

POLITECNICO
MILANO 1863

Iran First International Combustion School (ICS2019)
Tehran, 24-26 August 2019

Combustion Modeling

Presentation of short course on Combustion Modeling

Alberto Cuoci

About me...

Alberto Cuoci

Department of Chemistry, Materials and
Chemical Engineering
Politecnico di Milano
P.zza Leonardo da Vinci 32
20133 Milano (Italy)



Email: alberto.cuoci@polimi.it

Github: <https://github.com/acuoci>

Scopus ID: [55906162200](https://scopus.org/authorid/55906162200)

ResearchGate: https://www.researchgate.net/profile/Alberto_Cuoci

Linkedin: <https://www.linkedin.com/in/alberto-cuoci-61b1b827>

ORCID: <http://orcid.org/0000-0001-5653-0180>

About this course...

Objectives

- i. to introduce the **main methodologies and techniques** that constitute the basis of combustion modeling
- ii. to make the students more familiar with the **numerical implementation** of those techniques
- iii. to cover a range of **modern/advanced techniques for numerical modeling of combustion**, aiming to provide students with a general knowledge and understanding of the subject, including recommendations for further studies.

Organization

6 modules (1.5 or 2 hours) on Combustion Modeling

Material for training sessions is provided (see next slides)

Topics

governing equations of reacting flows, numerical methods for solving 1D and multidimensional reacting flows, advanced techniques for combustion modeling with emphasis on detailed chemistry, turbulent combustion modeling

About this course...

Slides and material about the training sessions are available at the following GitHub page:

<https://github.com/acuoci/ICS2019>

I will keep the repository online and active during the next months.

If you find errors in the published material, please send me an email, so I can fix them:

alberto.cuoci@polimi.it

The screenshot displays the GitHub interface for the repository `acuoci/ICS2019`. At the top, there are navigation tabs for Code, Issues, Pull requests, Projects, Wiki, Security, Insights, and Settings. Below these, the repository name and a 'Private' label are shown, along with statistics for Unwatch (1), Star (0), and Fork (0). The main section is titled 'Combustion Modeling - Iran First International Combustion School (ICS2019)'. It features a table with 14 commits, 1 branch, 0 releases, 1 contributor, and CC BY 4.0 license. The table lists recent commits by user 'acuoci', including 'Merge branch 'master' of https://github.com/acuoci/ICS2019', 'Create Lesson_6.pdf', 'Added kinetic mechanisms for training sessions', 'Initial commit' for .gitattributes, .gitignore, LICENSE, and README.md. Below the table, the README.md file is open, showing the title 'ICS2019', the subtitle 'Combustion Modeling - Iran First International Combustion School (ICS2019)', and the section 'Lessons on Combustion Modeling'. Under this section, 'Lesson 1: Governing equations, thermodynamics, kinetics, and transport properties (~1.5 h)' is listed with a bulleted list of topics: Presentation of the course, learning objectives, organization; Transport equations (Continuity and momentum equations, Conservation of species; diffusion fluxes (Stefan-Maxwell theory, Fick diffusion, Soret effect), Energy equation: enthalpy and temperature formulations; Basics of thermodynamics, kinetics, and transport properties (Enthalpy and specific heats, NASA polynomial formalism, Kinetic parameters, reaction rate, reversible reactions, equilibrium constant, examples of kinetic mechanisms in

- **Lesson 1:** Governing equations, thermodynamics, kinetics, and transport properties (~1.5 h)
- **Lesson 2:** Numerical algorithms for reactive flows (~2 h)
- **Lesson 3:** Numerical methods for 1D and multi-dimensional flames (~2 h)
- **Lesson 4:** Advanced techniques for reacting flows with detailed kinetics (~1.5 h)
- **Lesson 5:** Introduction to numerical modeling of turbulent reacting flows (~1.5 h)
- **Lesson 6:** Turbulent combustion modeling (~2 h)

- **Lesson 1:** Governing equations, thermodynamics, kinetics, and transport properties (~1.5 h)
- **Lesson 2:** Numerical algorithms for reactive flows (~2 h)
- **Lesson 3:** Numerical methods for 1D and multi-dimensional flames (~2 h)
Numerical methods for combustion
- **Lesson 4:** Advanced techniques for reacting flows with detailed kinetics (~1.5 h)
- **Lesson 5:** Introduction to numerical modeling of turbulent reacting flows (~1.5 h)
- **Lesson 6:** Turbulent combustion modeling (~2 h)

Syllabus

- **Lesson 1:** Governing equations, thermodynamics, kinetics, and transport properties (~1.5 h)
- **Lesson 2:** Numerical algorithms for reactive flows (~2 h)
- **Lesson 3:** Numerical methods for 1D and multi-dimensional flames (~2 h)
- **Lesson 4:** Advanced techniques for reacting flows with detailed kinetics (~1.5 h) **Combustion and detailed chemistry**
- **Lesson 5:** Introduction to numerical modeling of turbulent reacting flows (~1.5 h)
- **Lesson 6:** Turbulent combustion modeling (~2 h)

Syllabus

- **Lesson 1:** Governing equations, thermodynamics, kinetics, and transport properties (~1.5 h)
- **Lesson 2:** Numerical algorithms for reactive flows (~2 h)
- **Lesson 3:** Numerical methods for 1D and multi-dimensional flames (~2 h)
- **Lesson 4:** Advanced techniques for reacting flows with detailed kinetics (~1.5 h)
- **Lesson 5:** Introduction to numerical modeling of turbulent reacting flows (~1.5 h)
- **Lesson 6:** Turbulent combustion modeling (~2 h)

Turbulent Combustion

Training sessions (I)

No training sessions are scheduled during the short course on Combustion Modeling. However, material (detailed instructions, software, input files, short comments on results) for self-assessed training sessions is provided in the same GitHub repository.

Feel free to contact me during the course or later for additional explanations, comments, etc.

The training sessions are based on numerical tools developed in my research group and freely available on the web:

- OpenSMOKE++ Suite: <https://www.opensmokepp.polimi.it/> (registration is required)
- laminarSMOKE: <https://github.com/acuoci/laminarSMOKE> (it requires OpenFOAM)
- flameletsSMOKE: <https://github.com/acuoci/flameletSMOKE> (it requires OpenFOAM)

Training sessions (II)

Training Session 1 (OpenSMOKE++ Suite)

Pre-processing of kinetic mechanisms, thermodynamic equilibrium and adiabatic flame temperature

Training Session 2 (OpenSMOKE++ Suite)

Numerical simulation of 0D reacting systems: batch reactor (ignition delay times) and perfectly stirred reactor (speciation)

Training Session 3 (OpenSMOKE++ Suite)

Numerical modeling of 1D flames: laminar premixed flames and laminar flame speed

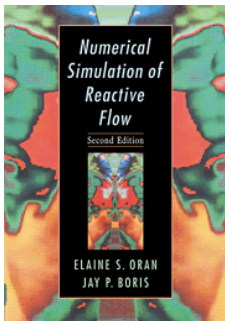
Training Session 4 (laminarSMOKE)

Simulation of a laminar coflow flame fed with a mixture of H₂/N₂ and air. Tutorial available at <https://github.com/acuoci/laminarSMOKE/tree/master/run/validation/ToroFlames/F3>

Training Session 5 (flameletSMOKE)

Simulation of Sandia CO/H₂/N₂ turbulent jet flame via Steady Laminar Flamelet model. Tutorial available at <https://github.com/acuoci/flameletSMOKE/tree/master/cases>

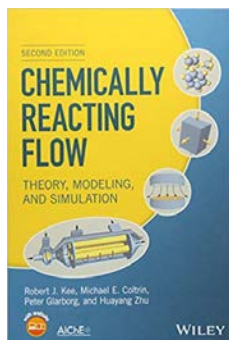
Textbooks on reacting flows



Oran E.S., Boris J.P

Numerical Simulation of Reactive Flow

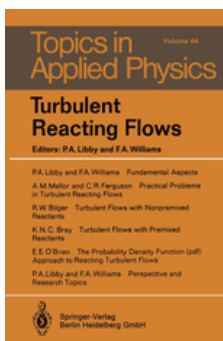
Cambridge University Press (2001)



R.J. Kee, M.E. Coltrin, P. Glarborg

Chemically Reacting Flow: Theory and Practice

Wiley, 2 edition, 2017

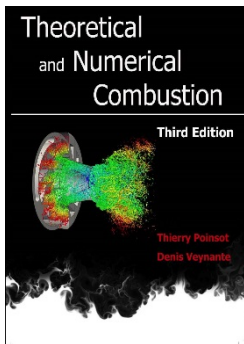


Libby A.L., Williams F. A.

Turbulent Reacting Flows

Academic Press, 1994

Textbooks on turbulent combustion modeling



Poinso T., Veynante D.

"Theoretical and Numerical Combustion"

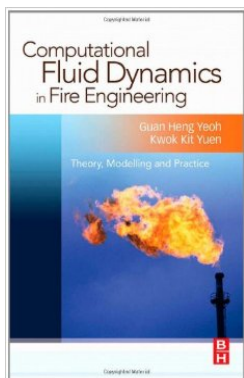
R.T. Edwards, 2nd Edition, 2005



Peters N.

"Turbulent Combustion"

Cambridge University Press, 2000



Yeoh G.H., Yuen K.K.

"Computational Fluid Dynamics in Fire Engineering Theory, Modelling and Practice"

Butterworth-Heinemann Ltd, 2009