AAE590 COMPUTATIONAL COMBUSTION ANS PROPULSION

(Spring 2023, T/Th)

(12:00pm - 1:15pm, ARMS 1021)

(This class is flipped. We meet online on Tuesdays and in person on Thursdays.)

PROFESSOR HAIFENG WANG

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Email: haifeng@purdue.edu
Office Hours: by email appointment only.

COURSE DESCRIPTION:

- Fundamentals of thermochemistry
- Chemical equilibrium and its calculation
- Chemical kinetics and auto-ignition.
- Laminar non-premixed flames and computation of an opposed jet flame.
- Laminar premixed flames and calculation of the laminar flame speed.
- Models for turbulent combustion (the flamelet model and the transported probability density function model).
- Turbulent non-premixed combustion and the modeling and simulation of a turbulent free jet flame.
- Turbulent partial premixed combustion and the modeling and simulation of a turbulent lifted jet flame.
- Computational propulsion and the modeling of a model rocket combustor
- [Tentative] Advanced topics on data-driven modeling and machine learning.

The course consists of lectures and computer projects.

PREREQUISITES:

Sufficient knowledge on fundamentals of combustion theory (ME525 or equivalent), turbulence (ME611, AAE626, or equivalent), computational fluid dynamics (AAE412, AAE512, or equivalent), and at least one modern programming language (MATLAB, FORTRAN, C/C++ etc.). Students who do not meet the prerequisites should get the instructor's permission to enroll.

COURSE GOALS:

Students are expected to learn the fundamentals and skills for performing combustion modeling and simulations, as well as the status of the frontier turbulent combustion research.

LEARNING OBJECTIVES:

- Calculate chemical equilibrium;
- Calculate rate of chemical reaction and compute auto-ignition process;
- Compute opposed jet flames and understand characteristics of non-premixed combustion;

- Compute laminar flame speed and understand characteristics of premixed combustion;
- Understand turbulent combustion problems and the advanced modeling approaches;
- Choose appropriate models for turbulent combustion problems and perform turbulent combustion simulations.

TEXTBOOKS AND OHER RESOURCES

It is recommended that you buy a modern text on combustion (e.g., Turns) and turbulence (e.g., Pope). All books are "recommended".

Combustion

S.R. Turns, *An Introduction to Combustion*, McGraw Hill
J. Warnatz, U. Maas and R.W. Dibble, *Combustion*, Springer

More Specialized

R.J. Kee, M.E. Coltrin and P. Glarborg, *Chemically Reacting Flow*, Wiley
T. Poinsot and D. Veynante, *Theoretical and Numerical Combustion*, Edwards
R.O. Fox, *Computational Models for Turbulent Reacting Flows*, Cambridge
S.B. Pope, *Turbulent Flows*, Cambridge

Numerical Methods

W.H. Press, S.A. Teukolsky, W.T. Vetterling and B. P. Flannery, *Numerical Recipes in Fortran*, Cambridge
K.E. Brenan, S.L. Campbell and L.R. Petzold, *Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations*, SIAM

TOPICS AND PROJECTS

There are in total 8 topics, each being covered in approximately 2-3 weeks, and with a project for it.

- Topic 1. Thermochemistry
- Topic 2. Chemical kinetics
- Topic 3. Premixed laminar flames
- Topic 4. Nonpremixed laminar flames
- Topic 5. Turbulence modeling of jet flames
- Topic 6. Simple models of non-premixed jet flames
- Topic 7. Transported PDF methods
- Topic 8. Computational propulsion

There are 25 lectures and 8 computer projects. All the lectures are provided as recorded videos (except Lecture 1). The computer projects will be done in ANSYS FLUENT. There are two learning pathways that can be followed as shown below to fulfil the course requirements. Learning Path 1 focuses more on advanced combustion modeling, and Learning Path 2 focuses more on computational propulsion. Every student must pick one and only one path and follow it.

Lecture Videos (LecV)	Computer Projects (CP)	Learning Path 1	Learning Path 2
Lecture 1: Introduction		◆	◆
Lecture 2: In compressible assumption		◆	◆
Lecture 3: Flame examples		◆	◆
Lecture 4: Thermodynamic properties		◆	◆
Lecture 5: Chemical equilibrium	Project 1 (finish Lecture 5)	◆	◆
Lecture 6: Chemical kinetics-I		◆	◆
Lecture 7: Chemical kinetics-II		◆	◆
Lecture 8: Chemical kinetics-III	Project 2 (finish Lecture 8)	◆	◆
Lecture 9: Laminar premixed flame I		◆	◆
Lecture 10: Laminar premixed flame II	Project 3 (finish Lecture 10)	◆	◆
Lecture 11: Laminar non-premixed flame I		◆	◆
Lecture 12: Laminar non-premixed flame II	Project 4 (finish Lecture 12)	◆	◆
Lecture 13: Turbulence modeling I		◆	◆
Lecture 14: Turbulence modeling II		◆	◆
Lecture 15: Turbulence modeling III	Project 5 (finish Lecture 15)	◆	◆
Lecture 16: Turbulent combustion with equilibrium chemistry model		◆	◆
Lecture 17: Turbulent combustion with flamelet model	Project 6 (finish Lecture 17)	◆	
Lecture 18: Turbulent combustion with PDF methods (composition space)		◆	
Lecture 19: Turbulent combustion with PDF methods (PDF transport equations)		◆	
Lecture 20: Turbulent combustion with PDF methods (model implementation)	Project 7 (finish Lecture 20)	◆	
Lecture 21: Turbulent combustion with PDF methods (efficient chemistry implementation)		◆	
Lecture 22*: Computational propulsion			◆
Lecture 23*: Computational propulsion	Project 8 (finish Lecture 23)		◆
Lecture 24*: Computational propulsion			◆
Lecture 25*: Computational propulsion			◆

CLASS ARRANGEMENT

This is a flipped classroom. The learning is done mostly outside of the class by watching the lecture videos (LecV) online. The class time is used for questions, discussions, project demonstration, project review, and additional topics not covered by the lecture videos.

The Tuesday's class is online and mainly used as Q/A office hour. The attendance is optional. The class will NOT be recorded. Please bring your questions to the meeting. I will NOT discuss anything other than answering questions. Please join the meeting through this LINK

The Thursday's class is in-person and will cover Q/A, free discussions, project demonstration, project review, and additional topics. The class will be recorded and made available online through BoilerCast.

COURSE WEBSITE AND TOOLS

Purdue Brightspace (https://purdue.brightspace.com) is used to organize the course contents such as announcements, course notes, homework assignments, grades, and solutions. Please check Brightspace frequently to get the latest update.

MISCELLANEOUS

General Course Policies

Students are required to take all the lectures online following their Learning Path choice. For questions or concerns arising from the course, students are encouraged to communicate with the instructor.

Absence

Attendence on Tuesday's online meeting is optional. Attendence on Thursday's class is recommended. The Thursday's class will be recorded and made available via BoilerCast.

Computer projects

The computer projects will be assigned approximately every one to two weeks. They may be assigned early if the topic has been finished. Plenty of time will be given to finish the project. You are encouraged to form groups to work on the project together and get help from each other. Your report, however, should be your own. Copying or duplicating other's work in your report is not allowed. Your reports need to be submitted before the due date. In general, no late reports will be accepted, so plan early and make sure that you will be able to hand in your report in time. All project reports should be submitted to Brightspace.

Software tools

The computer projects require MATLAB and ANSYS FLUENT. Please manage to get both. The AAE computer lab (ARMS2106) has all the required software for this course..

Exams and Grades

There will be no exams. There are computer projects in this course. Students are required to do these projects and submit written reports. The final grades are based on the submitted project reports.

Office Hours

There is no additional office hour. If a private meeting is needed, please email me. It is recommended to use the class time during the Tuesday's online meeting or Thursday's in-person meeting to ask questions.

Integrity and Code of Conduct

Students in this course are expected to abide by the Purdue University Statement of Integrity and Code of Conduct. Any work submitted by a student in this course for academic credit will be the student's own work. Purdue's student guide on Academic Integrity is available at http://www.purdue.edu/odos/aboutodos/academicintegrity.php.

Emergency

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Here are ways to get information about changes in this course. Brightspace web page, my email address:haifeng@purdue.edu, and my office phone: 494-4093.

The course syllabus is subject to change at the discretion of the instructor.

LecV=Lecture Video **CP=Computer Porject**
Q&A=Online Q&A Meeting **InpM=In-person Meeting**

	Mon	Tues	Wed	Thur	Fri
Week 1	January 9	January 10	January 11	January 12	January 13
		LecV1 (intro.), LecV2 (incompress.) InpM		LecV3 (flame examples) InpM	
Week 2	January 16	January 17	January 18	January 19	January 20
	MLK day (no class)	LecV4 (thermodynamic properties)/Q&A		LecV5 (Chem. Equil.) InpM CP1 demo	
Week 3	January 23	January 24	January 25	January 26	January 27
		LecV6 (chem. kinetics-I)/Q&A		LecV7 (chem. kinetics-II) InpM	
Week 4	January 30	January 31	February 1	February 2	February 3
		LecV8 (chem. kinetics-III) /Q&A		LecV9 (Lam. premixed I) InpM CP2 demo/CP1 due	
Week 5	February 6	February 7	February 8	February 9	February 10
		LecV10 (Lam. premixed II) /Q&A		LecV11 (Lam. non-premixed I) InpM CP3 demo	
Week 6	February 13	February 14	February 15	February 16	February 17
		LecV12 (Lam. non-premixed II) /Q&A		InpM CP4 demo/CP2 due	
Week 7	February 20	February 21	February 22	February 23	February 24
		LecV13 (Turbul. Model I)/Q&A		InpM CP3 due	
Week 8	February 27	February 28	March 1	March 2	March 3
		LecV14 (Turbul. Model II) /Q&A		LecV15 (Turbul. Model III) InpM CP5 demo/CP4	
Week 9	March 6	March 7	March 8	March 9	March 10
		LecV16 (Equil. Chem. Model) /Q&A		InpM	
Week 10	March 13	March 14	March 15	March 16	March 17
	SP VAC	SP VAC	SP VAC	SP VAC	SP VAC
Week 11	March 20	March 21	March 22	March 23	March 24
		LecV17 (Flamelet Model) LecV22* (Comp. Propulsion) /Q&A		InpM CP6 demo/CP5 due	
Week 12	March 27	March 28	March 29	March 30	March 31
		LecV18 (PDF - Composition Space) LecV23* (Comp. Propulsion) /Q&A		LecV19 (PDF – Equations) InpM CP8* demo	
Week 13	April 3	April 4	April 5	April 6	April 7
		LecV20 (PDF - Implementation) LecV24* (Comp. Propulsion) /Q&A		InpM CP7 demo/CP6 due	
Week 14	April 10	April 11	April 12	April 13	April 14
		LecV21 (Efficient Chem. Implementation) LecV25* (Com. Propulsion) /Q&A		InpM CP8* due	
Week 15	April 17	April 18	April 19	April 20	April 21
		/Q&A		InpM CP7 due	
Week 16	April 24	April 25	April 26	April 27	April 28
		Quiet Week		InpM /Quiet Week	
Week 17	May 1	May 2	May 3	May 4	May 5
		Final Exam Week		no Final Exam	