__Supporting Information 6__

Comprehensive Experimental and Kinetic Modeling Study of *n*-Tetradecane Combustion

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Table S1. A list of C_3 and larger species discussed in this work.

| Name	Formula	Structure	Name	Formula	Structure
n-tetradecane	*n*-$C_{14}H_{30}$	$CH_3(CH_2)_{12}CH_3$	1-tetradecyl	$C_{14}H_{29}X1$	$\bullet CH_2(CH_2)_{12}CH_3$
2-tetradecyl	$C_{14}H_{29}X2$	$CH_3(\bullet CH)(CH_2)_{11}CH_3$	3-tetradecyl	$C_{14}H_{29}X3$	$CH_3CH_2(\bullet CH)(CH_2)_{10}CH_3$
4-tetradecyl	$C_{14}H_{29}X4$	$CH_3(CH_2)_2(\bullet CH)(CH_2)_9CH_3$	5-tetradecyl	$C_{14}H_{29}X5$	$CH_3(CH_2)_3(\bullet CH)(CH_2)_8CH_3$
6-tetradecyl	$C_{14}H_{29}X6$	$CH_3(CH_2)_4(\bullet CH)(CH_2)_7CH_3$	7-tetradecyl	$C_{14}H_{29}X7$	$CH_3(CH_2)_5(\bullet CH)(CH_2)_6CH_3$
1-tridecyl	$C_{13}H_{27}X1$	$\bullet CH_2(CH_2)_{11}CH_3$	3-tridecyl	$C_{13}H_{27}X3$	$CH_3CH_2(\bullet CH)(CH_2)_9CH_3$
7-tridecyl	$C_{13}H_{27}X7$	$CH_3(CH_2)_5(\bullet CH)(CH_2)_5CH_3$	1-dodecyl	$C_{12}H_{25}X1$	$\bullet CH_2(CH_2)_{10}CH_3$
6-dodecyl	$C_{12}H_{25}X6$	$CH_3(CH_2)_4(\bullet CH)(CH_2)_5CH_3$	1-dodecene	1-$C_{12}H_{24}$	$CH_2=CH(CH_2)_9CH_3$
1-undecyl	$C_{11}H_{23}X1$	$\bullet CH_2(CH_2)_9CH_3$	5-undecyl	$C_{11}H_{23}X5$	$CH_3(CH_2)_3(\bullet CH)(CH_2)_5CH_3$
1-decyl	$C_{10}H_{21}X1$	$\bullet CH_2(CH_2)_8CH_3$	4-decyl	$C_{10}H_{21}X4$	$CH_3(CH_2)_2(\bullet CH)(CH_2)_5CH_3$
1-nonyl	$C_9H_{19}X1$	$\bullet CH_2(CH_2)_7CH_3$	3-nonyl	$C_9H_{19}X3$	$CH_3CH_2(\bullet CH)(CH_2)_5CH_3$
1-nonene	1-C_9H_{18}	$CH_2=CH(CH_2)_6CH_3$	1-octyl	$C_8H_{17}X1$	$\bullet CH_2(CH_2)_6CH_3$
1-octene	1-C_8H_{16}	$CH_2=CH(CH_2)_5CH_3$	1-heptyl	$C_7H_{15}X1$	$\bullet CH_2(CH_2)_5CH_3$
3-heptyl	$C_7H_{15}X3$	$CH_3CH_2(\bullet CH)(CH_2)_3CH_3$	1-hexyl	$C_6H_{13}X1$	$\bullet CH_2(CH_2)_4CH_3$
1,3-hexadiene	1,3-C_6H_{10}	$CH_2=CHCH=CHCH_2CH_3$	1-pentyl	$C_5H_{11}X1$	$\bullet CH_2(CH_2)_3CH_3$
1-pentene	1-C_5H_{10}	$CH_2=CH(CH_2)_2CH_3$	1,3-pentadiene	1,3-C_5H_8	$CH_2=CHCH=CHCH_3$
1-butyl	PXC_4H_9	$\bullet CH_2(CH_2)_2CH_3$	1-butene	1-C_4H_8	$CH_2=CHCH_2CH_3$
1,3-butadiene	1,3-C_4H_6	$CH_2=CHCH=CH_2$	2-butene	2-C_4H_8	$CH_3CH=CHCH_3$
1-propene	C_3H_6	$CH_2=CHCH_3$	1-propyl	NXC_3H_7	$\bullet CH_2CH_2CH_3$
allene	aC_3H_4	$CH_2=C=CH_2$	allyl	C_3H_5XA	$\bullet CH_2CH=CH_2$
propargyl	C_3H_3	$\bullet CH_2C\equiv CH$	propyne	pC_3H_4	$CH\equiv CCH_3$

1. Flow reactor pyrolysis of *n*-decane and *n*-tetradecane
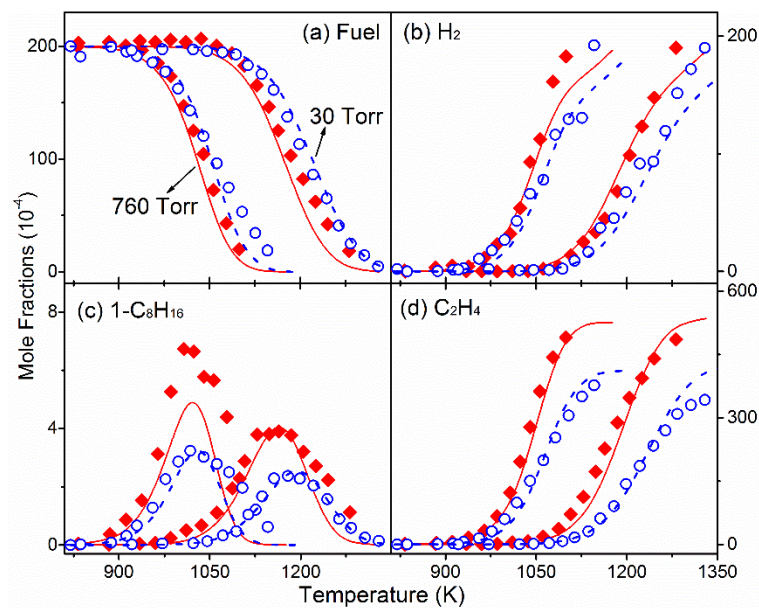
Figure S1 Experimental (symbols) and simulated (lines) mole fractions of (a) fuel, (b) H_2, (c) $1\text{-}C_8H_{16}$, and (d) C_2H_4 in the flow reactor pyrolysis of $n\text{-}C_{14}H_{30}$ and $n\text{-}C_{10}H_{20}$ at 30 Torr and 760 Torr, respectively. Experimental data (hollow circles) represent experiments of $n\text{-}C_{10}H_{20}$ from Zeng and coworkers[1], and experimental data (solid diamonds) represent experiments of $n\text{-}C_{14}H_{30}$ from present work. Solid lines, and dashed lines represent simulations by present model for the pyrolysis of $n\text{-}C_{14}H_{30}$, and $n\text{-}C_{10}H_{20}$, respectively. In Fig. (a), fuel in the $n\text{-}C_{10}H_{20}$ pyrolysis represents mole fraction of $n\text{-}C_{10}H_{20}$ and fuel in the $n\text{-}C_{14}H_{30}$ pyrolysis represents mole fraction of $n\text{-}C_{14}H_{30}$, respectively.

2. Validation of present model

Mzé-Ahmed and coworkers[2] investigated *n*-tetradecane oxidation in a jet stirred reactor at 10 bar, 560 to 1030 K, the residence time of 1 s and three equivalence ratios ($\phi = 0.5$, 1.0 and 2.0). Mole fractions were measured with gas chromatography and Fourier transformed infrared spectrometry. These literature data[2] were used to validate present model. Figures S2 and S3 provide experimental and simulated mole fractions at $\phi = 0.5$ and 1.0, respectively.
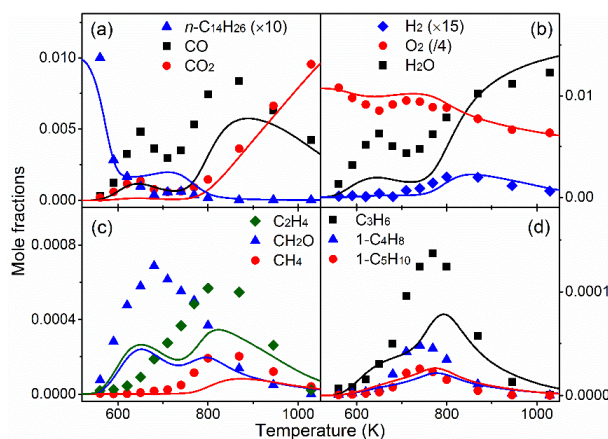
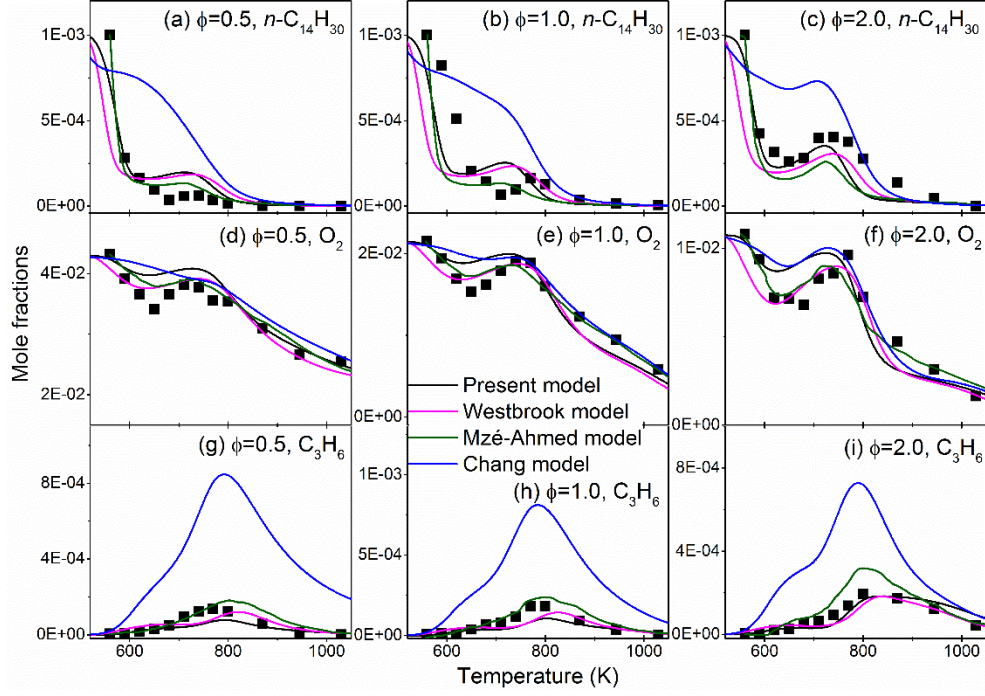**Figure S2** Mole fractions for *n*-tetradecane oxidation in a jet stirred reactor at 10 bar, $\tau = 1$ s and $\phi = 0.5$. Symbols represent literature experiments[2]. Solid lines represent simulations by present model.
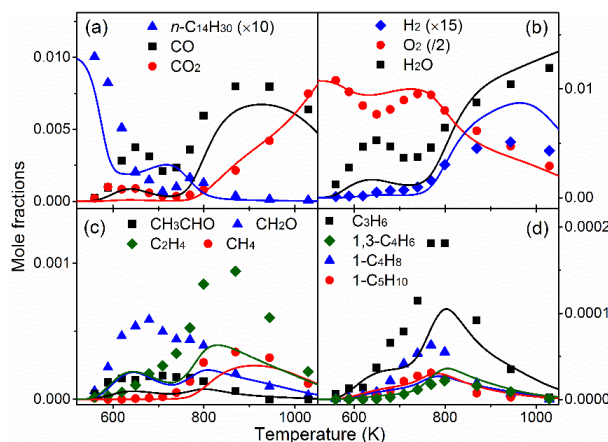
Figure S3 Mole fractions for *n*-tetradecane oxidation in a jet stirred reactor at 10 bar, $\tau = 1$ s and $\phi = 1.0$. Symbols represent literature experiments[2]. Solid lines represent simulations by present model.

Moreover, performances of literature models, *i.e.* Westbrook model[3], Mzé-Ahmed model[2], Chang model[4], and present model against literature JSR experimental data[2] are presented in Fig. S4.

Figure S4 Mole fractions for *n*-tetradecane oxidation in a jet stirred reactor at 10 bar, $\tau = 1$ s and $\phi = 0.5$, 1.0 and 2.0. Symbols represent literature experiments[2]. Solid lines represent simulations by present model, Westbrook model[3], Mzé-Ahmed model[2] and Chang model[4], respectively.

3. Ignition delay times of *n*-decane, *n*-dodecane and *n*-tetradecane

Shen and coworkers[5] investigated ignition delay times of *n*-decane/air mixtures, *n*-dodecane/air mixtures and *n*-tetradecane/air mixtures in a heated shock tube at $\phi = 0.5$ and 1.0 at similar experimental conditions. Both literature experiments of *n*-decane, *n*-dodecane and *n*-tetradecane as well as simulations by present model are shown in Fig. S5.
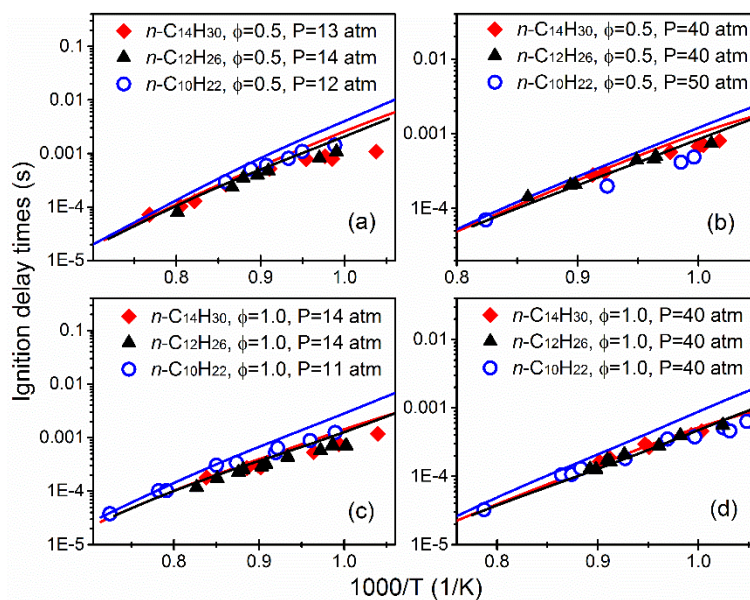
Figure S5 Ignition delay times of *n*-decane/air mixtures, *n*-dodecane/air mixtures and *n*-tetradecane/air mixtures. Symbols represent literature experimental ignition delay times from Shen and coworkers[5]. Lines represent simulations by present model.

References:

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(2) Mzé-Ahmed, A.; Dagaut, P.; Dayma, G.; Diévart, P.; Hadj-Ali, K. *Combust. Sci. Technol.* **2014**, *186*, 594-606.

(3) Westbrook, C.K.; Pitz, W.J.; Herbinet, O.; Curran, H.J.; Silke, E.J. *Combust. Flame* **2009**, *156*, 181-199.

(4) Chang, Y.C.; Jia, M.; Liu, Y.D.; Li, Y.P.; Xie, M.Z.; Yin, H.C. *Energy Fuels* **2013**, *27*, 3467-3479.

(5) Shen, H.P.S.; Steinberg, J.; Vanderover, J.; Oehlschlaeger, M.A. *Energy Fuels* **2009**, *23*, 2482-2489.