A Numerical and Experimental Investigation of Autoignition

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Summary

This body of research uses numerical and experimental investigative techniques to further the understanding of autoignition. Hydrogen/nitrogen and methane/air fuel configurations of turbulent lifted flames in a vitiated coflow burner are used as model flames for this investigation. Characterisation was undertaken to understand the impact of controlling parameters and the overall behaviour of the flames, and to provide a body of data for modelling comparisons.

Modelling of the flames was conducted using the PDF-RANS technique with detailed chemistry incorporated using In-situ Adaptive Tabulation (ISAT) within the commercial CFD package, FLUENT 6.2. From these investigations, two numerical indicators for autoignition were developed: convection-reaction balance in the species transport budget at the mean flame base; and the build-up of ignition precursors prior to key ignition species. These indicators were tested in well defined autoignition and premixed flame cases, and subsequently used with the calculated turbulent lifted flames to identify if these are stabilised through autoignition.

Based on learnings from the modelling, a quantitative, high-resolution simultaneous imaging experiment was designed to investigate the correlations of an ignition precursor (formaldehyde: CH_2O) with a key flame radical (OH) and temperature. Rayleigh scattering was used to measure temperature, while Laser Induced Fluorescence (LIF) was used to measure OH and CH_2O concentrations. The high resolution in the Rayleigh imaging permitted the extraction of temperature gradient data, and the product of the OH and CH_2O images was shown to be a valid and useful proxy for peak heat release rate in autoigniting and transient flames.

The experimental data confirmed the presence of formaldehyde as a precursor for autoignition in methane flames and led to the identification of other indicators. Sequenced images of CH_2O, OH and temperature show clearly that formaldehyde exists before OH and peaks when autoignition occurs, as confirmed by images of heat release. The CH_2O peaks decrease later while those of OH remain almost unchanged in the reaction zone.

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Lastly and most importantly I thank my wife, Larissa, for everything.

Contents

List of Figures

Nomenclature

Roman

Symbol	Definition	Units
a	Strain rate parameter	s^{-1}
A_{12}	Einstein coefficient of spontaneous emission	s^{-1}
b	Bias	
B_{12}	Einstein coefficient of absorption	$m^2.(J.s)^{-1}$
c	Constant	
$C_{\epsilon 1}$	First experimental constant from the ϵ transport equation	
$C_{\epsilon 2}$	Second experimental constant from the ϵ transport equation	
C_ϕ	Mixing model constant	
C_μ	Modelling constant from the turbulent viscosity model	
D	Diameter	m, mm
E	Error	
f	Mixture fraction	
f_b	Boltzmann fraction	
F	Fluorescence intensity	counts
$I_{Rayleigh}$	Rayleigh Image	
I	Laser Intensity	$J.cm^{-2}$
I	Turbulence intensity	%
k	Turbulent kinetic energy	$m^2.s^{-2}$
K_{refl}	Zero cross-section reflection image	
l	Turbulence length scale	m

Symbol	Definition	Units
m, MW	Molecular weight	kg.mol^{-1}
n	Refractive index	
N	Number of particles (mixing models)	
N_a	Avogadro's Number	
N_{PC}	Number of particles per cell	
N_{TA}	Number of steps in the time average	
N(f)	Scalar dissipation rate distribution in mixture fraction	
p	Pressure	kPa, Atm, Bar
P	Probability Density Function (PDF)	
Pr	Prandtl number	
Q_{24}	Quenching coefficient from ν'=0	
Q_{31}	Quenching coefficient from ν'=1	
r	Radial distance	m, mm
Re	Reynolds number	
R_u	Universal gas constant	J.K^{-1}.mol^{-1}
S	Chemical source term	
Sc	Schmidt number	
S_L	Laminar flame speed	m.s^{-1}
t	Time	s
T	Temperature	K
u	Velocity	m.s^{-1}
U	Velocity	m.s^{-1}
V_{ij}	Vibrational transfer coefficient	
V	Voltage	V
x	Axial distance	m, mm
X	Mole fraction	
Y	Composition array	

Symbol	Definition	Units
Y	Mass fraction	

Greek

Symbol	Definition	Units
α	Scattering angle	rad
δ_{ij}	Kronecker delta	
ϵ	Turbulent Dissipation Rate	$m^2.s^{-3}$
η	Throughput efficiency	
ϕ	Diameter	m
Φ	Equivalence ratio	
λ	Wavelength	nm, cm^{-1}
μ	Dynamic viscosity	$kg.(m.s)^{-1}$
ν	Vibrational state	
ν	Kinematic viscosity	$m^2.s^{-1}$
τ	Time scale	s^{-1}
ρ	Density	$kg.m^{-3}$
ρ_0	Depolarization ratio	
σ	RANS modelling constants	
σ_i	Relative Rayleigh cross-section for species i	
ξ	Uniform random number	
ψ	Composition array	
Ω	Solid angle	srad

Superscripts

^{0}	Original state
^{1}	New state

Subscripts

air	Values taken in room temperature air
coflow	Values taken in the coflow of the VCB
flame	Values taken in the flame
ϵ	Pertaining to turbulent dissipation rate
i	Value for species i
j	Values taken in the fuel jet of the VCB
k	pertaining to turbulent kinetic energy term, k
o	Excess velocity
stoich, s	Stoichiometric value
T, t	Turbulent
v	vertically polarised

Notation

$\langle p \rangle$	Conventional mean of p
$\langle p\|q \rangle$	Mean of p conditional on q
$[p]$	Concentration, mole fraction of p
$\triangle p$	Delta - difference or change in value in p
$\bigtriangledown p$	Gradient operator
$\overline{p}$	Average
$\widetilde{p}$	Favre average
$\dot{p}$	Rate operator

Abbreviations

2Sc	Two Scalar experiment
3Sc	Three Scalar experiment
BD	Beam Dump
BG	Black Glass
CCD	Charge Coupled Device
CDR	Convection, Diffusion, Reaction
CFD	Computational Fluid Dynamics
CL	Cylindrical Lens
CMC	Conditional Moment Closure
CNG	Compressed Natural Gas
DNS	Direct Numerical Simulation
EDC	Eddy Dissipation Concept
EMST	Euclidian Minimum Spanning Tree
FWHM	Full Width Half Maximum
HCCI	Homogenous Compressed Charge Ignition
HeO_2	Helium-Oxygen replacement for air
HRR	Heat Release Rate
ICCD	Intensified Charge Coupled Device
IEM	Interaction by Exchange with the Mean
I/I	Image Intensifier
IMG	Image
ISAT	In-situ Adaptive Tabulation
LDV	Laser Doppler Velocimetry
LES	Large Eddy Simulation
LHS	Left Hand Side
LIF	Laser Induced Fluorescence
LSF	Line Spread Function
MC	Modified Curl’s

Nd:YAG	Neodinium doped Yttrium Aluminium Garnet crystal laser
PAH	Polycyclic Aromatic Hydrocarbons
PDF	Probability Density Function
PDL	Pumped Dye Laser
PISO	Pressure-Implicit with Splitting of Operators
PMT	Photo Multiplier Tube
PRESTO!	PREssure STaggering Option
RANS	Reynolds Averaged Navier Stokes
QE	Quantum Efficiency
RHS	Right Hand Side
RMS	Root Mean Squared (square root of variance)
RR	Heat Release Rate
SHG	Second Harmonic Generator
SL	Spherical Lens
SLM	Standard Liters per Minute
SNR	Signal to Noise Ratio
SRF	Step Response Function
SS	Stainless Steel
Tant.	Tantalum
THG	Third Harmonic Generator
TLF	Turbulent Lifted Flame
TNF	Turbulent Nonpremixed Flame
UV	Ultra Violet
VCB	Vitiated Coflow Burner
VIS	Visible luminescence experiment