2018 CCEFP IEC Summit at the University of Minnesota

Modeling and Optimization of Trajectory-based HCCI Combustion

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Presentation Outline

- Motivation, Background and Objective
- Trajectory-based HCCI Combustion Control
  - *Chemical Kinetics Driven Model*
  - *Control-oriented Model*
  - *Optimization of Piston Trajectory*
- Controlled Trajectory Rapid Compression and Expansion Machine (CT-RCEM)
- Conclusions

Motivation

Large amount of energy is consumed by transportation sector annually:

- In the US, transportation sector consumes ~30% of total energy.
- There are 800 million passenger vehicles in the world now.
- The above number is projected to reach 2.8 billion by 2050.

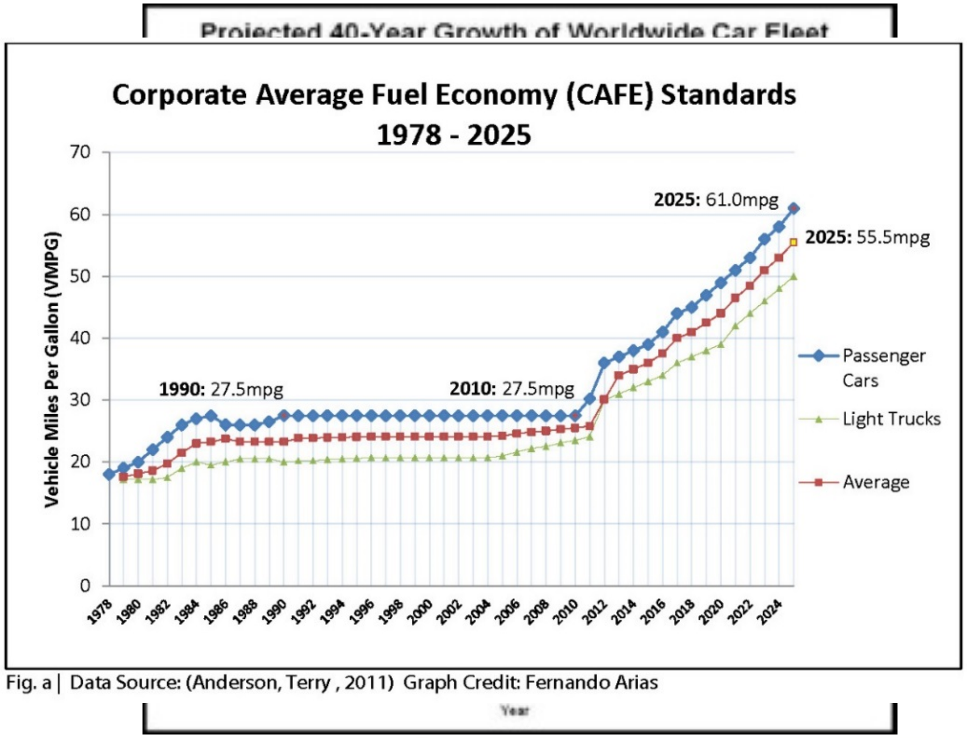
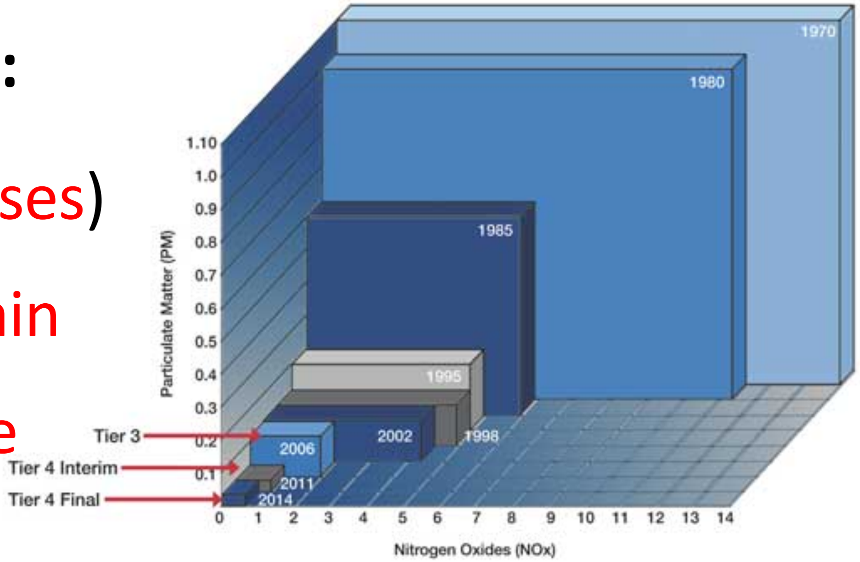


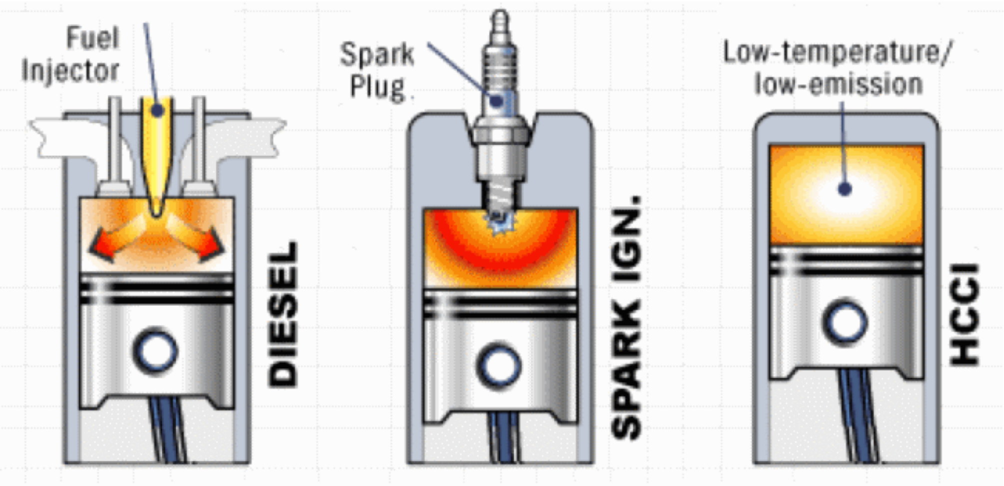
Fig. a | Data Source: (Anderson, Terry , 2011) Graph Credit: Fernando Arias

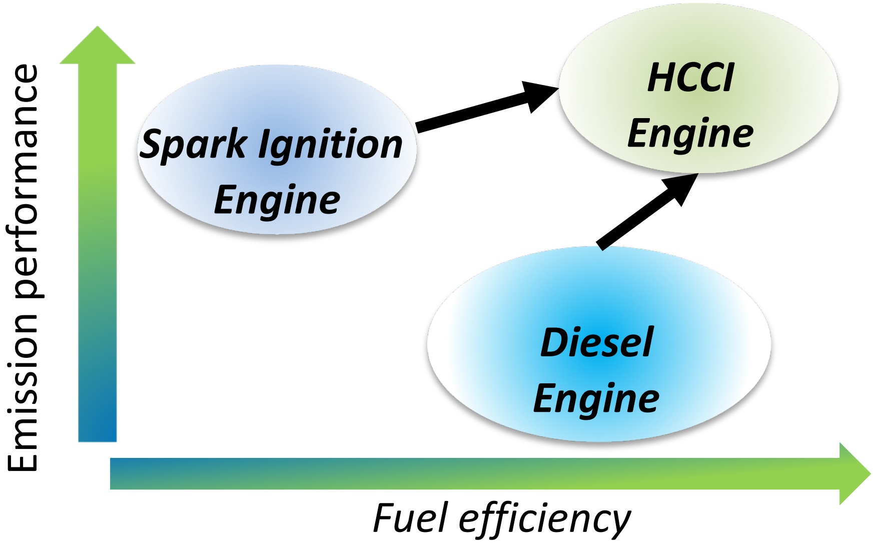
Environment and human health impact:

- CO_2 effect on climate (greenhouse gases)
- NOx emission forms smog and acid rain
- PM causes serious respiratory disease



Background – HCCI Combustion

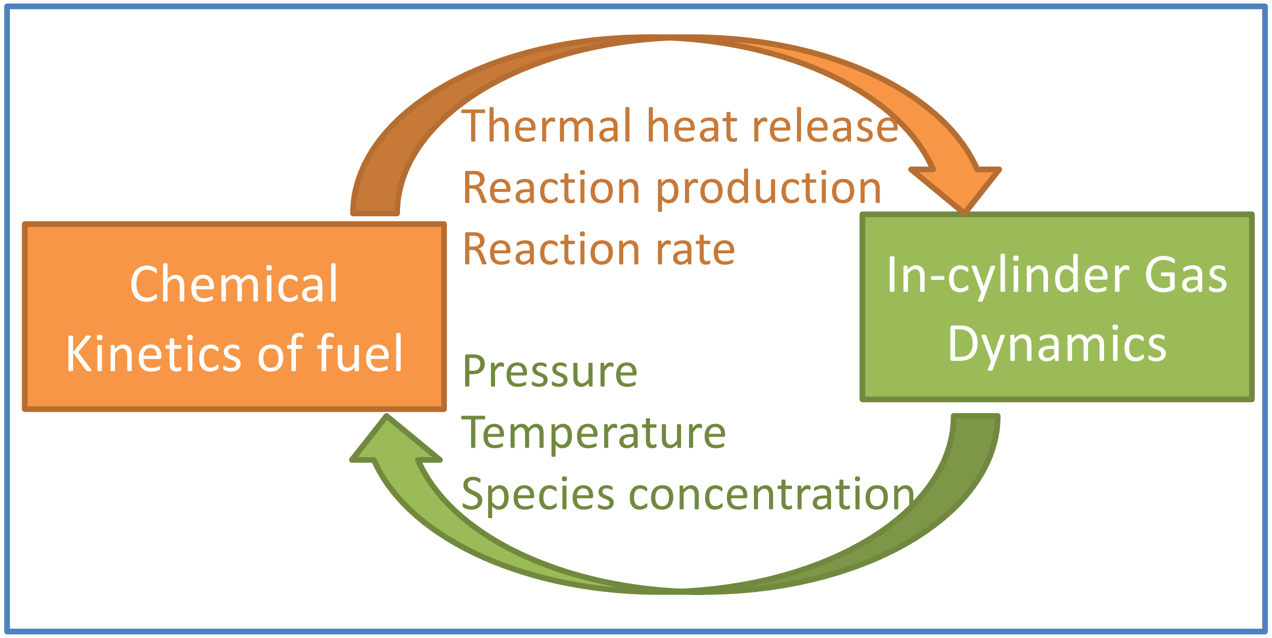




Spark Ignition Engine

HCCI Engine

Diesel Engine



Chemical Kinetics of fuel

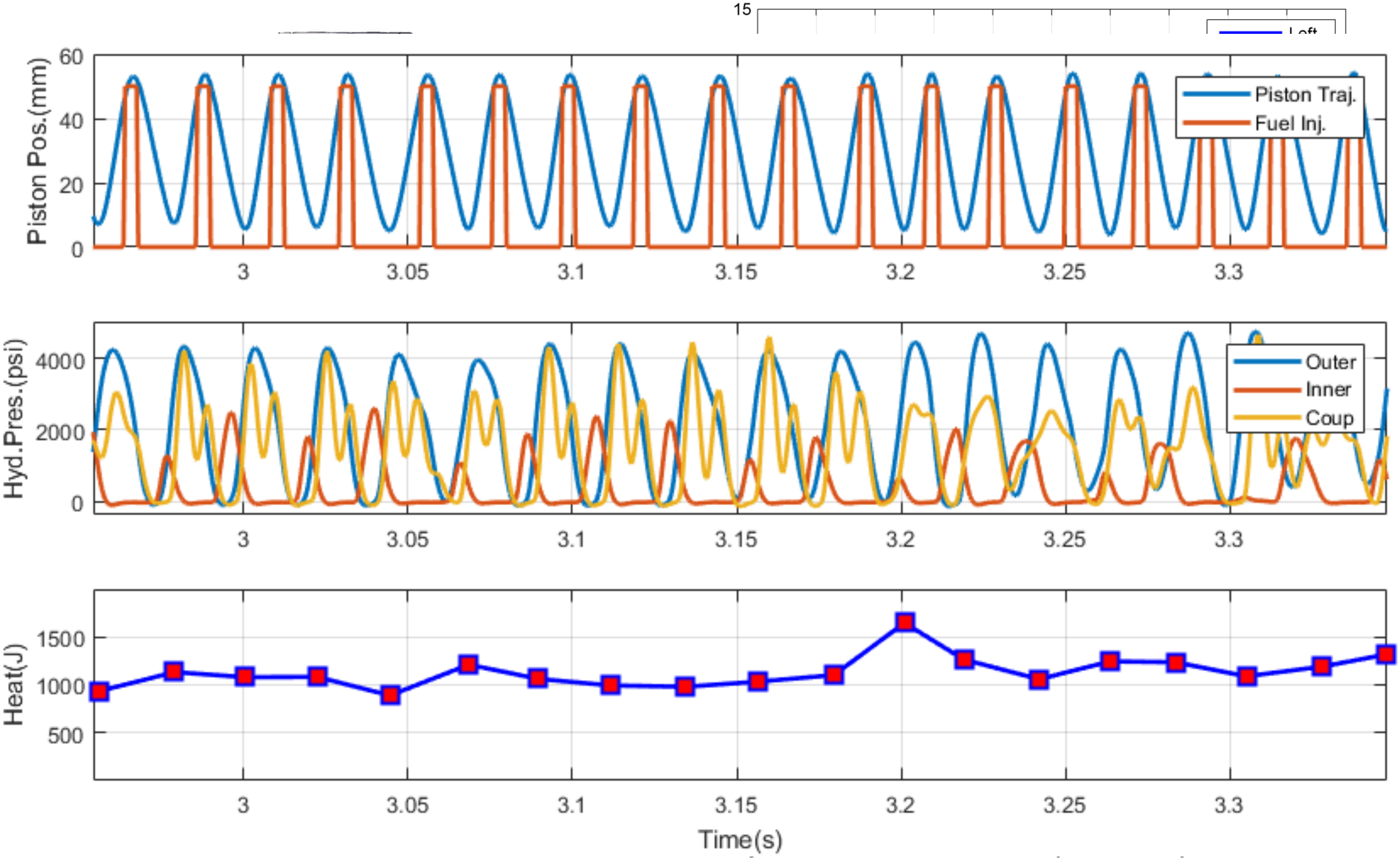
In-cylinder Gas Dynamics

Thermal heat release
Reaction production
Reaction rate

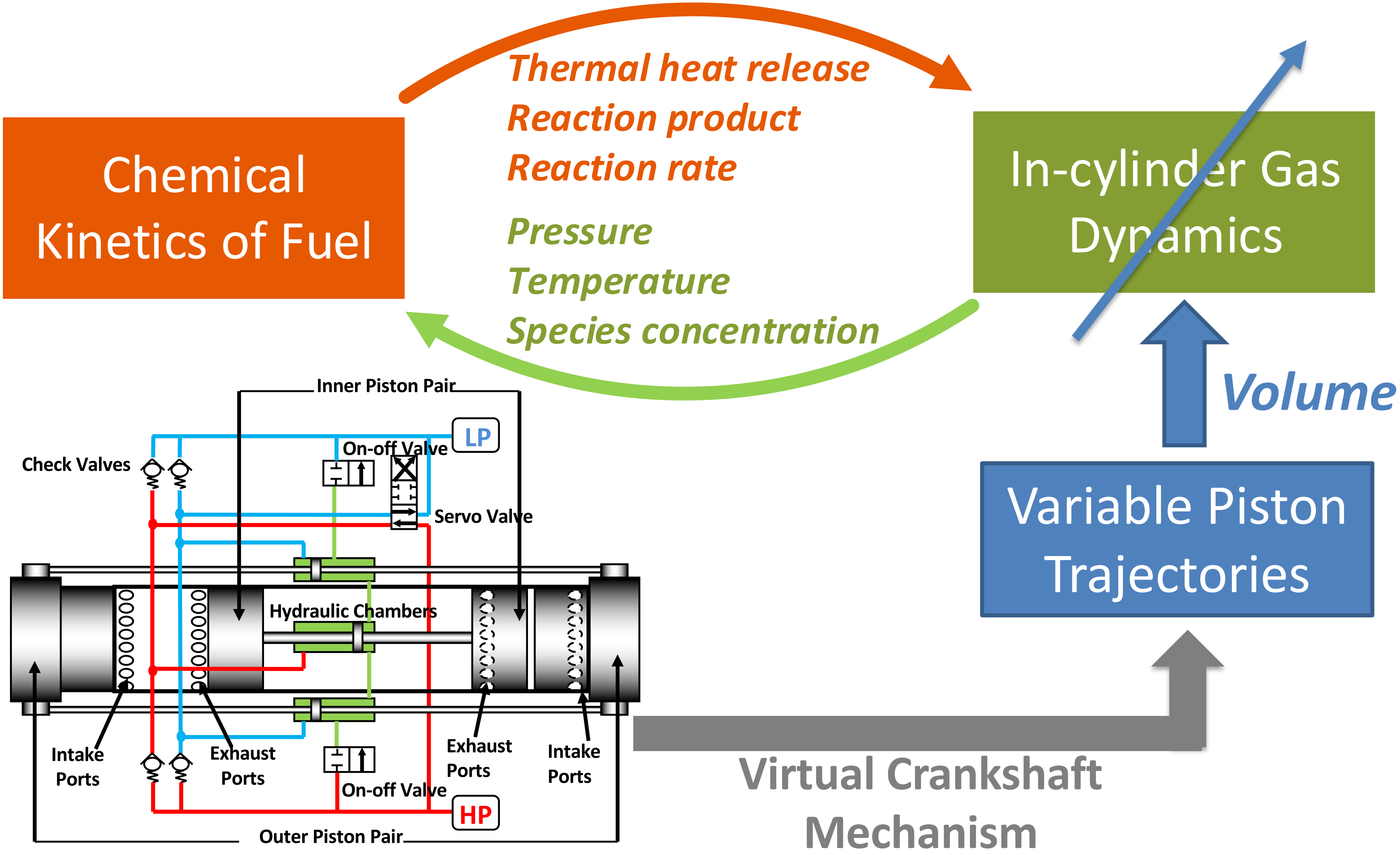
Pressure
Temperature
Species concentration

- ❖ Still short of controllability in ICE to adjust the HCCI combustion.
- ❖ Existing control methods, e.g. regulating exhaust gas recirculation (EGR), varying valve timing and stratifying charge, can only execute combustion control at specific time instants in each cycle.

Background – FPE in UMN



Trajectory-based Combustion Control



Chemical Kinetics of Fuel

Thermal heat release
Reaction product
Reaction rate

Pressure
Temperature
Species concentration

In-cylinder Gas Dynamics

Volume

Variable Piston Trajectories

Virtual Crankshaft Mechanism

Trajectory-based Combustion Control

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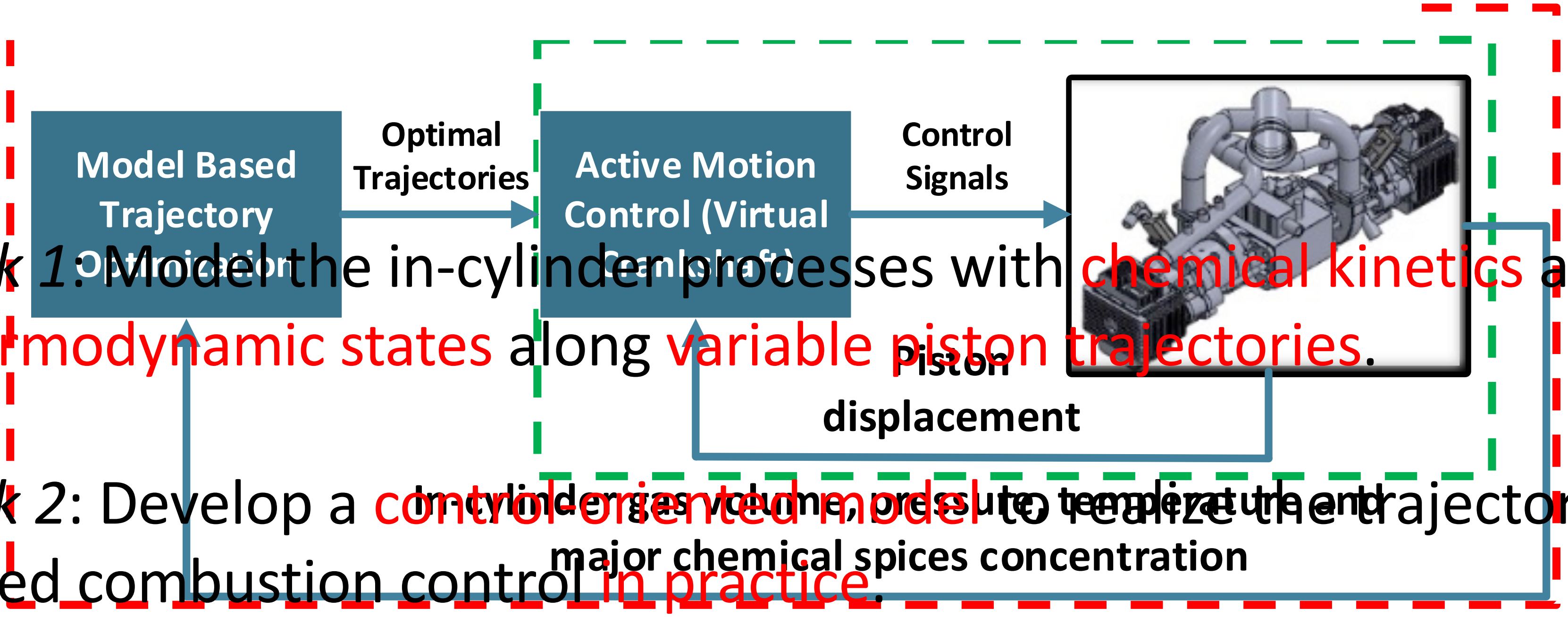
Task 1: Model the in-cylinder processes with chemical kinetics and thermodynamic states along variable piston trajectories.

Task 2: Develop a control-oriented model to realize the trajectory-based combustion control in practice.



Overall system configuration of trajectory based combustion control

Task 3: Based on the above models, design optimal piston trajectories by leveraging the dynamic between chemical kinetics and gas dynamics.

- ☐ ***Inner Loop:*** piston motion control - virtual crankshaft
- ☐ ***Outer Loop:*** Trajectory-based combustion control

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Chemical Kinetics Driven Model

The entire model is separated into 3 parts.

Cantera
Chemical Kinetics • Thermodynamics • Transport Processes

Heat Loss Submodel

$$\dot{Q}_{HT} = h \cdot A_{wall}(T - T_{wall})$$

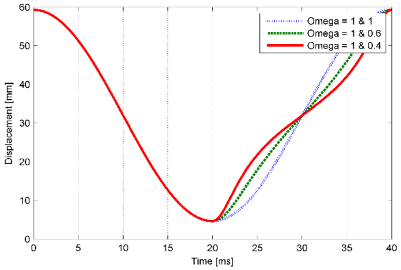
$$h = 3.26 \cdot b^{-0.2} P^{0.8} T^{-0.55} w^{0.8}$$

$\dot{Q}_{HT}$

P, T

A_{wall}

Variant Piston Trajectories



Geometric Model

$\frac{dV}{dt}, V$

Thermal Dynamics Submodel

$$\frac{dU}{dt} = -P\frac{dV}{dt} - \dot{Q}_{HT} + \dot{Q}_{Chem}$$

$$m\frac{d\omega_i}{dt} = \dot{m}_{i,chem}$$

$$P \cdot V = m \cdot R_{mass} \cdot T$$

$$\frac{dU}{dt} = \sum_{i=1}^{N_s} C_{v,i} \cdot m \cdot \omega_i \frac{dT}{dt} + \sum_{i=1}^{N_s} C_{v,i} \cdot m \cdot T \cdot \frac{d\omega_i}{dt}$$

Physics-based Model

T

$C_{v,i}$

T, ω_i

V

$\dot{Q}_{Chem}$

$\dot{m}_{i,chem}$

Thermal Data Part

NASA Polynomial Parametrization

$h_{i,m}, S_{i,m}$

Chemical Kinetics Part

$$\frac{d[A]}{dt} = n_a \cdot (-k_f [A]^{n_a}[B]^{n_b} + k_b [C]^{n_c}[D]^{n_d})$$

$$[A] = \frac{m \cdot \omega_A}{M_A \cdot V}$$

$$k_f = A \cdot T^n \cdot \exp^{(-\frac{E_a}{RT})} \qquad \frac{k_f}{k_b} = K_e = \exp^{(-\frac{\Delta G^o}{RT})}$$

$$v_A = \sum_{1}^{N_{rxn}} \frac{d[A]}{dt}$$

$$\dot{Q}_{Chem} = -V \cdot \sum_{i=1}^{N_s} v_i \cdot h_{i,m} \qquad \dot{m}_{i,chem} = V \cdot M_i \cdot v_i$$

Chemical Reaction Mechanism

Fuel	Number of species	Number of reactions	Resource
Methane	53	325	GRI-30
Propane	50	244	UC Santiago
Ethanol	57	383	LLNL[a]
DME	79	683	LLNL
Ammonia	23	98	Cal-tech
n-Heptane	160	1540	LLNL

NASA polynomial parametrization:

$$\frac{C_{v,i}(T)}{R} = a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 - 1$$

$$\frac{h_{i,m}(T)}{RT} = a_0 + \frac{a_1}{2}T + \frac{a_2}{3}T^2 + \frac{a_3}{4}T^3 + \frac{a_4}{5}T^4 + a_5$$

Combustion Phasing Control

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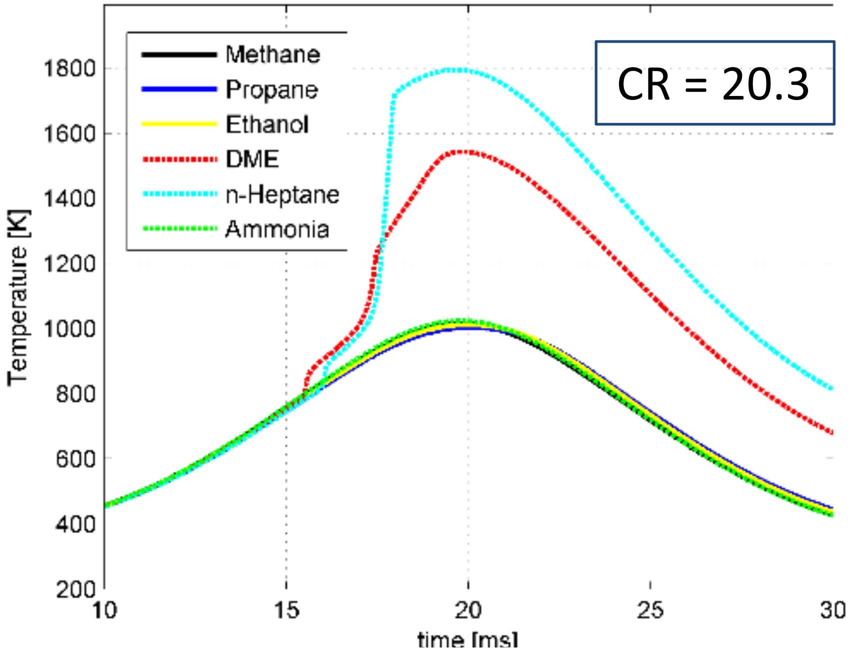
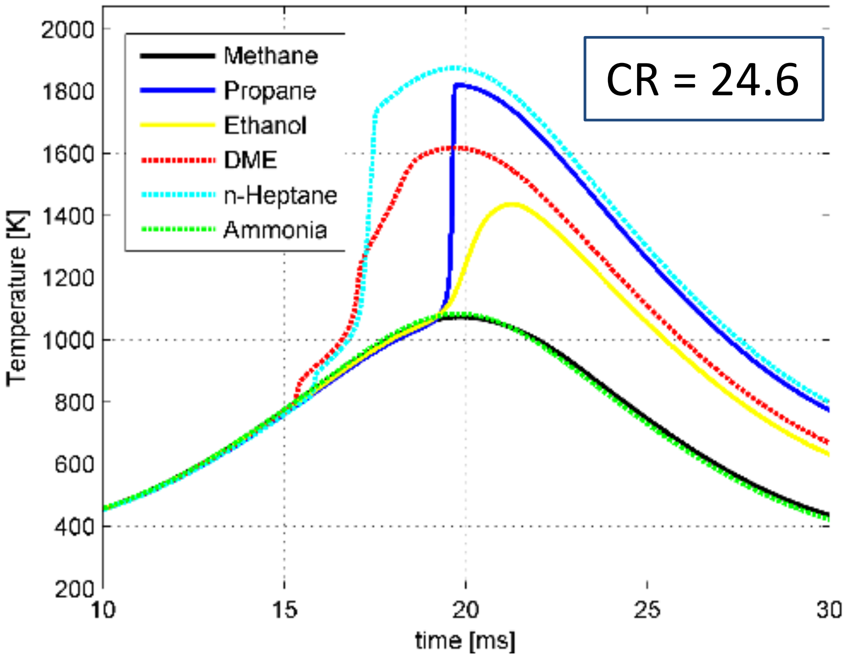
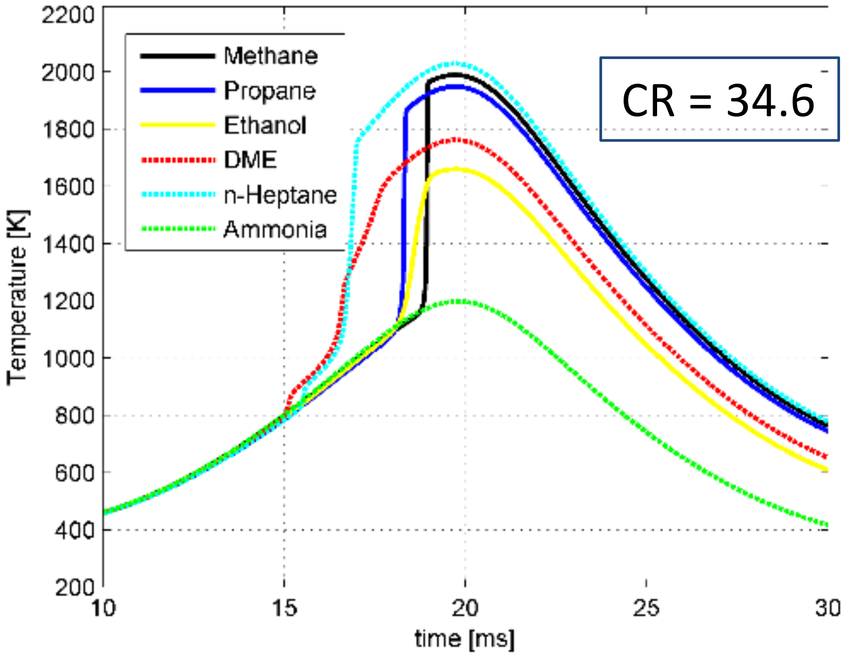


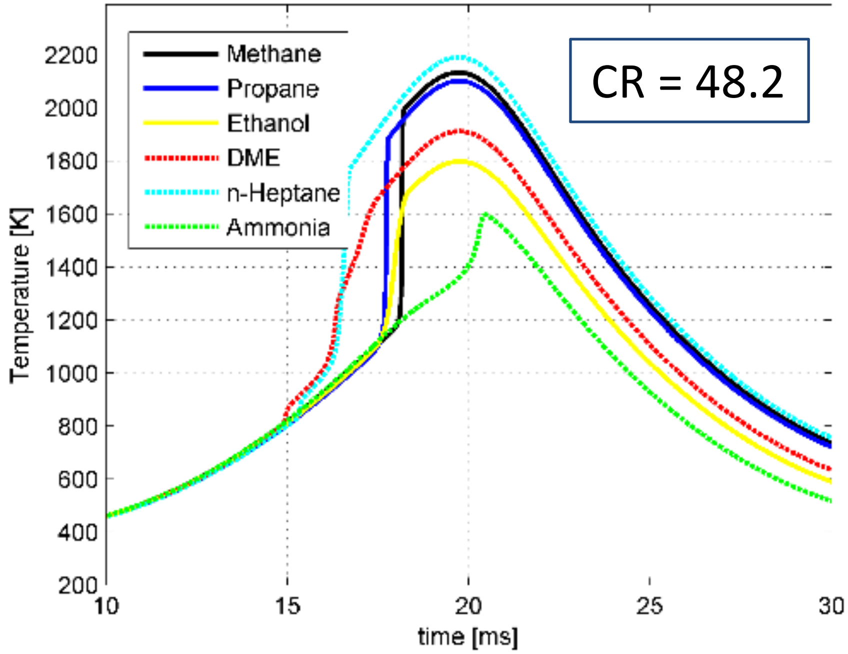
CR = 20.3



CR = 24.6

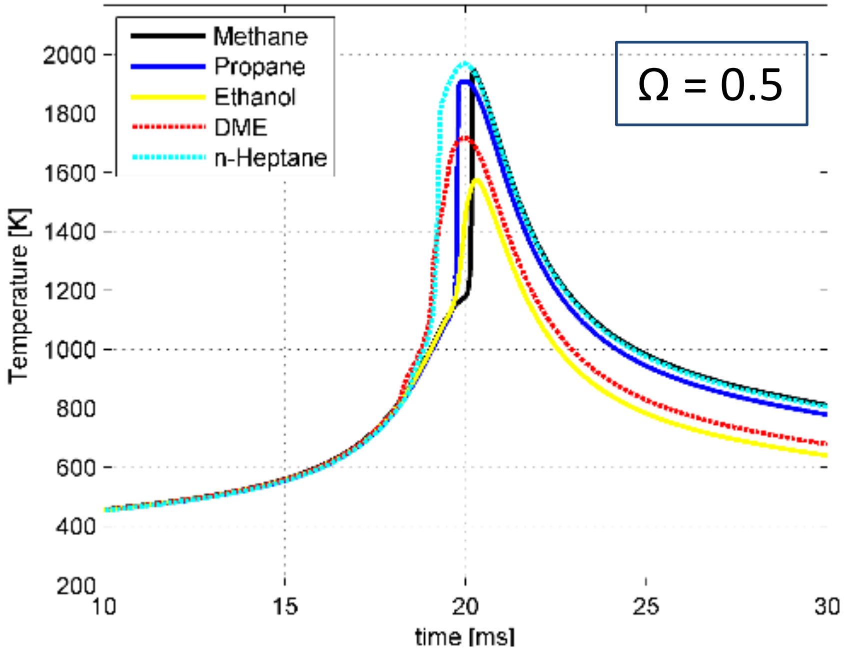


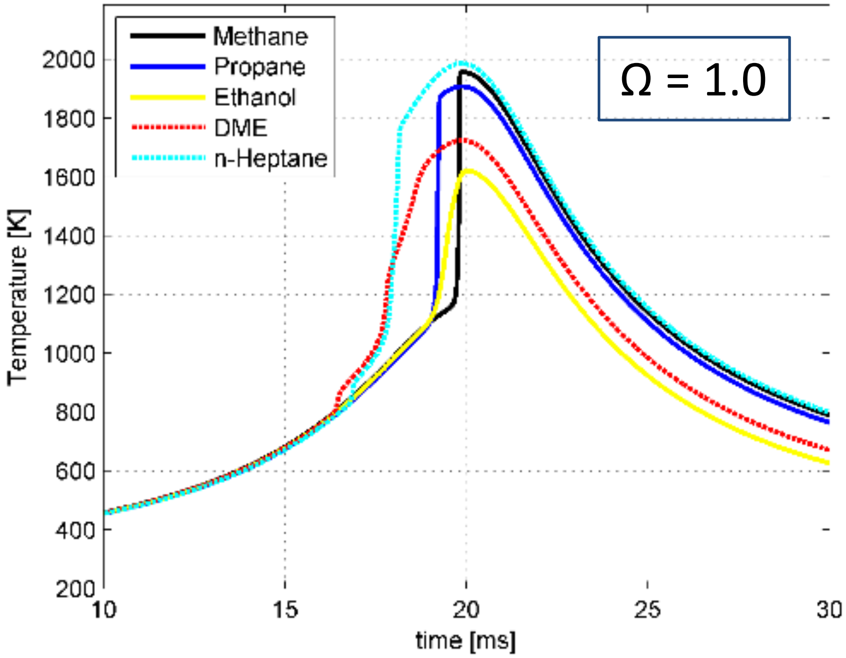
CR = 34.6

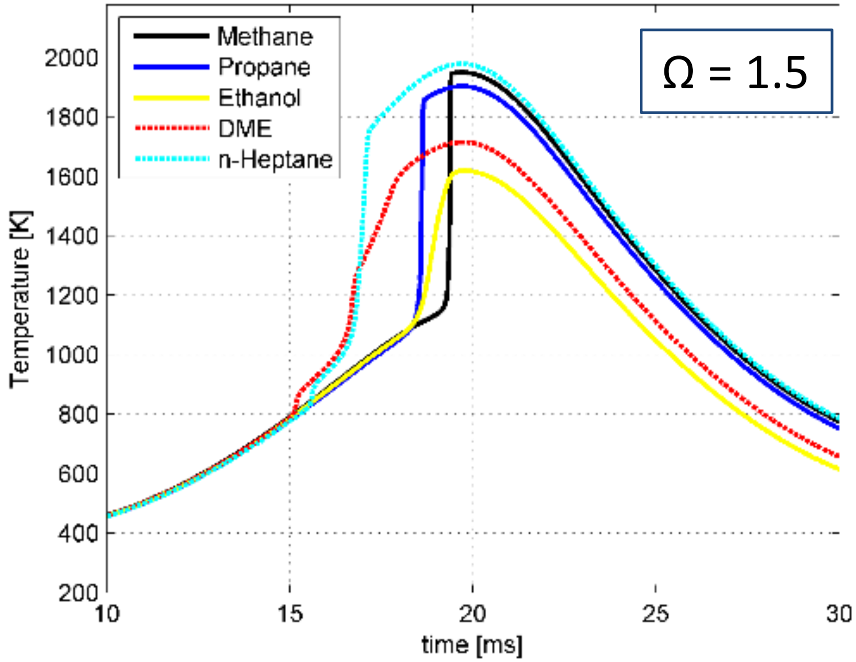


CR = 48.2

Combustion Phasing Control







- Increasing both the CR and the Ω can realize multiple fuels combustion in FPE
- Increasing CR and Ω can both advance the SOC timing
- A new control means is achieved for combustion phasing control – piston trajectory

Indicative Output Works

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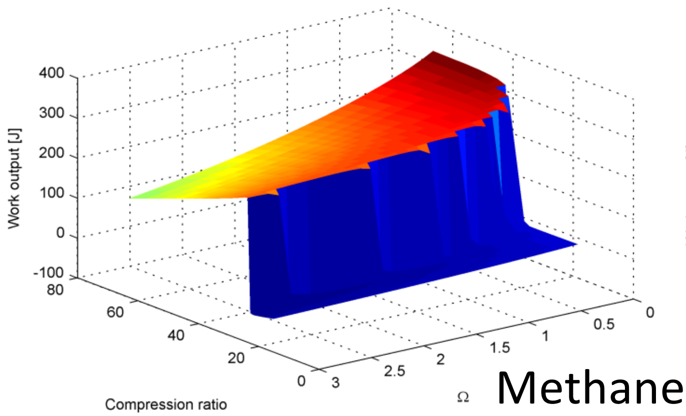
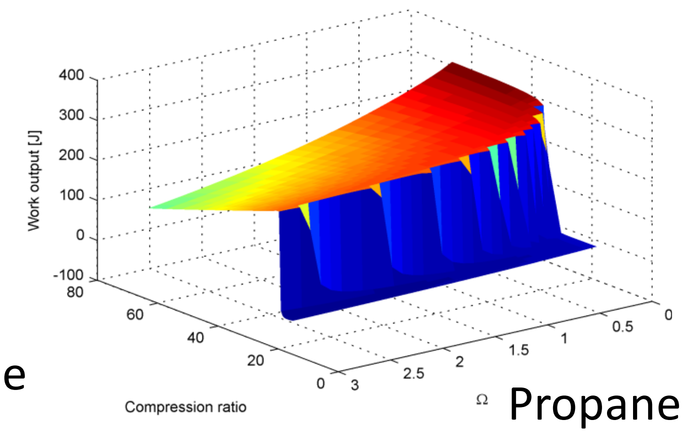
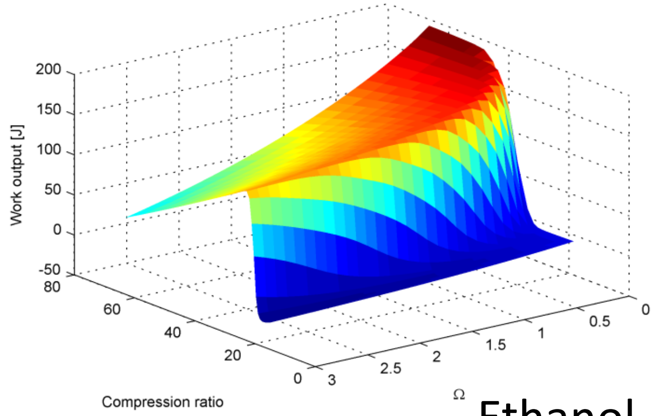


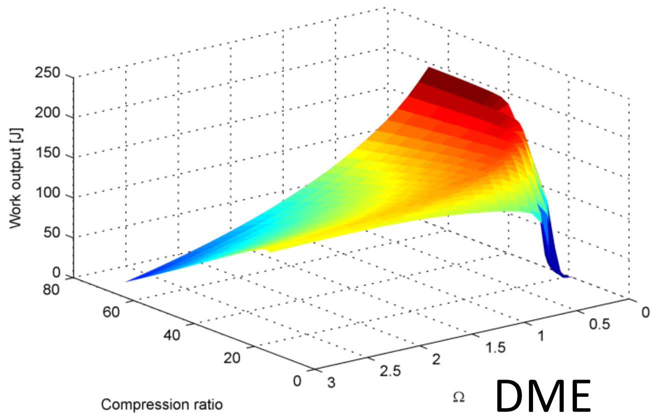
Methane



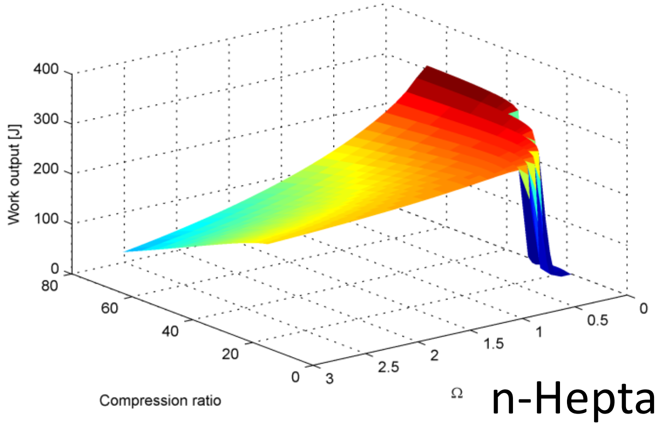
Propane



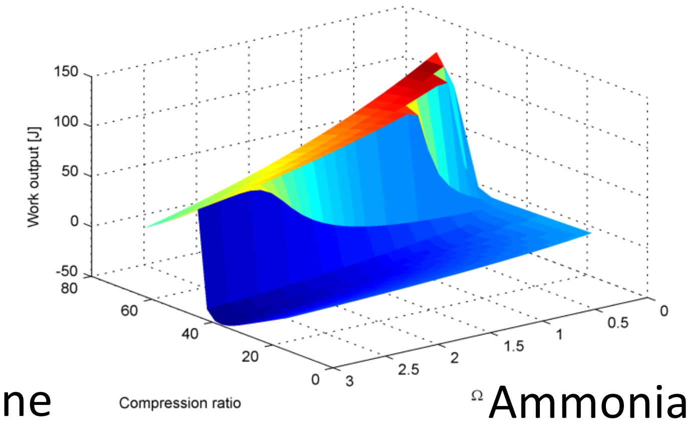
Ethanol



DME



n-Heptane

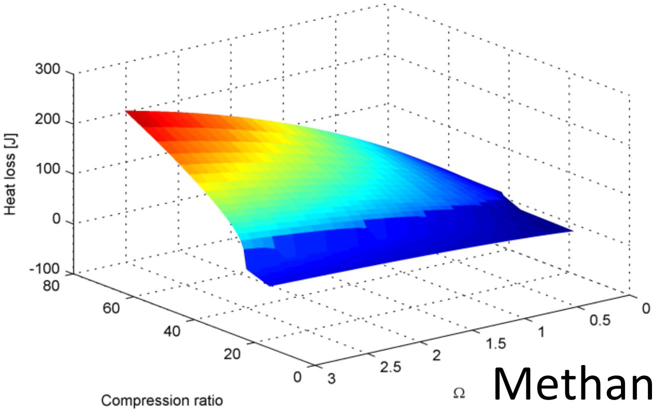


Ammonia

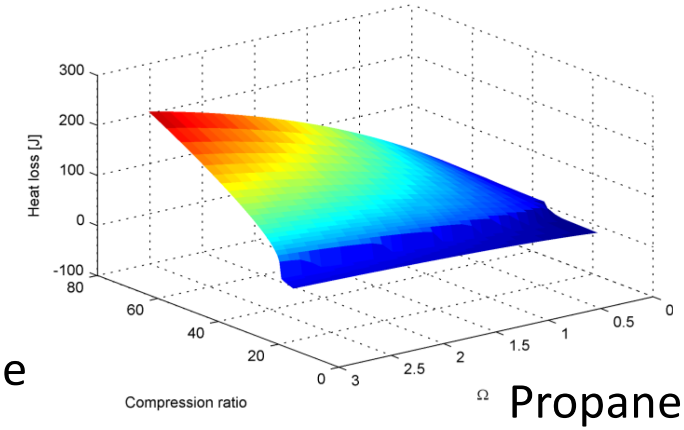
Both CR and Ω have direct effects on the amount of indicative work output

The peak of output work surface is located at zone with larger CR and smaller Ω

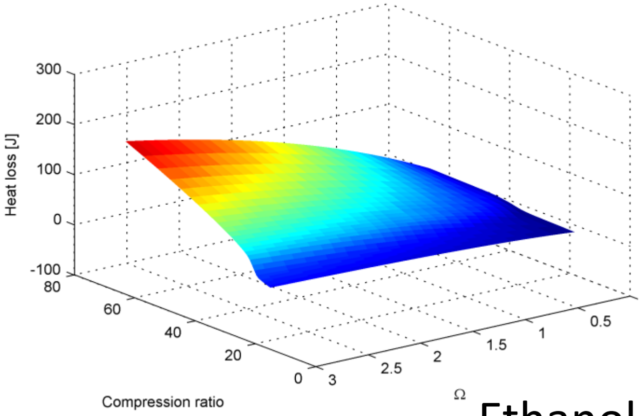
Heat loss amount



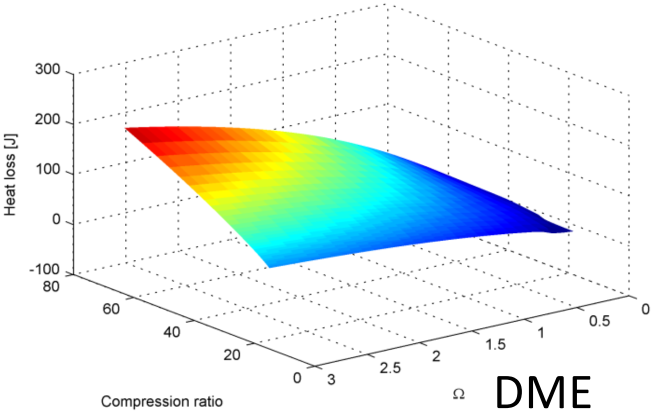
Methane



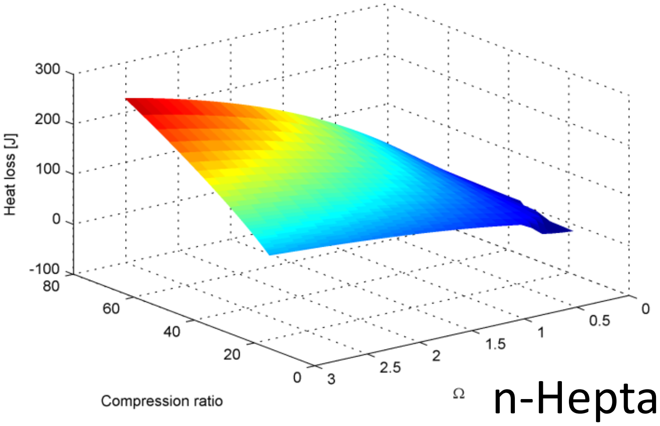
Propane



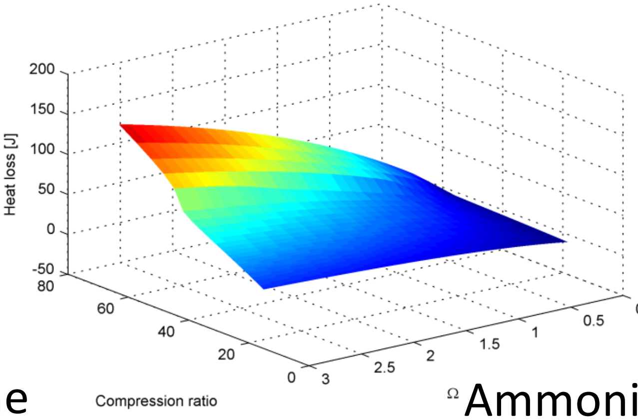
Ethanol



DME



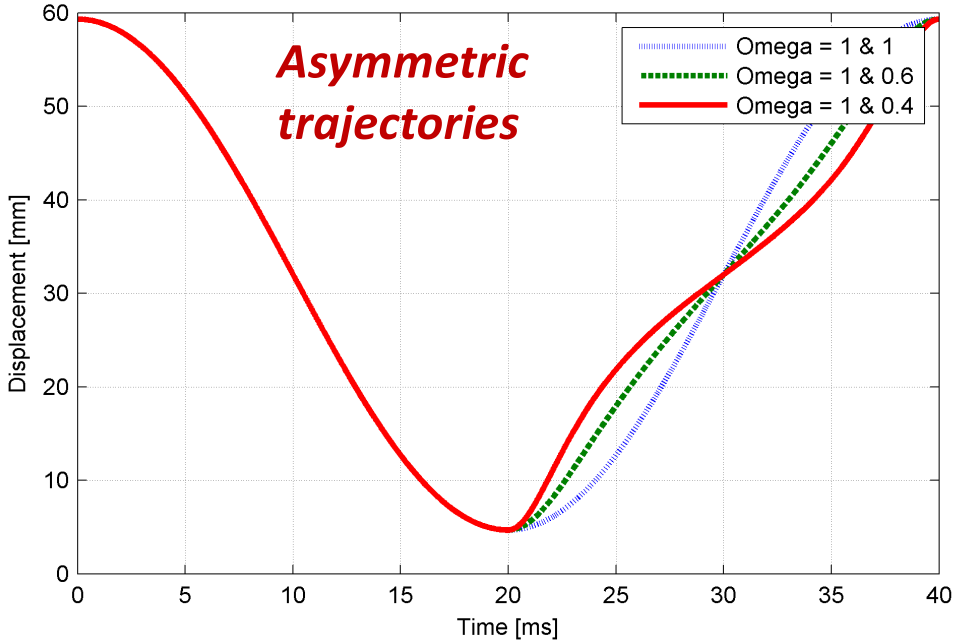
n-Heptane

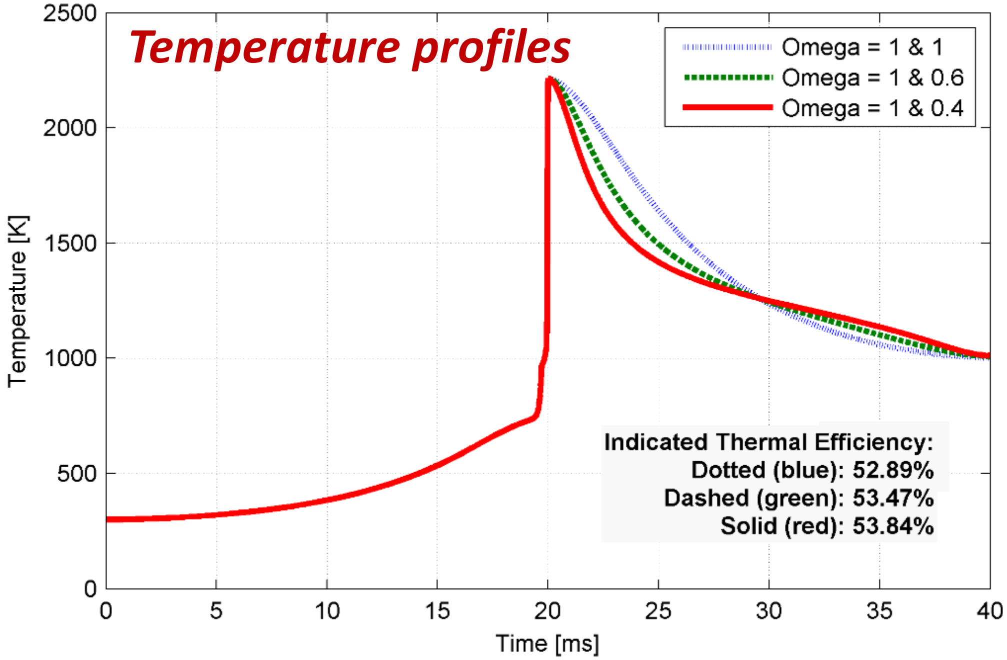


Ammonia

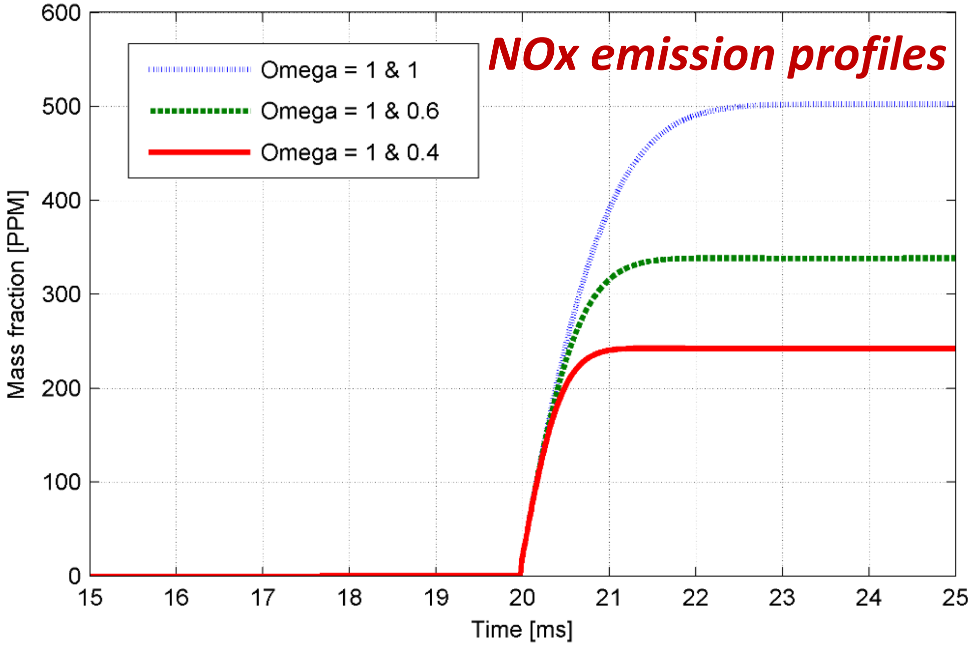
The peak of heat loss amount is located at zone with larger CR and larger Ω

NOx Emission


Asymmetric trajectories


Temperature profiles

Indicated Thermal Efficiency:
Dotted (blue): 52.89%
Dashed (green): 53.47%
Solid (red): 53.84%


NOx emission profiles

NOx emission

- The majority of NOx emission is produced after the major heat release.
- Quick expansion reduce the temperature and thus reduce the NOx emission.
- We can reduce NOx emissions and increase efficiency simultaneously.

Control-Oriented Model

Comprehensive model

- **Detailed** reaction mechanism
- **Higher** computational burden
- Control application

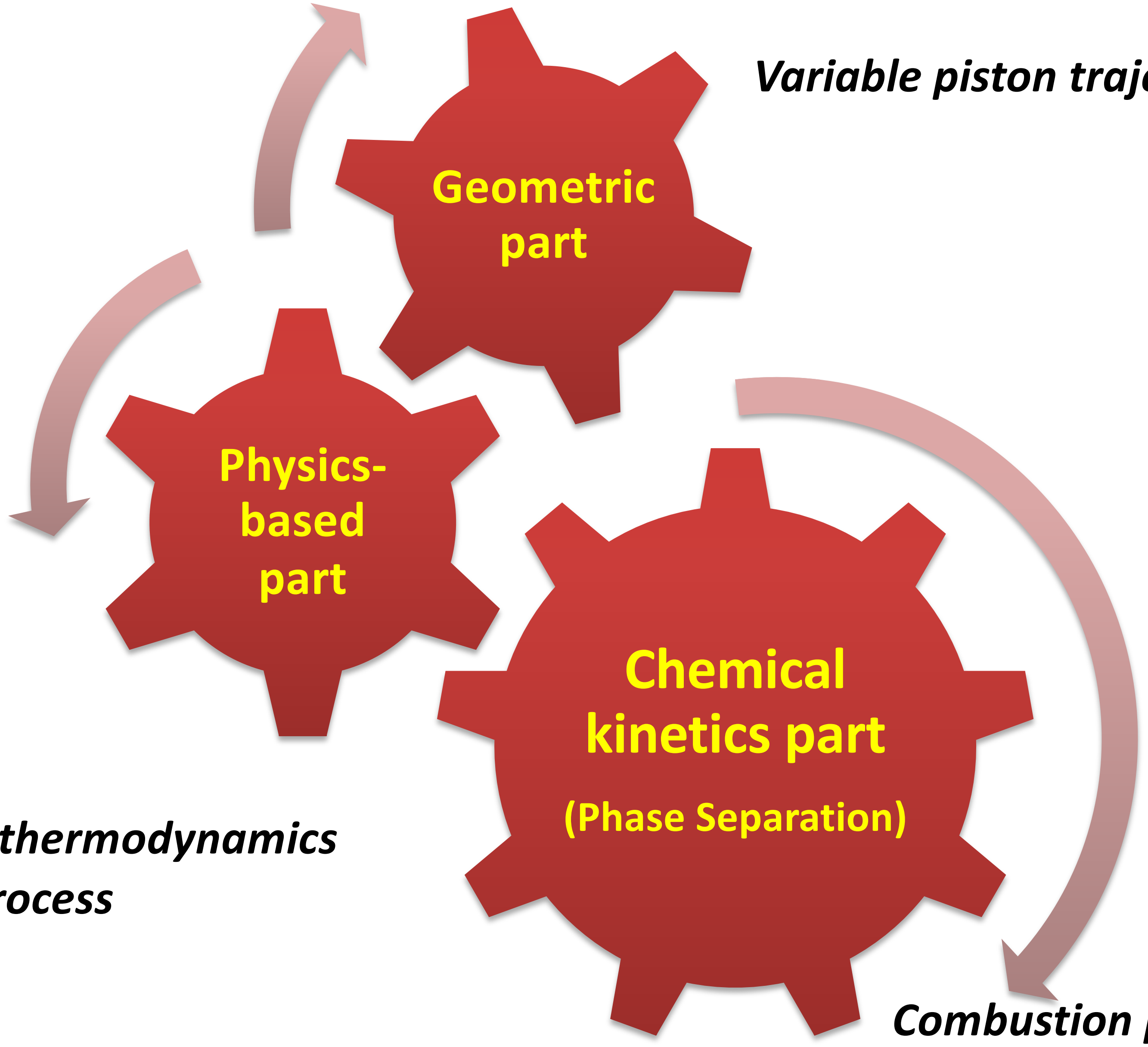
Existing control-oriented model

- **Over-simplifying** the chemical kinetics
- HCCI combustion simulation

New control-oriented model

- Best balance between **computational burden** and **prediction accuracy**

Modeling Approach



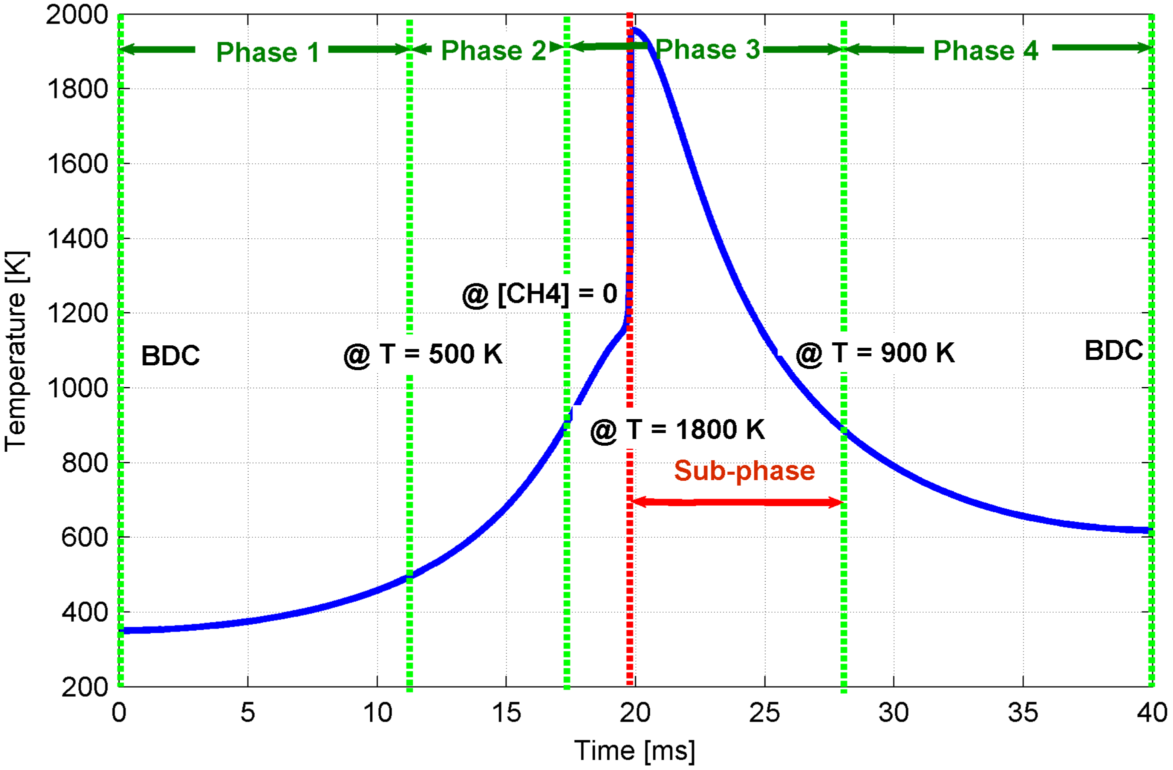
Variable piston trajectories

The first law of thermodynamics and heat loss process

Combustion process

Phase Separation Method

In order to reduce computational time and keep sufficient chemical kinetics information, the engine operation cycle is separated by several phases.



Phase separation within an engine cycle

Phase 1: Pure compression

Phase 2: Ignition phase

$$R_1 : CH_4 + 0.5O_2 \rightarrow CO + 2H_2$$

$$RR_1 = 4.4 \times 10^9 \cdot [CH_4]^{0.5} \cdot [O_2]^{1.25} \exp(-\frac{15095}{T})$$

Phase 3: Heat release phase

$$R_2 : CO + H_2O \rightarrow CO_2 + H_2$$

$$R_3 : H_2 + 0.5O_2 \rightarrow H_2O$$

$$RR_2 = 2.75 \times 10^7 \cdot [CO] \cdot [H_2O] \exp(-\frac{10065}{T})$$

$$RR_3 = 1.5 \times 10^9 \cdot [H_2][O_2]^{0.5} \exp(-\frac{17609}{T})$$

Sub-phase: NOx production

$$w_{NO_x} = \frac{6.0 \times 10^{16}}{T^{0.5}} [N_2][O_2]^{0.5} \exp(\frac{-69090}{T})$$

Phase 4: Pure expansion

Computational Cost

The proposed model is compared with the other two models:

Simplified model

- Entire chemical kinetics is represented by a global reaction.
- Assuming the heat release is instantaneous after the combustion.

Detailed model

- The chemical kinetics is represented by a detailed reaction mechanism includes 53 species and 325 reactions.

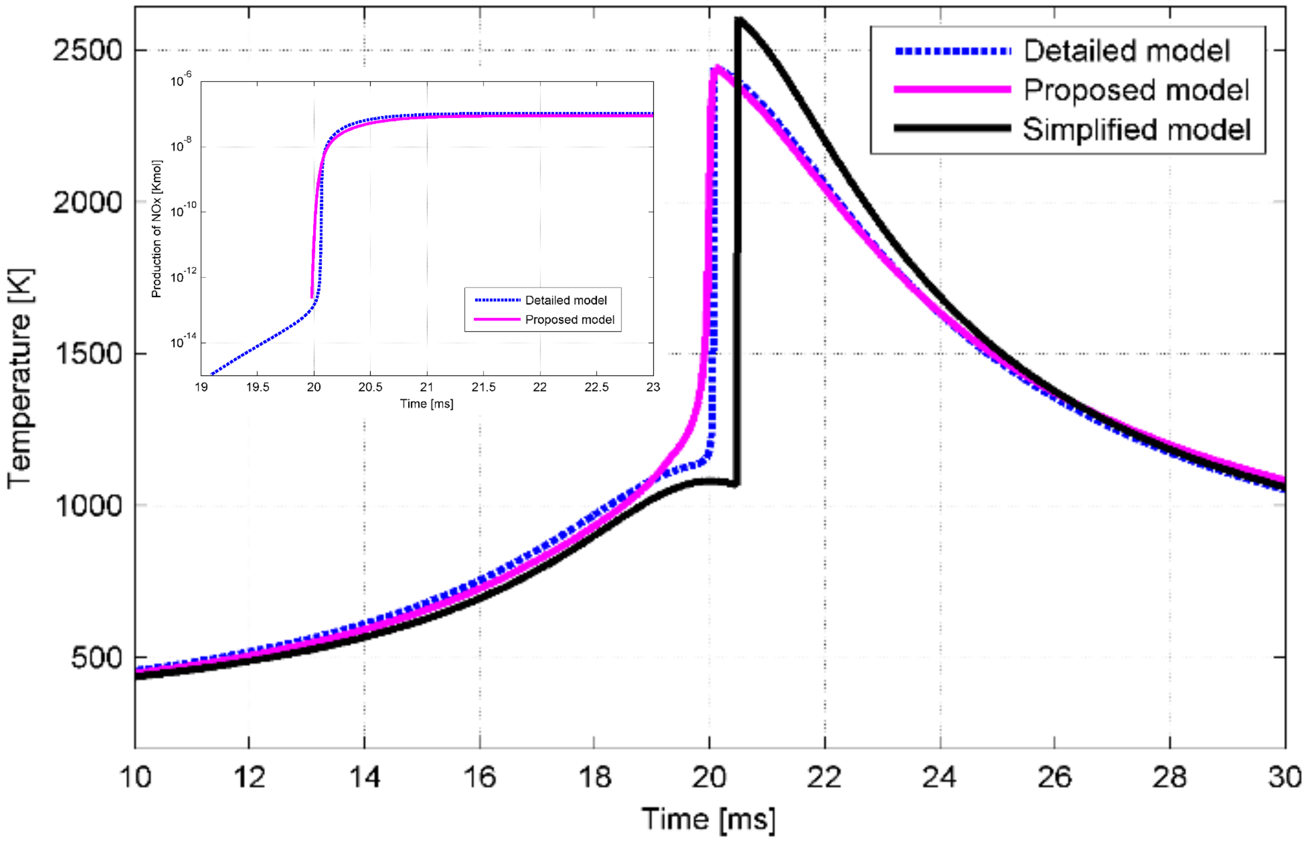
Utilized model	Computational time [ms]
Detailed model	2070
Proposed model	98
Simplified model	6

☐ The detailed model needs 2070 ms to simulate an engine cycle.

☐ The proposed model reduce the computational turnaround time by 95%.

☐ The simplified model only takes 6 ms.

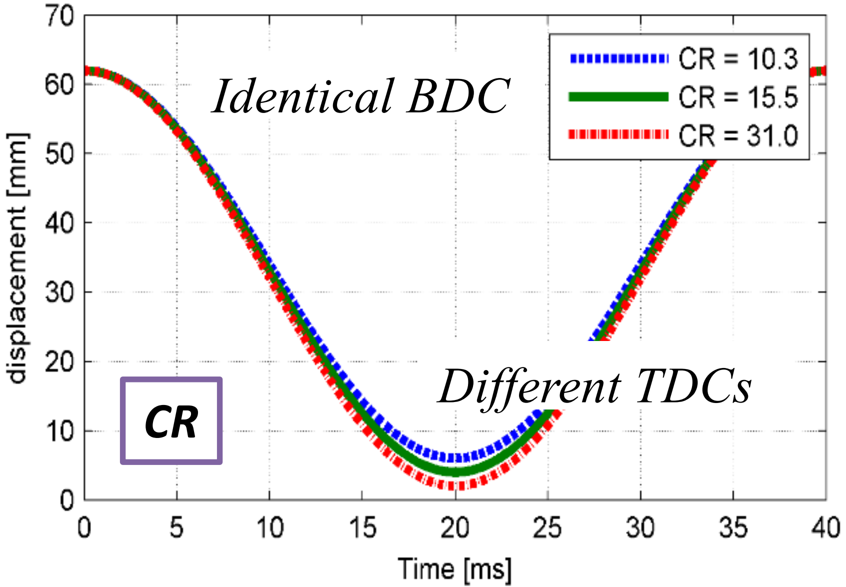
Prediction Accuracy

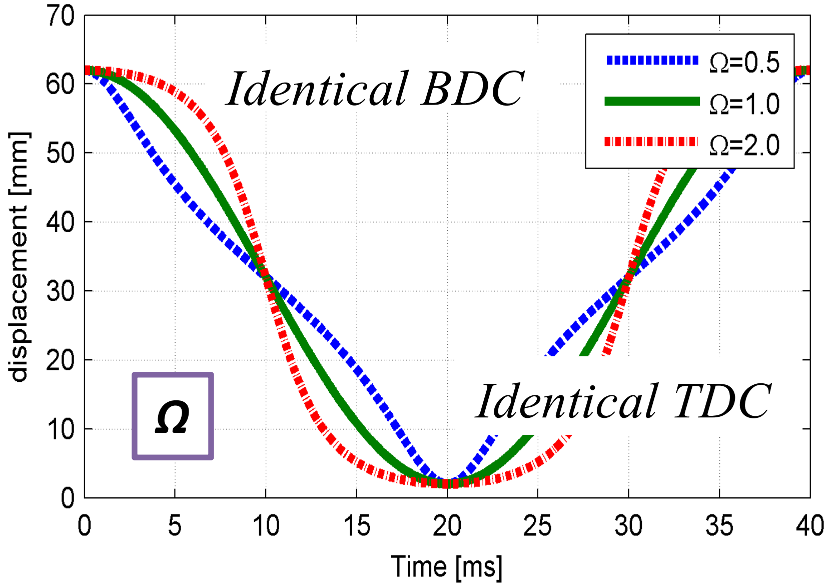


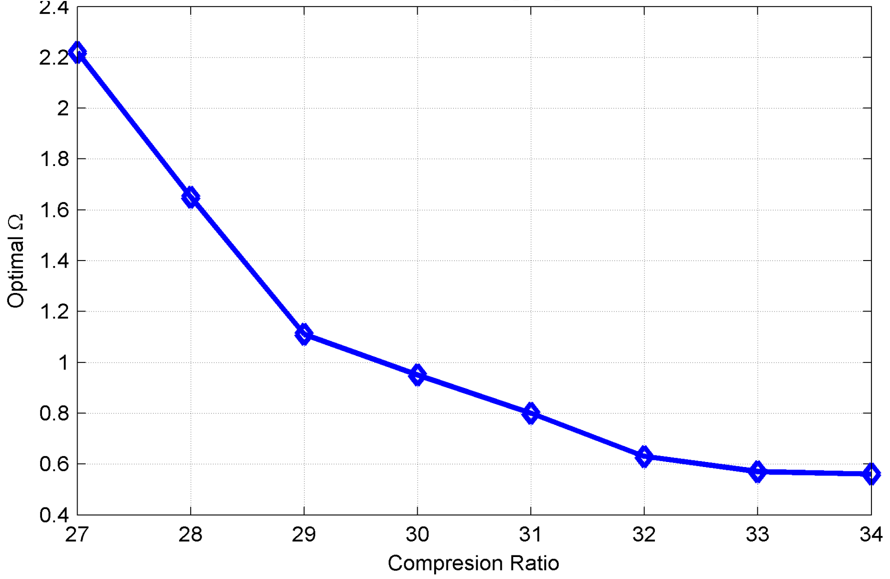
Comparison of the accuracy of the prediction – Temperature and NOx production (inserted)

- Good agreement between the proposed model and the detailed one.
- The simplified model fails to represent the combustion precisely due to its over-simplifying of the chemical kinetics.
    - later start of combustion
    - higher peak temperature
- Simplified model cannot provide any information on NOx emission while the others predicts similar results of NOx production.

Piston Optimization – one Ω





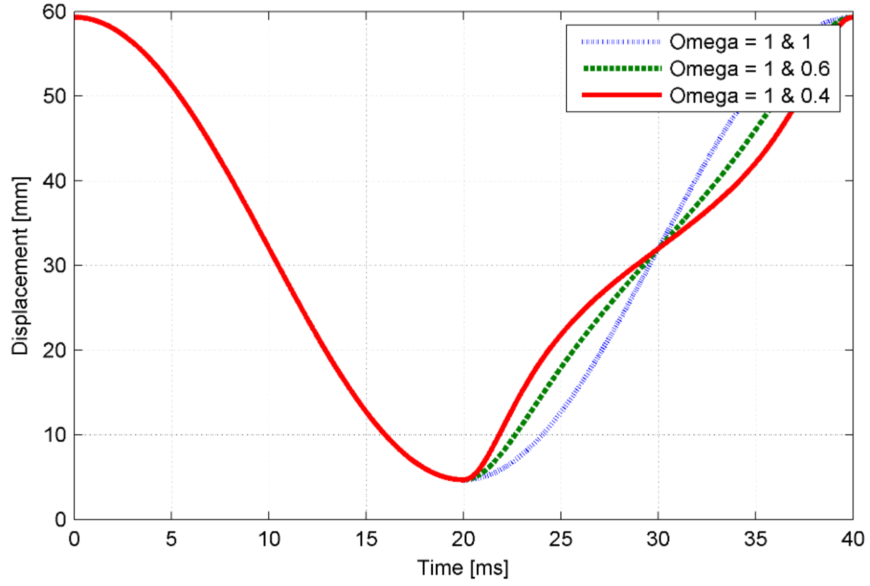


- At given *CR*, various piston trajectories as well as their output work can be presented as a function of *Ω*.

$$Maximize : J_1 = W_{ouput} = f(\Omega)$$

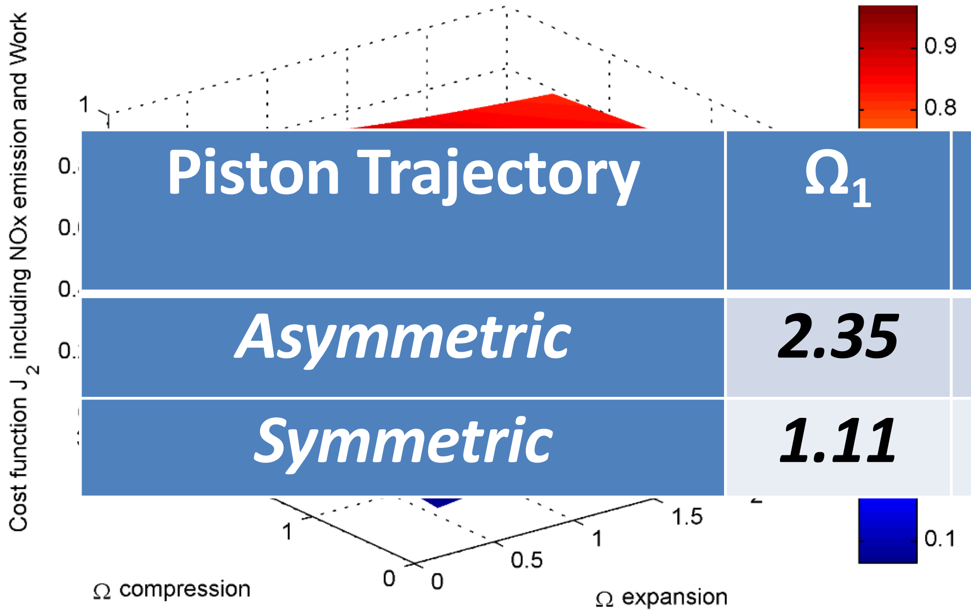
- Smaller *Ω* will result in *an incomplete combustion and larger Ω* will increase the heat loss.
- higher CR, lower optimal *Ω*.

Piston Optimization – two Ω



- ☐ Asymmetric trajectories
  - ○ Increase thermal efficiency
  - ○ Reduce NOx emissions
- ☐ Two Ωs represent compression and expansion trajectories respectively.
- ☐ Forming a two dimensional optimization problem at a fixed CR.

$$Maxmize: J_2 = w_1 \frac{W}{W_{\max}} - w_2 \frac{C(NOx)}{C_{\max}(NOx)} = f(\Omega_1, \Omega_2)$$



Piston Trajectory	Ω_1	Ω_2	Work [J]	NOx Emission [mol/m^3]
Asymmetric	***2.35***	***0.40***	***401.91***	***2.32e-6***
Symmetric	***1.11***	***1.11***	***398.28***	***4.07e-6***

❖ w_1 and w_2 are weight coefficients.

Piston Dynamic Optimization

Due to the repetitive nature of the FPE operation:

- the time differential equations in the model can be numerically solved in cycle base.
- It forms a mapping converting the piston trajectory (u) in each cycle to other states of the model.

$$\Phi\left(\begin{bmatrix} u_1 \\ u_2 \\ . \\ . \\ . \\ u_{n-1} \\ u_n \end{bmatrix}\right) = \begin{bmatrix} P_1 & T_1 & [X_{CH_4}]_1 & \dots & [X_{N_2}]_1 \\ P_2 & T_2 & [X_{CH_4}]_2 & \dots & [X_{N_2}]_2 \\ . & . & . & & . \\ . & . & . & & . \\ . & . & . & & . \\ P_{n-1} & T_{n-1} & [X_{CH_4}]_{n-1} & \dots & [X_{N_2}]_{n-1} \\ P_n & T_n & [X_{CH_4}]_n & \dots & [X_{N_2}]_n \end{bmatrix}$$

The original dynamic optimization problem is transformed into a static nonlinear programming problem and solved by SQP algorithm:

Minimize: **_Work output_** **_NOx emission_**

$$f(\Phi(u),u) = -\sum_{i=1}^{100} P_i \frac{(u_{i+1}-u_i)}{dt} + r\cdot\max(0,[X_{NO_x}]_{101} - 3e-6)$$

r works as a penalty if the final *NOx* emission > 3e-6 mol/m^3

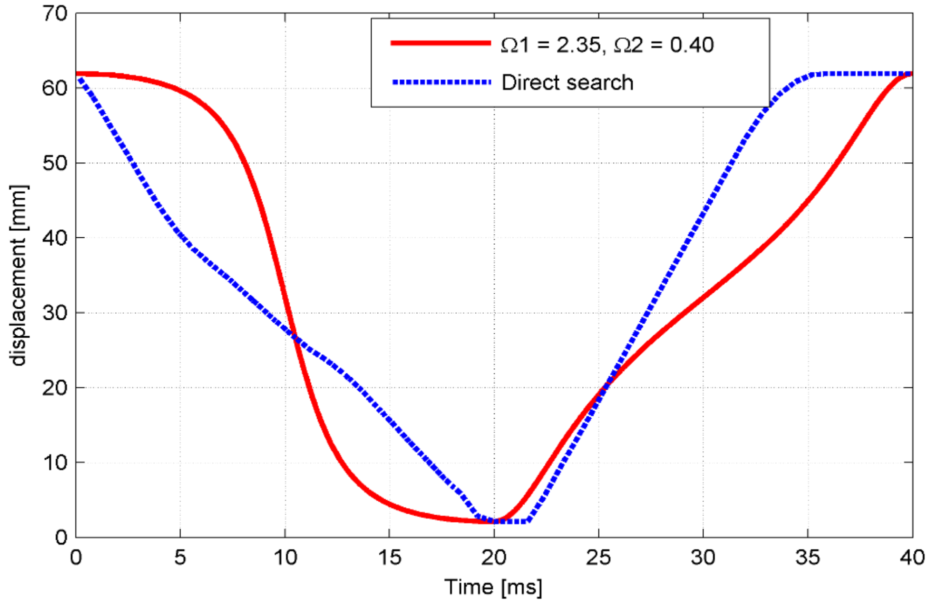
over $u \in R^{101}$

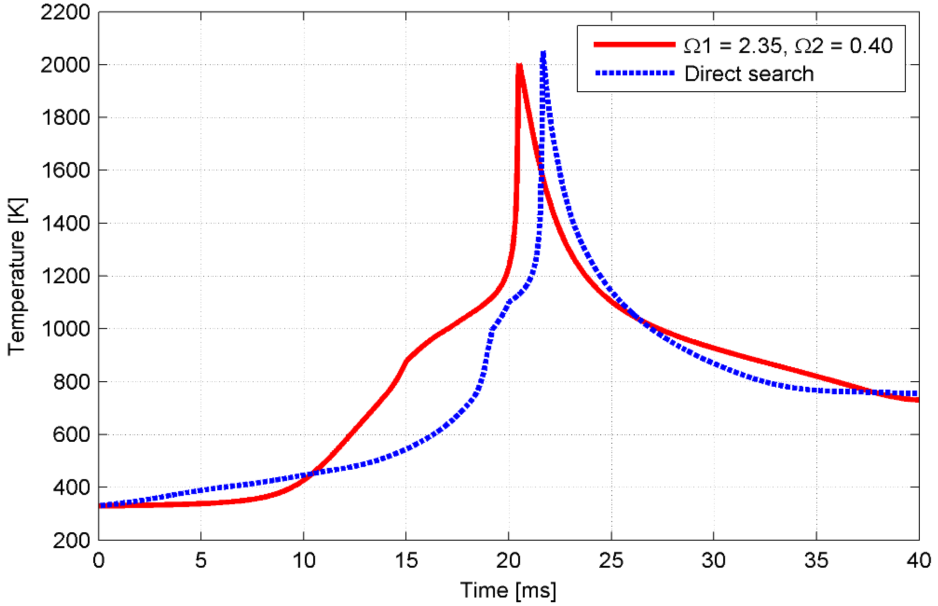
Subject to $h(u) = 0$ *h(u)* limits the start, middle and end points of the trajectory.

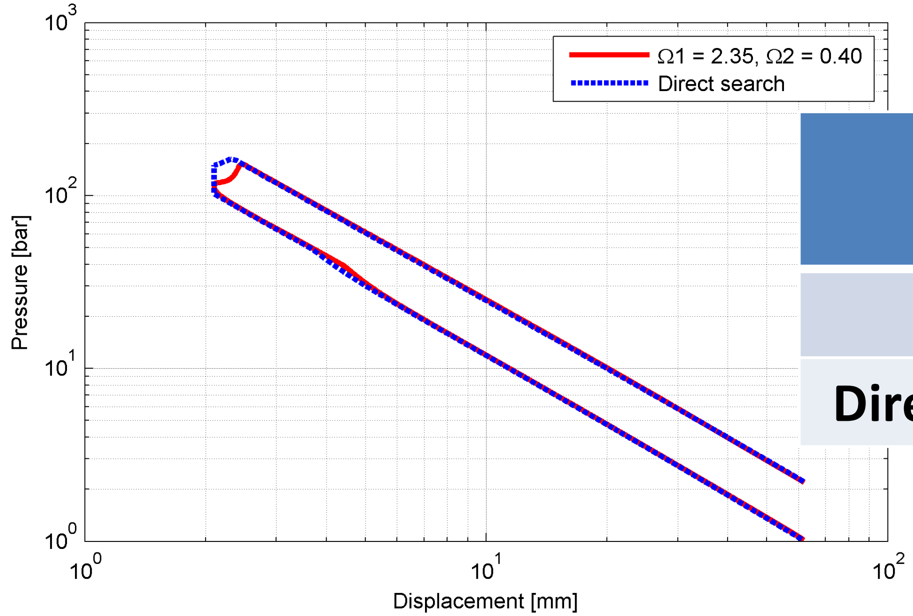
$g(u) \leq 0$ *g(u)* ensures the piston velocity < 8m/s.

$u^L \leq u \leq u^U$ u^L and u^U are the TDC point and the BDC point respectively.

Piston Dynamic Optimization







Trajectory	Work output [J]	NOx Emission [mol/m^3]
Asymmetric	**401.91**	**2.45e-6**
Direct Optimization	**416.70**	**2.31e-6**

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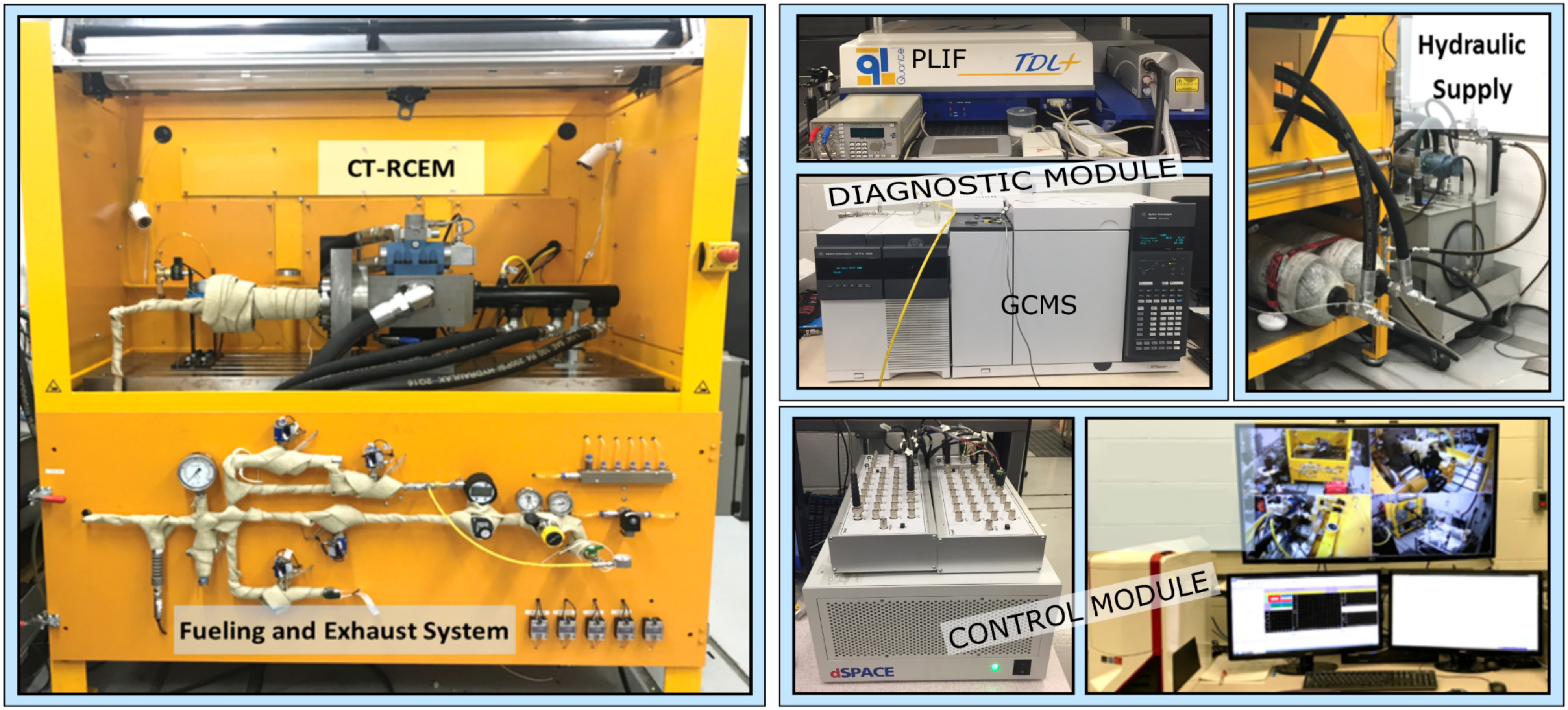
- Conclusions

Controlled Trajectory RCEM



Hydraulic actuator unit: high pressure accumulator, servo-valve

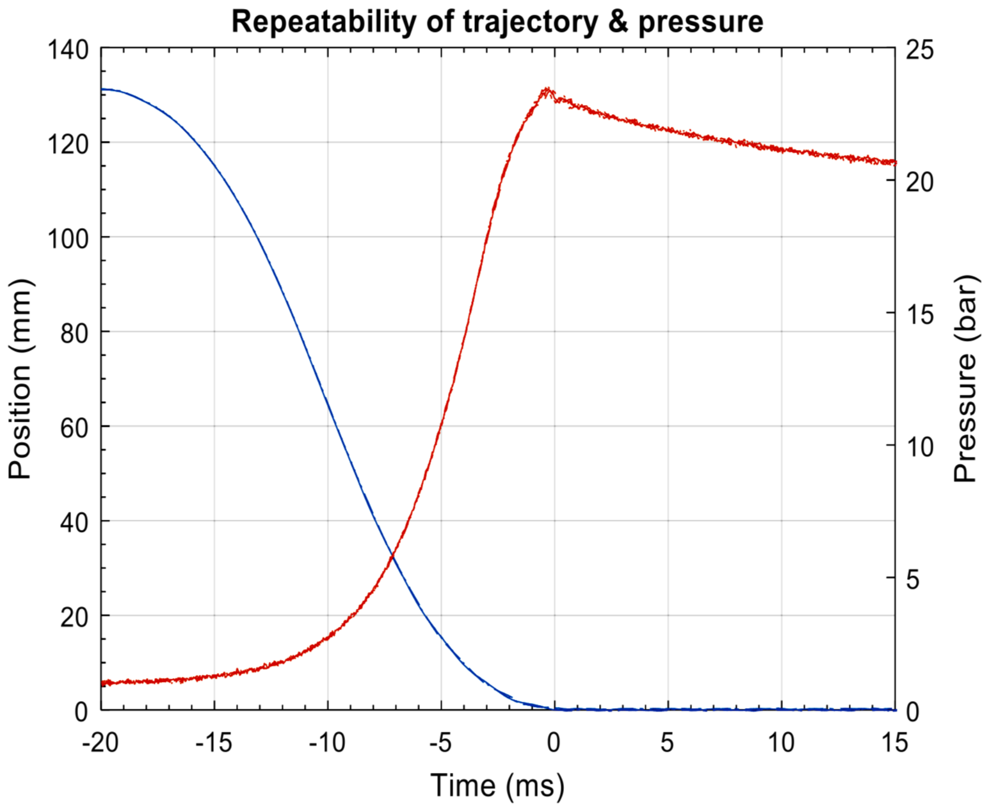
Combustion chamber unit: combustion cylinder with a creviced piston

Fueling and exhaust purging system: different set of check valves

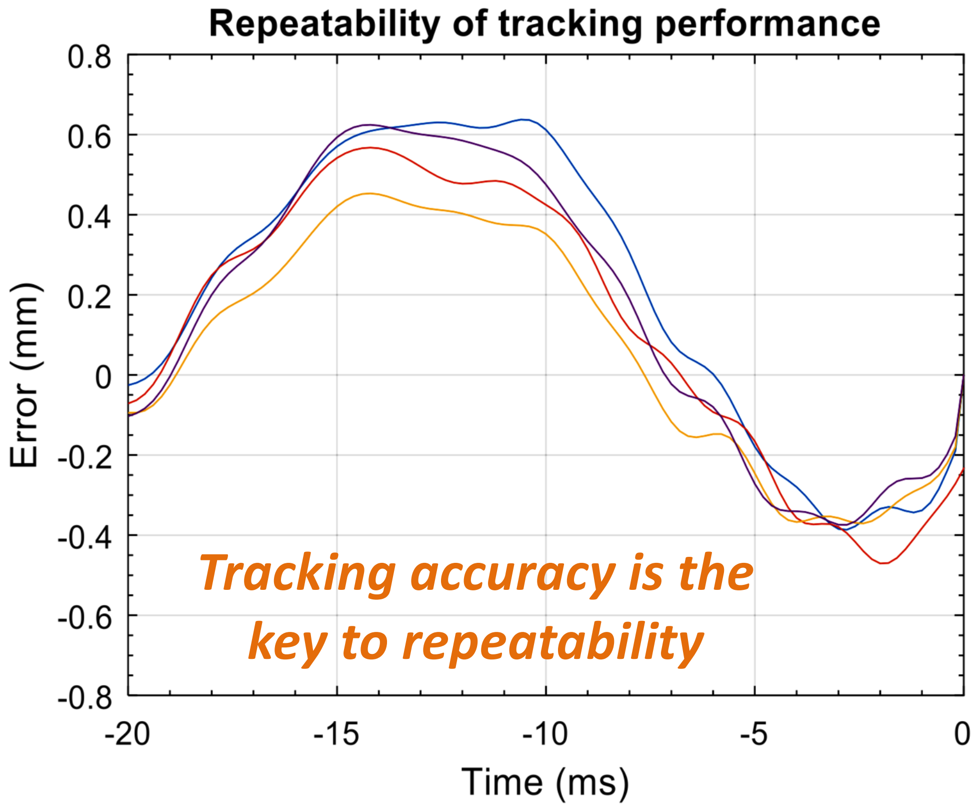
Control module: centralized data logging and motion control unit

Diagnostics system: GCMS and PLIF system

Characterization of CT-RCEM



Four repetitions for CR: 16.7, compression time 20ms.



Tracking accuracy is the key to repeatability

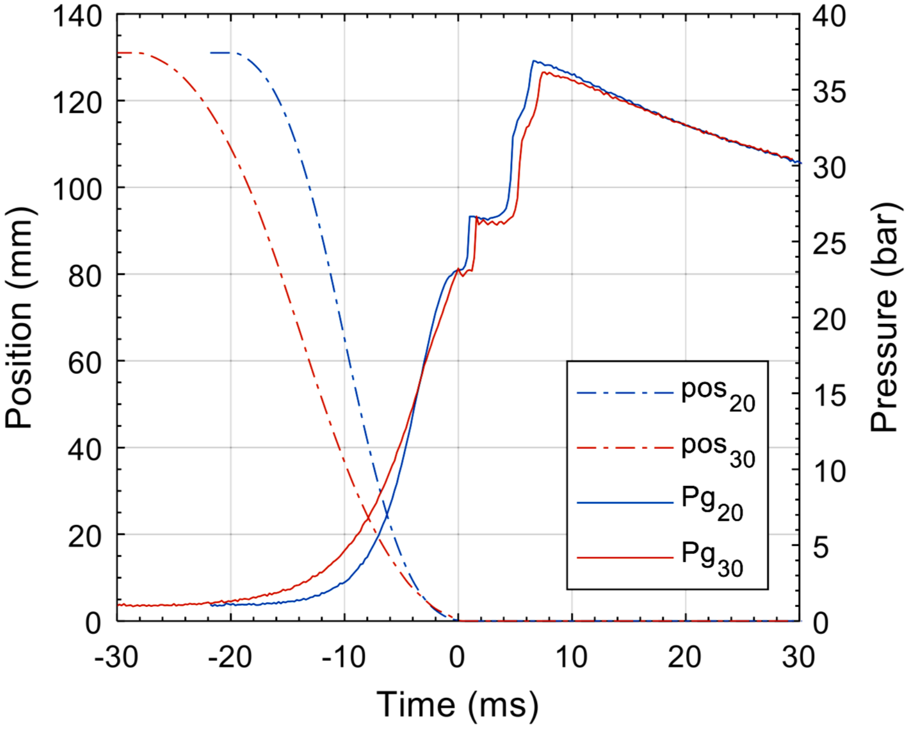
Repeatability Analysis for CR16.7

- *Stroke: 131 mm*
- *Compression time: 20ms*
- *Peak velocity: 12.5 m/s*
- *Average velocity: 7 m/s*
- *Peak tracking error: 0.6 mm*

Controlled Trajectory RCEM

Preliminary Case Study: trajectory effect on the auto-ignition of DME

- Identical air fuel mixtures were compressed (DME:O2:N2 = 1:4:40)
- The trajectories are with the same CR = 16.7, but different compression time (20ms and 30ms)
- The first-stage ignition delay is 0.9ms in 20ms case, while it is 1.6ms in 30ms case.



The CT-RCEM is a perfect facility to validate the trajectory-based combustion control:

- Precise and fast piston motion control
- Comprehensive information on fuel properties and the related emissions
- Accurate measurement on pressure and species concentration via the optical diagnostics system

Presentation Outline

- Motivation, Background and Objective
- Trajectory-based Combustion Control
  - *Chemical Kinetics Driven Model*
  - *Control-oriented Model*
  - *Optimization of Piston Trajectory*
- Controlled Trajectory Rapid Compression and Expansion Machine (CT-RCEM)
- Conclusions

Conclusion

- Proposed the trajectory-based combustion control to achieve real-time control on the combustion in the FPE
- Developed a dynamic model to systematically investigate the effectiveness of the proposed combustion control
- Realized the enhancement of the thermal efficiency and the reduction of NOx emission simultaneously as well as the combustion phasing control for multiple fuels
- Designed, manufactured and tested a unique CT-RCEM to enable the experimental validation of the proposed combustion control method
- Provided a new platform to realize co-optimization on both fuel production and engine performance