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Formation of NO_x and N_2O in a n-Heptane Fuelled HCCI Engine

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Background

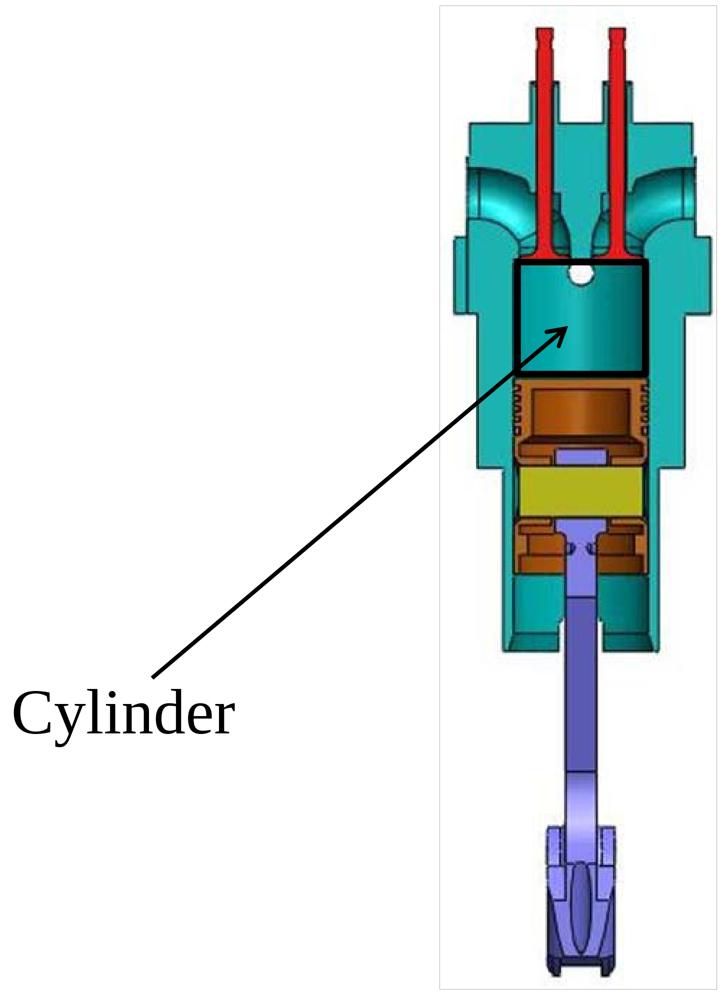
- HCCI combustion is usually highly diluted by high AFR or EGR, resulting in significantly low combustion temperature
- Mechanisms of NO_x formation in HCCI combustion may be different
- N_2O emissions may become significant in HCCI combustion
  - A numerical study (Guo et al., 2004) has shown that N_2O emissions become significant for lean premixed flames
  - HCCI experiments did show an increase in N_2O emission at near-misfire conditions
  - ***Why?***
- It is of interest to further investigate the fundamental mechanisms of NO_x and N_2O formation in HCCI combustion

Objectives

- To numerically investigate the fundamental mechanisms of NO_x and N_2O formation in a HCCI engine fuelled with n-heptane
- *Why n-heptane:* well developed kinetics

Engine Producing Experimental Data

- A CFR engine
  - Single cylinder
  - Variable compression ratio
  - Four-stroke

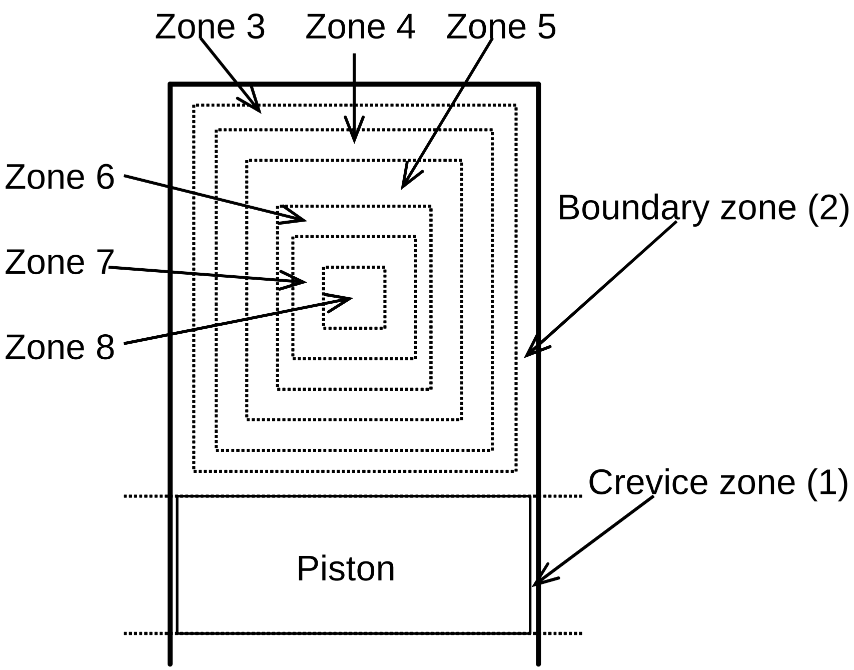


Numerical Model

- A multi-zone model
- Working fluid: ideal gas
- Simulation: starts from -360° and finishes at 360° ATDC
- Initial condition (at -360° ATDC):
  - Pressure: exhaust tank pressure
  - Residual composition: exhaust composition
- A combination of single and multi-zone models
  - -360° to IVC: single zone model, including intake and exhaust gas exchange
  - IVC to EVO: multi-zone model
  - EVO to 360° : single zone model, including exhaust gas exchange

Multi-Zone Model

- IVC ~ EVO
  - Crevice zone: (1) 2.5% of total mass, (2) reactions never happen
  - Boundary zone: exchanges heat with wall and zone next to it
  - Each core zone: (1) exchange heat with zones next to it by conduction, (2) exchanges heat with wall by radiation
- No mass exchange between zones



Chemistry

- A combination of LLNL mechanism and Gri Mech 3.0
  - N-heptane combustion: LLNL reduced mechanism (Seiser et al., Proc. Comb. Inst. 28, 2000)
  - NO_x: Gri Mech 3.0 (http://www.me.berkeley.edu/gri_mech/), including all possible NO formation mechanisms (thermal, prompt, N_2O and NNH)
- 177 species, 1638 reactions

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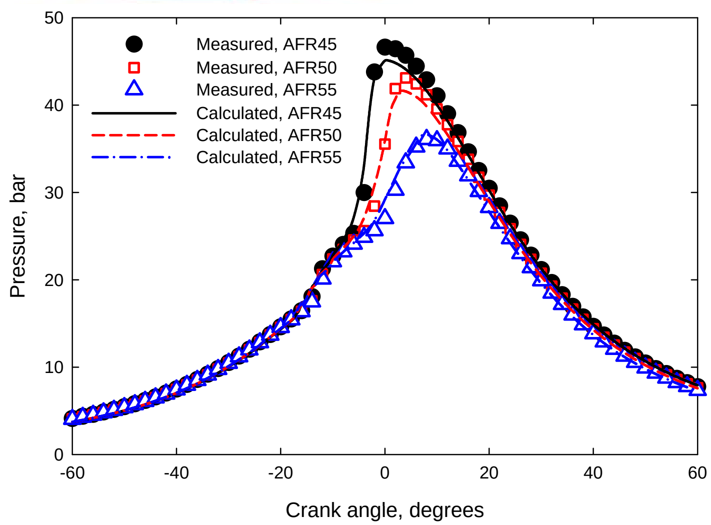
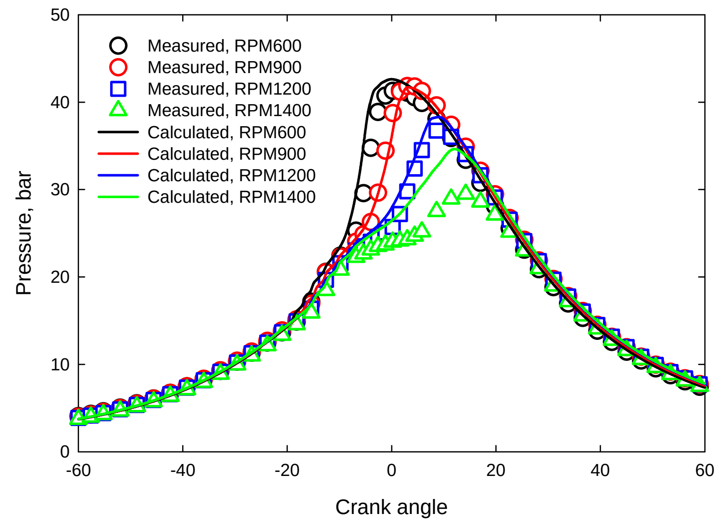
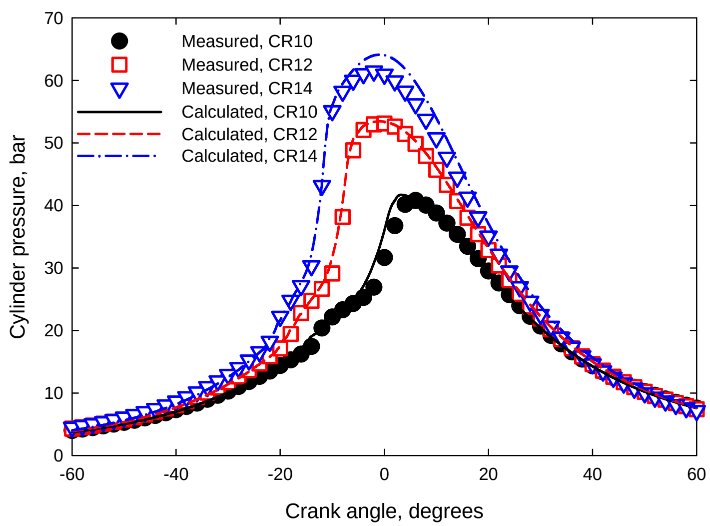
Model Validation – Pressure Prediction

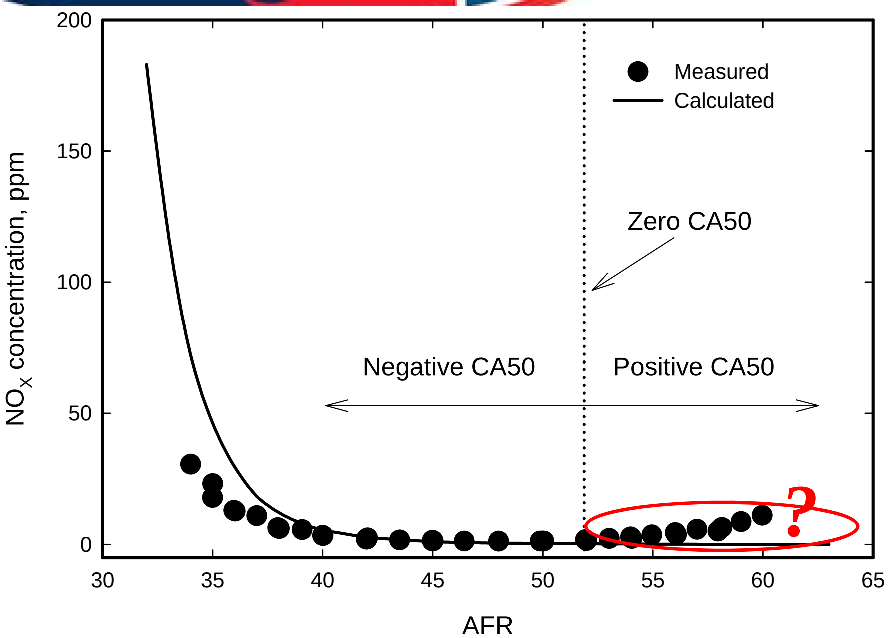


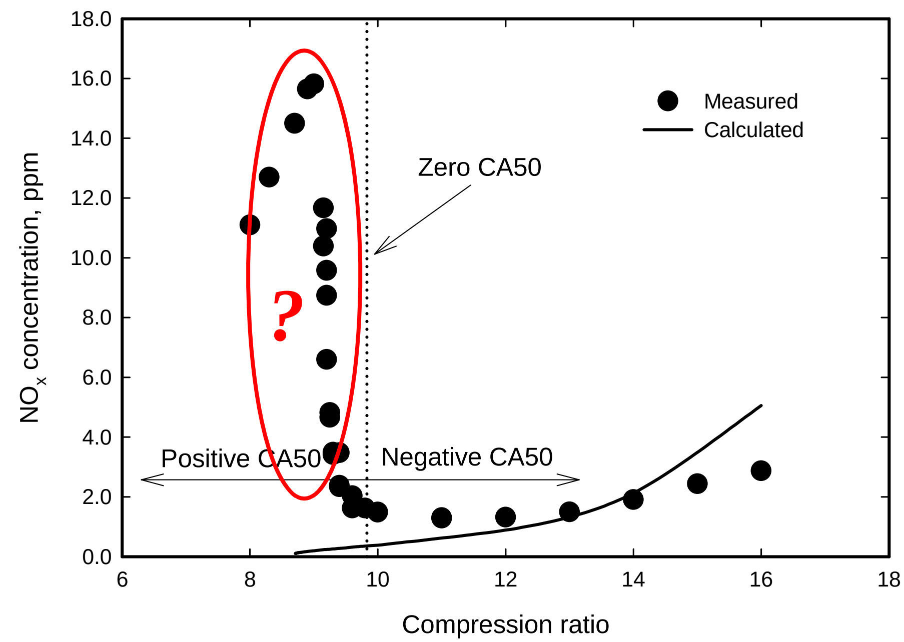




- Model predicts reasonable results

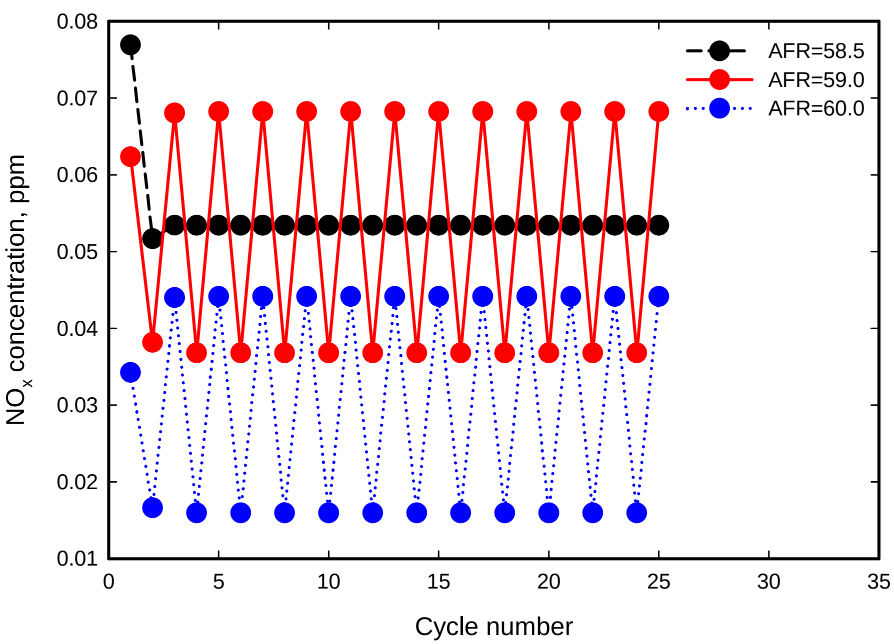
NO_x Emissions

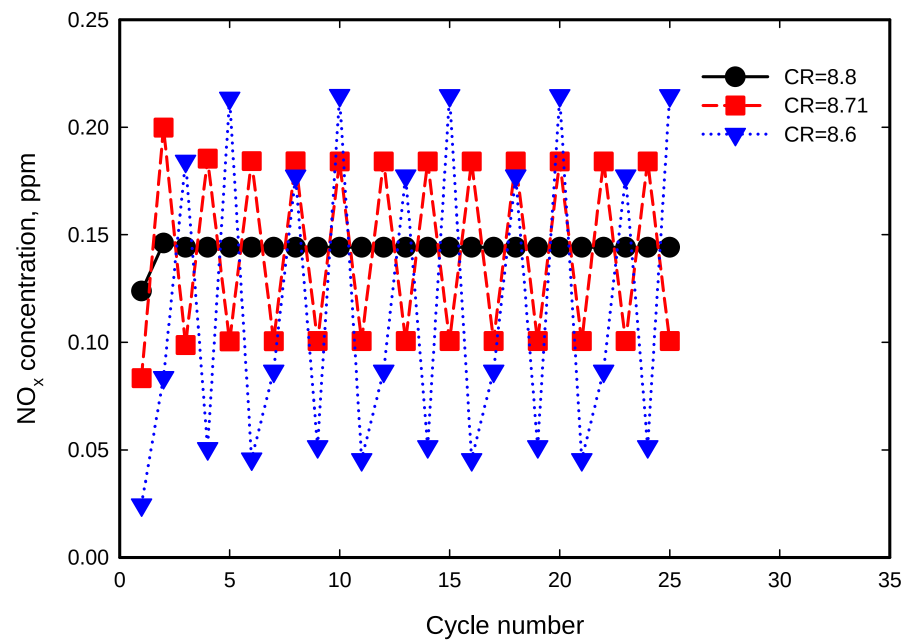




- Simulation captured the qualitative trend when AFR is smaller than 50 or CR is greater than 10
  - Increasing AFR or decreasing CR result in decreases in NO_x emission
- However, failed to predict the trend at higher AFR or lower CR when combustion phasing is retarded and misfire condition is approached

Cycle Variation Results in NO_x Increase at Misfire Conditions?



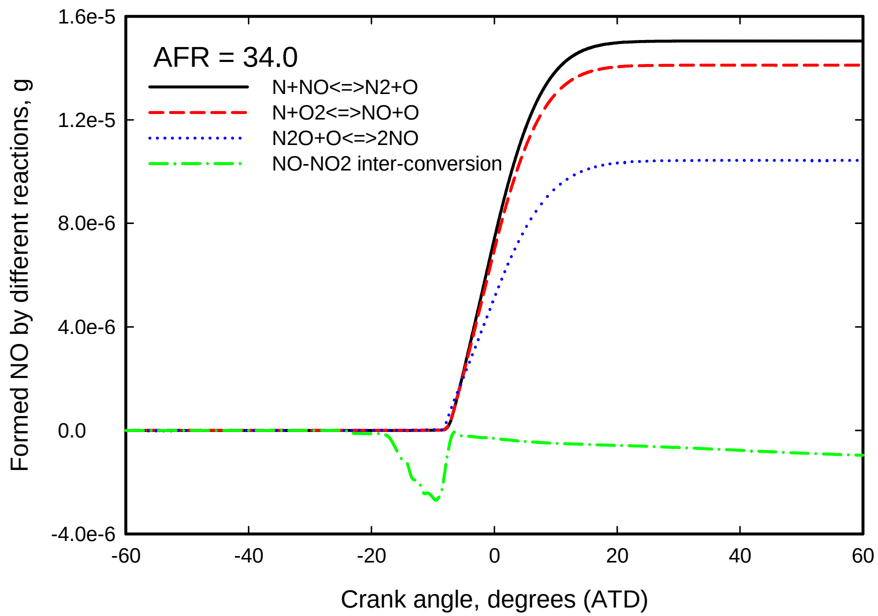


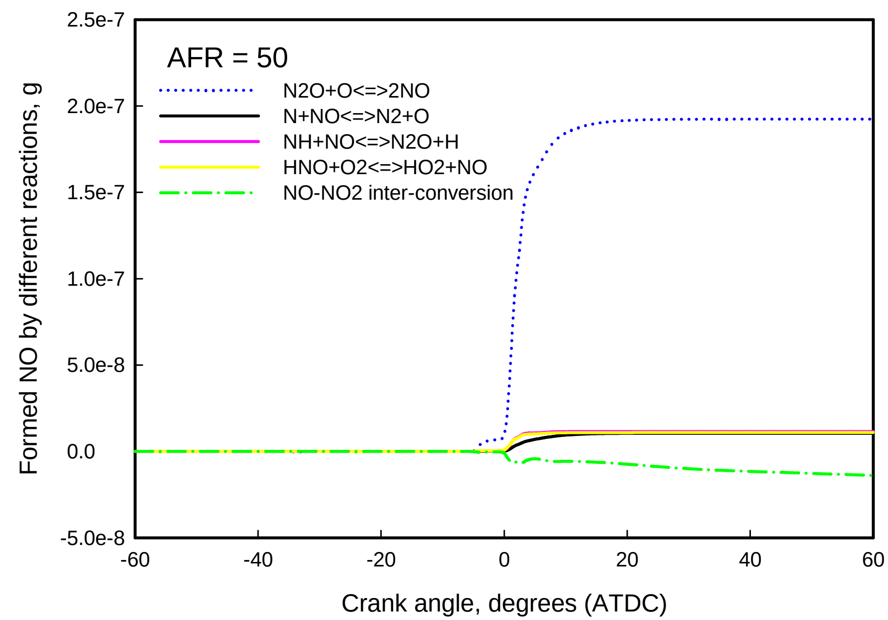
- Significant cycle-to-cycle variation does exist at higher AFR or lower CR
- However, average NO_x emissions decrease with increasing AFR or decreasing CR
- Further study is needed to understand the increase in NO_x emissions at near-misfire conditions

NO_x Formation Mechanisms

- NO formation dominates the formation of NO_x, since NO_2 comes from NO
- NO can be formed by four possible mechanisms
  - Thermal mechanism, dominating in conventional engines
  - Prompt mechanism, dominating in diffusion flames
  - N_2O intermediate route mechanism. N_2 is converted to N_2O first, and then N_2O is converted to NO
  - NNH intermediate route mechanism. N_2 is converted to NNH first, and then NNH is converted to NO
- ***Which mechanism dominates in HCCI combustion?***

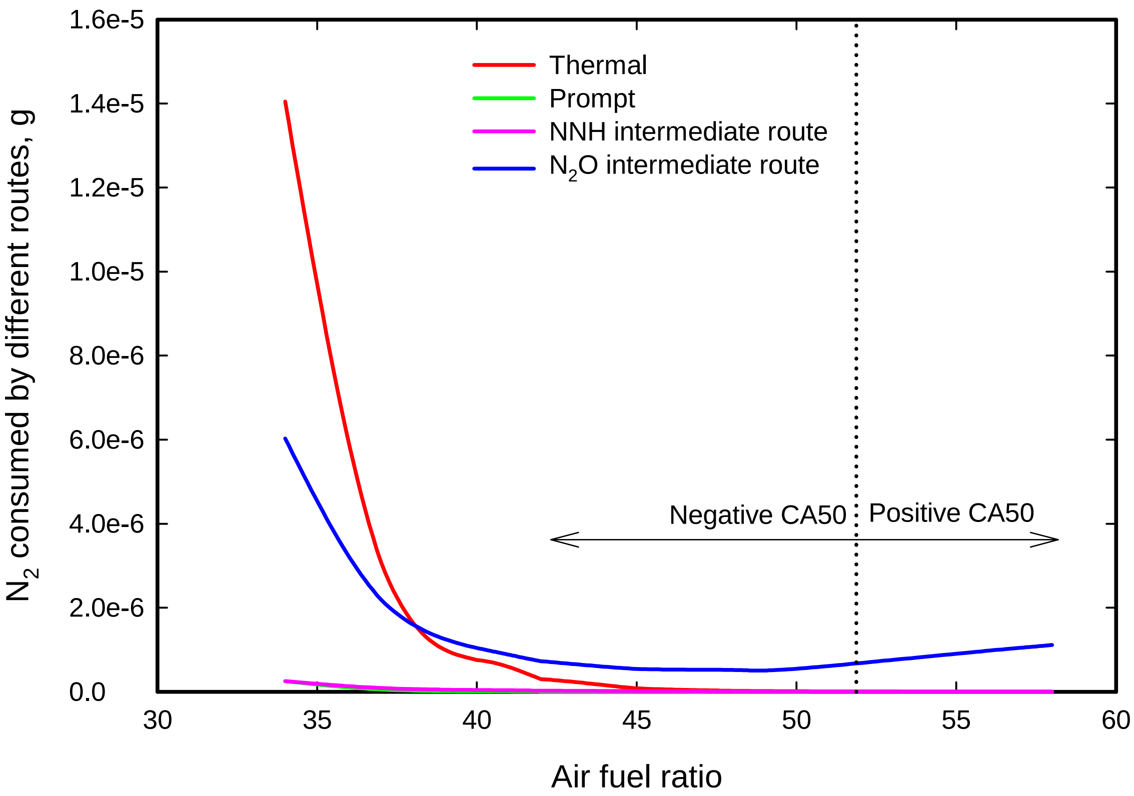
NO Formation by Various Reactions at Different AFRs





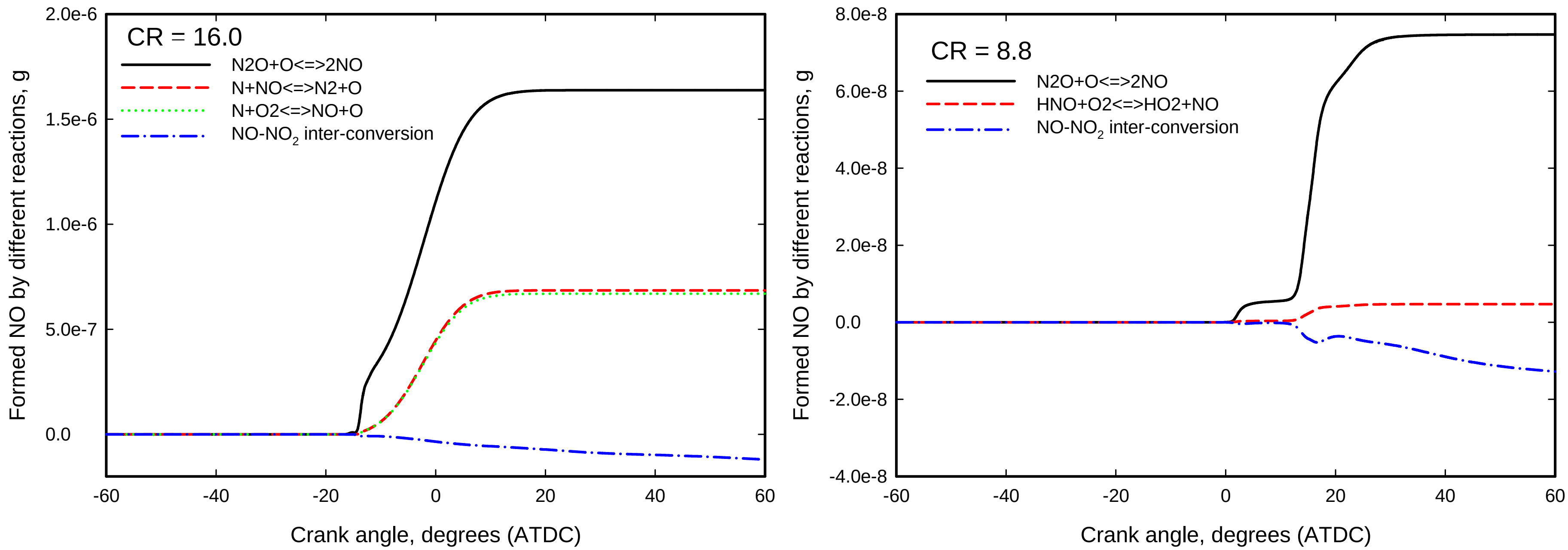
- At AFR = 34
  - **$N+NO \Leftrightarrow N_2+O$, $N+O_2 \Leftrightarrow NO+O$**, thermal mechanism
  - **$N_2O+O \Leftrightarrow 2NO$**, N_2O intermediate route
  - NO is primarily formed by the thermal mechanism at a lower AFR
- At AFR = 50
  - **$N_2O+O \Leftrightarrow 2NO$**
  - N_2O intermediate route dominates

N_2 Consumption by Different Routes



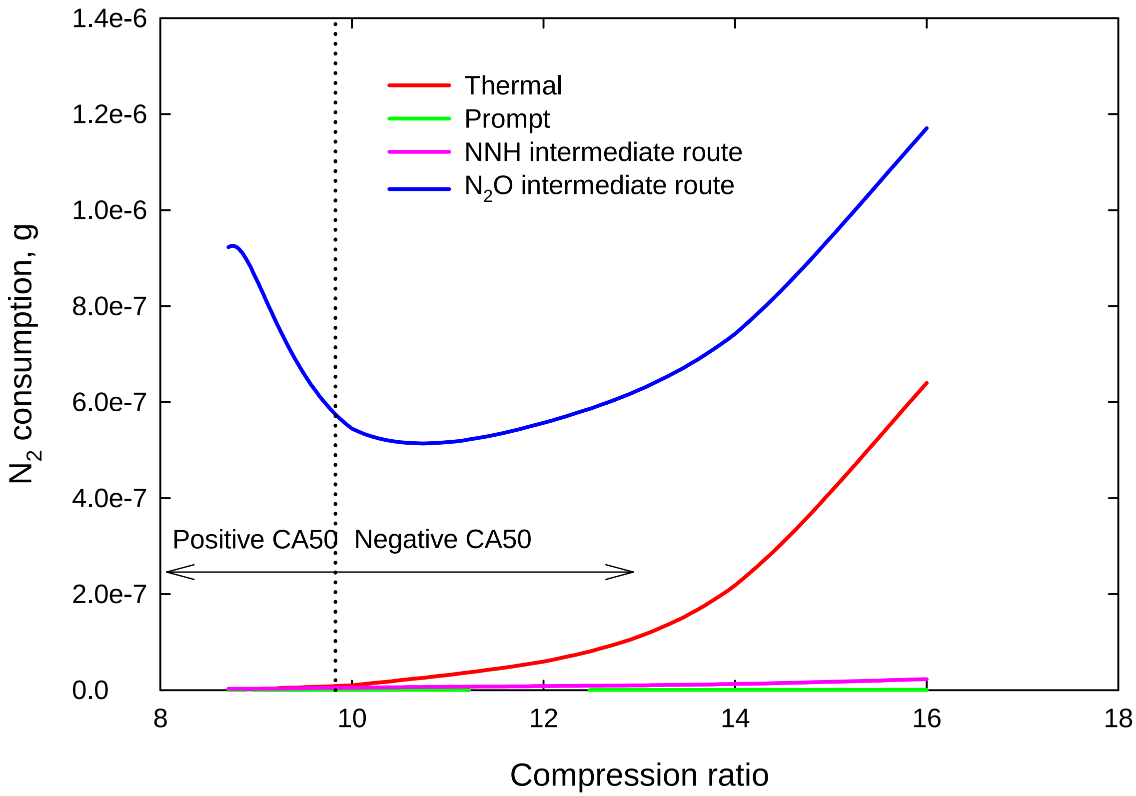
- At most AFRs, N_2 is primarily consumed by N_2O intermediate route
  - NO formation is dominated by N_2O intermediate route at most AFRs

NO Formation by Various Reactions at Different CRs



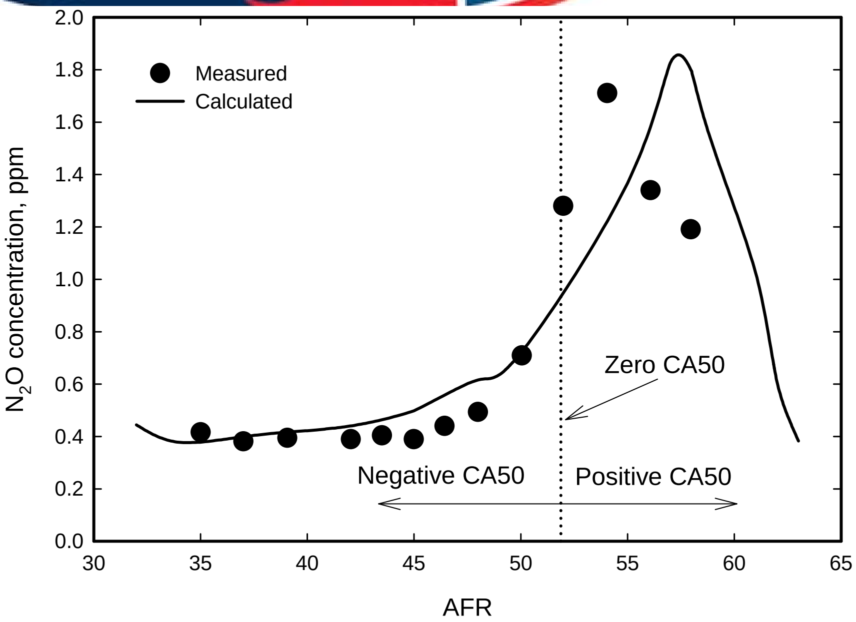
- At a lower CR, N_2O intermediate dominates the formation of NO
- At a higher CR, the contribution of thermal mechanism increases

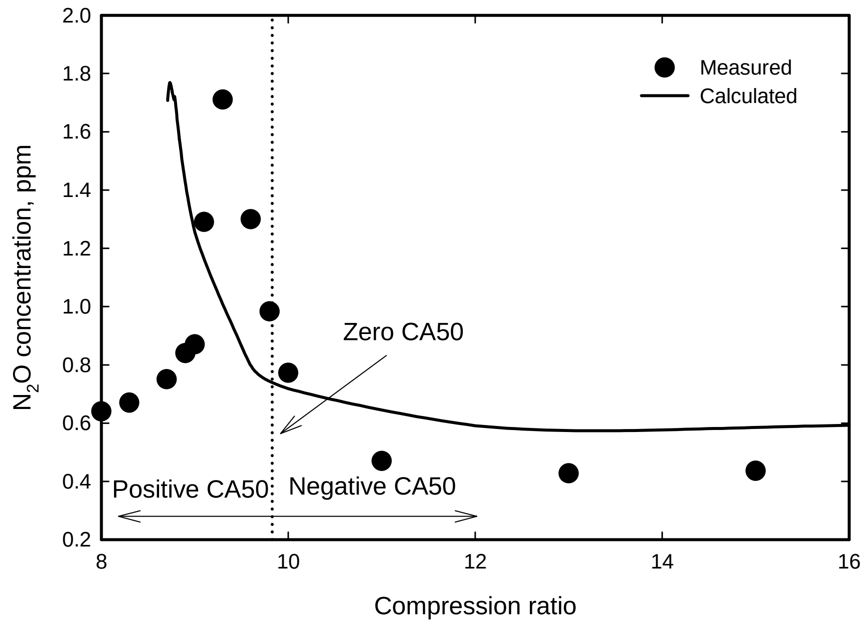
N_2 Consumption at Various CRs



- N_2 is primarily consumed by N_2O intermediate route as long as combustion phasing is not advanced too mush
  - N_2O intermediate route usually dominates NO formation in HCCI combustion

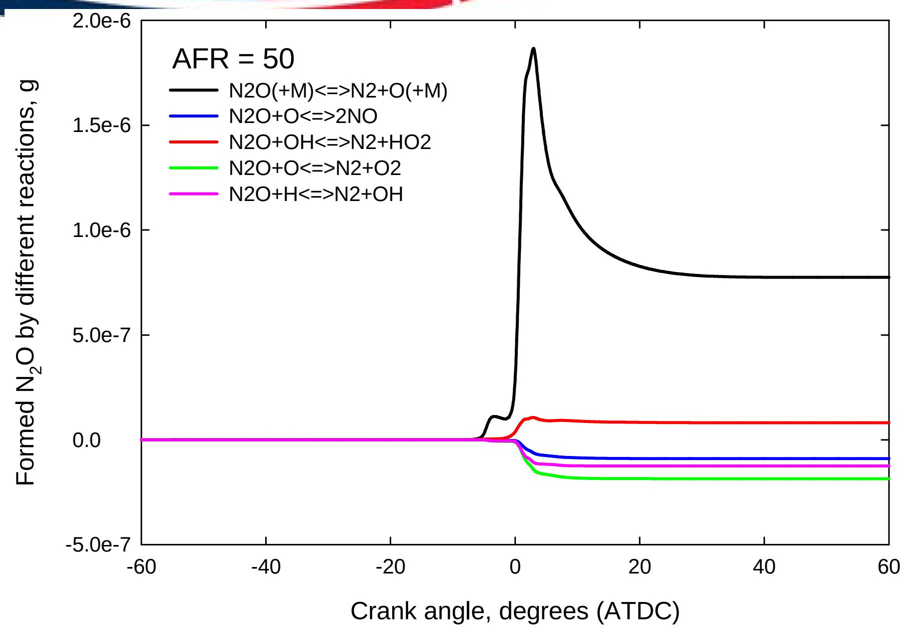
N_2O Emissions

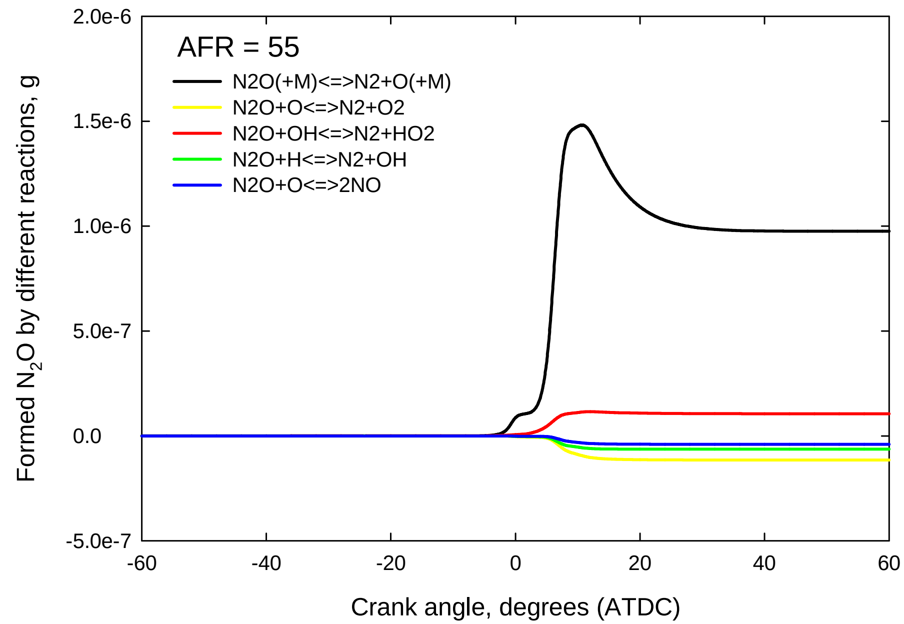




- N_2O emissions increase when misfire condition is approached, being similar to the observation for extremely lean premixed flames
  - N_2O is a concern in low temperature combustion
- *Why?*

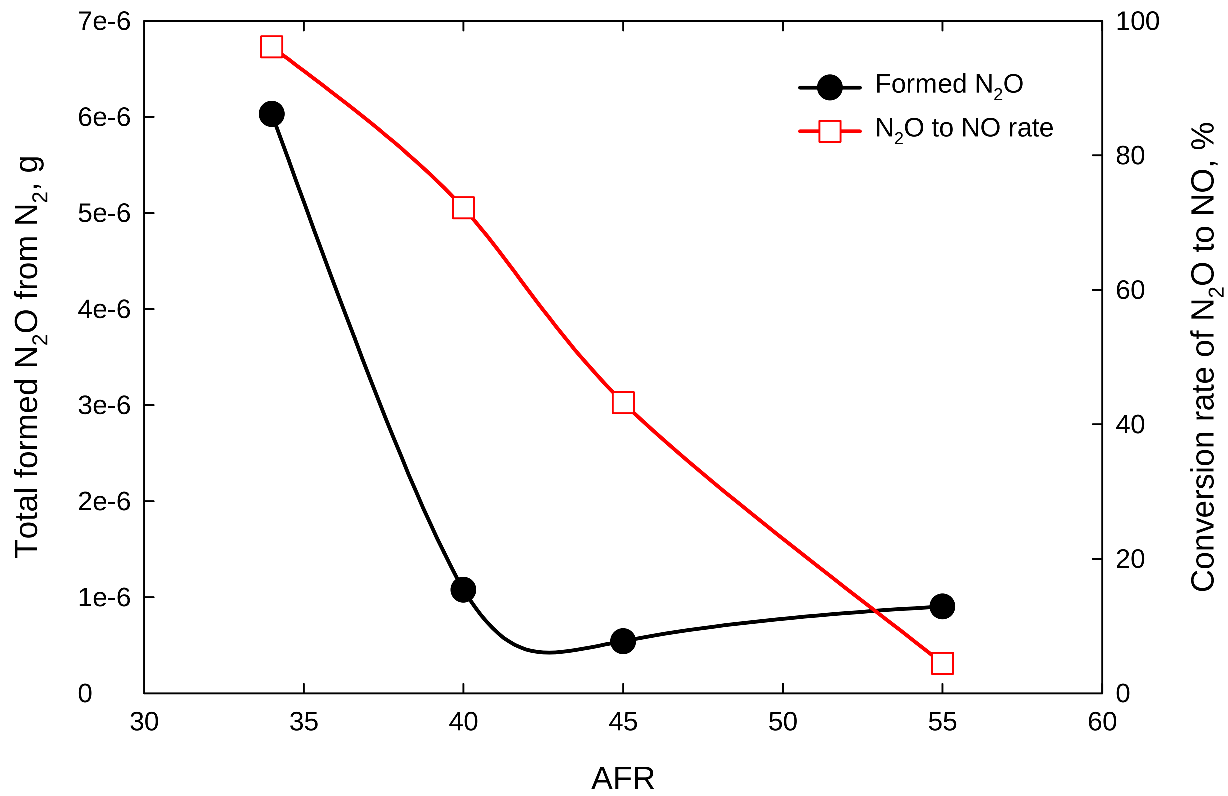
N_2O Formation by Various Reactions at Different AFRs





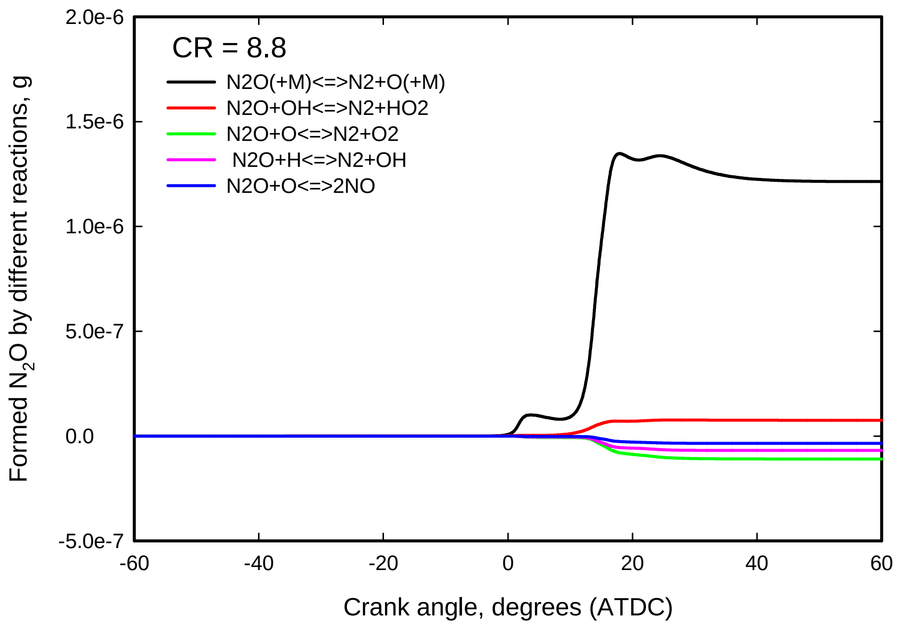
- Two factors result in the increase in N_2O emissions when AFR increases
  - The fraction of **N_2O => NO** decreases with the increase in AFR
  - The fraction of **N_2O formed in combustion stage => N_2 in expansion stroke** decreases with the increase in AFR, due to the shift of reaction **N_2O (+M) = N_2 +O (+M)** toward to reverse direction

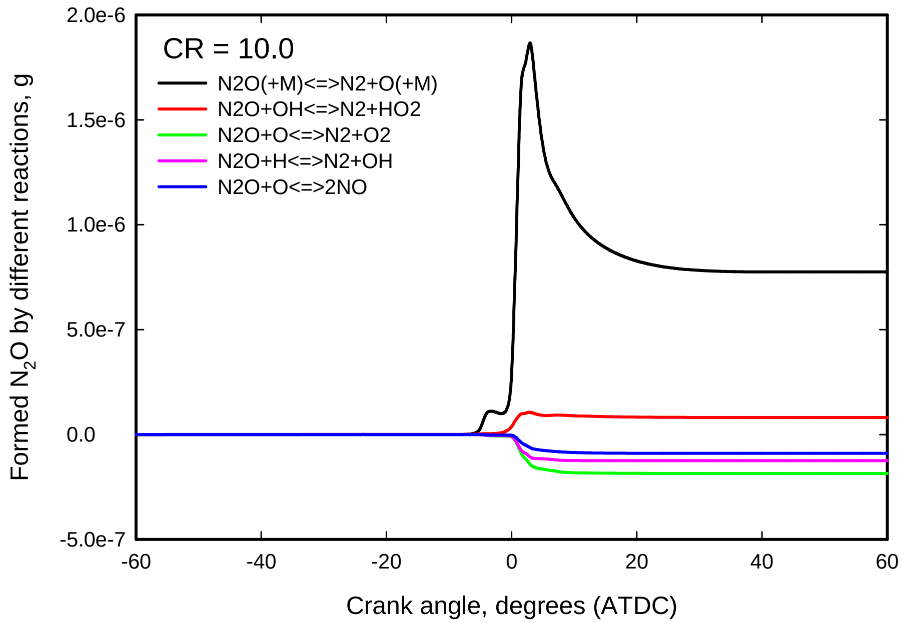
N_2O Formation and Destruction at Various AFRs



- The fraction of N_2O => NO decreases with increasing AFR
- The formed N_2O from N_2 slightly increases at higher AFRs, due to the shift of reaction **N_2O (+M) = N_2 +O (+M)** to the reverse direction

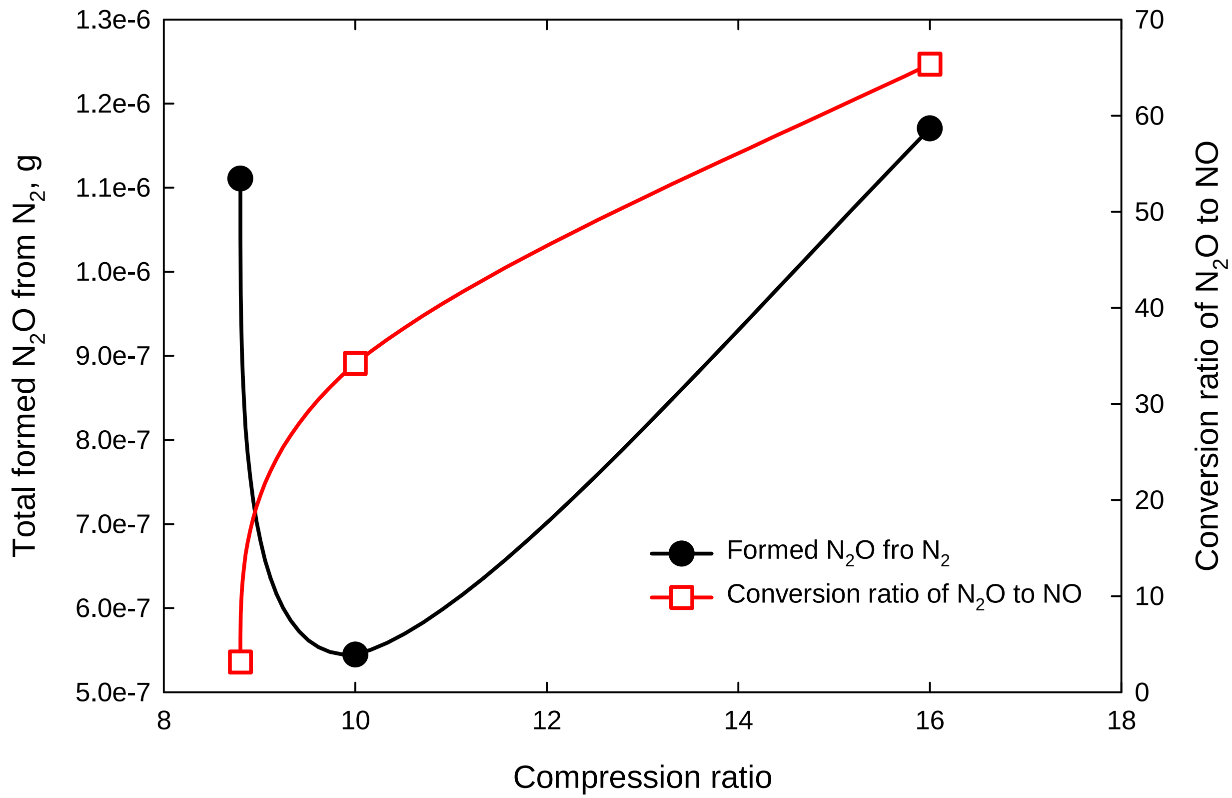
N_2O Formation by Various Reactions at Different CRs





- Two factors result in the increase in N_2O emissions when CR decreases
  - The fraction of **N_2O => NO** decreases
  - The fraction of **N_2O formed in combustion stage => N_2 in expansion stroke** decreases

N_2O Formation and Destruction at Various CRs

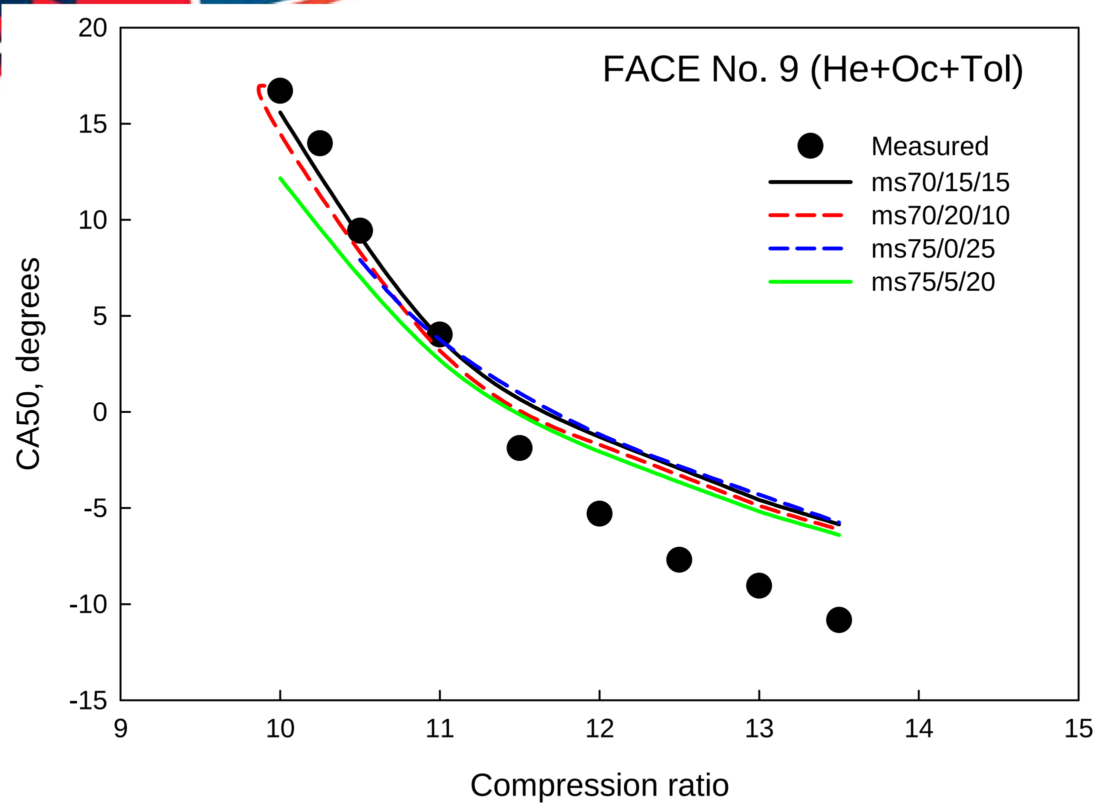


- The fraction of N_2O => NO decreases with decreasing CR
- The formed N_2O from N_2 increases at lower CRs

Conclusions

- The numerical model captured experimentally measured NO_x emissions trend at most conditions, but failed to capture the increase in NO_x emissions at near-misfire conditions
- NO_x formation in a HCCI engine at most operating conditions is dominated by the N_2O intermediate route mechanism, being different from in conventional engines
- The model successfully captured the increase in N_2O emissions at near-misfire conditions
- The increase in N_2O emissions at near-misfire conditions is due the decrease in the fraction of N_2O to NO and the shift of the reaction N_2O (+M) = N_2 + O (+M) toward the reverse direction

Next



- Modelling of diesel HCCI combustion by surrogate fuel
  - selection of appropriate surrogates
  - mechanism for surrogate fuels
  - improvement of zone model

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Thank you!

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