Reactivity Stratification Analysis (RSA) and Heat Release Shaping in Reactivity Controlled Compression Ignition (RCCI) Combustion

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Motivation
To investigate the effect of fuel properties and chemistry on RCCI combustion, and to determine engine performance and emission characteristics for specific fuel combinations at a range of loads, combustion phasing, and equivalence ratios. The research focuses on the stratification requirements of fuels with a range of reactivities to achieve thermodynamically favorable heat release profiles while simultaneously maintaining low noise and emissions.

RCCI Strategy and Laboratory Setup
Reactivity Controlled Compression Ignition (RCCI) is an LTC strategy involving in-cylinder blending of two fuels with different properties for simultaneous NOx and soot mitigation, as well as high efficiency. A port injection of low reactivity fuel establishes the background equivalence ratio, and multiple direct injections of high reactivity fuel control the stratification of equivalence ratio and reactivity for combustion phasing, combustion duration, heat release shape, and emissions control.

Reactivity Stratification Analysis (RSA)
The objective of the RSA is to provide a computationally inexpensive 0-D prediction of in-cylinder fuel distribution based on auto-ignition predictions from the temperature, pressure, and composition history of zones in the cylinder. The fuel chemistry is modeled via ignition delay predictions obtained from reduced kinetic mechanisms. These predictions are then correlated to the mass fraction burned (MFB) profile to determine the probability that mass in the cylinder is at a given reactivity and equivalence ratio. The RSA approach is limited to kinetically controlled combustion strategies as it does not consider flame propagation effects on combustion phasing and does not account for mixing or heat transfer between zones.

RSA Methodology
- Divide the air and premixed fuel mass into N zones in the cylinder each with a different reactivity and Φ (add DI fuel).
- 0-D analysis, no mass or spatial location initially associated with the zones.
- Define a temperature profile for unburned zones that includes compression heating from combustion elsewhere in the cylinder, but not heat transfer between zones.
- Bulk gas follows ideal gas law temperature and mixtures that cover the range of in-cylinder zones that includes compression heating due to spray cooling.
- Unburned gas follows polytropic relationship.
- Assumes pressure, temperature, and mixture properties like R and γ are uniform in the cylinder. Zones can have different temperature histories due to spray cooling.
- Populate a matrix of ignition delay values that cover the range of in-cylinder conditions (T, P, EGR, Φ, fuel ratios), and interpolate the matrix to determine ignition delay at each step.
- Use the Livengood-Wu autoignition integral to predict the location of autoignition of the zones based on ignition delay.
- Equate the crank angle of autoignition to experimental mass fraction burned crank angle assuming once a zone ignites it instantaneously burns.
- Determine cumulative and probability density functions (CDF, PDF) to establish the distribution of mass in the cylinder.

Heat Release Shaping
The RSA tools can be used to predict the necessary in-cylinder stratification to achieve thermodynamically favorable heat release profiles for given initial conditions (intake temperature, intake pressure, equivalence ratio) and specific fuel combinations.

Operational Conditions
- Speed: 1300 rpm
- Intake Temperature: 40°C
- Intake Pressure: 1.28 bar
- Exhaust Pressure: 1.41 bar
- Φ: 0.42
- IMEP: 6.5 bar

Fuels
- iC8H18/nC7H16
- CH4/nC7H16

Heat Release Shaping
The results of the RSA from experimental data were compared to non-reacting CFD spray cases from KIVA to validate the methodology. Diesel fuel was modeled as pure n-heptane, and physically as tetradecane in the CFD. The RSA showed good agreement with the CFD predictions for the cases tested.

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Future Work
- Continue to validate RSA methodology with CFD and experimental results for PRF fuels, methane, and alcohols.
- Determine desirable HR profiles from a thermodynamic and emissions perspective, and use RSA to predict fuel distribution.
- Utilize a 1-D spray model to determine the necessary injection strategy (pressure, timing, number of injections) to achieve the desired fuel distribution.