Classification of ignition regimes in thermally stratified n-heptane-air mixtures using computational singular perturbation

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University Consortium on HPLB Engine Research
**Motivation**

- **Gasoline Engine (Spark Ignition)**
- **Diesel Engine (Compression Ignition)**
- **HCCI Engine (Homogeneous Charge Compression Ignition)**

**DOE University Consortium of Advanced IC Engines**

**HCCI (Homogeneous Charge Compression Ignition) Engines**

- Promises in low emissions and high efficiencies
- Challenges in control of ignition and combustion phasing
- Thermal inhomogeneities can be utilized to control ignition and extend combustion duration
- Need fundamental understanding of ignition in stratified mixtures

[https://www-pls.llnl.gov/](https://www-pls.llnl.gov/)
**Classification of Ignition Regimes**

- Homogeneous/Spontaneous Ignition
- Front Propagation
  - Spontaneous Ignition Front Propagation
  - Deflagration Front Propagation

**Experimental Observations in Spark-Assisted HCCI Engines** (Zigler, Wooldridge *et al.*, 2007)

HIGH LOAD ($\Phi = 0.62$); LOW Tint (271C)

Spark assist with high load ($\Phi \sim 0.6$) and low T is dominated by flame (deflagration) type behavior.

LOW LOAD ($\Phi = 0.40$); HIGH Tint (321C)

Spark assist with low load ($\Phi \sim 0.4$) and high T shows mixed-mode (front/homogeneous) ignition.

**Need for Classification:** Development of ignition sub-models for large scale multi-dimensional simulations of HCCI combustion
Validation and identification of physical and chemical processes in autoignition problems

Given temporally and spatially resolved data, computational singular perturbation (CSP) provides an automated method to develop and validate reduced order models.

- Validation of temporal resolution for implementation of efficient time-integration schemes
  1) Temporal resolution and stiffness
- Validation of reduced chemical mechanisms and quasi-steady state approximations
  2) Insights into chemical pathways
- Reliable computational methods needed to enable feature detection and automate data reduction for analysis of intermittent combustion phenomena
  3) Feature-tracking
- Development of predictive combustion models for modern engines need fundamental insights into ignition regime detection
  4) Ignition regime detection

Heat release rate isocontours in n-heptane-air 2D DNS (Yoo et al, Combustion & Flame, 2011)

Workshop on Validation and Verification in Computational Science, 2011
Ignition problems are closely linked to singularly perturbed problems, i.e. they have solutions that vary on disparate time scales.

Take advantage of this separation of time scales to obtain reduced problems that are simpler than the original full problem.

Decouple the fast time scales from the slow time scales.
Geometrical Representation of Chemical Kinetics

Consider homogeneous ignition system
\[ y(t) = [y_1, y_2, \ldots, y_N, T] \]: solution vector
\( g(y) \): chemical reaction source

\[ \frac{dy}{dt} = g(y) \]

Optimal Projector \( P = ? \)
\[
\frac{dy}{dt} = g(y) \quad \ldots\ldots(1)
\]

**Differentiating (1) once w.r.t. time:**

\[
\frac{dg}{dt} = Jg \quad J = \frac{dg}{dy} \quad \ldots\ldots(2)
\]

**Optimal Projector (P)**
- Leads to complete mode decoupling

Consider basis vectors as the eigenvectors of the Jacobian, J

\[
J = A\Lambda B \quad BA = I \quad \ldots\ldots(3)
\]

from (2), (3), and realizing \( \frac{dB}{dt} \approx 0 \)

(J \approx \text{const} in the neighborhood of the fixed point)

\[
\frac{d(Bg)}{dt} = BA\Lambda(Bg) \quad \ldots\ldots(4)
\]

\[
\frac{df}{dt} = \Lambda f, \quad f = Bg \quad \ldots\ldots(5)
\]

\( \Lambda \) = diagonal

therefore, mode decoupling is achieved

*for individual modes*

\[
f^i = f_0 \exp(\lambda_i t)
\]

Mode amplitude \quad Mode timescale

\[
\tau_i = \frac{1}{|\lambda_i|}
\]

\( g = S_1r_1 + S_2r_2 + \ldots + S_Rr_R \)

**Physical Representation**

\[
g = a_1(b_1.g) + a_2(b_2.g) + \ldots + a_N(b_N.g)
\]

**Optimal Representation**

\[
(I-P)g \Rightarrow g_{\text{fast}} \quad Pg \Rightarrow g_{\text{slow}}
\]

**Workshop on Validation and Verification in Computational Science, 2011**
CSP : Extension to convective/diffusive systems

Extension of CSP from ODEs to PDEs

\[ \frac{\partial y}{\partial t} = g(y) + L_c(y) + L_d(y) \]

Transport terms are projected on the SIM through the “chemical” projector, \( P \)

\[ J = \frac{\partial g}{\partial y} \]
\[ P = a_{M+1}b_{M+1} + \ldots + a_NB_N \]

(includes transport contribution)

Diffusion and Convection of all species are considered as separate processes in the calculation of Importance and Participation Indices
CSP: Mode separation (M) and Importance Index

Mode timescales

\[ \tau_1 < \tau_2 < \tau_M < \tau_{M+1} < \tau_{M+2} < \tau_N \]

Specify \( \varepsilon_r \) and \( \varepsilon_a \)  

\[ \tau_{M+1} \left( \sum_{i=1}^{M} a_i^j f^i \right) \leq \varepsilon_r y^j + \varepsilon_a \rightarrow \text{get } M \]

Slow (or fast) Importance Index

How important is \( k^{\text{th}} \) process in slow (or fast) dynamics of \( i^{\text{th}} \) species

\[ (I^i_k)_{\text{slow}} = \frac{\sum_{s=M+1}^{N-N_p} a_s^i (b^s . S_k) r^k}{\sum_{j=1}^{N-N_p} \left| \sum_{s=M+1}^{N-N_p} a_s^i (b^s . S_j) r^j \right|} \]
Feature-tracking & ignition regime detection

Ignition regime identification using the importance index of transport processes

\[ I^T = \left| I^T_{(T-\text{Diffusion})_{\text{slow}}} \right| + \left| I^T_{(T-\text{Convection})_{\text{slow}}} \right| \]

The importance of diffusive and convective transport of heat (sensible enthalpy) on the slow dynamics of Temperature field

- Identify a reaction zone / ignition front by M profile
- Look for the distribution of \( I^T \) in the region just upstream of the front

\[ I^T \approx 1 \quad \text{Reaction zone propagates by virtue of diffusion & convection} \quad \text{– Deflagration} \]

\[ I^T \approx 0 \quad \text{Reaction zone propagates by virtue of chemical reactions} \quad \text{– Spontaneous Ignition} \]

\[ 0 < I^T < 1 \quad \text{Gives the relative strength of deflagrative behavior} \]
**Initial conditions:**
2D homogeneous isotropic turbulence turbulence with thermal inhomogeneities ($p=41\text{atm}$, $\varphi=0.1$)

- $\text{H}_2/$air detailed chemistry – Mueller et al (21 reactions, 9 species)

**DNS data obtained from G. Bansal, H.G. Im, Combustion & Flame (2011)**
Ignition regimes in turbulent mixture – 2D Analysis

50% heat release point \((\varepsilon_r = 10^{-3}, \varepsilon_a = 10^{-7})\)

Fronts tracked by M profile

Cyan – Highly Active Reaction Region
Red – Gives the direction of front propagation
Ignition regimes in turbulent mixture –– 2D analysis

Mixed-mode propagation for a closely connected front contour

\[ I_T = |I_{(T-Diffusion)_{\text{slow}}}^T| + |I_{(T-Convection)_{\text{slow}}}^T| \]
2D analysis – Classification of ignition regimes

H: Homogeneous kernel
F: Front
S: Spontaneous Ignition
D: Deflagration
2D analysis – Classification of ignition regimes

- **H**: Homogeneous kernel
- **F**: Front
- **S**: Spontaneous Ignition
- **D**: Deflagration

![Graph showing different regimes of ignition](image)
Autoignition of n-heptane/air mixture

Negative Temperature Coefficient (NTC)

Two-stage ignition behavior

Temporal resolution and stiffness

Homogeneous autoignition of n-heptane-air mixture
58 species mechanism (Yoo et al., Combustion & Flame, 2011)

\[ \varepsilon_r = 10^{-3}, \varepsilon_a = 10^{-9} \]

\[ \Delta t_{\text{integration}} < \tau_1 \]

850K, 40atm, \( \varphi = 0.3 \)

1st stage

2nd stage

Driving time-scale

17
Insights into chemical pathways

Fastest active mode: #15
CSP radical: HCO

Importance Index for HCO

\[
\begin{align*}
\text{CH}_2\text{O} + \text{OH} &= \text{HCO} + \text{H}_2\text{O} & (0.321) \\
\text{HCCO} + \text{O}_2 &= \text{CO}_2 + \text{HCO} & (0.202) \\
\text{HCO} + \text{O}_2 &= \text{CO} + \text{HO}_2 & (-0.319)
\end{align*}
\]

14 exhausted modes. Quasi-steady state species:

\[
\text{C}_3\text{H}_2, \text{C}_4\text{H}_7\text{O}, \text{nC}_3\text{H}_7\text{CO}, \text{C}_2\text{H}_5\text{CO}, \text{CH}_2(\text{s}), \text{C}_7\text{H}_{14}\text{OOH}4-2, \\
\text{C}_4\text{H}_8\text{OOH}1-3, \text{C}_7\text{H}_{14}\text{OOH}2-4, \text{C}_7\text{H}_{14}\text{OOH}3-5, \text{C}_7\text{H}_{14}\text{OOH}1-3, \\
\text{C}_7\text{H}_{15}-3, \text{C}_7\text{H}_{15}-4, \text{C}_7\text{H}_{15}-2, \text{CH}_3
\]
Constant volume 1D n-heptane-air autoignition, $P_{\text{init}} = 40 \text{ atm}$, $\varphi_{\text{init}} = 0.3$ \hspace{0.5cm} ($\varepsilon_r = 10^{-3}$, $\varepsilon_a = 10^{-7}$)

$0.4 \text{ ms}$

$1^{\text{st}}$ stage ignition front propagating in deflagration mode
Ignition fronts have reached the walls. M dips at the center implying reactions have started cooking up beyond the 1st stage of ignition.
M dips down further throughout the domain. The entire mixture is now undergoing homogeneous autoignition.
Spontaneous ignition fronts have now appeared; pertaining to both 1st and 2nd ignition stages.
Spontaneous ignition fronts have reached the walls. $M$ starts to increase at the center implying the system moving towards near-equilibrium.
M dips at the walls, suggesting end gas consumption
Effect of different initial mixture composition

a) Uniform

b) Positively correlated

c) Negatively correlated

a) Spontaneous ignition front  
b) Fronts propagating due to both transport and reactions  
c) Homogeneous autoignition
CSP analysis has been used as a tool in homogeneous & 1D laminar (n-heptane-air), and 2D turbulent (H₂-air) constant volume problems for:

Validation of temporal resolution requirements and stiffness
τ_{M+1}: driving time scale, τ_1: fastest time scale (among M exhausted modes)
More gap between the two means higher stiffness

Validation of chemical pathways
Identification of QSS species, rate-limiting reactions, reactions responsible for heat release, through relevant importance indices

Feature tracking
Number of exhausted modes (M) profile allows for automated detection of pre-ignition, ignition and post-ignition zones

Ignition regime detection
\[ I^T = |I_{(T-Diffusion)_{slow}}^T| + |I_{(T-Convection)_{slow}}^T| \]

In the region just upstream of the ignition front
\[ I^T \rightarrow 1 \text{ Deflagration} \quad I^T \rightarrow 0 \text{ Spontaneous ignition} \]