental Panel on Climate Change. Available online: www.ipcc.ch/pub/spm22-01.pdf, 2001.
- [113] Jordan T. Hydrogen as an energy carrier. A lecture presented at the First European Summer School on Hydrogen Safety, 15–24 August 2006.
- [114] Maugeri L. Oil: never cry wolf - why the petroleum age is far from over. *Science*, 304:1114–1115, 2004.
- [115] Ogden J. Hydrogen as an energy carrier: outlook for 2010, 2030 and 2050. Reprint from workshop proceedings, The 10-50 Solution: Technologies and Policies for a Low-Carbon Future. The Pew Center on Global Climate Change and the National Commission on Energy Policy, March 2004 UCD-ITS-RP-04-24, Institute of Transportation Studies University of California, Davis, 2004.
- [116] Sperling D. and Cannon J.S. *The hydrogen energy transition: moving toward the post petroleum age in transportation*. Elsevier, Amsterdam, 2004.
- [117] Wikipedia Encyclopedia. http://en.wikipedia.org/wiki/Hindenburg_disaster.
- [118] Wikipedia Encyclopedia. http://en.wikipedia.org/wiki/Peak_oil.
- [119] Janssen H., Bringmann J.C., Emonts B., and Schroeder V. Safety-related studies on hydrogen production in high-pressure electrolysers. *International Journal of Hydrogen Energy*, 29:759–770, 2004.
- [120] Grigorieva S.A., Millet P., Korobtsev S.V., Porembskiy V.I., Pepic M., Etievant C., Puyenchet C., and Fateev V.N. Hydrogen safety aspects related to high-pressure polymer electrolyte membrane water electrolysis. *International Journal of Hydrogen Energy*, 34:5986–5991, 2009.
- [121] Barnard J.A. and Bradley J.N. *Flame and Combustion*. Chapman and Hall, London, 1985.
- [122] Drysdale D. *An Introduction to Fire Dynamics*. John Wiley & Sons, Chichester, 1999.
- [123] Glassman I. *Combustion*. Academic Press, New York, third edition, 1996.
- [124] Griffiths J.F. and Barnard J.A. *Flame and Combustion*. Chapman & Hall, London, third edition, 1995.
- [125] Kanury A.M. *Introduction to combustion phenomena for fire, incineration, pollution and energy applications*. Gordon and Breach, New York, second edition, 1977.
- [126] Lewis B. and von Elbe G. *Combustion, Flames and Explosions of Gases*. Academic Press, third edition, 1987.
- [127] Poinot T. and Veynante D. *Theoretical and numerical combustion*. Edwards, Philadelphia, 2001.

- [128] Toong T.-Y. *Combustion dynamics: the dynamics of chemically reacting fluids*. McGraw-Hill, New York, 1983.
- [129] Williams F.A. *Combustion Theory: the fundamental theory of chemically reacting flow systems*. Combustion Science and Engineering Series. The Benjamin/Cummings Publishing Company, Menlo Park, California, second edition, 1985.
- [130] Lanz A., Heffel J., and Messer C. Hydrogen fuel cell engines and related technologies. College of the Desert, USA Energy Technology Training Center, 43-500 Monterey Avenue, Palm Desert, CA 92260, United States of America, 2001.
- [131] NASA. Safety Standard for Hydrogen and Hydrogen Systems. Guidelines for hydrogen system design, materials selection, operations, storage, and transportation. Technical Report NSS 1740.16, Office of Safety and Mission Assurance, Washington, 1997.
- [132] Zabetakis M.G. and Burgess D.S. Research on the hazards associated with the production and handling of liquid hydrogen. Bureau of Mines Report of Investigation RI 5707, US Department of Interior, 1961.
- [133] Barthelemy H. and Allidieres L. Gaseous hydrogen refuelling stations : Selection of materials for hydrogen high pressure fuelling connectors. Paper presented at the First International Conference on Hydrogen Safety, Pisa, Italy, 8–10 September 2005.
- [134] Barthelemy H. Compatibility of metallic materials with hydrogen. A lecture presented at the First European Summer School on Hydrogen Safety, 15–24 August 2006.
- [135] Rogante M., Battistella P., and Cesari F. Hydrogen interaction and stress-corrosion in hydrocarbon storage vessel and pipeline weldings. *International Journal of Hydrogen Energy*, 31:597–601, 2006.
- [136] Miller J.A., Mitchell R.E., Smooke M.D., and Kee R.J. Toward a comprehensive chemical kinetic mechanism for the oxidation of acetylene: comparison of model predictions with results from flame and shock tube experiments. In *Proceedings of the Nineteenth Symposium (International) on Combustion*, pages 181–196, Pittsburgh, 1982. The Combustion Institute.
- [137] Benson S.W. *The Foundations of Chemical Kinetics*. Malabar, Krieger, 1982.
- [138] Dainton F.S. *Chain Reactions, An Introduction*. Methuen and Co. Ltd., London, 1956.
- [139] Frank-Kamenetzky D.A. *Diffusion and heat transfer in chemical kinetics*. Nauka, Moscow, 1967.
- [140] W.J. Moore. *Basic physical chemistry*. Englewood Cliffs, New Jersey, fourth edition, 2000.
- [141] Westbrook C.K. Chemical-kinetics of hydrocarbon oxidation in gaseous detonation. *Combustion and Flame*, 46:191–216, 1982.

- [142] Williams F.A. Reduced chemistry for hydrogen combustion and detonation. A lecture presented at the First European Summer School on Hydrogen Safety, 15–24 August 2006.
- [143] Buckmaster J.D. and Ludford G.S.S. *Theory of Laminar Flames*. Cambridge University Press, Cambridge, United Kingdom, 1982.
- [144] Clavin P. Dynamic behavior of premixed flame fronts in laminar and turbulent flows. *Progress in Energy and Combustion Science*, 11:1–59, 1985.
- [145] Karlovitz B., Denniston D.W., and Wells F.E. Investigation of turbulent flames. *Journal of Chemical Physics*, 19(5):541–547, 1951.
- [146] Hottel H.C. and Hawthorne W.R. Diffusion in laminar flame jets. In *Proceedings of the Third Symposium (International) on Combustion*, pages 253–266, Baltimore, 1949. Williams and Wilkins.
- [147] McCaffrey B.J. Purely buoyant diffusion flames: Some experimental results. Technical Report NBSIR 79-1910, National Bureau of Standards, Washington DC, 1979.
- [148] Williams F.A. Urban and wildland fire phenomenology. *Progress in Energy and Combustion Science*, 8:317–354, 1982.
- [149] Buckmaster J., Clavin P., Linan A., Matalon M., Peters N., Sivashinsky G., and Williams F.A. Combustion theory and modeling. In *Proceedings of the Thirtieth Symposium (International) on Combustion*, pages 1–19, Pittsburgh, 2005. The Combustion Institute.
- [150] Abdel-Gayed R.G., Ali-Khishali K.J., and Bradley D. Turbulent burning velocity and flame straining in explosions. *Proceedings of the Royal Society of London, Series A: Mathematical and Physical Sciences*, 391:393–414, 1984.
- [151] Abdel-Gayed R.G., Bradley D., and Lawes M. Turbulent burning velocities: a general correlation in terms of straining rates. *Proceedings of the Royal Society of London, Series A: Mathematical and Physical Sciences*, 414:389–413, 1987.
- [152] Andrews G.E., Bradley D., and Lwakabamba S. B. Turbulence and turbulent flame propagation – A critical appraisal. *Combustion and Flame*, 24:285–304, 1975.
- [153] Bradley D., Lau A.K.C., and Lawes M. Flame stretch as a determinant of turbulent burning velocity. *Philosophical Transactions of the Royal Society of London, Series A: Mathematical and Physical Sciences*, 338:359–387, 1992.
- [154] Clavin P. and Williams F.A. Theory of premixed-flame propagation in large-scale turbulence. *Journal of Fluid Mechanics*, 90:589–604, 1979.
- [155] Damköhler G. Der Einfluss der Turbulenz auf die Flammgeschwindigkeit in Gasgemischen. *Zeitschrift für Elektrochemie*, 46:601–626, 1940.
- [156] Damköhler G. The effect of turbulence on the flame velocity in gas mixtures. Technical Memorandum NACA TM 1112, National Advisory Committee for Aeronautics, Washington, 1947.

- [157] Leason D.B. Turbulence and flame propagation in premixed gases. *Fuel*, 30:233–239, 1951.
- [158] Gouldin F.C. An application of fractals to modeling premixed turbulent flames. *Combustion and Flame*, 68:249–266, 1987.
- [159] Gülder Ö.L. Turbulent premixed flame propagation models for different combustion regimes. In *Proceedings of the Twenty-Third Symposium (International) on Combustion*, pages 743–750, Pittsburgh, 1990. The Combustion Institute.
- [160] Hamberger P., Schneider H., Jamois D., and Proust C. Correlation of turbulent burning velocity and turbulence intensity for starch dust air mixtures. Proceedings of the Third European Combustion Meeting, 11–13 April 2007, Chania, Greece, 2007.
- [161] Hentschel H.G.E. and Procaccia I. Relative diffusion in turbulent media: the fractal dimension of clouds. *Physical Review A*, 29:1461–1470, 1984.
- [162] Kerstein A.R. Pair-exchange model of turbulent premixed flame propagation. In *Proceedings of the Twenty-First Symposium (International) on Combustion*, pages 1281–1289, Pittsburgh, 1986. The Combustion Institute.
- [163] Kerstein A.R. Simple derivation of Yakhot’s turbulent premixed flamespeed formula. *Combustion Science and Technology*, 60:163–165, 1988.
- [164] Kerstein A.R., Ashurst W., and Williams F.A. Field equation for interface propagation in an unsteady homogeneous flow field. *Physical Review A*, 37:2728–2731, 1988.
- [165] Klimov A.M. Premixed turbulent flames – interplay of hydrodynamic and chemical phenomena. *Progress in Astronautics and Aeronautics*, 88:133–146, 1983.
- [166] Liu Y. and Lenze B. The influence of turbulence on the burning velocity of premixed CH₄–H₂ flames with different laminar burning velocities. In *Proceedings of the Twenty-Second Symposium (International) on Combustion*, pages 747–754, Pittsburgh, 1988. The Combustion Institute.
- [167] Leuckel W., Nastoll W., and Zarzalis N. Experimental investigation of the influence of turbulence on the transient premixed flame propagation inside closed vessels. In *Proceedings of the Twenty-Third Symposium (International) on Combustion*, pages 729–734, Pittsburgh, 1990. The Combustion Institute.
- [168] Lipatnikov A.N. and Chomiak J. Turbulent flame speed and thickness: phenomenology, evaluation, and application in multi-dimensional simulations. *Progress in Energy and Combustion Science*, 28:1–74, 2002.
- [169] Lovejoy S. The area-perimeter relation for rain and cloud areas. *Science*, 216:185–187, 1982.
- [170] Peters N. Laminar flamelet concepts in turbulent combustion. In *Proceedings of the Twenty-First Symposium (International) on Combustion*, pages 1231–1250, Pittsburgh, 1988. The Combustion Institute.

- [171] Poinso T. and Veynante D. *Theoretical and numerical combustion*. Edwards, Philadelphia, second edition, 2005.
- [172] Pope S.B. and Anand M.S. Flamelet and distributed combustion in premixed turbulent flames. In *Proceedings of the Twentieth Symposium (International) on Combustion*, pages 403–410, Pittsburgh, 1984. The Combustion Institute.
- [173] Schelkin K.I. On combustion in a turbulent flow. *Soviet Physics – Technical Physics*, 13:520–530, 1943.
- [174] Schelkin K.I. On combustion in a turbulent flow. NACA Technical Memorandum 1110, National Advisory Committee for Aeronautics, Washington, February 1947. Original: Jour. Tech. Phys. (USSR), vol. 13, nos. 9–10, 1943, pp. 520–530.
- [175] Schneider H. and Proust C. Determination of turbulent burning velocities of dust air mixtures with the open tube method. *Journal of Loss Prevention in the Processes Industries*, 20:470–476, 2007.
- [176] Shy S.S., Lin W.J., and Wei J.C. An experimental correlation of turbulent burning velocities for premixed turbulent methane-air combustion. *Proceedings of the Royal Society of London, Series A: Mathematical and Physical Sciences*, 456:1997–2019, 2000.
- [177] Sreenivasan K.R. and Meneveau C. The fractal facets of turbulence. *Journal of Fluid Mechanics*, 173:357–186, 1986.
- [178] Tucker M. Interaction of a free flame front with a turbulence field. Technical Note NACA TN 3407, National Advisory Committee for Aeronautics, Washington, March 1955.
- [179] Yakhot V. Propagation velocity of premixed turbulent flames. *Combustion Science and Technology*, 60:191–214, 1988.
- [180] Zimont V.L. and Lipatnikov A.N. A numerical model of premixed turbulent combustion of gases. *Chemical Physics Reports*, 14:993–1025, 1995.
- [181] Borghi R. Turbulent combustion modelling. *Progress in Energy and Combustion Science*, 14:245–292, 1988.
- [182] Makarov D.V. and Molkov V.V. Large eddy simulation of gaseous explosion dynamics in an unvented vessel. *Combustion, Explosion and Shock Waves*, 40:136–144, 2004.
- [183] Peters N. Length scales in laminar and turbulent flames. *Progress in Astronautics and Aeronautics*, 135:155–182, 1991.
- [184] Peters N. *Turbulent Combustion*. Cambridge University Press, Cambridge, United Kingdom, 2000.
- [185] Babrauskas V. Heat release rates. In P.J. DiNenno, D. Drysdale, C.L. Beyler, W.D. Walton, R.L.P. Custer, J.R. Hall, and J.M. Watts, editors, *SFPE Handbook of Fire Protection Engineering, Section 3: Hazard Calculations*, chapter 3-1, pages 3–1 – 3–37. National Fire Protection Association, Quincy, Massachusetts, third edition, 2002.

- [186] Spalding D.B. *Some Fundamentals of Combustion*. Butterworths, London, 1955.
- [187] Tewarson A. Generation of heat and chemical compounds in fires. In P.J. DiNenno, D. Drysdale, C.L. Beyler, W.D. Walton, R.L.P. Custer, J.R. Hall, and J.M. Watts, editors, *SFPE Handbook of Fire Protection Engineering, Section 4: Design Calculations*, chapter 3-4, pages 3–82 – 3–161. National Fire Protection Association, Quincy, Massachusetts, third edition, 2002.
- [188] Swain M.R. and Swain M.N. Passive ventilation systems for the safe use of hydrogen. *International Journal of Hydrogen Energy*, 21:823–835, 1996.
- [189] Swain M.R., Filoso P., Grilliot E.S., and Swain M.N. Hydrogen leakage into simple geometric enclosures. *International Journal of Hydrogen Energy*, 28:229–248, 2003.
- [190] Witcofsky R.D. and Chirivella J.E. Experimental and analytical analysis of the mechanisms governing the dispersion of flammable clouds formed by liquid hydrogen spills. *International Journal of Hydrogen Energy*, 9:425–435, 1984.
- [191] Lee J.H.S. and Berman M. Hydrogen combustion and its application to nuclear reactor safety. In G.A. Greene, J.P. Hartnett, T.F. Irvine Jr., and Y.I. Cho, editors, *Heat Transfer in Nuclear Reactor Safety*, volume 29 of *Advances in Heat Transfer*, chapter 2, pages 59–123. Academic Press, New York, 1997.
- [192] Drell I.L. and Belles F.E. Survey of hydrogen combustion properties. Report NACA 1383, National Advisory Committee for Aeronautics, Cleveland, Ohio, 1958.
- [193] Stamps D.W. and Berman M. High-temperature hydrogen combustion in reactor safety applications. *Nuclear Science and Engineering*, 109:39–48, 1991.
- [194] Tamm H., Ungurian M., and Kumar R.K. Effectiveness of thermal ignition devices in rich hydrogen -air-steam mixtures. Technical Report EPRI NP-5254, Electric Power Research Institute, Palo Alto, California, 1987.
- [195] Zabetakis M.G. Research on the combustion and explosion hazards of hydrogen-water vapor-air mixtures. Technical Report AECU-3327, U.S. Atomic Energy Commission Report, 1956.
- [196] Shepherd J.E. Hydrogen steam jet flame facility and experiments. Technical Report NUREG/CR-3638, SAND84-0060, Sandia National Laboratories, Albuquerque, New Mexico, 1985.
- [197] Bach G.G., Knystautas R., and Lee J.H.S. Direct initiation of spherical detonations in gaseous explosives. In *Proceedings of the Twelfth Symposium (International) on Combustion*, pages 853–864, Pittsburgh, 1969. The Combustion Institute.
- [198] Bull D.C., Elsworth J.E., and Hooper G. Initiation of spherical detonation in hydrocarbon/air mixtures. *Acta Astronautica*, 5:997–1008, 1978.
- [199] Clarke J.F., Kassoy D.R., and Riley N. On the direct initiation of a plane detonation wave. *Philosophical Transaction of the Royal Society of London, Series A:Mathematical and Physical Sciences*, 408:129–148, 1986.

- [200] Clarke J.F., Kassoy D.R., Meharzi N.E., Riley N., and Vasantha R. On the evolution of plane detonations. *Philosophical Transaction of the Royal Society of London, Series A: Mathematical and Physical Sciences*, 429:259–283, 1990.
- [201] Del Alamo G., Williams F.A., and Sanchez A.L. Hydrogen-oxygen induction times above crossover temperatures. *Combustion Science and Technology*, 176:1599–1626, 2004.
- [202] Dold J.W. and Kapila A.K. Comparison between shock initiations of detonation using thermally-sensitive and chain-branching chemical models. *Combustion and Flame*, 85:185–194, 1991.
- [203] Fickett K.K. and Davis W.C. *Detonation: theory and experiment*. Dover, New York, 2001.
- [204] He L. and Clavin P. On the direct initiation of gaseous detonation by an energy source. *Journal of Fluid Mechanics*, 277:227–248, 1994.
- [205] He L. and Lee J.H.S. The dynamic limit of one-dimensional detonations. *Physics of Fluids*, 7:1151–1158, 1995.
- [206] He L. Theoretical determination of the critical conditions for the direct initiation of detonations in hydrogen-oxygen mixtures. *Combustion and Flame*, 104:401–418, 1996.
- [207] Kapila A.K. Homogeneous branched-chain explosion: Initiation to completion. *Journal of Engineering Mathematics*, 12:221–235, 1978.
- [208] Lee J.H.S. Initiation of gaseous detonation. *Annual Reviews of Physical Chemistry*, 28:75–104, 1977.
- [209] Lee J.H.S. and Higgins A.J. Comments on criteria for direct initiation of detonations. *Philosophical Transaction of the Royal Society of London, Series A: Mathematical and Physical Sciences*, 357:3503–3521, 1999.
- [210] Nettleton M.A. *Gaseous Detonations: their nature, effects and control*. Chapman and Hall, 1987.
- [211] Nettleton M.A. Recent work on gaseous detonations. *Shock Waves*, 12:3–12, 2002.
- [212] Baker W.E., Cox P.A., Westine P.S., Kulesz J.J., and Strehlow R.A. *Explosion Hazards and Evaluation*, volume 5 of *Fundamental studies in engineering*. Elsevier Scientific Publishing Company, New York, 1983.
- [213] Bartknecht W. *Explosions: Course Prevention Protection*. Springer Verlag, 1981. Translation of the second edition of *Explosionen, Ablauf und Schutzmaßnahmen* by H. Burg and T. Almond.
- [214] Bradley D. and Mitcheson A. Mathematical solutions for explosions in spherical vessels. *Combustion and Flame*, 26:201–217, 1976.
- [215] Dahoe A.E. and de Goey L.P.H. On the determination of the laminar burning velocity of closed vessel explosions. *Journal of Loss Prevention in the Process Industries*, 16:457–478, 2003.

- [216] Dorofeev S.B., Kuznetsov M.S., Alekseev V.I., Efimenko A.A., and Breitung W. Evaluation of limits for effective flame acceleration in hydrogen mixtures. *Journal of Loss Prevention in the Processes Industries*, 14:583–589, 2001.
- [217] Dorofeev S.B. Flame acceleration and DDT in gas explosions. *Journal de Physique de France IV*, 12(7):3–10, 2002.
- [218] Eckhoff R.K. *Dust explosions in the process industries*. Gulf, Amsterdam, third edition, 2003.
- [219] Eckhoff R.K. Explosion hazards in the process industries, 2005. To appear in 2005.
- [220] Kuznetsov M., Alekseev V., Yankin Y., and Dorofeev S. Slow and fast deflagrations in hydrocarbon-air mixtures. *Combustion Science and Technology*, 174:157–172, 2002.
- [221] Makarov D.V. and Molkov V.V. Validation of large eddy simulations of stoichiometric h₂-air mixture deflagration against experiment in 2.3m diameter vessel. *Fire and Explosion Safety*, 11:10–17, 2004.
- [222] Kuznetsov M., Matsukov I., and Dorofeev S. Heat loss rates from hydrogen-air turbulent flames in tubes. *Combustion Science and Technology*, 174:75–93, 2002.
- [223] Tamanini F. Modeling of turbulent unvented gas/air explosions. *Progress in Aeronautics and Astronautics*, 154:3–30, 1993.
- [224] Lee J.H.S. Dynamic parameters of gaseous detonations. *Annual Reviews of Fluid Mechanics*, 16:311–336, 1984.
- [225] Chapman D.L. On the rate of explosion in gases. *Physics of Fluids*, 47:90–104, 1899.
- [226] Denisov Yu.N. and Troshin Ya.K. Pulsating and spinning detonation of gaseous mixtures in tubes. *Doklady Akademii Nauk USSR*, 125:110–113, 1959.
- [227] Doering W. On detonation processes in gases. *Annalen der Physik*, 43:421–436, 1943.
- [228] Dorofeev S.B., Efimenko A.A., Kochurko A.S., and Chaivanov B.B. Evaluation of the hydrogen explosions hazard. *Nuclear Engineering Design*, 148:305–316, 1995.
- [229] Dorofeev S.B., Bezmelnitsin A.V., and Sidorov V.P. Transition to detonation in vented hydrogen-air explosions. *Combustion and Flame*, 103:243–246, 1995.
- [230] Fujiwara T. and Reddy K.V. Propagation mechanism of detonation - three-dimensional phenomena. *Memoirs of the Faculty of Engineering, Nagoya University*, 41:1–18, 1989.
- [231] Jouguet E. On the propagation of chemical reactions in gases. *Journal de Mathematiques Pures et Appliquees*, 1:347–425, 1906.
- [232] Gavrikov A.I., Efimenko A.A., and Dorofeev S. B. A model for detonation cell size prediction from chemical kinetics. *Combustion and Flame*, 120:19–33, 2000.

- [233] Kailasanath K., Oran E.S., Boris J.P., and Young T.R. Determination of cell size and the role of transverse waves in two-dimensional detonations. *Combustion and Flame*, 61:199–209, 1985.
- [234] Kassoy D.R. and Clarke J.F. The structure of steady deflagration with a finite origin. *Journal of Fluid Mechanics*, 150:253–280, 1985.
- [235] Pintgen F., Eckett C.A., Austin J.M., and Shepherd J.E. Direct observations of reaction zone structure in propagating detonations. *Combustion and Flame*, 133:211–229, 2003.
- [236] Soloukhin R. Multiheaded structure of gaseous detonation. *Combustion and Flame*, 9:51–58, 1965.
- [237] Strehlow R.A., Liaugminas R., Watson R.H., and Eyman J. Transverse waves structure in detonations. In *Proceedings of the Eleventh Symposium (International) on Combustion*, pages 683–692, Pittsburgh, 1967. The Combustion Institute.
- [238] Strehlow R.A. Gas phase detonations: Recent developments. *Combustion and Flame*, 12:81–101, 1968.
- [239] Strehlow R.A. Gas phase detonations: recent developments. *Progress in Aeronautics and Astronautics*, 14:539–548, 1969.
- [240] Strehlow R.A. Multi-dimensional wave structure. *Progress in Aeronautics and Astronautics*, 15:345–357, 1970.
- [241] Strehlow R.A. *Combustion Fundamentals*. McGraw-Hill Series In Energy. McGraw-Hill, New York, 1984.
- [242] Neumann J. von. Theory of detonation waves. In A.H. Taub, editor, *John von Neumann, Collected Works*, volume 6 of *Theory of games, astrophysics, hydrodynamics and meteorology*. Pergamon, Oxford, 1942.
- [243] Williams D.N., Bauwens L., and Oran E.S. Structure and propagation of three-dimensional detonations. In *Proceedings of the Twenty-Sixth Symposium (International) on Combustion*, pages 2991–2998, Pittsburgh, 1996. The Combustion Institute.
- [244] Williams D.N., Bauwens L., and Oran E.S. Numerical study of the mechanisms of self-reignition in low-overdrive detonations. *Shock Waves*, 6:93–110, 1996.
- [245] White D.R. Turbulent structure of gaseous detonation. *Physics of Fluids*, 4:465–480, 1961.
- [246] Yao J. and Scott-Stewart D. On the dynamics of multi-dimensional detonation. *Journal of Fluid Mechanics*, 309:225–275, 1996.
- [247] Zeldovich Ya.B. and Kompaneets S.A. *Theory of Detonations*. Academic Press, New York, 1960.
- [248] Alekseev V.I., Kuznetsov M.S., Yankin Y. G., and Dorofeev S.B. Experimental study of flame acceleration and DDT under conditions of transverse venting. *Journal of Loss Prevention in the Processes Industries*, 14:591–596, 2001.

- [249] Dorofeev S.B., Sidorov V.P., Kuznetsov M.S., Matsukov I.D., and Alekseev V.I. Effect of scale on the onset of detonations. *Shock Waves*, 10:137–149, 2000.
- [250] Urtiew P.A. and Oppenheim A.K. Experimental observations of transition to detonation in explosive gas. *Philosophical Transactions of the Royal Society of London, Series A: Mathematical and Physical Sciences*, 295:13–38, 1966.
- [251] Whitehouse D.R., Greig D.R., and Koroll G.W. Combustion of stratified hydrogen-air mixtures in the 10.7 m³ combustion test facility cylinder. *Nuclear Engineering and Design*, 166:453–462, 1996.
- [252] Zeldovich Ya.B. On the theory of the propagation of detonation in gaseous systems. *Journal of Experimental and Theoretical Physics*, 10:542–568, 1940.
- [253] Dorofeev S.B. Blast effect of confined and unconfined explosions. In B. Sturtevant, J. Shepherd, and H. Hornung, editors, *Shock Waves, Proceedings of the 20th ISSW*, volume 1, pages 77–86, Singapore, 1996. World Scientific Publishing Co.
- [254] Dorofeev S.B., Sidorov V.P., and Dvoinishnikov A.E. Blast parameters from unconfined gaseous detonations. In B. Sturtevant, J. Shepherd, and H. Hornung, editors, *Shock Waves, Proceedings of the 20th ISSW*, volume 1, pages 673–678, Singapore, 1996. World Scientific Publishing Co.
- [255] Tang M.J. and Baker Q.A. A new set of blast curves from vapor cloud explosion. *Process Safety Progress*, 18:235–240, 1999.
- [256] Committee for the Prevention of Disasters. *Methods for the calculation of physical effects due to releases of hazardous materials (liquids and gases)*, CPR14E. Publication Series on Dangerous Substances. The Dutch Ministry of the Interior and Kingdom Relations, The Hague, The Netherlands, third edition, 2005. Yellow Book, 2005 revision of the third edition published in 1997.
- [257] Groethe M., Colton J., Chiba S., and Sato Y. Hydrogen deflagrations at large scale. WHEC, 2004.
- [258] Molkov V.V. Guidelines for venting of deflagrations in enclosures with inertial vent covers. In D. Bradley, D. Drysdale, and V. Molkov, editors, *Fire and Explosion Hazards, Proceedings of the 4th International Seminar, 8-12 September 2003, Londonderry, United Kingdom*, page 41, Newtownabbey, Northern Ireland, United Kingdom, 2003. FireSERT, University of Ulster.
- [259] Khan F.I. and Amyotte P.R. How to make inherent safety practice a reality. *Canadian Journal of Chemical Engineering*, 81:2–16, 2003.
- [260] AIAA G-095-2004. Guide to safety of hydrogen and hydrogen system, ANSI/AIAA standard. American Institute for Aeronautics and Astronautics, Reston, Virginia, 2004.
- [261] Kalyanam K.M. and Hay D.R. Safety guide for hydrogen. NRC Publication 27406, National Research Council of Canada, Ottawa, 1987.

- [262] Molkov V.V., Dobashi R., Suzuki M., and Hirano T. Modeling of vented hydrogen-air deflagrations and correlations for vent sizing. *Journal of Loss Prevention in the Process Industries*, 12:147–156, 1999.
- [263] NFPA 68. Venting of deflagrations, 2002 edition. National Fire Protection Association, Quincy, MA, United States of America, 2002.
- [264] Molkov V.V. Unified correlations for vent sizing of enclosures against gaseous deflagrations at atmospheric and elevated pressures. loss prevention in the process industries. *Journal of Loss Prevention in the Process Industries*, 14:567–574, 2001.
- [265] Molkov V.V. Accidental gaseous deflagrations: modelling, scaling and mitigation. *Journal de Physique de France IV*, 12(7):19–30, 2002.
- [266] Grigorash A., Eber R., and Molkov V. Theoretical model of vented gaseous deflagrations in enclosures with inertial vent covers. In D. Bradley, D. Drysdale, and V. Molkov, editors, *Fire and Explosion Hazards, Proceedings of the 4th International Seminar, 8-12 September 2003, Londonderry, United Kingdom*, pages 445–456, Newtownabbey, Northern Ireland, United Kingdom, 2004. FireSERT, University of Ulster.
- [267] Korzhavin A.A., Klimenko A.S., and Babkin V.S. Inert porous media as an effective tool for explosion-proofing of closed technological equipment. In D. Bradley, D. Drysdale, and V. Molkov, editors, *Fire and Explosion Hazards, Proceedings of the 4th International Seminar, 8-12 September 2003, Londonderry, United Kingdom*, pages 893–904, Newtownabbey, Northern Ireland, United Kingdom, 2004. FireSERT, University of Ulster.
- [268] Cox G. *Combustion Fundamentals of Fire*. Academic Press, New York, 1995.
- [269] Cox G. and Kumar S. Modelling enclosure fires using CFD. In P.J. DiNenno, D. Drysdale, C.L. Beyler, W.D. Walton, R.L.P. Custer, J.R. Hall, and J.M. Watts, editors, *SFPE Handbook of Fire Protection Engineering, Section 3: Hazard Calculations*, chapter 3-8, pages 3–194 – 3–218. National Fire Protection Association, Quincy, Massachusetts, third edition, 2002.
- [270] Ferziger J.H. and Peric M. *Computational Methods for Fluid Dynamics*. Springer, New York, third edition, 2002.
- [271] Patankar S.V. *Numerical Heat Transfer and Fluid Flow*. Hemisphere Publishing Corporation, Taylor & Francis Group, New York, 1980.
- [272] Roy G.D., Frolov S.M., and Givi P. *Advanced Computation and Analysis of Combustion*. ENAS Publishers, Berlin, 1997.
- [273] Warsi Z.U.A. *Fluid Dynamics: Theoretical and Computational Approaches*. CRC Press, London, second edition, 1999.
- [274] AIAA G-077-1998. Guide for the verification and validation of computational fluid dynamics simulations, 1998.
- [275] Veynante D. and Vervisch L. Turbulent combustion modeling. *Progress in Energy and Combustion Science*, 28:193–266, 2002.

- [276] Bourlioux A. and Majda A.J. Theoretical and numerical structure for unstable two-dimensional detonations. *Combustion and Flame*, 90:211–229, 1992.
- [277] Oran E.S., Boris J.P., Young T.R., Flanigan M., Burks T., and Picone M. Numerical simulations of detonations in hydrogen-air and methane-air mixtures. In *Proceedings of the Eighteenth Symposium (International) on Combustion*, pages 1641–1649, Pittsburgh, 1981. The Combustion Institute.
- [278] Quirk J.J. Godunov-type schemes applied to detonation flows. In J. Buckmaster, T. Jackson, and A. Kumar, editors, *Combustion in High Speed Flows*, pages 575–596, Dordrecht, The Netherlands, 1994. Kluwer.
- [279] Taki S. and Fujiwara T. Numerical analysis of two-dimensional nonsteady detonations. AIAA-paper 76-404, 1978.
- [280] Choudhuri A.R. and Gollahalli S.R. Intermediate radical concentrations in hydrogen-natural gas blended fuel jet flames. *International Journal of Hydrogen Energy*, 29:1291–1302, 2004.
- [281] Barlow R.S., Dibble R.W., Chen J.-Y., and Lucht R.P. Effect of Damkohler number on superequilibrium OH concentration in turbulent nonpremixed jet flames. *Combustion Science and Technology*, 82:235–251, 1990.
- [282] Cox G. On radiation heat transfer from turbulent flames. *Combustion Science and Technology*, 1:75–78, 1977.
- [283] Barlow R.S., Smith N.S.A., Chen J.-Y., and Bilger R.W. Nitric oxides formation in dilute hydrogen jet flames: isolation of the effects of radiation and turbulent-chemistry submodels. *Combustion and Flame*, 117:4–31, 1999.
- [284] Kim S.H., Kim M., Yoon Y., and Jung I.-S. The effect of flame radiation on the scaling of nitrogen oxide emission in turbulent hydrogen non-premixed flames. In *Proceedings of the Twenty-Ninth Symposium (International) on Combustion*, pages 1951–1956, Pittsburgh, 2002. The Combustion Institute.
- [285] Chelin P. and Pina V. Investigative method for radiative properties of water vapour in the 0.8 μ m region by optical diagnostic of h₂-air combustion. *Combustion Science and Technology*, 174:215–229, 2002.
- [286] Iibas M. The effect of thermal radiation and radiation models on hydrogen-hydrocarbon combustion modelling. *International Journal of Hydrogen Energy*, 30:1113–1126, 2005.
- [287] Faeth G.M., Jeng S.M., and Gore J. Radiation from fires. In C.K. Law, W.W. Yuen, and K. Miyasaka, editors, *Heat Transfer in Fire and Combustion Systems*, volume 45, pages 137–151. ASME, New York, 1985.
- [288] Liu L.H., Xu X., Chen Y.L., and Wang H.F. Fluctuating characteristics of radiative source term in hydrogen turbulent jet diffusion flame. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 87:193–201, 2004.

- [289] Baek S.W., Kim J.J., Kim H.S., and Kang S.H. Effects of addition of solid particles on thermal characteristics in hydrogen-air flame. *Combustion Science and Technology*, 174:99–116, 2002.
- [290] Blinov V.I. and Khudiakov G.N. Certain laws governing diffusive burning of liquids. *Academiia Nauk, SSSR Doklady*, 113:1094–1098, 1957. US Army translation, NTIS no. 296762, 1961.
- [291] Burgess D.S., Strasser A., and Grumer J. Diffusive burning of liquid fuels in open trays. *Fire Res. Abs. and Rev.*, 3:177, 1961.
- [292] Burgess D.S. and Hertzberg M. Radiation from pool flames. In N.H. Afgan and J.M. Beer, editors, *Heat transfer in flames*, chapter 27. Scripta Book Co., Washington, DC, 1974.
- [293] McGratten K.B., Baum H.R., and Hamins A. Thermal radiation from large pool fires. Technical Report NISIR 6546, National Institute of Standards and Technology, 2000.
- [294] Greiner M. and Suo-Anttila A. Validation of the isis-3d computer code for simulating large pool fires under a variety of wind conditions. *Journal of Pressure Vessel Technology, Transactions of the ASME*, 126:360–368, 2004.
- [295] Venetsanos A.G., Huld T., Adams P., and Bartzis J.G. Source, dispersion and combustion modelling of an accidental release of hydrogen in an urban environment. *Journal of Hazardous Materials*, A105:1–25, 2003.
- [296] Sathiah P., Komen E., and Roekaerts D. The role of CFD combustion modeling in hydrogen safety management - I: Validation based on small scale experiments. *Nuclear Engineering and Design*, 248:93–107, 2012.
- [297] Sathiah P., van Haren S., Komen E., and Roekaerts D. The role of CFD combustion modeling in hydrogen safety management - II: Validation based on homogeneous hydrogen-air experiments. *Nuclear Engineering and Design*, 252:289–302, 2012.
- [298] Abdo D., Magnaud H., Paillere H., Studer E., and Bachellerie E. Experimental and numerical studies of inerting efficiency for H₂-risk mitigation. Proceedings of the International Topical Meeting on Nuclear Thermal-Hydraulics, NURETH-10, Seoul, Korea, 5-9 October 2003, 2003.
- [299] Beccantini A. and Pailhories P. Use of a finite volume scheme for simulation of hydrogen explosions. IAEA/NEA Technical meeting on use of CFD for safety analysis of reactor systems, including containment. Pisa, Italy, 11-13 November 2002, 2002.
- [300] Bielert U., Breitung W., Kotchourko A., Royl P., Scholtyssek W., Vesper A., Beccantini A., Dabbene F., Paillere H., Studer E., Huld T., Wilkening H., Edlinger B., Poruba C., and Mohaved M. Nuclear engineering and design. *Journal of Loss Prevention in the Processes Industries*, 209:165–172, 2001.
- [301] US Department of Energy. Guidance for safety aspects of proposed hydrogen projects. Hydrogen, Fuel Cells & Infrastructure Technologies Program, August 2004.

- [302] Lees F.P. *Loss Prevention in the Process Industry*, volume 1. Butterworth, London, second edition, 1996.
- [303] Lees F.P. *Loss Prevention in the Process Industry*, volume 2. Butterworth, London, second edition, 1996.
- [304] Lees F.P. *Loss Prevention in the Process Industry*, volume 3. Butterworth, London, second edition, 1996.
- [305] Newsholme G. The management of risk. A lecture contributed to Module Principles of Hydrogen Safety of the Postgraduate Certificate in Hydrogen Safety Engineering. The Health and Safety Executive, Bootle, United Kingdom, 2007.
- [306] Pasmaan H.J. The challenge of risk control in a hydrogen based economy. A lecture presented at the First European Summer School on Hydrogen Safety, 15–24 August 2006.
- [307] European Commission. Directive 94/9/EC of the European Parliament and of the Council of 23 March 1994 on the approximation of the laws of the Member States concerning equipment and protective systems intended for use in potentially explosive atmospheres. *Official Journal of the European Union*, series L100, volume 37(19.04.1994):1–33, 1994. EU ATEX 100.
- [308] European Commission. Corrigendum to Directive 94/9/EC of the European Parliament and of the Council of 23 March 1994 on the approximation of the laws of the Member States concerning equipment and protective systems intended for use in potentially explosive atmospheres. *Official Journal of the European Union*, series L21, volume 43(26.01.2000):42–44, 2000. EU ATEX 100.
- [309] European Commission. Corrigendum to Directive 94/9/EC of the European Parliament and of the Council of 23 March 1994 on the approximation of the laws of the Member States concerning equipment and protective systems intended for use in potentially explosive atmospheres. *Official Journal of the European Union*, series L304, volume 43(05.12.2000):19, 2000.
- [310] European Commission. Directive 1999/92/EC of the European Parliament and of the Council of 16 December 1999 on minimum requirements for improving the safety and health protection of workers potentially at risk from explosive atmospheres (15th individual Directive within the meaning of Article 16(1) of Directive 89/391/EEC). *Official Journal of the European Union*, series L23, volume 43(28.01.2000):57–64, 2000. EU ATEX 137.
- [311] European Commission. Corrigendum to Directive 1999/92/EC of the European Parliament and of the Council of 16 December 1999 on minimum requirements for improving the safety and health protection of workers potentially at risk from explosive atmospheres (15th individual Directive within the meaning of Article 16(1) of Directive 89/391/EEC). *Official Journal of the European Union*, series L134, volume 43(07.06.2000):36, 2000.
- [312] van den Braken - van Leersum A.M. Safety distances - a space oddity. Process Safety and Industrial Explosion Protection, International ESMG Symposium, Nurnberg, Germany, 11-13 October 2005.

- [313] Newsholme G. Hydrogen Safety and Regulation. A lecture contributed to Module Applied Hydrogen Safety of the Postgraduate Certificate in Hydrogen Safety Engineering. The Health and Safety Executive, Bootle, United Kingdom, 2007.
- [314] European Commission, Directorate General Enterprise and Industry. Guidelines on the Application of Council Directive 94/9/EC of the European Parliament and of the Council of 23 March 1994 on the approximation of the laws of the Member States concerning equipment and protective systems intended for use in potentially explosive atmospheres, Second Edition, July 2007.
- [315] European Commission. Council Directive 89/336/EEC of 3 May 1989 on the approximation of the laws of the Member States concerning electromagnetic compatibility. *Official Journal of the European Union*, series L139, volume 32(23.05.1989):19–26, 1989.
- [316] European Commission. Council Directive 92/31/EEC of 28 April 1992 amending Directive 89/336/EEC on the approximation of the laws of the Member States concerning electromagnetic compatibility. *Official Journal of the European Union*, series L126, volume 53(12.05.1992):11, 1992.
- [317] European Commission. Council Directive 93/68/EEC of 22 July 1993 amending Directives 87/404/EEC (simple pressure vessels), 88/378/EEC (safety of toys), 89/106/EEC (construction products), 89/336/EEC (electromagnetic compatibility), 89/392/EEC (machinery), 89/686/EEC (personal protective equipment), 90/384/EEC (non-automatic weighing instruments), 90/385/EEC (active implantable medicinal devices), 90/396/EEC (appliances burning gaseous fuels), 91/263/EEC (telecommunications terminal equipment), 92/42/EEC (new hot-water boilers fired with liquid or gaseous fuels) and 73/23/EEC (electrical equipment designed for use within certain voltage limits). *Official Journal of the European Union*, series L220, volume 36(30.08.1993):1–22, 1993.
- [318] Department of Trade and Industry. Electrical Equipment (implementing the Low Voltage Directive), Guidance notes on UK Regulations. Technical Report URN 00/588, Department of Trade and Industry, London, United Kingdom, July 1995. Reprinted with corrections, February 2000.
- [319] European Commission. Directive 98/37/EC of the European Parliament and of the Council of 22 June 1998 on the approximation of the laws of the Member States relating to machinery. *Official Journal of the European Union*, series L207, volume 41, 23.07.1998:1–46, 1998.
- [320] EN 61511-1. Functional safety – Safety instrumented systems for the process industry sector – Part 1: Framework, definitions, system, hardware and software requirements. European Committee for Electrotechnical Standardization, CENELEC, Reference number EN 61511-1:2004 E, 2004. European Standard, Covers IEC 61511-1:2003 + corrigendum 2004.
- [321] EN 61511-2. Functional safety – Safety instrumented systems for the process industry sector – Part 2: Guidelines for the application of IEC 61511-1. European Committee for Electrotechnical Standardization, CENELEC, Reference number EN 61511-2:2004 E, 2004. European Standard, IEC 61511-2:2.

- [322] EN 61511-3. Functional safety – Safety instrumented systems for the process industry sector – Part 3: Guidance for the determination of the required safety integrity levels. European Committee for Electrotechnical Standardization, CENELEC, Reference number EN 61511-3:2004 E, 2004. European Standard, Covers IEC 61511-3:2003 + corrigendum 2004.
- [323] PD IEC/TR 61508-0. Functional safety of electrical/electronic/programmable electronic safety-related systems - Part 0: Functional safety and IEC 61508. International Electrotechnical Commission, IEC, Reference number CEI/IEC/TR 61508-0:2005, 2005. Guide for EN 61508-1 to EN 61508-7.
- [324] EN 61508-1. Functional safety of electrical/electronic/programmable electronic safety-related systems - Part 1: General requirements. European Committee for Electrotechnical Standardization, CENELEC, Reference number EN 61508-0:2001 E, 2001. European Standard, Covers IEC 61508-1:1998 + corrigendum 1999.
- [325] EN 61508-2. Functional safety of electrical/electronic/programmable electronic safety-related systems - Part 2: Requirements for electrical/electronic/programmable electronic safety-related systems. European Committee for Electrotechnical Standardization, CENELEC, Reference number EN 61508-2:2001 E, 2001. European Standard, Covers IEC 61508-2:2000.
- [326] EN 61508-3. Functional safety of electrical/electronic/programmable electronic safety-related systems - Part 3: Software requirements. European Committee for Electrotechnical Standardization, CENELEC, Reference number EN 61508-3:2001 E, 2001. European Standard, Covers IEC 61508-3:1998 + corrigendum 1999.
- [327] EN 61508-4. Functional safety of electrical/electronic/programmable electronic safety-related systems - Part 4: Definitions and abbreviations. European Committee for Electrotechnical Standardization, CENELEC, Reference number EN 61508-4:2001 E, 2001. European Standard, Covers IEC 61508-4:1998 + corrigendum 1999.
- [328] EN 61508-5. Functional safety of electrical/electronic/programmable electronic safety-related systems - Part 5: Example of methods for the determination of safety integrity levels. European Committee for Electrotechnical Standardization, CENELEC, Reference number EN 61508-5:2001 E, 2001. European Standard, Covers IEC 61508-5:1998 + corrigendum 1999.
- [329] EN 61508-6. Functional safety of electrical/electronic/programmable electronic safety-related systems - Part 6: Guidelines on the application of IEC 61508-2 and IEC 61508-3. European Committee for Electrotechnical Standardization, CENELEC, Reference number EN 61508-6:2001 E, 2001. European Standard, Covers IEC 61508-6:2000.
- [330] EN 61508-7. Functional safety of electrical/electronic/programmable electronic safety-related systems - Part 7: Overview of techniques and measures. European Committee for Electrotechnical Standardization, CENELEC, Reference number EN 61508-7:2001 E, 2001. European Standard, Covers IEC 61508-7:2000.
- [331] AIChE CCPS. Guidelines for chemical process quantitative risk analysis, second edition. American Institute of Chemical Engineers, Center for Chemical Process Safety, New York, 2000.

- [332] Bedford T. and Cooke R. *Probabilistic Risk Analysis, Foundations and Methods*. Cambridge University Press, Cambridge, United Kingdom, 2001.
- [333] AIChE CCPS. Plant guidelines for technical management of chemical process safety. American Institute of Chemical Engineers, Center for Chemical Process Safety, New York, 1992.
- [334] Pasmaan H.J., Körvers P.M.W., and Sonnemans P.J.M. Some recent developments in process safety tools - Part II Precursor analysis. *Chemical Engineering Transactions*, 5:7–12, 2004.
- [335] Crawley F., Preston M., and Tyler B. HAZOP: Guide to best practice, guidelines to best practice for the process and chemical industries. IChemE, Warwickshire, United Kingdom, 2000.
- [336] Pasmaan H.J. and Vrijling J.K. Social risk assessment of large technical systems. *Human Factors and Ergonomics in Manufacturing*, 13:305–316, 2003.
- [337] AIChE CCPS. Layer of protection analysis, Simplified process risk assessment. American Institute of Chemical Engineers, Center for Chemical Process Safety, New York, 2001.
- [338] Pasmaan H.J., Schupp B., and Lemkowitz S.M. Complementing layer of protection analysis with economics. In *AIDIC Conference Series*, volume 6, pages 237–246. AIDIC & Reed Business Information, 2003.
- [339] Ooms G. A new method for the calculation of the plume path of gases emitted by a stack. *Atmospheric Environment*, 6:899–909, 1972.
- [340] Ooms G., Mahieu A.P., and Zelis F. The plume path of vent gases heavier than air. In C.H. Buschmann, editor, *International Symposium on Loss Prevention and Safety Promotion in the Process Industries, Delft, The Netherlands, 17–21 April, 1974*, pages 211–219, Amsterdam, 1974. Elsevier.
- [341] Ooms G. and Mahieu A.P. A comparison between a plume path model and a virtual point source model for a stack plume. *Applied Scientific Research*, 36:339–356, 1980.
- [342] Sluman T.J., van Maanen H.R.E., and Ooms G. Atmospheric boundary layer simulation in a wind-tunnel, using air injection. *Applied Scientific Research*, 36:289–307, 1980.
- [343] Li X.Y., Leijdens H., and Ooms G. An experimental verification of a theoretical model for the dispersion of a stack plume heavier than air. *Atmospheric Environment*, 20:1087–1094, 1986.
- [344] Casal J. *Evaluation of the effects and consequences of major accidents in industrial plants*. Industrial Safety Series. Elsevier, Amsterdam, 2008.
- [345] Perry R.H. and Green D.W. *Perry's Chemical Engineers' Handbook*. McGraw-Hill, New York, seventh edition, 1997.

- [346] Hauptmanns U. Semi-quantitative fault tree analysis for process plant safety using frequency and probability ranges. *Journal of Loss Prevention in the Process Industries*, 17:339–345, 2004.
- [347] Khan F.I. and Abbasi S.A. Analytical simulation and PROFAT II: A new methodology and a computer automated tool for fault tree analysis in chemical process industries. *Journal of Hazardous Materials*, 75:1–27, 2000.
- [348] Committee for the Prevention of Disasters. *Methods for the determination of possible damage to people and objects resulting from releases of hazardous materials, CPR 16E*. Publication Series on Dangerous Substances. The Dutch Ministry of the Interior and Kingdom Relations, The Hague, The Netherlands, first edition, 1992. Green Book, 2005 revision of the first edition published in 1992.