Combustion Group

CTR Summer Program 2014

Group members:
Thierry Poinsot, Emilien Courtine, Luc Vervisch, Benjamin Farcy, Franck Nicoud, Michael Bauerheim, Matthew Juniper, Luca Magri, Wolfgang Polifke, Camilo Silva, Benedicte Cuenot, Peter Hamlington, Colin Towery, Alexei Poludnenko, Evatt Hawkes, Shahram Karami
Introduction

Energy consumption

- Fossil and hydrocarbon-based fuels remain major energy source for transportation and power-generation
  - Current energy supply from fossil fuel sources: >70%
  - Energy consumption by transportation sector: 30%
Introduction

Research needs

- Rapidly increasing energy consumption in emerging markets
- Increasingly stringent emission regulations: GHG, NOx, Soot
- Emerging fuel sources: biofuels, renewable fuels, fuel-flexible engine and propulsion systems
- New combustion and energy-conversion concepts
Introduction

Combustion research thrusts

- Combustion Dynamics and Flame-Stabilization
- Combustion Physics
- Combustion Modeling and Numerical Methods
- Pollutants, Emissions, and Soot Formation
- Uncertainty Quantification and System Identification
- Reaction Chemistry and Chemical Mechanisms

Research objectives

- Obtain fundamental understanding of combustion-physical processes
- Control and mitigation of pollutant emissions
- Develop combustion models for prediction of
  - Combustor performance and efficiency
  - Pollutant formation
  - Stability and combustion dynamics; lean operation; flame stabilization
- Enable utilization of alternative and bio-renewable fuels
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Research focus

- Assess closure models for low-order modeling of thermo-acoustics instabilities
- Adjoint sensitivity analysis of coupling between hydrodynamic and thermo-acoustic instabilities in confined combustor systems
- Develop methods for robust evaluation of flame-transfer function in presence of combustion noise and flow-field perturbations
- Determine propensity of thermo-acoustic instabilities using uncertainty quantification
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Research focus

- Fundamental analysis of energy transfer from small-to-large scales in turbulent premixed flames; characterization of backscattering and assessment of multiscale effects on SGS-models
- Development of closure models for premixed flames: baroclinic torque
- Analysis of flame-stabilization in premixed flames and development of closure models using leading-edge point theory
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Research focus

- Develop LES soot-models for application to real combustors; assess model approximations and coupling between chemistry, turbulence and soot production
- Characterization of soot/radiation interaction
- Analysis of DeNOx configurations under consideration of coupling between turbulence, spray, and NO-oxidation using ammonia

![Graph showing Take-Off Landing-Cycle NOx emissions over years 1970, 1980, and 1990 with pressure ratio on the x-axis and NOx emissions on the y-axis.]
Introduction

CTR Summer Program

- 10 Research projects
- Contributions from: France, Germany, USA, UK, Australia, Canada

Stanford Hosts

- Graduate students: Jeff O’Brien, Peter Ma, Chris Ivy
- Post-docs/Research associates: Benedetta Franzelli, Yee Chee See, Javier Urzay

Tutorials:

- Iain Boyd: Radiation Modeling
  Location: Braun Lecture Hall, 4:00 – 5:30pm, 7/18/2014
- Matthew Juniper: Combustion Instabilities
  Location: Braun Lecture Hall, 4:00 – 5:30pm, 7/30/2014
Research Topics

Thermoacoustic Instabilities

- **Thierry Poinso, Emilien Courtine (Host: Matthias):** Causality of flame transfer function concepts for combustion instability models
- **Matthew Juniper, Luca Magri (Host: Yee Chee See):** Adjoint sensitivity analysis of hydrodynamic/thermoacoustic instability in turbulent combustion chambers
- **Wolfgang Polifke, Camilo Silva (Host: Jeff O’Brien, Matthias):** Identification of combustion noise source strength and acoustic scattering coefficients of enclosed flames
- **Franck Nicoud, Michael Bauerheim (Host: Gianluca):** Uncertainty quantification of thermoacoustic instabilities in annular combustors

Soot and Emissions

- **Benedicte Cuenot (Host: Benedetta Franzelli):** Towards the prediction of soot in aero- engine combustors with large-eddy simulation
- **Alireza Najafi-Yazdi (Host: Benedetta Franzelli):** Radiation effects on soot and NOx interaction in turbulent nonpremixed flames
- **Luc Vervisch, Benjamin Farcy (Host: Matthias):** Large-Eddy simulation of nitric oxide emission control in burners by injection of ammonia

Turbulent Combustion Modeling

- **Peter Hamlington, Colin Towery (Host: Javier Urzay, Jeff O’Brien):** Multiscale interactions and backscatter in turbulent reacting flows
- **Alexei Poludnenko (Host: Jeff O’Brien, Javier Urzay):** Stability and self-acceleration of premixed turbulent flames in the thin reaction zones regimes
- **Evatt Hawkes, Shahram Karami (Host: Matthias):** The dynamics of edge flames using an existing comprehensive DNS database modeling turbulent slot and round lifted jet flames
Thermoacoustic Instabilities
Causality of flame transfer function concepts for combustion instability models
T. Poinrot and E. Courtine, IMF Toulouse, CNRS. M. Ihme, CTR

Background

- Combustion instabilities (CI) are a major issue in most combustors
- A large class of models for CI relies on a model called n-tau where fluctuations of heat release are assumed to be controlled by inlet velocity fluctuations into the combustor
- This model has causality problems: the velocity fluctuations contain acoustic waves which propagate upstream, away from the chamber and should not affect combustion

Research Issue

- If the n-tau approach is valid, recent work at TU Munich and TU Eindhoven show that certain flames can be ‘intrinsically unstable’: they can oscillate in a purely anechoic system without any acoustic feedback
- Both questions (n-tau validity and intrinsic modes) are essential for thermoacoustics approaches

Research Approach and Methods

- Will use DNS of a simple laminar flame, forced by upstream or downstream waves and verify if the n-tau relation holds or not
- Study causality relations extracted from the DNS to understand why the n-tau relation holds if it does.
- Will use thermoacoustics theory to compute the same flame

Expected Outcome

- Either the n-tau model is NOT valid and 95 percent of the literature on thermoacoustics is wrong...
- Or it is valid and then we should see intrinsic instability in flames, something which most thermoacoustics experts have never considered up to now.
Adjoint sensitivity analysis of hydrodynamic/thermoacoustic instability in turbulent combustion chambers
Matthew Juniper, Luca Magri, Matthias Ihme, Yee Chee See

Background
- Thermo-acoustic instability occurs when heat release fluctuations in a combustion chamber synchronize with acoustic fluctuations.
- It causes noise and can cause catastrophic failure of the engine.
- It is one of the biggest and most persistent problems facing gas turbine and rocket engine manufacturers.

Research Issue
- Adjoint sensitivity analysis can, in very few calculations, identify the parts of a flow or system that most influence an instability.
- It has mainly been applied to hydrodynamic stability. We will apply it to thermo-acoustics.
- It will help identify the physical mechanisms that cause the instability and show how to control them, either by addition of a passive device or by changing part of the system.

Research Approach and Methods
- Our approach is numerical. We derive direct and adjoint equations for infinitesimal perturbations around a given base flow.
- For the flame, we use the Low Mach Number Navier–Stokes equations (LMN). For the acoustics we solve the Helmholtz equation.
- We will use the method of multiple scales in order to combine these approaches.
- We have already used simplified versions of this approach for adjoint sensitivity analysis.

Expected Outcome
- After examining simple systems, we will apply this to the model gas turbine combustor simulated at Stanford.
- We will identify the wavemaker region and mechanism of thermoacoustic instability.
- We will identify the best way to actively control this thermoacoustic instability.
- Through base state sensitivity, we will identify the changes to the system that will stabilize the oscillations.
Identification of combustion noise source strength and acoustic scattering coefficients of enclosed flames
Camilo Silva and Wolfgang Polifke (TUM), Host: Matthias Ihme

Background
- Identification of transfer function of turbulent premixed flames (FTF) with LES & SysID is currently possible only if combustion noise has low amplitude
- Combustion noise is not just “noise” – it is of significant technological interest. But: In SysID with correlation analysis, noise is suppressed, but not identified.

Research Issue
- Robust techniques to compute the flame transfer function in the presence of significant noise levels
- Quantify uncertainty of “noisy” results
- Identify combustion noise source strength

Research Approach and Methods
- DNS / LES & advanced SysID, e.g. polynomial models (Box-Jenkins)
- Study the response of a laminar premix flame to simultaneous perturbation of $u'$, $Θ'$, $T'$ (input vs. fake noise)
- Explore the role of
  - correlation between input /noise
  - spectral distribution of input signals

Expected Outcome
- Better understand how input signal design and statistical properties of noise influence estimation quality of the FTF.
- Collaboration with Jeff O'Brien and Matthias Ihme to characterize a turbulent swirl flame with new methods
# UQ of Thermo-acoustic instabilities in annular combustors

M. Bauerheim (SNECMA), F. Nicoud, S. Moreau, T. Poinsot, A. Ndiaye + M. Ihme

## Background
- When acoustic waves and flames interact, large amplitude pressure oscillations sometimes appear
- LES accurate but remains quite expensive
- Acoustic solvers more suitable for parametric studies / design purposes
- Major improvements obtained during CTR SPs 04, 06, 08,12
  e.g.: Motheau et al., JFM 2014

## Research Issue
- CIs are very sensitive to many physical parameters (regime, manufacturing tolerances, fuel changes, loss, …)
- Typical combustion instabilities analysis lead to a binary answer: stable / unstable
- Introducing UQ is necessary to obtain a more useful answer like instability risk factor
- Large dimension: Typical combustor contain 10-20 turbulent flames, each with its own uncertain response (amplitude + time delay).

## Research Approach and Methods
- Academic 19-burner combustor with 38 uncertain parameters
- Obtain the exact instability risk factor from the ATACAMAC analytical tool for annular combustors + Monte-Carlo method
- Apply UQ methods suitable for large dimensions
- Minimum # of runs to get a reasonable answer?
- Redo the exercise with a 3D Helmholtz solver (if feasible)

## Expected Outcome
- Do we really need 38 uncertain parameters?
- What does it cost to provide a instability risk factor for each mode instead of just and only a decay/growth rate?
- Expected collaborations:
  - G. Iaccarino (UQ), P. Constantine (active subspace), S. Ghili (low rank algorithm)
  - W. Polifke, C. Silva (CIs)
- Anyone interested??
Soot Formation and Emissions
Towards the prediction of soot on aero-engine combustors with LES
[B. Cuenot & E. Riber (CERFACS) CTR-Host B. Franzelli]

Background
- Soot prediction is still very challenging due to complex chemistry, particle dynamics and thermal radiation
- Existing works are either DNS with detailed chemistry in academic configurations, or RANS in real configurations
- LES prediction of soot in real combustors is still difficult and expensive (Mueller & Pitsch 2013)

Research Issue
- The objective is to evaluate simple models for soot prediction in LES of real combustors, and to identify possible improvement compatible with a reasonable cost
- This research will contribute to the modeling of soot in real combustors, and give first results on the coupled chemistry/dynamics mechanisms of soot production in complex flows

Research Approach and Methods
- LES will be performed with the code AVBP in a complex configuration. Soot are described by using a two-equations model. Two reduced chemical description for the gaseous phase (fuel oxidation + PAH formation) will be considered: hybrid TFLES/tabulation (Lecocq et al. 2014) or full tabulation of flame and soot chemistry
- The geometry is the experimental burner of DLR (Geigle et al. 2013)
- Preliminary results: reacting flow LES

Expected Outcome
- Expected accomplishments are the LES predictions of soot in a real burner, and comparison with measurements. This will allow to evaluate the level of accuracy of the tested soot models for real burners and to determine the most important weaknesses.
- The simulation with fully tabulated model will be made with the help of CTR host. Collaboration is also expected with participants at the Summer Program, by providing data on soot distribution in a real geometry.
Large Eddy Simulation of Nitric Oxide Emission Control in Burners by Injection of Ammonia
B. Farcy, L. Vervisch and P. Domingo Normandy University, INSA & CNRS CORIA, Rouen France
M. Ihme Center for Turbulence Research, Stanford

Background
- Legislations are evolving toward very strict regulation of Nitrous Oxides (NOx) emission.
- NOx are produced by combustion systems, but also during the processing of industrial waste containing large amount of nitrogen.
- NOx may be transformed by ammonia (NH₃) or Urea (CO(NH₂)₂) in Selective Non Catalytic Reduction (SNCR), i.e. spraying ammonia in the fumes.

Research Issue
- Ammonia transforms NO within the temperature range 1150 K – 1300 K:
  \[ NH_3 + NO + \frac{1}{4}O_2 \rightarrow N_2 + \frac{3}{2}H_2O \]
- But ammonia also produces NO above 1300K:
  \[ NH_3 + \frac{5}{4}O_2 \rightarrow NO + \frac{3}{2}H_2O \]
- Turbulent fluctuations of species concentrations and temperature must be kept under perfect control to secure the process efficiency.

Research Approach and Methods
- The process is highly sensitive to spray, turbulence and chemistry interactions.
- LES is performed including multicomponent spray evaporation and reduced chemistry optimized from the Klippenstein et al. detailed scheme (Combust. Flame 158: 774-789 (2011), Farcy et al. Fuel 118: 291-299 (2014)).
- The geometry of a full system under operation by SOLVAY is simulated.
- YALES2 flow solver is used.

Expected Outcome
- A detailed analysis of the coupling between flow physics and chemistry of nitric oxide emission and its control based on injection of ammonia.
- List of generic scaling rules and best practice guide for ammonia DeNOx design using turbulent flows.
- Interactions with Combustion group on multicomponent spray modeling and its coupling with chemistry.
Turbulent Combustion Modeling
Multi-Scale Interactions and Backscatter in Turbulent Reacting Flows
Peter Hamlington and Colin Towery, University of Colorado at Boulder
Hosts: Matthias Ihme, Jeff O’Brien and Javier Urzay

Background
- Multi-scale interactions and backscatter between premixed flames and turbulence are currently not well understood.
- No studies have directly measured turbulence spectra through premixed flames or have determined the direction of energy transfer occurring in the flow.
- Multi-scale interactions and backscatter pose considerable challenges for SGS models in LES. The extent to which existing SGS models are able to capture this multi-scale transfer has yet to be fully evaluated.

Research Issue
- **Objective**: Quantitatively characterize multi-scale interactions and backscatter between turbulence and premixed flames.
- **Hypothesis**: Energy is transferred from small to large scales in premixed flames via heat release and fluid expansion.
- **Hypothesis**: Backscatter of energy is more pronounced in the reaction zone of premixed flames and for less intense turbulence.
- **Hypothesis**: Existing SGS models fail to accurately capture multi-scale interactions and backscatter of energy in premixed combustion.

Research Approach and Methods
- There will be two primary research tasks:
  (i) Characterization of Multi-Scale Interactions in Premixed Combustion
  (ii) Testing of Multi-Scale Effects in SGS Models
- The multi-scale analysis will be based on both existing and new DNS of premixed flames.
- New conditional diagnostics will be developed in order to address variations in the turbulent scales of motion through the flame itself.
- The capability of existing SGS models to capture combustion-induced energy backscatter will be assessed using the DNS data.

Expected Outcome
- New DNS and diagnostics will be used to determine dynamical processes associated with multi-scale energy transfer in premixed combustion, and to evaluate the validity of classical theories of turbulence such as the Kolmogorov hypotheses.
- Based on the results of the SGS model analysis, approaches for improving existing models will be identified (if necessary).
- The research will be carried out at CTR with Matthias Ihme, Jeff O’Brien, Javier Urzay, Alexei Poludnenko, and other program participants.
Stability and Self-Acceleration of Premixed Turbulent Flames in the Thin Reaction Zones Regime
Alexei Poludnenko, Naval Research Laboratory, Washington, DC
Hosts: Matthias Ihme and Javier Urzay

Background
- Recent fully-resolved calculations of the interaction of driven, high-speed turbulence (Da ~ 1, Ka >> 1) with a premixed flame have demonstrated the importance of a baroclinic torque (Poludnenko 14, Hamlington et al. 11, also H. Kolla & J. Chen, private communication).
- Such action of the baroclinic term can result, in certain regimes, in a significant anisotropic turbulence amplification inside the flame brush.
- This can lead to a substantial flame acceleration and can significantly alter the flame dynamics from the nominal regime determined based on the upstream flow.

Research Issue
- **Objective**: Quantitatively characterize multi-scale effects of the baroclinic torque on the turbulent flow inside the flame brush.
- **Question**: What is the spectral structure of the resulting turbulent flow?
- **Question**: What is the magnitude of turbulence amplification and what are its effects on the flame dynamics?
- **Hypothesis**: Existing SGS models fail to accurately capture multi-scale effects of the baroclinic torque in premixed combustion.

Research Approach and Methods
- Previous analysis of the effects of the baroclinic torque was done either with a simplified single-step chemistry (Poludnenko 14), or in a highly non-steady turbulent flow (Hawkes et al. 12).
- The new analysis will use DNS calculations incorporating the detailed kinetics for the premixed, stoichiometric H\textsubscript{2}-air (2014 San Diego mechanism) in a steadily-driven turbulent flow.
- Calculations will have a sufficiently large dynamical range of scales to demonstrate the multi-scale effects of the baroclinic torque on the energy cascade.
- The capability of existing SGS models to capture the effects of the baroclinic torque on the resulting reacting turbulence will be assessed using the DNS data.

Expected Outcome
- First-principles analysis of the effects of the baroclinic torque on the high-speed reacting turbulence will be performed using large-scale DNS of premixed H\textsubscript{2}-air flames.
- Based on the results of the SGS model analysis, approaches for improving existing models will be identified (if necessary).
- The research will be carried out at CTR with Matthias Ihme, Javier Urzay, Peter Hamlington, and other program participants.
Edge flame dynamics in turbulent lifted jet flames
Evatt Hawkes, Shahram Karami, Mohsen Talei, Matthias Ihme, Ankit Bhagatwala, Jackie Chen

Background
- Lifted flames occur in many applications including gas turbines, industrial furnaces, and diesel engines.
- The stabilisation mechanism affects emissions and overall combustion stability.
- The stabilisation mechanism is still not understood, but partially premixed edge flames are believed to play a key role.

Research Issue
- We have shown that edge flames generate conditional fluctuations at the flame base.
- The dynamic behaviour of edge flames at the flame base will therefore be studied.
- The work will focus on the velocity of the leading edge points, to understand how it depends on other variables, such as strain rate, scalar dissipation, curvature, etc.

Research Approach and Methods
- A large DNS database has been generated modelling lifted flames.
- One step chemistry is employed with adjusted activation energy to achieve the correct dependence of flame speed on mixture fraction.
- Parameter space is comparable to experimentally measured flames.
- A large set of runs has been performed with parameter variations.

Expected Outcome
- The outcome will be a greatly improved understanding of edge flame dynamics in turbulent, lifted flames.
- This will lead to a better overall understanding of lifted flame stabilisation.
- The findings may feed into a new closure approach based on burning-conditioned flame surface density.
- Expected collaborations: interactions with others in the combustion group would be most welcomed.
- Additional possible areas of collaboration include: high Karlovitz number premixed combustion and solar radiation interactions in particle-laden flows.
DNS of soot/NOx/radiation interaction in turbulent flames
Alireza Najafi-Yazdi & Heinz Pitsch, RWTH Aachen University, Host: Benedetta Franzelli

Background
- Soot is a major contributor to flame radiative heat transfer
  - visible to infra-red range
  - Candle light is in fact soot radiation
- Radiative heat transfer can effect NOx formation (cf. M. Ihme & H. Pitsch, Physics of Fluids 2008)
- Soot formation/NOx formation and radiative heat transfer have relatively large time scales leading to potential strong interactions
- Strong soot radiation may cause flame quenching

Research Issue
- DNS of soot/radiation interaction in a 3D periodic jet configuration
- Effect of radiation time scale compared to flow and chemistry time scales (Radiation number)
- Determining the range of realistic Radiation numbers in combustors.
- Effect of soot radiation on NOx
- Effect of soot radiation on flame quenching

Research Approach and Methods
- DNS of soot/radiation/turbulence interaction in an n-heptane flame
- Detailed chemistry (65 species and 491 reactions): including NOx and PAHs submechanism
- Phenomenological Soot model (HMOM)
- Preliminary results:
  - DNS of 2D temporal jet
  - PAH mass fraction is significantly sensitive to radiative heat transfer
  - Soot volume fraction can decrease by a factor of 3

Expected Outcome
- Better understanding of soot/NOx/radiation interaction in turbulent flames
- A high quality dataset for subgrid modeling
- Collaboration with Dr. Franzelli and Dr. Cuenot to determine realistic radiation numbers in a typical combustor