

## Supplementary Material:

### *Uncertainty Analysis:*

An uncertainty analysis was performed on all measurements and calculations. For all measured values, the random uncertainty was calculated using 95% confidence intervals ( $2 \times$  the standard error,  $\sigma_{\bar{r}}$ ) [26]. The random uncertainty is defined as

$$R_x = 2 * \sigma_{\bar{r}} = \frac{2\sigma_r}{\sqrt{N}}, \quad (1)$$

where  $x$  is the measured value,  $N$  is the number of cycles, and  $\sigma_x$  is the standard deviation. The standard deviation is defined as

$$\sigma_x = \left( \frac{1}{N-1} \sum_{i=1}^n (x_i - \bar{x})^2 \right)^{1/2} \quad (2)$$

where  $\bar{x}$  is the mean of the measured value.

The general formula for error propagation in an equation with multiple variables was calculated using [27]

$$U_r = \sqrt{\left( \frac{dr}{dx_1} U_{x_1} \right)^2 + \left( \frac{dr}{dx_2} U_{x_2} \right)^2 + \dots + \left( \frac{dr}{dx_n} U_{x_n} \right)^2}, \quad (3)$$

where  $U_r$  is the uncertainty of some value  $r$  and  $x_n$  are independent variables with measured uncertainties.

### In-Cylinder Pressure

As mentioned in section 3.4.1, the in-cylinder pressure was measured using a 6052B Kistler piezoelectric pressure transducer in conjunction with a 5044A Kistler charge amplifier. The systematic error for the transducer,  $B_p$ , is listed as 0.2 bar. Random uncertainty in the pressure data were calculated using equation 1 and a minimum of 300 cycles.

Using the random uncertainty and the systematic error in the pressure, the total uncertainty in pressure can be calculated using [26]

$$U_p = \sqrt{R_p^2 + B_p^2}. \quad (4)$$

### Volume

The volume at each crank angle degree can be calculated by [27]

$$V = V_c + \frac{\pi B^2}{4} \left( l + a - a \cos \theta - \left( l^2 - a^2 \sin^2 \theta \right)^{1/2} \right), \quad (5)$$

where  $V_c$  is the clearance volume,  $B$  is the bore,  $l$  is the connecting rod length, and  $a$  is the crank radius [24]. Top Dead Center (TDC) of the motoring traces was calculated using the method outlined by Tunestal [28]. The uncertainty in crank angle degree, using Tunestal's method to find TDC, is  $0.05^\circ$ . The uncertainty in volume can be determined using

$$U_v = \left( \frac{dV}{d\theta} U_\theta \right), \quad (6)$$

where

$$\frac{dV}{d\theta} = \frac{\pi B^2}{4} \left( a \sin \theta + \frac{a^2 \sin \theta \cos \theta}{\sqrt{l^2 - a^2 \sin^2 \theta}} \right). \quad (7)$$

### Specific Heat Ratio

Uncertainty in the specific heat ratio was determined using 95% confidence intervals, similar to the pressure data.

### Net Heat Release Rate

Uncertainty in the net heat release rate was determined using 95% confidence intervals.

### Cumulative Net Heat Release

From the first law of thermodynamics, the net heat release per CAD can be defined as

$$\frac{dQ}{d\theta} = \frac{\gamma}{\gamma-1} P \frac{dV}{d\theta} + \frac{1}{\gamma-1} V \frac{dP}{d\theta}. \quad (8)$$

Because pressure is measured discretely, numerically differentiating the pressure will amplify the signal noise.

To avoid differentiating the pressure, equation 8 can be rewritten using  $\frac{d(PV)}{d\theta} = P \frac{dV}{d\theta} + V \frac{dP}{d\theta}$ ,

$$\frac{dQ}{d\theta} = P \frac{dV}{d\theta} + \frac{1}{\gamma-1} \frac{d(PV)}{d\theta}. \quad (9)$$

Using equation 9, Q can be computed as a finite sum instead of a continuous integral

$$Q_i = \frac{1}{\gamma-1} (P_i V_i - P_0 V_0) + \sum_{j=0}^i P_j (\Delta V)_j. \quad (10)$$

The uncertainty calculation for  $Q_i$  was performed by dividing equation 10 into two terms A,

$$A = \frac{1}{\gamma-1} (P_i V_i - P_0 V_0), \quad (11)$$

and B,

$$B = \sum_{j=0}^i P_j (\Delta V)_j . \quad (12)$$

The uncertainty in A can be found using equation 3 which yields,

$$\begin{aligned} U_A^2 &= \left( \frac{\partial A}{\partial \gamma} U_\gamma \right)^2 + \left( \frac{\partial A}{\partial P_i} U_{P_i} \right)^2 + \left( \frac{\partial A}{\partial V_i} U_{V_i} \right)^2 + \left( \frac{\partial A}{\partial P_0} U_{P_0} \right)^2 + \left( \frac{\partial A}{\partial V_0} U_{V_0} \right)^2 \\ &= \left( -\frac{P_i V_i - P_0 V_0}{\gamma - 1} U_\gamma \right)^2 + \left( \frac{V_i}{\gamma - 1} U_{P_i} \right)^2 + \left( \frac{P_i}{\gamma - 1} U_{V_i} \right)^2 + \left( -\frac{V_0}{\gamma - 1} U_{P_0} \right)^2 + \left( -\frac{P_0}{\gamma - 1} U_{V_0} \right)^2 . \end{aligned} \quad (13)$$

Similarly, the uncertainty in B is found to be,

$$\begin{aligned} U_B^2 &= \left( \frac{\partial B}{\partial P_1} U_{P_1} \right)^2 + \left( \frac{\partial B}{\partial \Delta V_1} U_{\Delta V_1} \right)^2 + \left( \frac{\partial B}{\partial P_2} U_{P_2} \right)^2 + \left( \frac{\partial B}{\partial \Delta V_2} U_{\Delta V_2} \right)^2 + \dots \left( \frac{\partial B}{\partial P_i} U_{P_i} \right)^2 + \left( \frac{\partial B}{\partial \Delta V_i} U_{\Delta V_i} \right)^2 \\ &= (\Delta V_1 U_{P_1})^2 + (P_1 U_{\Delta V_1})^2 + (\Delta V_2 U_{P_2})^2 + (P_2 U_{\Delta V_2})^2 + \dots (\Delta V_i U_{P_i})^2 + (P_i U_{\Delta V_i})^2 . \end{aligned} \quad (14)$$

After computing the uncertainty in the first and second terms, the uncertainty in  $Q_i$  is found by

[27]

$$U_{Q_i} = \sqrt{U_A^2 + U_B^2} . \quad (15)$$

### CA50

CA50 is defined as the crank angle position  $\theta_{Q50\%}$  where

$$\theta_{Q50\%} = 1/2 * (Q_{\max} - Q_{\min}) . \quad (16)$$

Uncertainty in the CA50 was determined using [27]

$$U_{CA50} = \left| \theta(Q_{50\%} + U_{Q50\%}) - \theta_{Q50\%} \right| . \quad (16)$$

### *28-species Reduced Mechanism:*

Presented below is the summary of the reduced chemistry mechanism for DME developed in this paper. The reduced mechanism contains 28 species and 24 reaction steps. The associated Chemkin files reduced.mec and reduced.ckwyp are included.

Units: cm<sup>3</sup>, mol, sec, K

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! SUMMARY OF REDUCED MECHANISM:
! TOTAL NUMBER OF SPECIES= 28 WITH 24 STEPS
! TOTAL NUMBER OF STEADY SPECIES= 25
! ( 1) H + O2 = O + OH
! ( 2) H2 + O = H + OH
! ( 3) H2 + OH = H + H2O
! ( 4) H2 = 2H
! ( 5) H + O2 = HO2
! ( 6) 2HO2 = O2 + H2O2
! ( 7) O + CO = CO2
! ( 8) CH2O = 2H + CO
! ( 9) CH3 + CH2O = H + CH4 + CO
! (10) CH3 + O = H + CH2O
! (11) 2CH3 = C2H6
! (12) H2O + C2H4 = H + CH3 + CH2O
! (13) H2O + C2H4 + CH2O = H + CH3 + CO + CH3OH
! (14) 2CH3 = H + C2H5
! (15) CH2 + CH4 = 2CH3
! (16) C2H4 = H2 + C2H2
! (17) CO + CH3OCH3 = 2CH3 + CO2
! (18) H2 + CH3OCH2O2 = H + CH3OCH2O2H
! (19) HO2 + CH3OCH3 = H2 + OH + CH3OCHO
! (20) H + O2 + CH3OCH3 = H2 + CH3OCH2O2
! (21) 2CH3OCH2O2 = O2 + CH3OCHO + CH3OCH2OH
! (22) 2CH2O + O2 = HO2CH2OCHO
! (23) HO2CH2OCHO = OH + HOCH2OCO
! (24) HOCH2OCO = H + CO + HCOOH
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