2EL1440 – Modeling and numerical simulation of reactive media

Instructors: Benoît Fiorina
Department: DÉPARTEMENT MÉCANIQUE ENERGÉTIQUE PROCÉDÉS
Language of instruction: ANGLAIS
Campus: CAMPUS DE PARIS - SACLAY
Workload (HEE): 60
On-site hours (HPE): 35,00
Elective Category : Engineering Sciences
Advanced level : No

Description

Reactive media cover a vast field of studies that fit perfectly into the current energy and environmental context. From a scientific point of view, reactive media include combustion and plasmas. From one side, combustion accounts for 80% of primary energy conversion, and is present in the energy, transport and process sectors. On the other side, plasmas represent more than 99% of the visible matter in the universe. Plasma are used in a wide range of industrial applications: energy, semiconductor manufacturing, transformation and treatment processes, and health.

The aim of this course is to introduce fundamentals of combustion and plasmas. It focuses on the importance of numerical modelling, which is a key element of research and development strategies in reactive systems engineering. To illustrate the field of application of reactive media in the field of energy, students will build a multi-physics numerical tool to simulate an emerging and promising technology based on plasma-assisted combustion of a hydrogen turbine.

Quarter number

SG6

Prerequisites (in terms of CS courses)

none

Syllabus

1. General introduction. Industrial applications and scientific challenges
    a. Combustion - (1h30)

b. Plasmas – (1h30)

2. Description of a reactive system
   a. Lecture (1h30)
      i. Chemical thermodynamics
      ii. Mixture equivalence ratio
      iii. Computation of burnt gases temperature
   b. Class Work (1h30) “Decreasing CO2 emissions by addition of di-hydrogen”

3. Numerical tools
   a. Matlab initiation (1h30)
      i. Using Matlab basic functions
      ii. Using the chemical package
   b. Class Work (1h30) “Computation of adiabatic combustion temperature of H2-O2 and H2-air reactive systems under global-step reaction assumption ”

4. Thermodynamical equilibrium
   a. Lecture (1h30)
      i. Second law of thermodynamic
      ii. Methods for computing chemical equilibrium state
   b. Class Work (1h30) “Computation of equilibrium composition in H2-O2 and H2-air reactive systems ”

5. Combustion chemical kinetics
   a. Lecture (1h30)
   b. Class Work (1h30) “Computation of auto-ignition in a constant pressure reactor”

6. Plasma production from electric discharges
   a. Lecture (1h30)
   b. Class Work and experimental demonstration (1h30)

7. Two temperature chemical kinetics in plasma
   a. Lecture (1h30)
   b. Class Work (1h30)

8. Optimization of energy in plasma discharges
   a. Lecture (1h30)
   b. Class Work (1h30)

9. Plasma assisted combustion
   a. Experiments and models (0h45)
   b. Simulations (0h45)
   c. EM2C visit and mini-project presentation (1h30)

10. Mini-project : numerical simulation of plasma-assisted combustion (3h00)

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Class components (lecture, labs, etc.)
Lecture, tutorial and computer work

Grading
Restitution of the work carried out in TD and during the mini-project in the form of an oral presentation

Course support, bibliography
Nasser Darabiha, Emile Esposito, François Lacas et Denis Veynante, Poly de combustion de CentraleSupélec.
- Kenneth Kuo, Principle of Combustion, published by John Wiley & Son, 2005
- Principles of Plasma Discharges and Materials Processing, Michael A. Lieberman and Allan J. Lichtenberg, John Wiley and Sons, New York, 2nd edition, 2005
- Partially Ionized Gases, M. Mitchner and C.H. Kruger, John Wiley & Sons, New York, 1973.
- Gas Discharge Physics, Yu. P. Raizer, Springer Verlag, Berlin, 1997

Resources
Teaching team: Pr. Benoît Fiorina and Pr. Christophe Laux.

Learning outcomes covered on the course

To dimension reactive systems, an engineer has to make approximations and calculate orders of magnitude. He has to calculate mass, chemical species and energy balances. He must determine the thermochemical equilibrium of a reactive system and know how to exploit thermochemical imbalances. In particular, this course provides the following skills:

- Understand the industrial, energy and environmental stakes of combustion and plasmas.
- Be able to establish the fundamental equations for dimensioning combustion and plasma systems
- Characterize the thermodynamic and chemical transient and equilibrium states of a reactive system

-Be able to program (under Matlab environment) a numerical simulation tool for chemical reactors with detailed kinetics. The code developed by the student will be based on a MATLAB library of pre-existing thermochemical functions.

Description of the skills acquired at the end of the course

To design reactive systems, engineers must make approximations and calculate orders of magnitude. They must carry out mass, chemical and energy balances. They must determine the thermo-chemical equilibrium of a reactive system and know how to exploit thermo-chemical imbalances. This course provides for that purpose the following skills:
- Understand the industrial, energy and environmental challenges of combustion and plasmas
- Establish the fundamental equations for designing combustion and plasma systems
- Characterize the thermochemical transient and equilibrium states of a reactive system
- Program (under Matlab environment) a numerical tool for chemical reactors with detailed kinetics. The code developed by the students will be based on a pre-existing MATLAB library of thermochemical functions.