uc3m Universidad Carlos III de Madrid

Combustion

Academic Year: (2021 / 2022) Review date: 10-06-2021

Department assigned to the subject: Thermal and Fluids Engineering Department

Coordinating teacher: VERA COELLO, MARCOS

Type: Electives ECTS Credits: 6.0

Year: 1 Semester: 2

REQUIREMENTS (SUBJECTS THAT ARE ASSUMED TO BE KNOWN)

Ordinary Differential Equations / Dynamic Systems
Partial Differential Equations
The student should have studied, or be studying, the Basic Modeling course

OBJECTIVES

COMPETENCES

Possess and understand knowledge that provides a basis or opportunity to be original in the development and/or application of ideas, often in a research context, knowing how to translate industrial needs in terms of R&D projects in the field of Industrial Mathematics:

Know how to apply acquired knowledge and problem solving skills in new or unfamiliar environments within broader contexts, including the ability to integrate into multidisciplinary R&D teams in the business environment;

Know how to communicate the conclusions, together with the latest knowledge and reasons that support them, to specialized and non-specialized audiences in a clear and unambiguous way;

Have the learning skills that allow the student to continue studying in a way that will be largely self-directed or autonomous, and able to undertake successful doctoral studies.

Achieve a basic knowledge in an area of ¿¿Engineering / Applied Sciences, as a starting point for an adequate mathematical modeling, both in well established contexts and in new or little known environments within broader and multidisciplinary contexts.

To model specific ingredients and make the appropriate simplifications in the model that facilitate their numerical treatment, maintaining the degree of precision, according to previously established requirements.

To be able to validate and interpret the obtained results, comparing with visualizations, experimental measures and / or functional requirements of the corresponding physical / engineering system.

Know how to model complex elements and systems or in poorly established fields, leading to well thought out / formulated problems.

LEARNING OUTCOMES

Understand some of the most complex problems of an application field in the field of Engineering and Applied Sciences Know how to model complex elements in this field of application, including the degree of approximation made.

Understand the difficulties that both the numerical simulation and the analysis of these models poses.

DESCRIPTION OF CONTENTS: PROGRAMME

- 1. Introduction
- Historical Perspective
- The science of combustion
- Future Developments

2. Conservation equations for reactive flows

- Multicomponent mixtures
 - * Mass fractions
 - * Molar fractions
 - * Molar concentrations
- Equations of state for ideal gas mixtures
 - * Thermal equation of state
 - * Caloric equation of state
- Molecular transport in multicomponent mixtures
 - * Diffusion velocities
 - * Multicomponent transport
 - * Usual simplifications in combustion problems
- Conservation equations
 - * Mass
 - * Linear momentum
 - * Species
 - * Energy
- Characteristic scales and dimensionless numbers

3. Thermochemistry

- The assumption of complete combustion
 - * Stoichiometric mixture
 - * Equivalence ratio
 - * Composition of the product mixture in complete combustion
 - + Lean combustion
 - + Rich combustion
- Adiabatic flame temperature
 - * Definition
 - * Heat of combustion
 - * Calculation of the adiabatic flame temperature
 - + Variable cp
 - + Constant cp
- Complete combustion vs. incomplete combustion
 - * Major and minor species
- Chemical equilibrium in reactive mixtures
 - * The equilibrium constant
 - * Dissociation of the major species
 - * Effect of temperature and pressure

4. Combustion kinetics

- Chemical kinetics
 - * Types of elementary reactions
 - * Detailed and reduced mechanisms
 - * One-step mechanism
 - * The limit of high activation energy
- Rate of heat release by chemical reaction
- Steady state assumption
- Partial equilibrium assumption
- Examples
 - * Hydrogen combustion
 - * Hydrocarbon combustion
 - * Zeldovich analysis for the production of NOx

5. Combustion in systems with homogeneous composition

- Conservation equations for systems with homogeneous composition
- Adiabatic combustion in a well-stirred reactor. Steady solutions
 - * The number of Damköhler
 - * Ignition and extinction: The S-shaped curve
- Frank-Kamenetskii theory of thermal explosions
- Chain-branching explosions
 - * Explosion limits in H2-O2 mixtures
 - * Explosion limits in HC-O2 mixtures

- Spontaneous ignition in a combustion chamber with variable volume
- Other ignition processes
- 6. Fronts reagents: Detonation and deflagration
- Rankine-Hugoniot relations
- Detonation
 - * ZND Structure
 - * Galloping "detonations"
 - * Actual structure of detonations
- Deflagrations or premixed flames
 - * Internal structure
 - * Laminar flame speed
 - + Variation with pressure and equivalence ratio
 - * Minimum Ignition Energy
 - * Quenching distance
 - * Flammability limits

7. Diffusion Flames

- non-premixed combustion
- Relevant thermochemical parameters
- The limit of infinitely fast reaction
- Finite-rate effects
 - * Counterflow diffusion flames
 - * Ignition and extinction: The S-shaped curve
- Examples
 - * Jet diffusion flames
 - * Non-premixed flame-vortex interactions
- 8. Evaporation and combustion of droplets and sprays
- Droplet evaporation
- Droplet combustion
- Homogenised description of spray combustion
- 9. Combustion instabilities
- Flame stretch and curvature
- Thermo-diffusive instability
- Hydrodynamic instability
- Thermoacoustic instability
- 10. Turbulent combustion
- Premixed turbulent combustion
 - * Characteritis scales
 - * Diagram of regimes
 - * Turbulent flame speed
- Non-premixed turbulent combustion
 - * Characteritis scales
 - * Diagram of regimes
 - * Turbulent jet diffusion flames

LEARNING ACTIVITIES AND METHODOLOGY

Use of board for discussion of theoretical concepts and illustrative examples.

ASSESSMENT SYSTEM

The students must show sufficient command of theoretical and applied concepts. The grade will be based on the solution of 4 homeworks related to the course contents.

In the extraordinary call the students can submit those works that have not been delivered during the continuous assessment, or have obtained a grade of less than 5 out of 10.

% end-of-term-examination:	60
% of continuous assessment (assigments, laboratory, practicals):	40

BASIC BIBLIOGRAPHY

- A. Liñán & F. A. Williams Fundamental Aspects of Combustion, Oxford University Press, 1993
- D. A. Frank-Kamenetskii Diffusion and Heat Transfer in Chemical Kinetics, Plenum Press, 1969
- D. E. Rosner Transport Processes in Chemically Reacting Flow Systems, Dover, 2000
- F. A. Williams Combustion Theory, Benjamin-Cummings, 1985
- N. Peters Turbulent Combustion, Cambridge University Press, 2000