uc3m Universidad Carlos III de Madrid

Aero-thermochemical Systems

Academic Year: (2023 / 2024) Review date: 03-10-2023

Department assigned to the subject: Thermal and Fluids Engineering Department

Coordinating teacher: HUETE RUIZ DE LIRA, CESAR

Type: Compulsory ECTS Credits: 6.0

Year: 4 Semester: 2

REQUIREMENTS (SUBJECTS THAT ARE ASSUMED TO BE KNOWN)

Calculus I, II
Physics I, II
Chemical Fundaments of Engineering
Writing and Communication Skills
Programming
Thermal Engineering
Engineering Fluid Mechanics

SKILLS AND LEARNING OUTCOMES

CB1. Students have demonstrated possession and understanding of knowledge in an area of study that builds on the foundation of general secondary education, and is usually at a level that, while relying on advanced textbooks, also includes some aspects that involve knowledge from the cutting edge of their field of study.

CB2. Students are able to apply their knowledge to their work or vocation in a professional manner and possess the competences usually demonstrated through the development and defence of arguments and problem solving within their field of study.

CB3. Students have the ability to gather and interpret relevant data (usually within their field of study) in order to make judgements which include reflection on relevant social, scientific or ethical issues.

CB4. Students should be able to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences.

CB5. Students will have developed the learning skills necessary to undertake further study with a high degree of autonomy.

CG2. Apply computational and experimental tools for analysis and quantification of energy engineering problems

CG4. Being able to do design, analysis, calculation, manufacture, test, verification, diagnosis and maintenance of energetic systems and devices.

CG10. Being able to work in a multi-lingual and multidisciplinary environment

CE1 Módulo TE. Applied knowledge on thermal engineering.

CE14 Módulo TE. Knowledge of thermal power production machines and plants, as well as their industrial and environmental range.

CT1. Ability to communicate knowledge orally as well as in writing to a specialized and non-specialized public.

CT2. Ability to establish good interpersonal communication and to work in multidisciplinary and international teams.

CT3. Ability to organize and plan work, making appropriate decisions based on available information, gathering and interpreting relevant data to make sound judgement within the study area.

CT4. Motivation and ability to commit to lifelong autonomous learning to enable graduates to adapt to any new situation.

By the end of this content area, students will be able to have:

RA1.1 knowledge and understanding of the scientific principles underlying advanced issues in thermal engineering and fluid mechanics.

RA1.2 a systematic understanding of the key aspects and concepts of heat transfer.

RA1.3 coherent knowledge of their branch of engineering including some at the forefront of thermal engineering and fluid mechanics.

RA1.4 awareness of the wider multidisciplinary context of engineering.

RA2.1 the ability to apply their knowledge and understanding to identify, formulate and solve advanced problems within the field of thermal engineering and fluid mechanics using established methods.

- RA2.3 the ability to select and apply relevant analytic and modelling methods in the field of thermal engineering and fluid mechanics.
- RA3.1 the ability to apply their knowledge and understanding to develop and realise designs to meet defined and specified requirements within the field of thermal engineering and fluid mechanics.
- RA3.2 an understanding of design methodologies, and an ability to use them.
- RA4.1 the ability to conduct searches of literature, and to use data bases and other sources of information.
- RA5.1 the ability to select and use appropriate equipment, tools and methods.
- RA5.3 an advanced understanding of applicable techniques and methods within the field of thermal engineering and fluid mechanics, and of their limitations;
- RA6.1 function effectively as an individual and as a member of a team.

OBJECTIVES

The objective of this course is to provide the student a basic understanding of the science and technology of aerothermochemical systems.

Knowledge mastered in this course:

- Conservation equations for chemically reactive systems.
- Thermochemistry.
- Combustion kinetics.
- Knowledge of the main features of homogeneous reactive systems (critical extinction/ignition conditions, thermal and chain branching explosions, etc.).
- Fenomenologycal knowledge of flames.
- Mass energy balance on boilers and HRSG and performance analysis.
- Fossil Fuel-Fired Power Generation.
- Operational consideration on boilers and HRSG design, effects of Boilers and HRSG on plant efficiency.
- Determine the adequate methodology to obtain the required variables in an engineering problem (calculus, experiments, etc.).
- Present results in a rational manner, in terms of the relevant parameters.
- Comprehension of basic terminology to understand technical documentation and specific literature.

Specific capacities:

- Characterization of the composition of a mixture of ideal gases in terms of i) species mass fractions, ii) mole fractions and iii) molar concentrations.
- Determination of the composition of a chemically reacting ideal gas mixture in terms of the equivalence ratio.
- Determination of the adiabatic flame temperature of a chemically reactive mixture using atomconservation equations and chemical equilibrium conditions for the product gases.
- Determination of reduced reaction mechanisms by sistematic application of the steady state approximation to full detailed mechanism.
- Determination of the critical ignition and extinction conditions for steady combustion in a well-stirred adiabatic reactor.
- Solution of convection problems involving solid-liquid and solid-vapor systems where takes place a change in phase of a fluid.
- Solution of radiation heat transfer problems in the presence of participating media.
- Thermal design of Coal Fired boilers.
- Thermal design of HRSG.

General capabilities:

- Analysis based on scientific principles.
- Multidisciplinar approach (use knowledge from several disciplines: Thermodynamics,

Engineering Fluid Mechanics, Thermal Engineering, etc.)

Capacity to locate and understand basic literature on the subject.

Attitudes:

- Analytical attitude.
- Critical attitude.
- Cooperative attitude.

DESCRIPTION OF CONTENTS: PROGRAMME

The Aero-thermochemical Systems course is divided into two different parts: the first (Part I) deals with the fundamental aspects of the Aero-thermochemical conversion processes, mostly combustion reactions, and the second (Part II) adresses the study of conversion processes in the context of Aero-

thermochemical systems with industrial application.

- 1. The science of aerothermochemistry. (Part I)
- Historical perspective.
- Combustion as a science.
- Current developments.
- 2. Multicomponent mixtures. (Part I)
- Composition.
 - * Mass fractions.
 - * Molar fractions.
 - * Concentrations.
- Equations of state for ideal gas mixtures.
 - * The thermal equation of state.
 - * The caloric equation of state.
- 3. Thermochemistry. (Part I)
- Stoichiometric mixture.
- The equivalence ratio.
 - * Product composition for complete combustion.
 - + Lean combustion.
 - + Rich combustion.
- Adiabatic flame temperature.
 - * Definition.
 - * Heat of combustion.
- Sample calculations.
 - * Lean hydrogen-air combustion.
 - * Lean methane-air combustion.
- Complete vs. incomplete combustion.
 - * Major vs. minor species.
- Chemical equilibrium in reactive systems.
 - * The equilibrium constant.
 - * Dissociation of major species.
 - * Effect of temperature and pressure.
- Sample calculations.
 - * Dissociation of air.
 - * Adiabatic flame temperature and product composition of stoichiometric/rich H2 and HC-air mixtures.
- 4. Conservation equations for reactive systems in integral form. (Part I)
- Mass conservation equation.
- Species conservation equation.
- Momentum conservation equation.
- Energy conservation equation.
 - * Conservation equation of thermal enthalpy.
 - * The constant cp approximation.
 - * The rate of heat release.

- 5. Power systems and steam generators. (Part II)
- Transition from science to combustion technology.
- Fossil Fuel-Fired Power Generation (hereogeneous combustion of coal).
- Traditional and advanced burning technologies (IGCC, Chemical looping, Fuel cells, energy penalties of CO2 capture).
- Fundamentals on new process for power production.
- Environmental aspects.
 - * CO2 capture.
- Steam Generator as a way to reduce CO2 emissions.
- 6. Design of reactors for thermal conversion. (Part II)
- Fundamentals on material and energy balances

- Fundamentals on Thermal systems and reactor design for thermal conversion.
- General procedure for Material & Energy Balance Problems.
- Case Study.
- 7. Boilers and heat recovery steam generators (HRSG). (Part II)
- Principles of boiler operation.
- Classification of boilers.
 - * Water tube-boilers.
 - * Fire/smoke tube boilers.
- Boiler Specifications.
- Fundamentals of boiler heat transfer design.
- Fuel type.
- Boiler slagging and fouling.
- Fuel ash corrosion.
- Definitions used in boiler efficiency calculations.
- Heat absorption and efficiency calculations (Heat fired, steam generator efficiency direct and indirect method) (offdesign example)
- Pseudoadiabatic flame temperature.
- Combine cycle and cogeneration application of HRSG and waste heat boilers.
- Gas turbine HRSGs.
- Flue gas composition, gas pressure, fired and unfired modes.
- Design temperature profile calculations.
- Emission Control in HRSGs.
- Improving the HRSG efficiency.
- 8. Heat transfer in boilers and HRSGs. (Part II)
- Liquid side:
 - * Phase equilibrium and dimensional parameters in boiling and condensation.
 - * Boiling heat transfer.
 - * Boiling modes (The boiling curve).
 - * Pool boiling.
 - * Forced convection boiling (external, internal).
- * Special topic on Heat transfer in Fossil Fuel-Fired Power Generation: HEAT TRANSFER IN CONDENSERS: CLOSED FEEDWATER HEATERS, cFWH¿s.
- Gas side:
 - * Fundamentals.
 - + Gas side heat transfer in boilers and HRSGs.
 - + Gas radiation (nonluminous).
 - + Absorption coefficient and optical thickness.
 - + Absorptivity and emissivity.
 - + Radiative exchange in a gas filled enclosure.
 - + Particle matter radiation (luminous).
 - Heat radiation in furnaces, boilers and HRSGs.
 - + Heat Radiation models in Furnaces.
 - The speckled enclosure.
 - + Convective heating surfaces in boilers and HRSGs.
 - Finned and bare tubes.
 - Convection radiation problems in convective surfaces.
- 9. Thermal design of boilers and HRSG. (Part II)
- Coal-fired boilers design.
 - * Principles of Boiler Operation.
 - * Major steam-water boiler components.
 - * Steam Drum and steam water system.
 - * Furnace thermal design.
 - * The well-stirred combustion chamber model.
- HRSG boilers design.
 - * Water tube HRSG boiler design consideration.
 - * HRSG design issues.
 - * Thermal design aspects of unfired HRSG.
 - * Sizing of HRSG¿s.
 - * Case study.

- 10. Combustion kinetics. (Part I)
- Chemical kinetics
 - * The Law of mass action.
 - * The Arrhenius equation and the limit of high activation energy.
 - * Reaction constants and equilibrium constant.
- Global vs. elementary reactions in combustion processes
 - * Detailed and reduced mechanisms.
 - * One-step irreversible models.
 - * The characteristic reaction time.
 - * Hydrogen combustion. Types of elementary reactions.
 - * Hydrocarbon combustion.
- The steady state approximation.
 - * Combustion of hydrogen with chlorine
 - * Zel'dovich analysis of thermal NO production.
- 11. Combustion in homogeneous systems. (Part I)
- Steady combustion in a well-stirred adiabatic reactor.
 - * The Damköhler number.
 - * Ignition and extinction: The S-shaped curve.
- 12. Flames. (Part I)
- Premixed vs. Non-premixed flames.
- Premixed vs. Non-premixed flames.
- Non-premixed flames.

LEARNING ACTIVITIES AND METHODOLOGY

Teaching methodology will incluye:

- 1. Lectures: The students will be provided with lecture notes and recommended bibliography.
- 2. Problem solving sessions related with the course topics.
- 3. Homework problems aiming at student self-evaluation.
- 4. Development and interactive presentation of guided works, including three lab sessions as direct application of theory.

Additionally, collective tutorship could be included in the programme.

ASSESSMENT SYSTEM

ORDINARY CALL:

- Continuous evaluation (70% of the total grade)
- Final exam (30% of the total grade)

Contents:

- Practical problems that cover the topics of the subject
- Brief theoretical questions
- Test questions
- Laboratory reports

A minimum grade of 4 will be required in Part I and Part II to pass the course.

EXTRAORDINARY CALL:

- Final evaluation

Contents:

- Final exam of Part I (45% of the total grade)
- Delivery of problems and reports from Parts I and II (55% of the total grade)

A minimum grade of 4 will be required in Part I and Part II to pass the course.

% end-of-term-examination:	30

% of continuous assessment (assignments, laboratory, practicals...): 70

BASIC BIBLIOGRAPHY

- C. K. Law Combustion Physics, Cambridge Univ. Press, 2006
- F. P. Incropera Introduction to heat transfer, John Wiley & Sons, 2006
- G. F. Hewitt Process heat transfer, CRC Press, 1994
- I. Glassman Combustion, Academic Press, 1985
- K. K. Kuo Principles of Combustion, John Wiley & Sons, 1986
- K. Rayaprolu Boilers for power and process, CRC, 2009
- R. A. Strehlow Combustion Fundamentals, McGraw-Hill, 1985
- S. R. Turns An Introduction to Combustion, Mc. Graw Hill, 1996
- V. Ganapathy Industrial boilers and heat recovery steam generators: design, applications, and calculations, CRC Press, 2002

ADDITIONAL BIBLIOGRAPHY

- F. A. Williams Combustion Theory (2nd ed), Benjamin/Cummings, 1985
- J. D. Buckmaster & G. S. S. Ludford Theory of Laminar Flames, Cambridge Univ. Press, 1982
- R. C. Flagan & J. H. Seinfeld Fundamentals of Air Pollution Engineering, Prentice-Hall, 1988
- Y.B. Zeldovich, G.I. Barenblatt, V.B. Librovich & G.M. Makhviladze The Mathematical Theory of Combustion and Explosions, Consultants Bureau, 1985

BASIC ELECTRONIC RESOURCES

- Biblioteca E.T.S.I.Aeronáuticos (UPM) . Aerothermochemistry, 50 años de su publicación, Gregoria Millán y el grupo de combustión: http://aerobib.aero.upm.es/millan/Index.htm
- Chris Morley . GasEq: http://www.gaseq.co.uk/
- N. Peters . Fifteen Lectures on Laminar and Turbulent Combustion: http://decane.itv.rwthaachen.de/fileadmin/LehreSeminar/Combustion/SummerSchool.pdf
- NASA . ThermoBuild: http://www.grc.nasa.gov/WWW/CEAWeb/ceaThermoBuild.htm