Characterization of Turbulence-induced Non-idealities in Rapid Compression Machines (RCMs)

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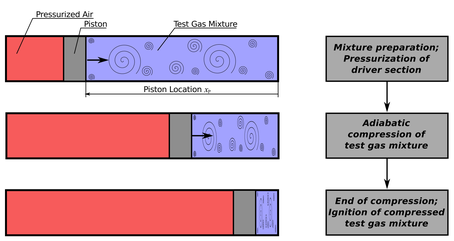
Motivation

- Integrated gasification combined cycle (IGCC) gas turbines provide attractive alternative to conventional coal-fired power plants:
  - Utilization of syngas as primary fuel component
  - Removal of impurities during gas-reforming process enables significant reduction of pollutant emissions
- Challenges in operating IGCCs using syngas
  - Variations in syngas composition: H_2/CO-ratio, H_2O/CO_2 content
  - High-pressure ($\leq$ 30 bar), intermediate temperature ($\leq$ 1000 K), and fuel-lean premixed operating conditions
  - Low density and high diffusivity of hydrogen affect flame-speed and flammability limits
- Recent comparisons between experiments and computations showed significant discrepancies in ignition delays; Reasons for this were attributed to
  - Limited validation data at gas-turbine relevant conditions
  - Incomplete reaction mechanisms
  - Sensitivity of rate constants to operating conditions
  - Hydrodynamic effects: Heat-losses and mixing processes
  - Inhomogeneities and surface-catalytic effects

$\Longrightarrow$ So far, role of turbulence as source of *systematic facility error* has not been systematically evaluated

Rapid Compression Machine

RCM Operation



Sources of Turbulence in RCMs

During RCM compression phase, different mechanisms for generation of turbulence and production of mixture/temperature inhomogeneities can be identified:

- **Filling process:** Generation of small-scale turbulence fluctuations during RCM-filling process
- **Corner vortices:** Piston motion leads to generation of large-scale vortical structures and roll-up of corner vortices, leading to entrainment of cold fluid into core region
- **Boundary-layer generated turbulence:** Piston-induced mean-flow motion leads to formation of turbulent boundary-layer; boundary-layer generated turbulence is transported into core-region
- **Compressive strain:** Amplification of turbulence due to piston-induced mean strain

$\Longrightarrow$ Effects of turbulence on scalar mixing and ignition dynamics in RCMs are currently not characterized

Objectives

- Develop low-order model to identify potential sources of systematic errors in RCM-measurements and to enable systematic investigation of critical process parameters on ignition dynamics in RCMs
- Identify regime-criterion for RCM-operating envelope

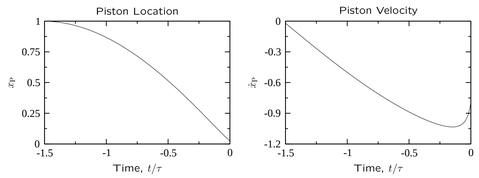
Computational Model

- Mathematical model is derived from conservation equations for mass, momentum, energy, and species, describing
  - Piston motion
  - Generation and amplification of turbulence and fluctuations in temperature and mixture composition during compression phase
  - Ignition and combustion

Piston Motion

- Equation for piston motion, $\dot{x}_P$, is obtained from dynamic force-balance on piston

$$\underbrace{\ddot{x}_P}_{\text{Acceleration}} + \underbrace{p_{2,s} - p_{1,s}x_P^{-\gamma}}_{\text{Pressure Force}} + \underbrace{\varepsilon\dot{x}_P}_{\text{Friction}} = 0$$



- Piston motion induces a time-dependent mean strain rate on fluid, $\alpha = \dot{x}_P/x_P$, which leads to amplification of turbulence and fluctuations in temperature and scalar perturbations
- Amplification of flow-field perturbations during compression phase is described using Rapid Distortion Theory (RDT)

Compression Phase

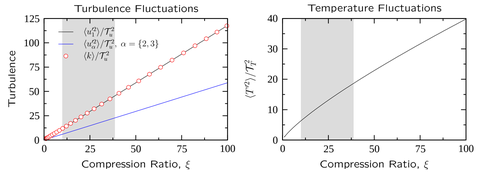
- Response of mixture-field to time-dependent mean strain is described by solution of linearized perturbation equations

$$\text{Turbulence:}\quad \partial_t u_i' + \alpha x_1 \partial_1 u_i' + \alpha u_1' \delta_{1i} = -\frac{1}{\bar{\rho}}\partial_i p'$$
$$\text{Species:}\quad \partial_t \boldsymbol{Y}' + \alpha x_1 \partial_1 \boldsymbol{Y}' + \beta u_1' = 0$$
$$\text{Temperature:}\quad \partial_t T' + \alpha x_1 \partial_1 T' = -(\gamma-1)\alpha T'$$

- RDT-analysis identifies six controlling parameters that affect temporal evolution of turbulence and species/temperature fluctuations in RCMs

Compression Ratio	ξ
Turbulence Intensity	$\mathcal{T}_u$
Initial Species Fluctuations	$\mathcal{T}_Y$
Initial Temperature Fluctuations	$\mathcal{T}_T$
Mixture Stratification	β
Wall Heat Losses	$T_\downarrow, \tau_\downarrow$

- Turbulence and temperature perturbations at end of compression phase are directly dependent on RCM-compression ratio



- Amplification of initial turbulence level can exceed a *factor of 50* for RCMs with high compression ratios

Ignition and Combustion

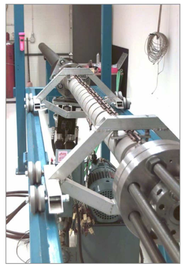
- Ignition and combustion is modeled as Partially Stirred Reactor (PaSR)

$$d_t\begin{pmatrix}\boldsymbol{Y}\\ T\end{pmatrix} = \underline{\underline{A}}\begin{pmatrix}\langle\boldsymbol{Y}\rangle - \boldsymbol{Y}\\ \langle T\rangle_\downarrow - T\end{pmatrix} + \begin{pmatrix}\dot{\boldsymbol{\omega}}\\ \dot{q}\end{pmatrix}$$

- Drift matrix $\underline{\underline{A}}$ accounts for turbulent mixing and wall heat losses
- Non-adiabatic effects are considered through volume expansion model

Application: Experimental Setup

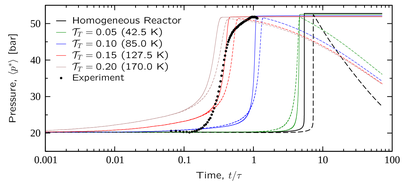
- Parametric investigation considers UM Rapid Compression Machine
- Geometric parameters
  - Compression ratio: $\xi = 35$
  - Charact. time-scale: $\tau = 70$ ms
  - Length of driven section: 2.7 m
  - External mixture preparation
- Syngas mixture
  - IGCC-relevant conditions
  - Fuel: H_2/CO-ratio = 3/2
  - Equivalence ratio: $\phi = 0.3$
  - Pressure: $p_0 =$ 10–20 atm
  - Temperature: $T_0 =$ 600–1200 K
  - Reaction mech.: Li et al. (2007)



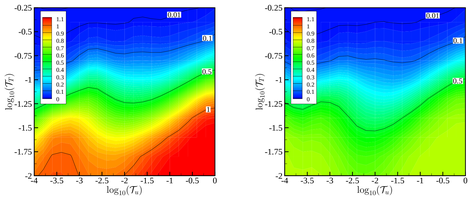
Results

Heat Loss Effects

- Entrainment of cold boundary layer fluid into adiabatic core region leads to temperature stratification
- Parametric studies are performed to quantify effects of wall-heat losses on ignition and combustion (*solid lines: adiabatic; dashed lines: no-adiabatic*)
- Composition: $H_2/O_2/CO_2/O_2/N_2$ = 7.33/9.71/1.98/17.01/63.97, $\phi = 0.5$, $\langle p_1^*\rangle$ =20 bar, $\langle T_1^*\rangle$ = 850 K, $\mathcal{T}_u = 0.1$



- Ratio between ignition delay time from RCM-model and homogeneous reactor simulation, τ_{ig}/τ_{ig}^{HR}, as function of turbulence level $\mathcal{T}_u$ and temperature perturbations $\mathcal{T}_T$

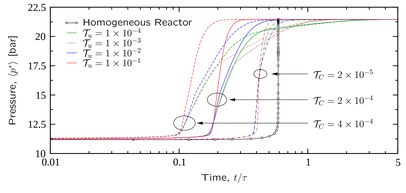


- Effects of wall-heat losses most prominent in post-ignition phase
- Depending on turbulence level, wall heat losses can either reduce or prolong ignition

$\Longrightarrow$ Overall, wall-heat losses are secondary in affecting onset of ignition

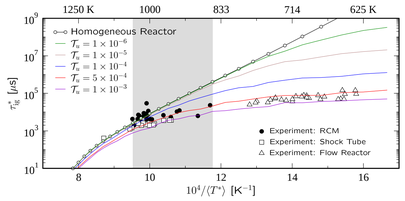
Variations in Test Gas Mixture

- Incomplete mixing, mixture segregation, or internal mixture preparation can lead to inhomogeneities in mixture composition
- Consider effects of compositional variations on ignition delay



Ignition Delay

- Parametric investigation of effects of turbulence and mixture inhomogeneities over temperature range of 600 K $\leq \langle T^* \rangle \leq$ 1300 K

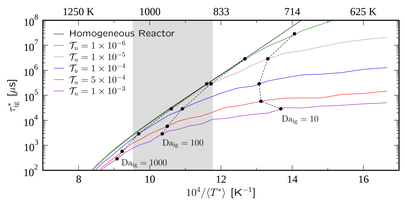


Damköhler Ignition Criterion

- Significance of turbulence in RCMs can be characterized using Damköhler criterion

$$\text{Da}_{ig} = \frac{\tau_{turb}}{\tau_{ign}} \propto \frac{1}{\xi^{3/2}}\frac{1}{\mathcal{T}_u}\frac{\tau}{\tau_{ig}}$$

- Large Da_{ig} : Turbulence effects are irrelevant; Chemistry much faster than hydrodynamics ("Homogeneous Reactor" limit)
- Small Da_{ig} : Turbulence has sufficient time to interact with reaction chemistry ("Partially Stirred Reactor" limit)

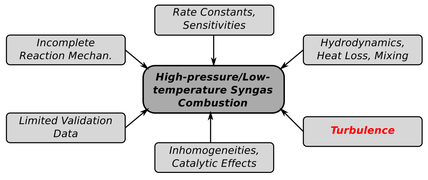


$\Longrightarrow$ Turbulence/chemistry interaction becomes increasingly relevant for low temperature conditions (extended ignition delay times)

$\Longrightarrow$ Turbulent Damköhler number provides metric to characterize low-temperature RCM operating regime

Conclusions

- Developed low-order model to characterize significance of turbulence/chemistry interaction in RCMs
- Model identified key parameters (ξ, $\mathcal{T}_u$, $\mathcal{T}_T$, $\mathcal{T}_Y$, β) that affect ignition process in RCMs
- Parametric studies indicate that turbulence/chemistry interaction can play equally important role in affecting syngas ignition than previously identified sources of non-idealities in RCMs



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References

[1] Ihme, M. AIAA-paper 2011-511, 2011.
[2] Chaos, M. and Dryer, F.L., Combust. Sci. Tech, 180:1053, 2008.
[3] Petersen, E.L. et al., Combust. Flame, 149:244, 2007.
[4] Donovan, M.T. et al., Combust. Flame, 137:351, 2004.
[5] Walton, S.M., et al., Proc. Combust. Inst., 3:3147, 2007.
[6] Li, J. et al., Int. J. Chem. Kinet., 39:1009, 2007.